



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:32 AM UTC

PDB ID : 6WI2 / pdb_00006wi2
Title : Structure of human mitochondrial complex Nfs1-ISCU2-ISD11 with E.coli ACP1 at 1.95 Å resolution (NIAU)2. N-terminal mutation of ISCU2 (L35) traps Nfs1 Cys loop in the active site of ISCU2 without metal present.
Authors : Boniecki, M.T.; Cygler, M.
Deposited on : 2020-04-08
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

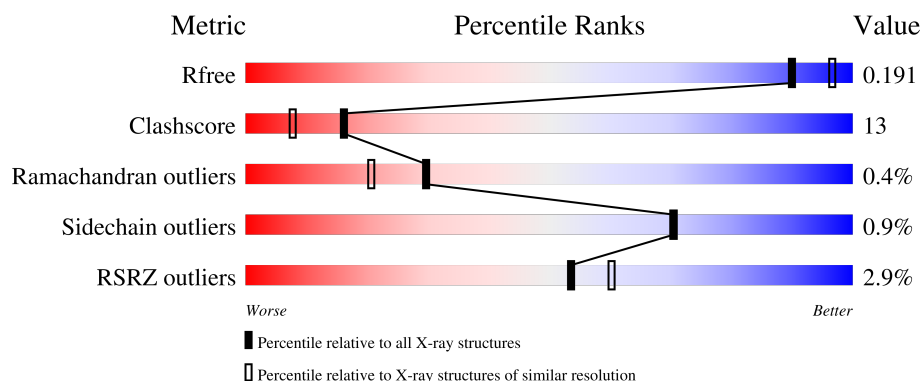
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	406	3% 78% 18% ...
2	B	91	2% 78% 8% 9%
3	C	77	5% 86% 9% ...
4	D	143	% 71% 17% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ETE	A	526	-	-	X	-
11	PGE	A	535	-	-	X	-
6	EDO	A	509	-	-	X	-
6	EDO	A	516	-	-	X	-
8	PEG	B	1607	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 6127 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	402	Total	C	N	O	S	0	9	0
			3143	1978	548	596	21			

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	83	Total	C	N	O	S	0	7	0
			727	457	147	122	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	1	0
			552	343	85	123	1			

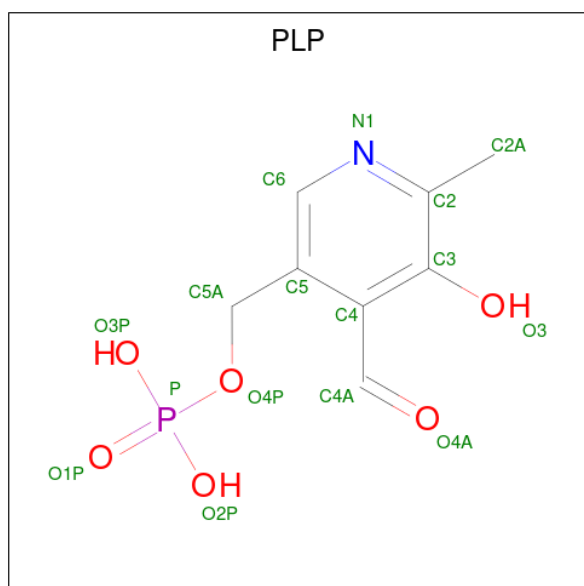
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	126	Total	C	N	O	S	1	3	0
			926	582	155	181	8			

There are 10 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

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



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

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

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



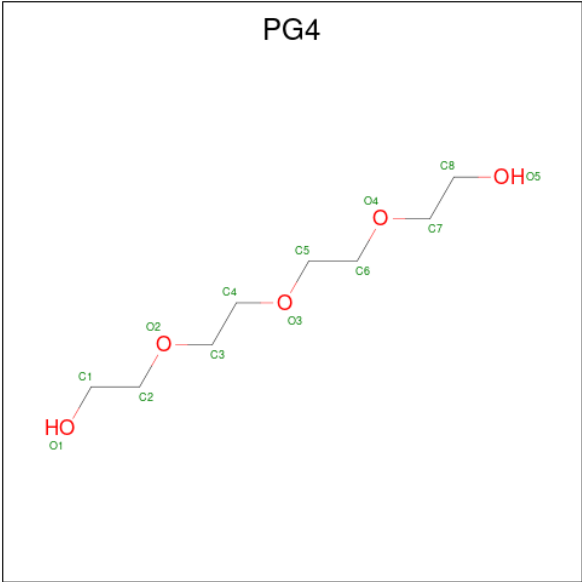
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



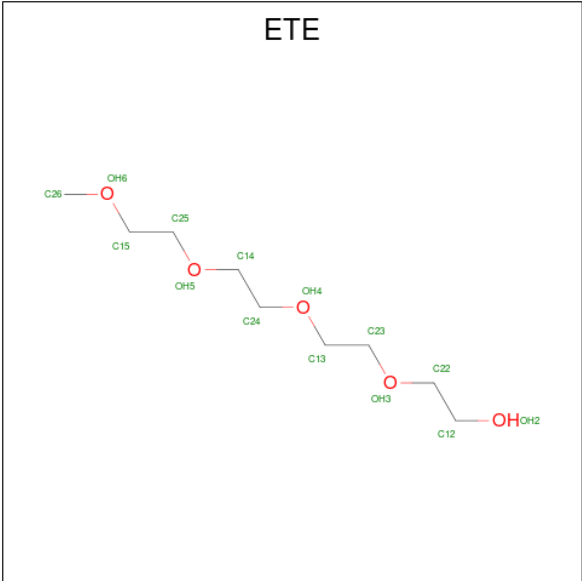
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



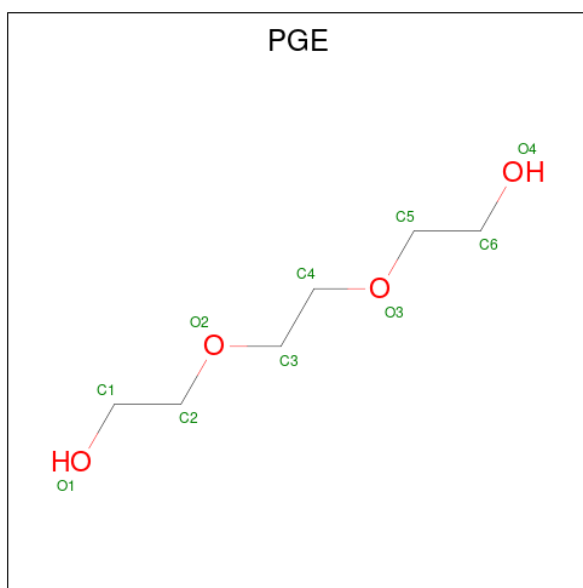
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is 2-{2-[2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



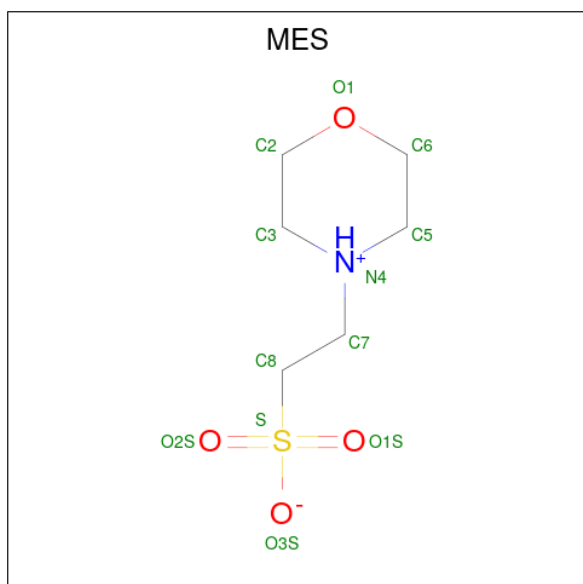
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



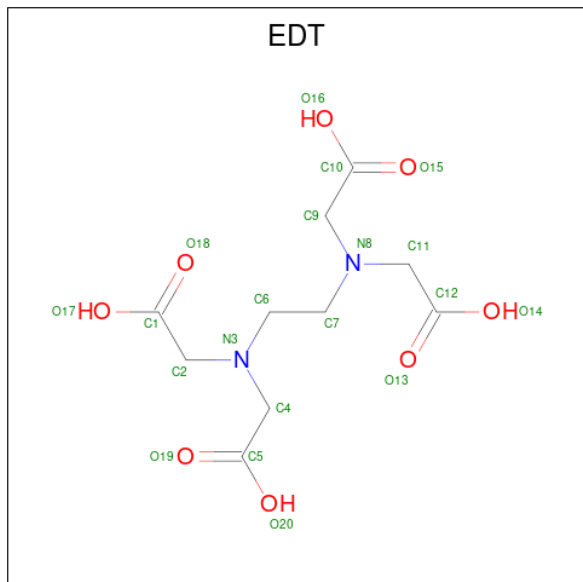
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



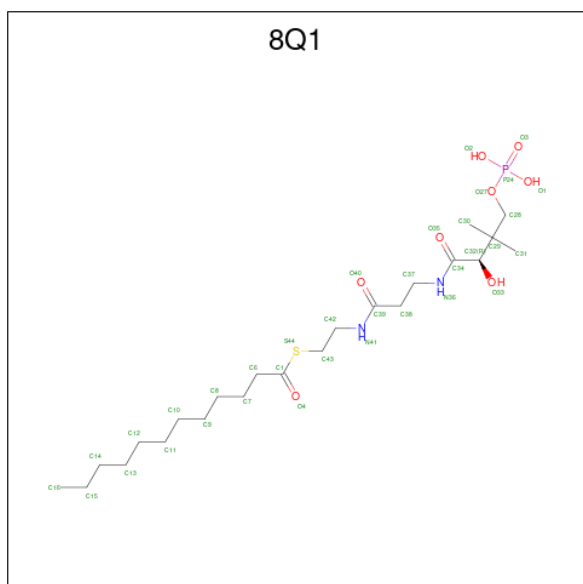
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



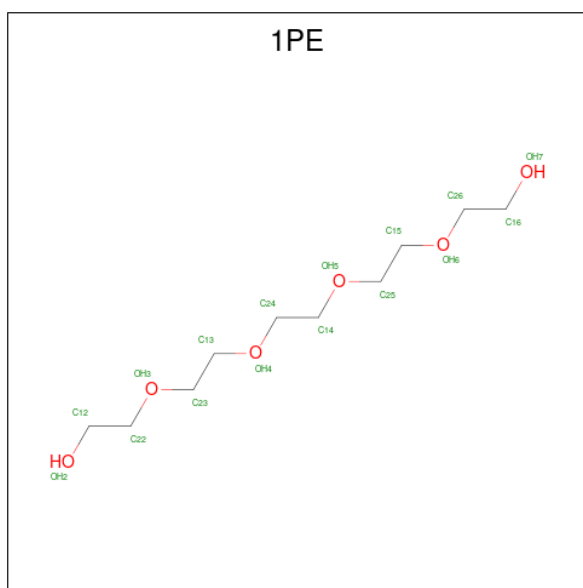
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 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 PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	281	Total	O	0	0
			281	281		
16	B	63	Total	O	0	0
			63	63		
16	C	17	Total	O	0	0
			17	17		
16	D	42	Total	O	0	0
			42	42		

- Molecule 1: Cysteine desulfurase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.43Å 86.43Å 246.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 1.95 49.01 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.01-1.95) 100.0 (49.01-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.150 , 0.185 0.166 , 0.191	Depositor DCC
R_{free} test set	3451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, EDO, PEG, PG4, 8Q1, PLP, MES, ETE, EDT, GOL, 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	1.38	24/3224 (0.7%)	1.21	22/4366 (0.5%)
2	B	1.63	8/757 (1.1%)	1.31	10/1014 (1.0%)
3	C	0.48	0/559	0.76	1/762 (0.1%)
4	D	0.98	5/947 (0.5%)	0.92	0/1284
All	All	1.29	37/5487 (0.7%)	1.14	33/7426 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	5
All	All	0	9

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24[A]	SER	CA-C	11.36	1.68	1.52
2	B	24[B]	SER	CA-C	11.36	1.68	1.52
2	B	27[A]	ASN	CA-C	11.26	1.68	1.52
2	B	27[B]	ASN	CA-C	11.26	1.68	1.52
2	B	37[A]	ARG	CA-C	11.22	1.68	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432[A]	ARG	N-CA-C	11.15	123.44	111.28
1	A	432[B]	ARG	N-CA-C	11.15	123.44	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27[A]	ASN	N-CA-C	10.52	123.74	111.11
2	B	27[B]	ASN	N-CA-C	10.52	123.74	111.11
3	C	6	ARG	N-CA-C	-10.42	99.83	112.54

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432[A]	ARG	Mainchain
1	A	432[B]	ARG	Mainchain
1	A	69[A]	LEU	Mainchain
1	A	69[B]	LEU	Mainchain
2	B	24[B]	SER	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3143	0	3136	84	0
2	B	727	0	764	19	0
3	C	552	0	489	9	0
4	D	926	0	926	30	0
5	A	15	0	7	0	0
6	A	96	0	140	27	0
6	B	24	0	36	4	0
6	C	8	0	12	1	0
6	D	16	0	24	3	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	63	0	90	8	0
8	B	7	0	10	5	0
9	A	26	0	36	2	0
10	A	14	0	20	9	0
11	A	10	0	14	13	0
12	B	12	0	13	1	0
13	B	17	0	10	5	0
14	C	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	D	16	0	22	3	0
16	A	281	0	0	13	0
16	B	63	0	0	5	0
16	C	17	0	0	0	0
16	D	42	0	0	3	0
All	All	6127	0	5773	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 151 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:1609:EDT:H061	1.22	0.99
1:A:105[B]:ARG:HG2	6:A:513:EDO:H11	1.55	0.88
1:A:371:LYS:HD3	6:A:509:EDO:H22	1.53	0.88
4:D:95:CYS:SG	4:D:135:LYS:NZ	2.50	0.85
4:D:51:SER:H	6:D:203:EDO:H11	1.42	0.83

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	409/406 (101%)	399 (98%)	8 (2%)	2 (0%)	24	16
2	B	88/91 (97%)	87 (99%)	1 (1%)	0	100	100
3	C	74/77 (96%)	68 (92%)	5 (7%)	1 (1%)	9	3
4	D	127/143 (89%)	125 (98%)	2 (2%)	0	100	100
All	All	698/717 (97%)	679 (97%)	16 (2%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ALA
1	A	450	LYS
3	C	5	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/346 (98%)	337 (99%)	3 (1%)	70	70
2	B	76/80 (95%)	74 (97%)	2 (3%)	40	33
3	C	54/66 (82%)	54 (100%)	0	100	100
4	D	98/118 (83%)	96 (98%)	2 (2%)	48	43
All	All	568/610 (93%)	561 (99%)	7 (1%)	70	61

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41[A]	ARG
2	B	41[B]	ARG
4	D	157	GLN
4	D	47	ARG
1	A	149[B]	LEU

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

Mol	Chain	Res	Type
1	A	109	GLN
1	A	194	GLN
1	A	444	GLN
3	C	24	ASN
3	C	73	ASN

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 ⓘ

58 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	$\# Z > 2$
6	EDO	B	1606	-	3,3,3	0.43	0	2,2,2	0.47	0
6	EDO	A	531	-	3,3,3	0.47	0	2,2,2	0.82	0
6	EDO	B	1603	-	3,3,3	0.45	0	2,2,2	0.55	0
6	EDO	A	532	-	3,3,3	0.41	0	2,2,2	0.16	0
6	EDO	D	206	-	3,3,3	0.45	0	2,2,2	0.28	0
6	EDO	C	302	-	3,3,3	0.42	0	2,2,2	0.37	0
8	PEG	A	505	-	6,6,6	0.56	0	5,5,5	0.45	0
8	PEG	A	527	-	6,6,6	0.49	0	5,5,5	0.30	0
6	EDO	A	502	-	3,3,3	0.49	0	2,2,2	0.11	0
6	EDO	A	511	-	3,3,3	0.70	0	2,2,2	0.93	0
10	ETE	A	526	-	13,13,13	0.65	0	12,12,12	0.81	0
6	EDO	B	1605	-	3,3,3	0.46	0	2,2,2	0.21	0
14	8Q1	C	301	-	28,33,34	2.18	7 (25%)	32,40,43	1.67	8 (25%)
6	EDO	A	514	-	3,3,3	0.27	0	2,2,2	0.67	0
6	EDO	A	517	-	3,3,3	0.52	0	2,2,2	0.07	0
6	EDO	A	534	-	3,3,3	0.46	0	2,2,2	0.25	0
6	EDO	A	530	-	3,3,3	0.48	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	D	202	-	3,3,3	0.46	0	2,2,2	0.21	0
8	PEG	A	537	-	6,6,6	0.51	0	5,5,5	0.49	0
11	PGE	A	535	-	9,9,9	0.31	0	8,8,8	0.88	0
6	EDO	A	510	-	3,3,3	0.51	0	2,2,2	0.58	0
6	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.13	0
6	EDO	A	507	-	3,3,3	0.58	0	2,2,2	0.64	0
6	EDO	A	509	-	3,3,3	1.43	1 (33%)	2,2,2	1.42	0
6	EDO	D	201	-	3,3,3	0.44	0	2,2,2	0.38	0
7	GOL	A	508	-	5,5,5	0.93	0	5,5,5	1.41	2 (40%)
15	1PE	D	204	-	15,15,15	0.57	0	14,14,14	0.38	0
6	EDO	A	512	-	3,3,3	0.47	0	2,2,2	0.13	0
8	PEG	A	540	-	6,6,6	0.51	0	5,5,5	0.29	0
6	EDO	B	1601	-	3,3,3	0.63	0	2,2,2	0.86	0
8	PEG	A	519	-	6,6,6	0.57	0	5,5,5	0.79	0
6	EDO	A	528	-	3,3,3	0.55	0	2,2,2	0.19	0
6	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.14	0
6	EDO	A	524	-	3,3,3	0.43	0	2,2,2	0.58	0
9	PG4	A	521	-	12,12,12	0.59	0	11,11,11	0.49	0
8	PEG	A	539	-	6,6,6	0.53	0	5,5,5	0.60	0
12	MES	B	1604	-	12,12,12	2.06	4 (33%)	15,16,16	1.89	4 (26%)
6	EDO	A	518	-	3,3,3	0.70	0	2,2,2	0.65	0
6	EDO	B	1608	-	3,3,3	0.47	0	2,2,2	0.32	0
8	PEG	B	1607	-	6,6,6	0.58	0	5,5,5	0.85	0
7	GOL	D	205	-	5,5,5	0.70	0	5,5,5	0.34	0
8	PEG	A	522	-	6,6,6	0.42	0	5,5,5	0.67	0
6	EDO	A	523	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	A	515	-	3,3,3	0.45	0	2,2,2	0.40	0
6	EDO	A	533	-	3,3,3	0.42	0	2,2,2	0.36	0
6	EDO	A	536	-	3,3,3	0.48	0	2,2,2	0.17	0
6	EDO	A	538	-	3,3,3	0.47	0	2,2,2	0.25	0
6	EDO	D	203	-	3,3,3	0.39	0	2,2,2	0.33	0
8	PEG	A	506	-	6,6,6	0.49	0	5,5,5	0.40	0
8	PEG	A	529	-	6,6,6	0.50	0	5,5,5	0.37	0
6	EDO	B	1602	-	3,3,3	0.51	0	2,2,2	0.53	0
6	EDO	A	525	-	3,3,3	0.44	0	2,2,2	0.33	0
7	GOL	A	504	-	5,5,5	0.48	0	5,5,5	0.44	0
6	EDO	A	516	-	3,3,3	1.30	0	2,2,2	1.63	1 (50%)
6	EDO	A	513	-	3,3,3	0.44	0	2,2,2	0.65	0
13	EDT	B	1609	-	16,16,19	1.17	0	19,20,24	1.42	4 (21%)
9	PG4	A	520	-	12,12,12	0.57	0	11,11,11	0.58	0
5	PLP	A	501	-	15,15,16	1.67	3 (20%)	21,22,23	1.14	1 (4%)

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
6	EDO	B	1606	-	-	0/1/1/1	-
6	EDO	A	531	-	-	1/1/1/1	-
6	EDO	B	1603	-	-	1/1/1/1	-
6	EDO	A	532	-	-	0/1/1/1	-
6	EDO	D	206	-	-	0/1/1/1	-
6	EDO	C	302	-	-	1/1/1/1	-
8	PEG	A	505	-	-	3/4/4/4	-
8	PEG	A	527	-	-	2/4/4/4	-
6	EDO	A	502	-	-	0/1/1/1	-
6	EDO	A	511	-	-	1/1/1/1	-
10	ETE	A	526	-	-	3/11/11/11	-
6	EDO	B	1605	-	-	1/1/1/1	-
14	8Q1	C	301	-	-	0/38/40/41	-
6	EDO	A	514	-	-	1/1/1/1	-
6	EDO	A	517	-	-	0/1/1/1	-
6	EDO	A	534	-	-	0/1/1/1	-
6	EDO	A	530	-	-	1/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
8	PEG	A	537	-	-	4/4/4/4	-
11	PGE	A	535	-	-	3/7/7/7	-
6	EDO	A	510	-	-	0/1/1/1	-
6	EDO	C	303	-	-	1/1/1/1	-
6	EDO	A	507	-	-	0/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
7	GOL	A	508	-	-	0/4/4/4	-
15	1PE	D	204	-	-	9/13/13/13	-
6	EDO	A	512	-	-	0/1/1/1	-
8	PEG	A	540	-	-	1/4/4/4	-
6	EDO	B	1601	-	-	0/1/1/1	-
8	PEG	A	519	-	-	1/4/4/4	-
6	EDO	A	528	-	-	1/1/1/1	-
6	EDO	A	503	-	-	1/1/1/1	-
6	EDO	A	524	-	-	1/1/1/1	-
9	PG4	A	521	-	-	4/10/10/10	-
8	PEG	A	539	-	-	2/4/4/4	-
12	MES	B	1604	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	518	-	-	1/1/1/1	-
6	EDO	B	1608	-	-	0/1/1/1	-
8	PEG	B	1607	-	-	3/4/4/4	-
7	GOL	D	205	-	-	1/4/4/4	-
8	PEG	A	522	-	-	2/4/4/4	-
6	EDO	A	523	-	-	1/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	A	533	-	-	1/1/1/1	-
6	EDO	A	536	-	-	0/1/1/1	-
6	EDO	A	538	-	-	1/1/1/1	-
6	EDO	D	203	-	-	0/1/1/1	-
8	PEG	A	506	-	-	2/4/4/4	-
8	PEG	A	529	-	-	2/4/4/4	-
6	EDO	B	1602	-	-	0/1/1/1	-
6	EDO	A	525	-	-	0/1/1/1	-
7	GOL	A	504	-	-	4/4/4/4	-
6	EDO	A	516	-	-	1/1/1/1	-
6	EDO	A	513	-	-	0/1/1/1	-
13	EDT	B	1609	-	-	13/17/17/21	-
9	PG4	A	520	-	-	7/10/10/10	-
5	PLP	A	501	-	-	0/6/6/8	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	C39-N41	5.28	1.45	1.33
14	C	301	8Q1	C34-N36	4.91	1.45	1.33
14	C	301	8Q1	C6-C1	4.67	1.55	1.50
12	B	1604	MES	C8-S	4.63	1.84	1.77
5	A	501	PLP	C3-C2	-3.68	1.37	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1604	MES	O3S-S-O2S	-4.41	100.37	111.40
14	C	301	8Q1	C37-N36-C34	-4.01	115.34	122.55
12	B	1604	MES	O1S-S-C8	3.48	111.98	106.73
14	C	301	8Q1	C38-C37-N36	-3.43	104.70	112.00
14	C	301	8Q1	C42-N41-C39	-3.28	116.71	122.82

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

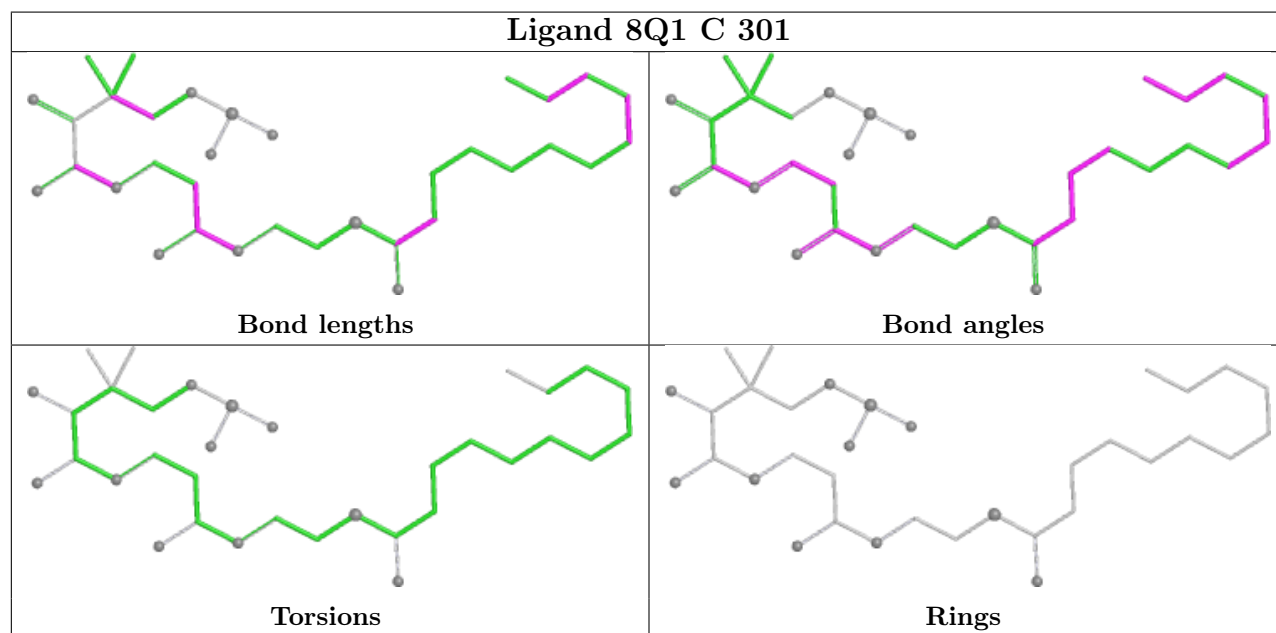
Mol	Chain	Res	Type	Atoms
12	B	1604	MES	C8-C7-N4-C3
13	B	1609	EDT	C7-C6-N3-C4
13	B	1609	EDT	C12-C11-N8-C7
13	B	1609	EDT	C6-C7-N8-C9
8	B	1607	PEG	C1-C2-O2-C3

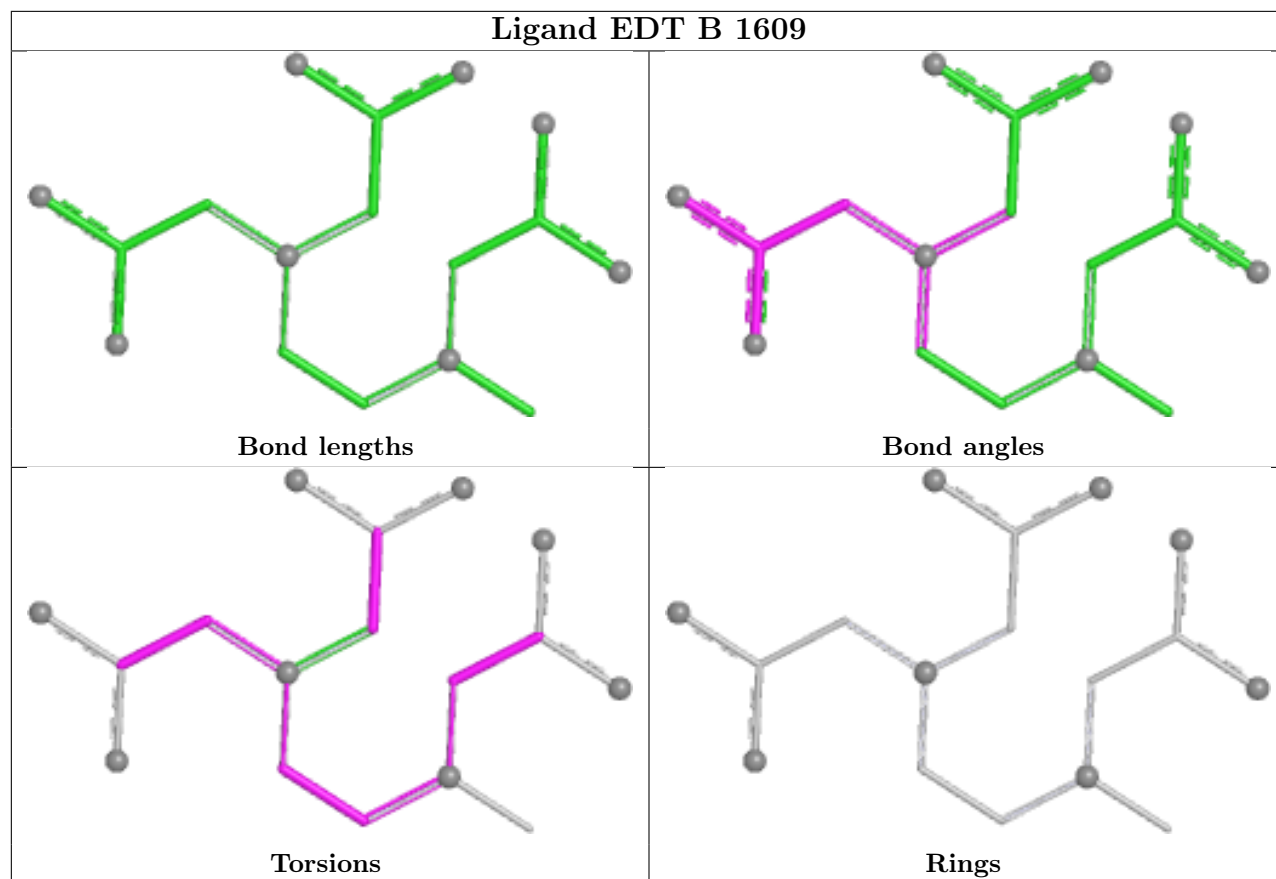
There are no ring outliers.

32 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1606	EDO	1	0
6	A	532	EDO	1	0
6	C	302	EDO	1	0
6	A	502	EDO	1	0
10	A	526	ETE	9	0
6	A	534	EDO	2	0
6	A	530	EDO	2	0
11	A	535	PGE	13	0
6	A	507	EDO	1	0
6	A	509	EDO	6	0
15	D	204	1PE	3	0
6	A	512	EDO	1	0
8	A	540	PEG	1	0
6	B	1601	EDO	3	0
8	A	519	PEG	1	0
6	A	528	EDO	1	0
6	A	503	EDO	1	0
6	A	524	EDO	2	0
8	A	539	PEG	2	0
12	B	1604	MES	1	0
6	A	518	EDO	1	0
8	B	1607	PEG	5	0
8	A	522	PEG	1	0
6	A	523	EDO	1	0
6	A	538	EDO	2	0
6	D	203	EDO	3	0
8	A	506	PEG	2	0
8	A	529	PEG	1	0
6	A	516	EDO	4	0
6	A	513	EDO	1	0
13	B	1609	EDT	5	0
9	A	520	PG4	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 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	402/406 (99%)	-0.23	12 (2%) 52 59	14, 28, 60, 97	16 (3%)
2	B	83/91 (91%)	0.01	2 (2%) 59 66	14, 30, 57, 85	7 (8%)
3	C	75/77 (97%)	0.69	4 (5%) 32 37	28, 68, 111, 138	1 (1%)
4	D	126/143 (88%)	0.17	2 (1%) 70 77	27, 45, 73, 83	4 (3%)
All	All	686/717 (95%)	-0.02	20 (2%) 53 60	14, 33, 77, 138	28 (4%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	ALA	6.6
2	B	3	ALA	5.4
1	A	385	SER	5.3
1	A	455	THR	5.1
1	A	386	LEU	4.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	524	4/4	0.61	0.18	63,63,63,63	4
12	MES	B	1604	12/12	0.61	0.20	121,122,127,128	0
6	EDO	A	525	4/4	0.67	0.21	84,84,85,85	0
6	EDO	A	533	4/4	0.68	0.17	85,85,85,85	0
9	PG4	A	521	13/13	0.69	0.24	88,95,102,102	0
6	EDO	B	1603	4/4	0.72	0.24	76,80,84,87	0
8	PEG	A	506	7/7	0.72	0.24	93,97,99,99	0
6	EDO	D	206	4/4	0.76	0.16	80,80,80,81	0
6	EDO	A	502	4/4	0.77	0.23	60,72,74,77	0
6	EDO	A	531	4/4	0.78	0.25	51,51,53,53	4
6	EDO	D	201	4/4	0.78	0.18	91,91,92,93	0
6	EDO	D	202	4/4	0.78	0.20	73,75,77,78	0
6	EDO	D	203	4/4	0.78	0.16	59,60,68,70	0
8	PEG	A	540	7/7	0.79	0.19	88,89,89,89	0
8	PEG	A	527	7/7	0.79	0.20	72,75,83,84	0
8	PEG	A	537	7/7	0.79	0.18	53,69,77,78	0
6	EDO	A	523	4/4	0.80	0.22	45,45,46,48	4
6	EDO	A	530	4/4	0.80	0.18	56,58,58,58	4
6	EDO	A	517	4/4	0.80	0.19	66,67,68,68	0
13	EDT	B	1609	17/20	0.80	0.21	54,70,75,77	17
8	PEG	B	1607	7/7	0.81	0.20	39,52,61,63	0
6	EDO	A	536	4/4	0.81	0.20	68,76,78,80	0
9	PG4	A	520	13/13	0.82	0.22	55,64,67,67	13
8	PEG	A	539	7/7	0.82	0.18	65,72,76,77	0
7	GOL	D	205	6/6	0.82	0.17	49,52,56,56	6
6	EDO	B	1602	4/4	0.82	0.19	67,68,71,72	0
6	EDO	B	1608	4/4	0.83	0.17	71,74,76,77	0
6	EDO	A	528	4/4	0.83	0.20	41,43,44,45	4
10	ETE	A	526	14/14	0.83	0.19	36,83,90,90	0
6	EDO	A	532	4/4	0.83	0.16	79,80,80,80	0
6	EDO	B	1606	4/4	0.83	0.18	73,73,74,74	0
8	PEG	A	505	7/7	0.84	0.20	58,66,76,76	0
6	EDO	B	1605	4/4	0.84	0.15	54,63,67,71	0
6	EDO	A	510	4/4	0.84	0.15	60,63,65,68	0
6	EDO	A	534	4/4	0.85	0.16	59,63,66,68	0
6	EDO	A	515	4/4	0.85	0.14	56,58,62,62	0
7	GOL	A	504	6/6	0.85	0.18	74,88,89,90	0
6	EDO	A	512	4/4	0.85	0.16	63,68,68,69	0
8	PEG	A	519	7/7	0.86	0.16	53,57,60,62	0
7	GOL	A	508	6/6	0.86	0.15	20,31,37,40	6
8	PEG	A	529	7/7	0.86	0.17	78,81,83,83	0
6	EDO	C	302	4/4	0.86	0.15	47,50,55,57	4
15	1PE	D	204	16/16	0.86	0.14	65,80,82,82	0

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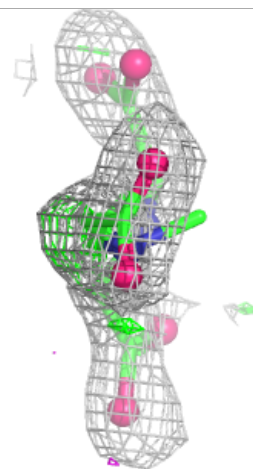
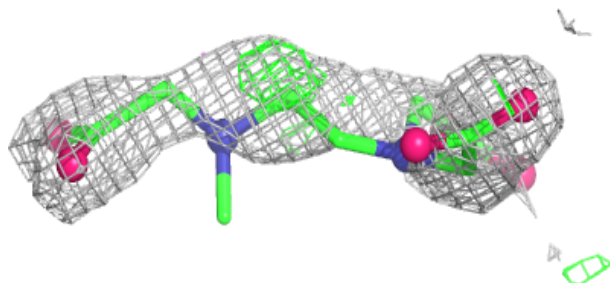
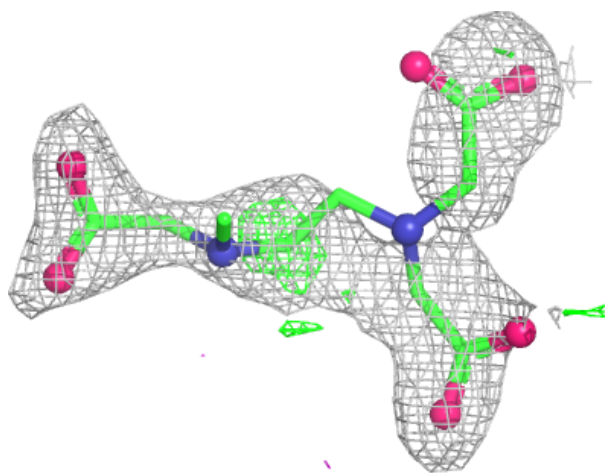
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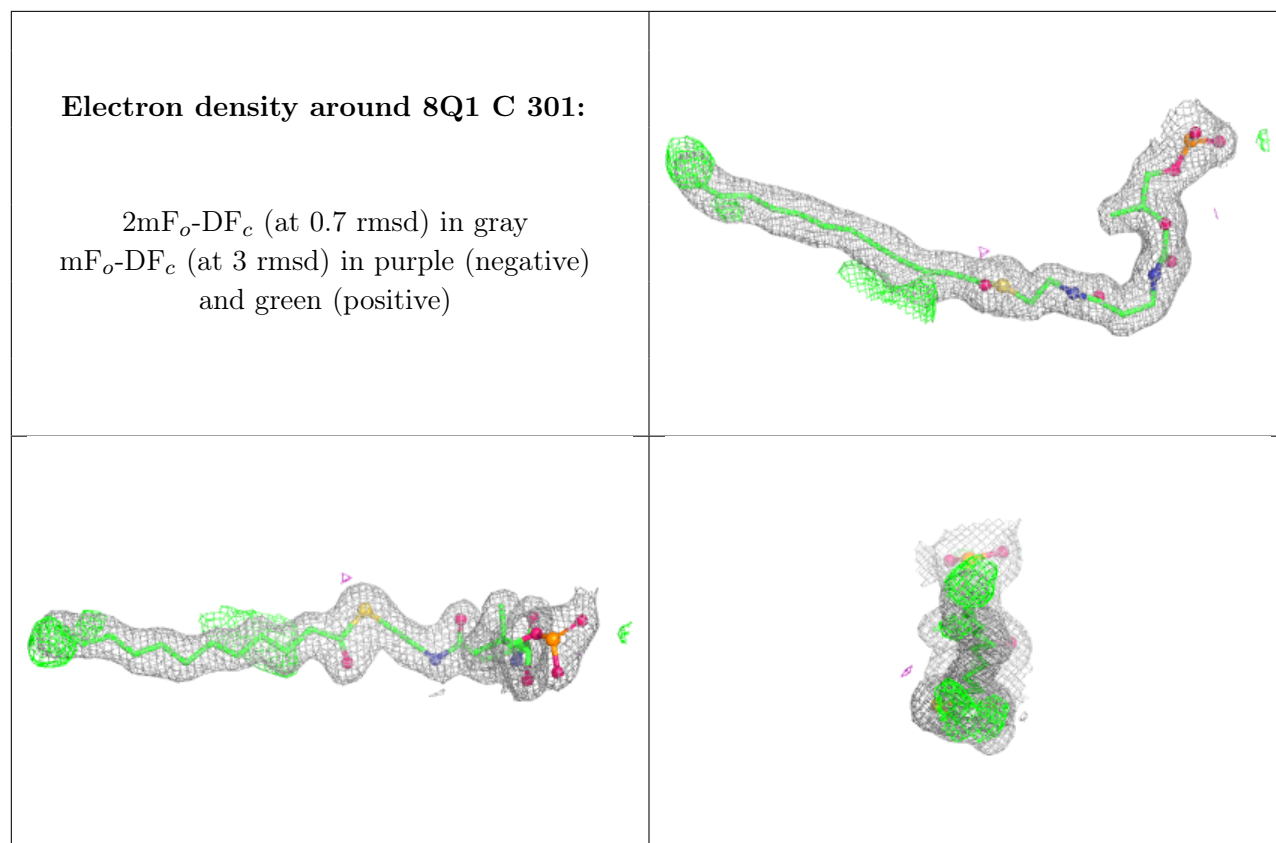
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	538	4/4	0.87	0.15	59,63,68,70	0
6	EDO	C	303	4/4	0.87	0.16	79,81,82,82	0
11	PGE	A	535	10/10	0.88	0.18	35,51,59,59	10
6	EDO	A	514	4/4	0.88	0.17	42,42,45,49	4
6	EDO	A	507	4/4	0.89	0.27	45,46,54,62	0
6	EDO	A	513	4/4	0.90	0.12	42,42,45,46	4
8	PEG	A	522	7/7	0.91	0.11	55,57,63,67	0
6	EDO	A	511	4/4	0.91	0.17	41,46,51,52	4
6	EDO	B	1601	4/4	0.92	0.20	44,47,50,59	0
6	EDO	A	518	4/4	0.92	0.11	25,31,33,33	4
6	EDO	A	503	4/4	0.93	0.16	43,51,52,55	0
14	8Q1	C	301	34/35	0.95	0.09	31,40,48,50	0
6	EDO	A	516	4/4	0.95	0.10	21,24,25,27	4
6	EDO	A	509	4/4	0.96	0.11	17,18,22,25	4
5	PLP	A	501	15/16	0.99	0.03	18,23,29,31	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 1609:

$2mF_o-DF_c$ (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.