



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:42 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 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)
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

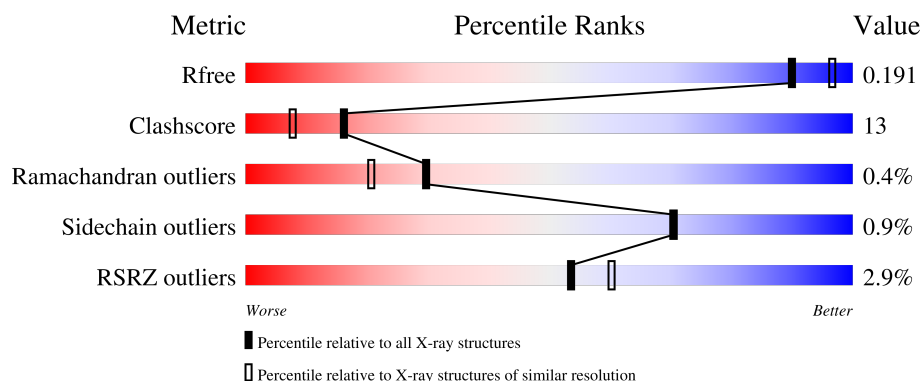
1 Overall quality at a glance

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

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			

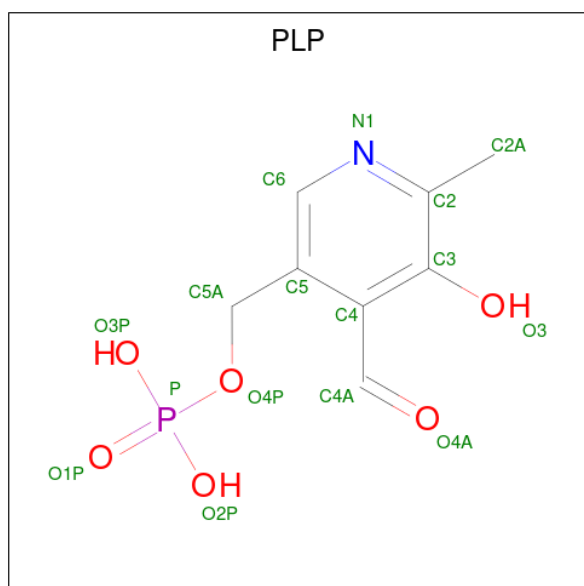
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

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 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	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	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	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

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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: $C_3H_8O_3$).



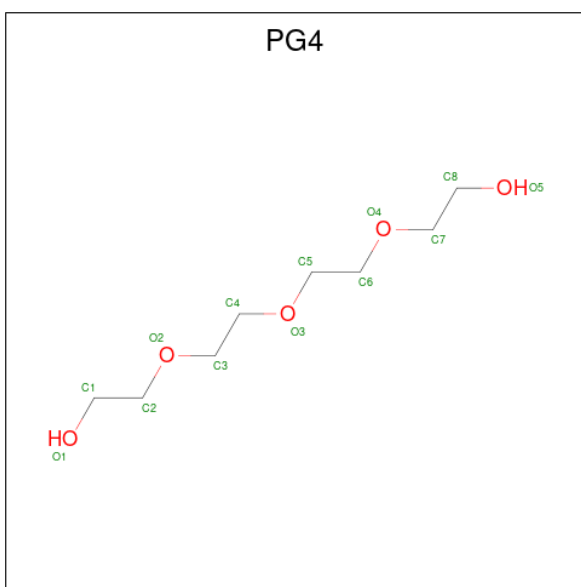
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

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



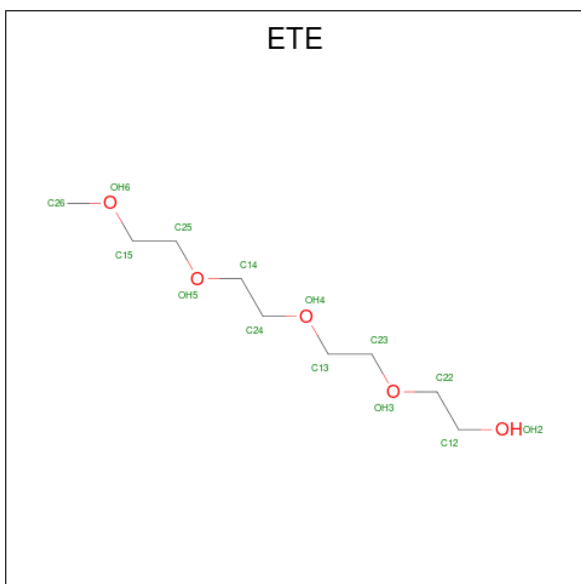
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



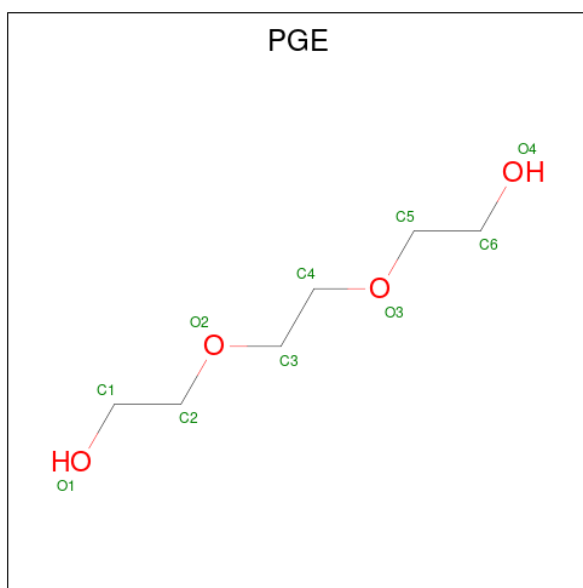
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is 2-{2-[2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: $C_9H_{20}O_5$).



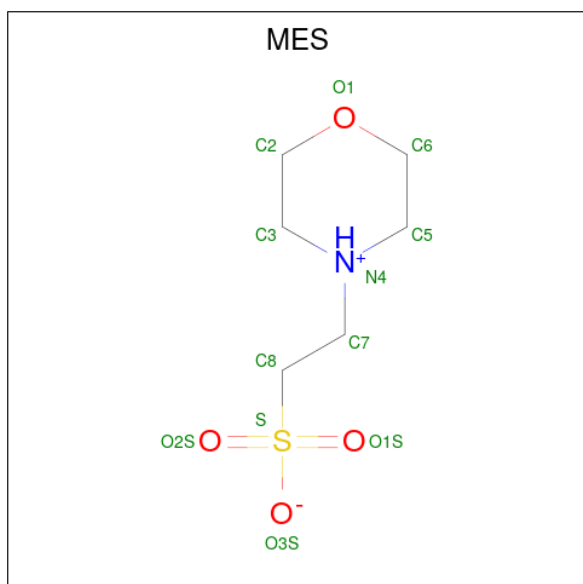
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			14	9	5		

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



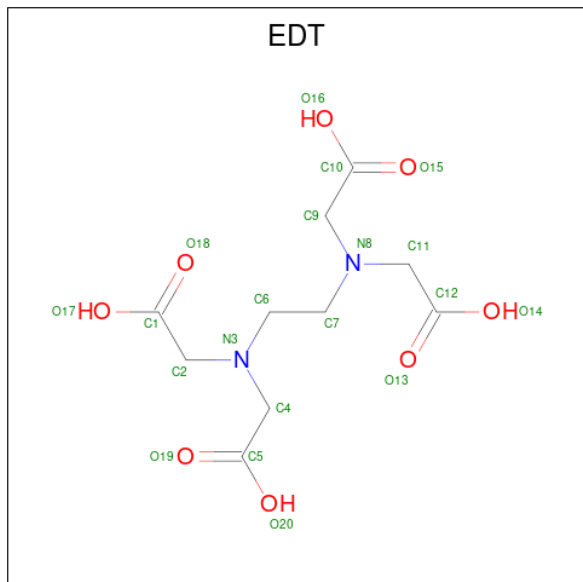
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			10	6	4		

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



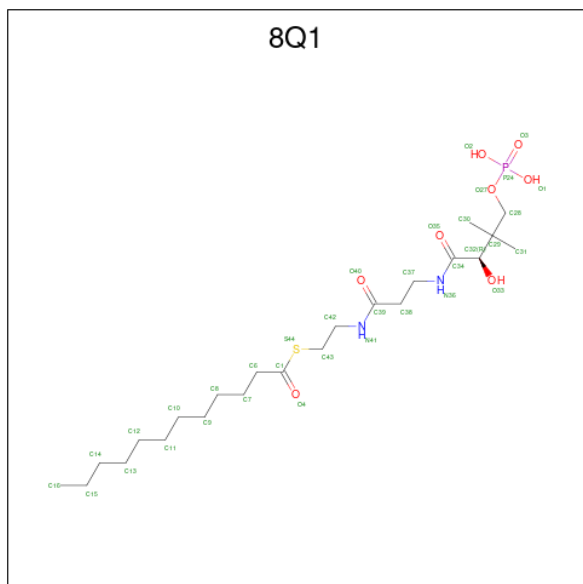
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



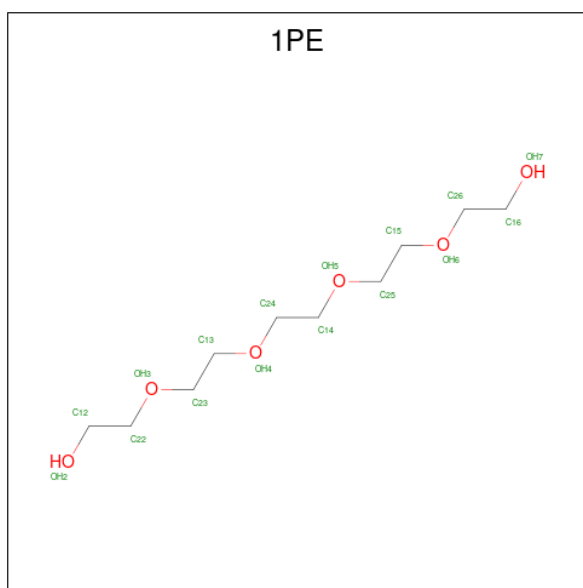
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			17	9	2	6		

- 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

All (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
2	B	37[B]	ARG	CA-C	11.22	1.68	1.52
1	A	149[A]	LEU	N-CA	9.50	1.57	1.45
1	A	149[B]	LEU	N-CA	9.50	1.57	1.45
2	B	34[A]	ARG	CA-C	7.97	1.63	1.52
2	B	34[B]	ARG	CA-C	7.97	1.63	1.52
4	D	69[A]	CYS	CA-C	7.92	1.63	1.52
4	D	69[B]	CYS	CA-C	7.92	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432[A]	ARG	CA-C	7.92	1.63	1.52
1	A	432[B]	ARG	CA-C	7.92	1.63	1.52
1	A	69[A]	LEU	N-CA	7.34	1.55	1.46
1	A	69[B]	LEU	N-CA	7.34	1.55	1.46
1	A	79	PRO	C-O	-6.96	1.15	1.24
1	A	299	PRO	C-O	-6.53	1.16	1.24
1	A	58	PRO	C-O	-6.35	1.16	1.23
1	A	241	PRO	C-O	-6.27	1.16	1.23
1	A	69[A]	LEU	CA-C	6.17	1.61	1.52
1	A	69[B]	LEU	CA-C	6.17	1.61	1.52
1	A	346	PRO	C-O	-6.12	1.16	1.24
1	A	195	PRO	C-O	-6.09	1.16	1.24
1	A	262	PRO	C-O	-5.72	1.17	1.23
1	A	297	PRO	C-O	-5.56	1.16	1.24
4	D	46	PRO	C-O	-5.54	1.17	1.23
1	A	88	PRO	C-O	-5.32	1.16	1.24
4	D	69[A]	CYS	N-CA	5.32	1.53	1.46
4	D	69[B]	CYS	N-CA	5.32	1.53	1.46
1	A	351	PRO	C-O	-5.29	1.17	1.24
1	A	307	ALA	C-O	-5.28	1.18	1.24
1	A	78	LEU	C-O	-5.25	1.19	1.24
1	A	416	GLU	C-O	-5.11	1.18	1.24
1	A	82	ILE	C-O	-5.09	1.18	1.24
1	A	341	VAL	C-O	-5.09	1.19	1.24
1	A	207	ASN	C-O	-5.01	1.17	1.24

All (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
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
2	B	37[A]	ARG	N-CA-C	10.28	123.53	111.71
2	B	37[B]	ARG	N-CA-C	10.28	123.53	111.71
2	B	24[A]	SER	N-CA-C	9.08	122.15	111.71
2	B	24[B]	SER	N-CA-C	9.08	122.15	111.71
1	A	69[A]	LEU	CB-CA-C	-8.57	97.41	110.26
1	A	69[B]	LEU	CB-CA-C	-8.57	97.41	110.26
1	A	291[A]	MET	N-CA-C	8.56	123.54	113.18
1	A	291[B]	MET	N-CA-C	8.56	123.54	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105[A]	ARG	CA-C-O	8.45	129.69	120.82
1	A	105[B]	ARG	CA-C-O	8.45	129.69	120.82
1	A	417[A]	GLU	CA-C-O	6.91	127.91	120.10
1	A	417[B]	GLU	CA-C-O	6.91	127.91	120.10
1	A	417[A]	GLU	N-CA-C	6.90	119.68	111.33
1	A	417[B]	GLU	N-CA-C	6.90	119.68	111.33
1	A	149[A]	LEU	CA-C-O	-6.29	114.00	121.11
1	A	149[B]	LEU	CA-C-O	-6.29	114.00	121.11
2	B	37[A]	ARG	CA-C-O	-5.89	113.44	120.10
2	B	37[B]	ARG	CA-C-O	-5.89	113.44	120.10
2	B	34[A]	ARG	N-CA-C	5.87	118.15	111.11
2	B	34[B]	ARG	N-CA-C	5.87	118.15	111.11
1	A	149[A]	LEU	N-CA-C	5.76	118.93	109.72
1	A	149[B]	LEU	N-CA-C	5.76	118.93	109.72
1	A	105[A]	ARG	N-CA-C	5.41	116.86	111.07
1	A	105[B]	ARG	N-CA-C	5.41	116.86	111.07
1	A	69[A]	LEU	CA-C-O	-5.30	114.43	120.58
1	A	69[B]	LEU	CA-C-O	-5.30	114.43	120.58
1	A	69[A]	LEU	N-CA-C	5.19	117.75	109.96
1	A	69[B]	LEU	N-CA-C	5.19	117.75	109.96

There are no chirality outliers.

All (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
2	B	27[A]	ASN	Mainchain
2	B	27[B]	ASN	Mainchain
2	B	37[A]	ARG	Mainchain
2	B	37[B]	ARG	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
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.

All (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
6:A:509:EDO:H11	4:D:44:GLU:HG2	1.62	0.81
2:B:68:ARG:HH11	8:B:1607:PEG:H22	1.49	0.75
4:D:41:ASP:OD2	16:D:301:HOH:O	2.06	0.72
4:D:114:VAL:O	4:D:118:LEU:CD2	2.38	0.71
4:D:112:LYS:HD3	15:D:204:1PE:H222	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:CYS:SG	4:D:135:LYS:NZ	2.64	0.71
3:C:3:ILE:O	3:C:6:ARG:HG3	1.89	0.70
2:B:41[B]:ARG:NH2	3:C:41:GLU:OE1	2.23	0.70
2:B:37[B]:ARG:NH1	16:B:1701:HOH:O	2.24	0.68
10:A:526:ETE:H132	16:A:813:HOH:O	1.92	0.68
1:A:175:TYR:HD1	6:A:503:EDO:H22	1.59	0.68
1:A:340:VAL:O	10:A:526:ETE:H151	1.95	0.67
1:A:117:ASP:HA	8:A:506:PEG:H41	1.76	0.67
1:A:381:CYS:SG	4:D:135:LYS:CE	2.83	0.67
4:D:80:ASP:OD2	16:D:302:HOH:O	2.12	0.66
1:A:109:GLN:HE22	11:A:535:PGE:C6	2.09	0.66
1:A:413:PHE:HB2	6:B:1601:EDO:H11	1.77	0.65
2:B:29:ARG:NH2	13:B:1609:EDT:H061	2.05	0.65
1:A:337:LEU:O	10:A:526:ETE:H261	1.96	0.65
1:A:248:LYS:HE3	6:A:523:EDO:H22	1.79	0.64
3:C:4:GLU:C	3:C:6:ARG:H	2.06	0.64
4:D:118:LEU:CD2	4:D:150:LEU:HD13	2.28	0.63
1:A:142:TYR:CZ	1:A:228:TYR:HE2	2.17	0.63
1:A:149[A]:LEU:HD12	1:A:199:LEU:HB3	1.80	0.62
4:D:51:SER:H	6:D:203:EDO:C1	2.11	0.62
4:D:114:VAL:O	4:D:118:LEU:HD22	1.99	0.61
4:D:113:THR:OG1	4:D:116:GLU:HG3	2.01	0.61
1:A:340:VAL:HB	10:A:526:ETE:H263	1.83	0.60
6:A:502:EDO:H11	2:B:34[A]:ARG:HE	1.65	0.60
1:A:241:PRO:HD3	8:A:522:PEG:H21	1.84	0.60
3:C:29:VAL:HG21	6:C:302:EDO:H12	1.83	0.60
1:A:181:SER:HB2	1:A:345:ASP:HB2	1.84	0.60
1:A:381:CYS:SG	4:D:135:LYS:HE2	2.42	0.60
1:A:339:ASP:HA	10:A:526:ETE:H241	1.82	0.60
1:A:109:GLN:HE22	11:A:535:PGE:H5	1.67	0.59
1:A:384:ALA:HB3	1:A:386:LEU:HG	1.84	0.59
9:A:520:PG4:H71	16:A:769:HOH:O	2.02	0.59
1:A:179:GLN:NE2	16:A:601:HOH:O	2.08	0.59
1:A:105[A]:ARG:NH2	11:A:535:PGE:H6	2.17	0.59
1:A:109:GLN:HE22	11:A:535:PGE:H62	1.66	0.59
10:A:526:ETE:H252	16:A:756:HOH:O	2.01	0.59
8:A:519:PEG:H22	16:A:858:HOH:O	2.02	0.58
2:B:34[B]:ARG:NE	16:B:1702:HOH:O	2.34	0.58
1:A:109:GLN:HE22	11:A:535:PGE:C5	2.17	0.58
4:D:118:LEU:HD22	4:D:150:LEU:HD13	1.85	0.57
1:A:196:ASP:OD1	1:A:196:ASP:N	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HE2	16:A:659:HOH:O	2.06	0.56
1:A:371:LYS:CD	6:A:509:EDO:H22	2.31	0.55
1:A:420:ASP:OD2	6:A:530:EDO:H11	2.07	0.55
1:A:432[A]:ARG:HH12	8:A:539:PEG:H42	1.72	0.54
1:A:432[B]:ARG:HE	6:A:534:EDO:C2	2.21	0.53
8:A:540:PEG:H21	16:A:856:HOH:O	2.08	0.53
2:B:67:ARG:HB3	8:B:1607:PEG:H41	1.91	0.53
11:A:535:PGE:H2	16:B:1755:HOH:O	2.09	0.53
2:B:27[B]:ASN:ND2	6:B:1601:EDO:O2	2.31	0.52
4:D:50:GLY:HA3	6:D:203:EDO:H12	1.91	0.52
3:C:3:ILE:HG23	3:C:5:GLU:HB2	1.92	0.52
2:B:68:ARG:HD3	8:B:1607:PEG:H22	1.91	0.51
1:A:349:HIS:H	6:A:538:EDO:H21	1.75	0.51
1:A:421:TYR:OH	16:A:602:HOH:O	2.16	0.51
4:D:38[B]:GLN:CD	4:D:38[B]:GLN:H	2.18	0.51
1:A:400:ASP:N	1:A:400:ASP:OD1	2.42	0.51
2:B:41[A]:ARG:NH1	12:B:1604:MES:O1S	2.43	0.51
1:A:432[B]:ARG:HE	6:A:534:EDO:H21	1.75	0.50
1:A:160:LEU:O	1:A:164:ARG:HD3	2.11	0.50
1:A:292:ARG:NH1	6:A:516:EDO:H11	2.26	0.50
1:A:321[A]:ARG:HD3	16:A:754:HOH:O	2.11	0.50
3:C:4:GLU:C	3:C:6:ARG:N	2.70	0.49
1:A:306:ALA:CB	11:A:535:PGE:H52	2.43	0.49
4:D:38[B]:GLN:NE2	4:D:130:CYS:HB2	2.28	0.48
2:B:41[B]:ARG:NE	16:B:1707:HOH:O	2.47	0.48
4:D:114:VAL:HG13	4:D:150:LEU:HD22	1.96	0.48
1:A:284:GLY:HA3	1:A:293:SER:HB3	1.96	0.48
1:A:164:ARG:HH22	6:A:512:EDO:H12	1.78	0.48
1:A:371:LYS:HD3	6:A:509:EDO:C2	2.35	0.47
1:A:68:PRO:HG3	6:B:1601:EDO:H22	1.97	0.47
4:D:134:VAL:HG13	16:D:336:HOH:O	2.13	0.47
1:A:105[A]:ARG:HH22	11:A:535:PGE:H6	1.79	0.47
2:B:29:ARG:HE	13:B:1609:EDT:H091	1.79	0.47
4:D:133:PRO:HA	4:D:136:LEU:HG	1.96	0.47
1:A:339:ASP:OD1	10:A:526:ETE:H131	2.14	0.47
4:D:114:VAL:O	4:D:118:LEU:HD23	2.15	0.46
4:D:112:LYS:HD3	15:D:204:1PE:C22	2.43	0.46
1:A:105[A]:ARG:CZ	11:A:535:PGE:H6	2.46	0.46
1:A:432[A]:ARG:NH1	8:A:539:PEG:H42	2.31	0.46
6:A:509:EDO:H12	4:D:43:TYR:CE2	2.50	0.45
1:A:350:TYR:CD1	1:A:351:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLN:HB3	1:A:195:PRO:CD	2.46	0.45
6:A:509:EDO:H12	4:D:43:TYR:CD2	2.52	0.44
1:A:137:GLY:HA3	1:A:278:VAL:CG1	2.48	0.44
1:A:360:TYR:CD2	1:A:440:TRP:HE3	2.36	0.44
1:A:183:ILE:HD12	6:A:518:EDO:H21	2.00	0.44
1:A:201:SER:HA	1:A:230:HIS:O	2.18	0.44
1:A:329:LEU:C	1:A:329:LEU:HD23	2.41	0.44
2:B:71[B]:HIS:CE1	16:B:1705:HOH:O	2.70	0.44
8:A:529:PEG:H31	8:A:529:PEG:H12	1.79	0.44
1:A:367:LEU:HD11	1:A:377:SER:HB3	1.98	0.44
4:D:112:LYS:HB3	4:D:116:GLU:HB2	2.00	0.44
1:A:250:ASP:HB3	1:A:276:VAL:HG21	1.99	0.43
3:C:5:GLU:C	3:C:7:VAL:N	2.73	0.43
1:A:384:ALA:HB3	1:A:386:LEU:CD1	2.47	0.43
4:D:112:LYS:HE3	15:D:204:1PE:H142	2.00	0.43
1:A:449:LEU:C	1:A:451:SER:H	2.26	0.43
11:A:535:PGE:H5	11:A:535:PGE:H32	1.76	0.43
1:A:299:PRO:HG2	6:A:507:EDO:H12	2.01	0.43
1:A:413:PHE:HB3	2:B:27[A]:ASN:HB3	2.00	0.43
6:A:538:EDO:H22	16:A:841:HOH:O	2.18	0.43
6:B:1606:EDO:O1	8:B:1607:PEG:H32	2.19	0.43
1:A:272:ARG:HH12	6:A:524:EDO:H21	1.84	0.43
1:A:339:ASP:HA	10:A:526:ETE:C24	2.48	0.43
1:A:428:GLN:O	1:A:432[B]:ARG:HG3	2.19	0.42
9:A:520:PG4:H12	16:A:635:HOH:O	2.19	0.42
1:A:109:GLN:NE2	11:A:535:PGE:H5	2.33	0.42
1:A:164:ARG:HD2	1:A:175:TYR:OH	2.19	0.42
1:A:384:ALA:HB3	1:A:386:LEU:CG	2.48	0.42
2:B:5:SER:O	2:B:9:VAL:HG23	2.20	0.42
1:A:306:ALA:HB2	11:A:535:PGE:H52	2.02	0.42
8:A:506:PEG:H42	6:A:528:EDO:H12	2.01	0.42
13:B:1609:EDT:H072	13:B:1609:EDT:O14	2.19	0.42
1:A:186:LEU:HD21	1:A:214:PRO:HG2	2.01	0.42
1:A:292:ARG:CZ	6:A:516:EDO:H11	2.50	0.42
3:C:11:ILE:HD13	3:C:65:VAL:HG22	2.02	0.42
3:C:4:GLU:O	3:C:7:VAL:HG23	2.20	0.41
1:A:151:THR:OG1	1:A:155:GLU:HG3	2.20	0.41
4:D:87:ASP:HA	4:D:110:LYS:HD3	2.03	0.41
1:A:417[B]:GLU:HA	6:A:530:EDO:H12	2.02	0.41
1:A:424:GLU:CD	6:A:532:EDO:H12	2.45	0.41
2:B:35:ARG:HD2	2:B:35:ARG:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD12	1:A:122:ILE:N	2.35	0.41
1:A:208:GLU:OE1	1:A:389:SER:OG	2.25	0.41
1:A:292:ARG:HH12	6:A:516:EDO:C2	2.34	0.41
13:B:1609:EDT:H062	13:B:1609:EDT:H092	1.22	0.41
1:A:105[B]:ARG:HD3	16:A:604:HOH:O	2.20	0.41
1:A:119:ARG:HH12	6:A:524:EDO:H12	1.86	0.41
1:A:321[A]:ARG:NH1	2:B:34[A]:ARG:CZ	2.84	0.41
11:A:535:PGE:H62	16:A:712:HOH:O	2.19	0.41
2:B:68:ARG:HH11	8:B:1607:PEG:C2	2.28	0.41
4:D:118:LEU:HD21	4:D:150:LEU:HD13	2.03	0.41
1:A:340:VAL:H	10:A:526:ETE:C26	2.34	0.41
4:D:118:LEU:HD22	4:D:118:LEU:N	2.36	0.40
1:A:142:TYR:CE1	1:A:228:TYR:HE2	2.39	0.40
1:A:386:LEU:HB2	1:A:387:GLU:H	1.47	0.40
1:A:292:ARG:NH2	6:A:516:EDO:H11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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

Mol	Chain	Res	Type
1	A	143	ARG
1	A	149[A]	LEU
1	A	149[B]	LEU
2	B	41[A]	ARG
2	B	41[B]	ARG
4	D	47	ARG
4	D	157	GLN

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

All (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
14	C	301	8Q1	C12-C13	-3.04	1.36	1.51
5	A	501	PLP	C2A-C2	3.00	1.55	1.50
12	B	1604	MES	C7-N4	2.65	1.53	1.47
12	B	1604	MES	O1S-S	2.54	1.52	1.45
14	C	301	8Q1	C15-C14	-2.48	1.36	1.51
5	A	501	PLP	C6-N1	2.41	1.39	1.34
12	B	1604	MES	C7-C8	2.11	1.57	1.52
14	C	301	8Q1	C38-C39	2.08	1.55	1.51
14	C	301	8Q1	C28-C29	2.06	1.56	1.52
6	A	509	EDO	O1-C1	-2.01	1.31	1.42

All (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
12	B	1604	MES	O2S-S-C8	3.04	111.32	106.73
14	C	301	8Q1	O40-C39-N41	-2.91	117.31	123.03
13	B	1609	EDT	C11-N8-C9	2.53	117.59	111.66
13	B	1609	EDT	O14-C12-O13	-2.45	117.03	123.33
14	C	301	8Q1	C8-C7-C6	-2.44	104.17	113.13
12	B	1604	MES	O3S-S-C8	2.43	110.75	106.00
13	B	1609	EDT	O14-C12-C11	2.37	122.73	113.38
13	B	1609	EDT	C11-N8-C7	2.37	117.62	111.91
14	C	301	8Q1	C16-C15-C14	2.19	128.13	113.36
14	C	301	8Q1	C11-C12-C13	2.17	125.36	114.37
7	A	508	GOL	C3-C2-C1	-2.16	103.87	111.80
6	A	516	EDO	O2-C2-C1	-2.13	96.20	112.39
5	A	501	PLP	C5-C6-N1	-2.11	120.41	123.83
14	C	301	8Q1	C7-C6-C1	2.09	116.89	112.27
7	A	508	GOL	O2-C2-C1	2.07	117.74	109.18

There are no chirality outliers.

All (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
8	A	539	PEG	C4-C3-O2-C2
8	A	505	PEG	C1-C2-O2-C3
13	B	1609	EDT	O18-C1-C2-N3
13	B	1609	EDT	O17-C1-C2-N3
13	B	1609	EDT	O16-C10-C9-N8
10	A	526	ETE	OH4-C13-C23-OH3
15	D	204	1PE	OH6-C15-C25-OH5
9	A	521	PG4	O2-C3-C4-O3
10	A	526	ETE	OH6-C15-C25-OH5
9	A	521	PG4	O3-C5-C6-O4
15	D	204	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
13	B	1609	EDT	O15-C10-C9-N8
8	A	537	PEG	O2-C3-C4-O4
9	A	521	PG4	O1-C1-C2-O2
11	A	535	PGE	C3-C4-O3-C5
13	B	1609	EDT	N3-C6-C7-N8
8	A	505	PEG	O2-C3-C4-O4
9	A	520	PG4	O1-C1-C2-O2
9	A	520	PG4	O4-C7-C8-O5
7	A	504	GOL	O1-C1-C2-C3
7	A	504	GOL	C1-C2-C3-O3
8	A	519	PEG	O1-C1-C2-O2
8	A	522	PEG	O1-C1-C2-O2
8	A	522	PEG	O2-C3-C4-O4
8	A	537	PEG	O1-C1-C2-O2
7	A	504	GOL	O1-C1-C2-O2
7	A	504	GOL	O2-C2-C3-O3
6	C	302	EDO	O1-C1-C2-O2
11	A	535	PGE	O2-C3-C4-O3
13	B	1609	EDT	C7-C6-N3-C2
8	A	539	PEG	O1-C1-C2-O2
8	A	529	PEG	O2-C3-C4-O4
6	A	503	EDO	O1-C1-C2-O2
6	A	511	EDO	O1-C1-C2-O2
6	A	514	EDO	O1-C1-C2-O2
6	A	516	EDO	O1-C1-C2-O2
6	A	528	EDO	O1-C1-C2-O2
6	A	531	EDO	O1-C1-C2-O2
6	B	1605	EDO	O1-C1-C2-O2
12	B	1604	MES	C8-C7-N4-C5
15	D	204	1PE	OH7-C16-C26-OH6
9	A	520	PG4	O3-C5-C6-O4
9	A	520	PG4	C4-C3-O2-C2
9	A	520	PG4	C6-C5-O3-C4
15	D	204	1PE	C15-C25-OH5-C14
9	A	520	PG4	C5-C6-O4-C7
8	B	1607	PEG	C4-C3-O2-C2
8	A	537	PEG	C1-C2-O2-C3
9	A	521	PG4	C5-C6-O4-C7
15	D	204	1PE	C24-C14-OH5-C25
8	A	506	PEG	O1-C1-C2-O2
8	A	537	PEG	C4-C3-O2-C2
15	D	204	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
8	A	540	PEG	C4-C3-O2-C2
8	A	527	PEG	C1-C2-O2-C3
8	A	529	PEG	C1-C2-O2-C3
6	A	515	EDO	O1-C1-C2-O2
6	A	533	EDO	O1-C1-C2-O2
6	C	303	EDO	O1-C1-C2-O2
8	B	1607	PEG	O1-C1-C2-O2
13	B	1609	EDT	C12-C11-N8-C9
10	A	526	ETE	C23-C13-OH4-C24
11	A	535	PGE	O1-C1-C2-O2
6	A	538	EDO	O1-C1-C2-O2
6	A	509	EDO	O1-C1-C2-O2
9	A	520	PG4	C3-C4-O3-C5
7	D	205	GOL	O1-C1-C2-O2
13	B	1609	EDT	N8-C11-C12-O13
6	A	523	EDO	O1-C1-C2-O2
6	A	524	EDO	O1-C1-C2-O2
6	A	530	EDO	O1-C1-C2-O2
6	B	1603	EDO	O1-C1-C2-O2
13	B	1609	EDT	C1-C2-N3-C4
15	D	204	1PE	OH5-C14-C24-OH4
13	B	1609	EDT	N8-C11-C12-O14
15	D	204	1PE	C23-C13-OH4-C24
6	A	518	EDO	O1-C1-C2-O2
15	D	204	1PE	C14-C24-OH4-C13
8	A	527	PEG	O1-C1-C2-O2
8	A	505	PEG	O1-C1-C2-O2
8	A	506	PEG	C4-C3-O2-C2

There are no ring outliers.

32 monomers are involved in 79 short contacts:

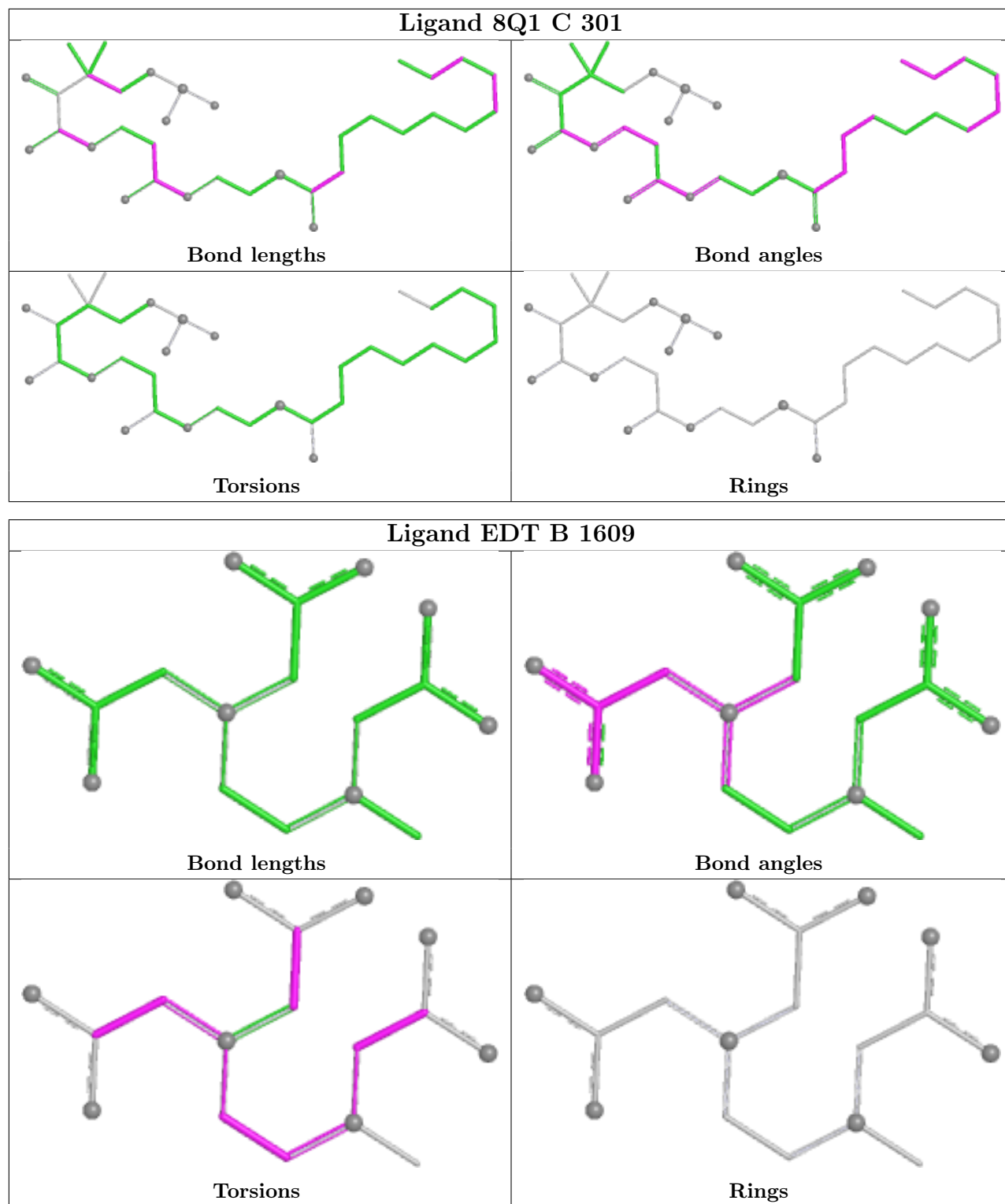
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1606	EDO	1	0
6	A	532	EDO	1	0
6	C	302	EDO	1	0
6	A	502	EDO	1	0
10	A	526	ETE	9	0
6	A	534	EDO	2	0
6	A	530	EDO	2	0
11	A	535	PGE	13	0
6	A	507	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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%)

All (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
4	D	159	PRO	4.5
4	D	158	GLU	4.3
1	A	383	SER	3.6
3	C	3	ILE	3.2
3	C	2	THR	3.0
1	A	54	SER	2.9
1	A	387	GLU	2.7
1	A	450	LYS	2.6
1	A	378	GLY	2.5
3	C	5	GLU	2.5
3	C	22	VAL	2.5
1	A	400	ASP	2.4
2	B	85	ASN	2.2
1	A	388	PRO	2.1
1	A	402	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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

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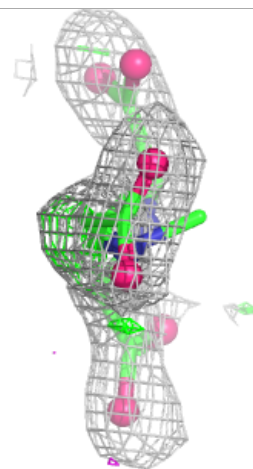
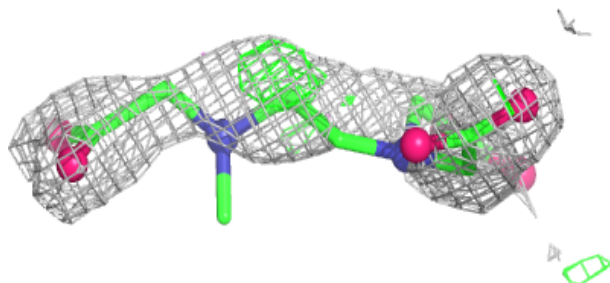
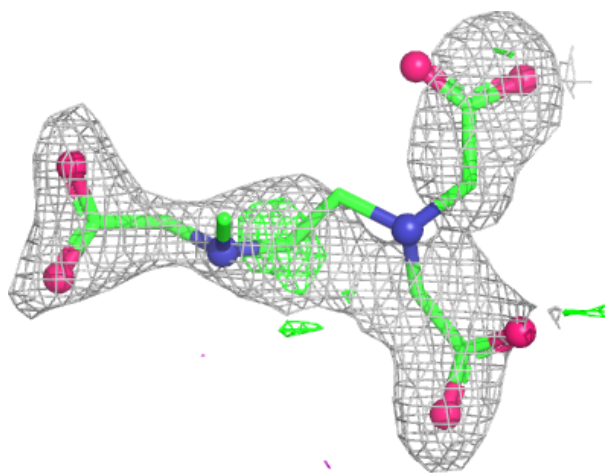
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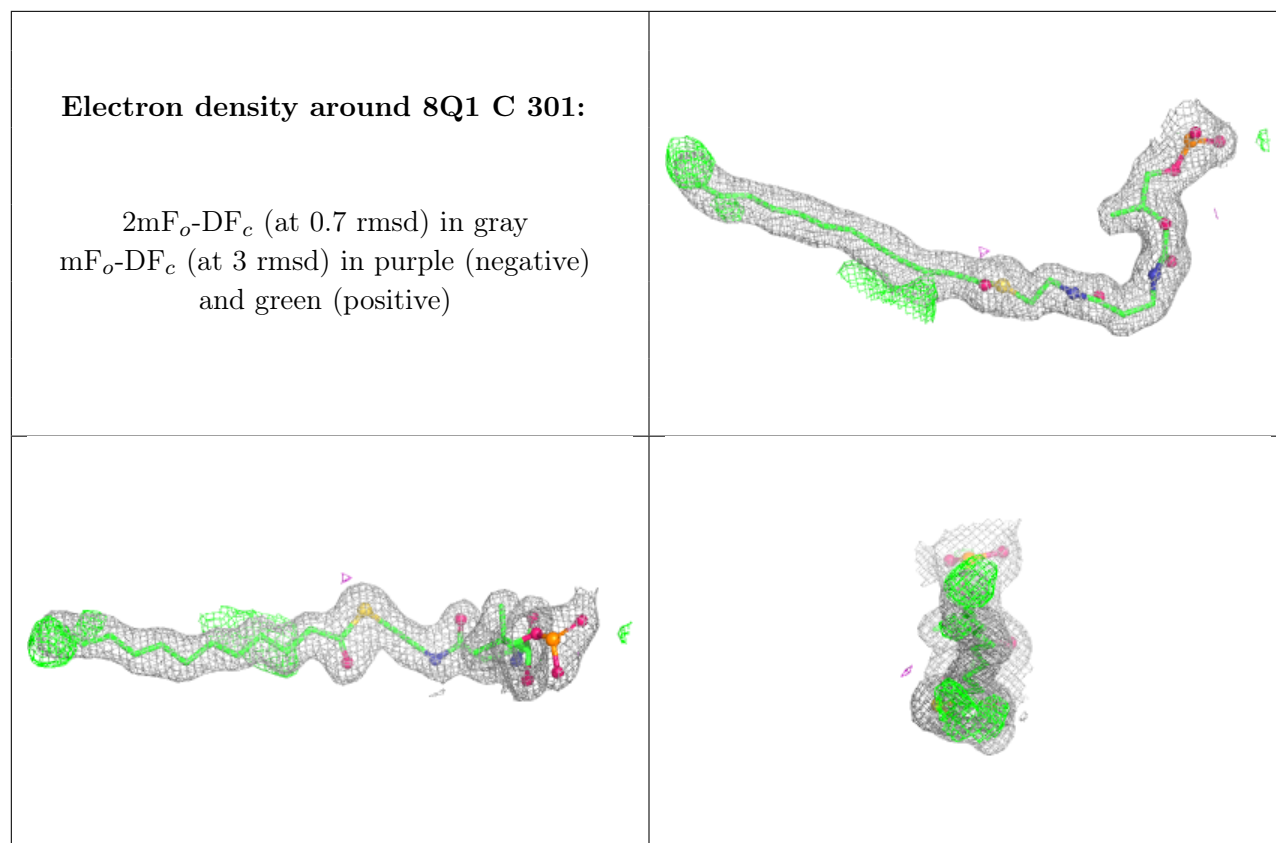
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	528	4/4	0.83	0.20	41,43,44,45	4
10	ETE	A	526	14/14	0.83	0.19	36,83,90,90	0
6	EDO	A	532	4/4	0.83	0.16	79,80,80,80	0
6	EDO	B	1606	4/4	0.83	0.18	73,73,74,74	0
8	PEG	A	505	7/7	0.84	0.20	58,66,76,76	0
6	EDO	B	1605	4/4	0.84	0.15	54,63,67,71	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
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.