



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:08 PM UTC

PDB ID : 8QEU / pdb_00008qeu
Title : Crystal structure of ornithine transcarbamylase from Arabidopsis thaliana (AtOTC) in complex with ornithine
Authors : Nielipinski, M.; Pietrzyk-Brzezinska, A.; Sekula, B.
Deposited on : 2023-09-01
Resolution : 1.50 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)
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

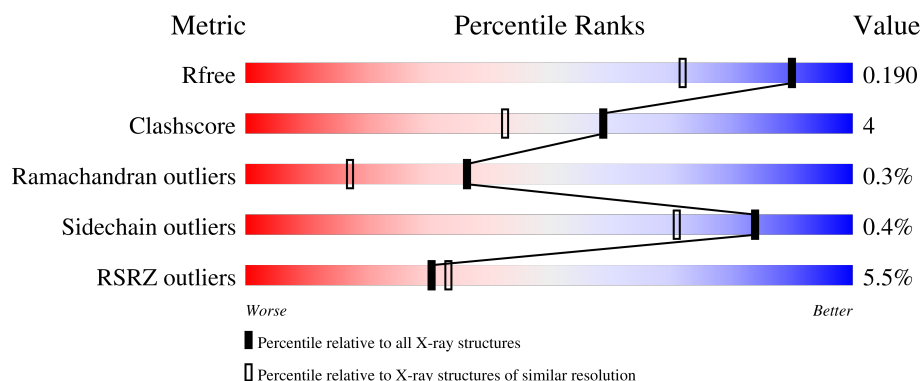
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

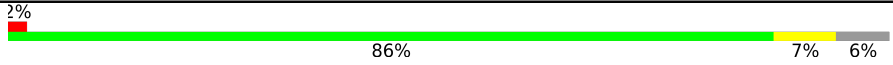
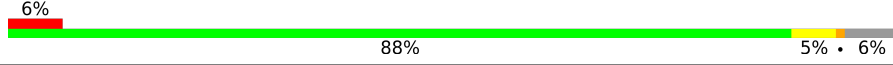
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	324	
1	B	324	
1	C	324	

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
2	ORN	C	404	-	-	X	-
4	EDO	A	408	-	-	X	-
4	EDO	B	403	-	-	X	-
4	EDO	C	403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8700 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.

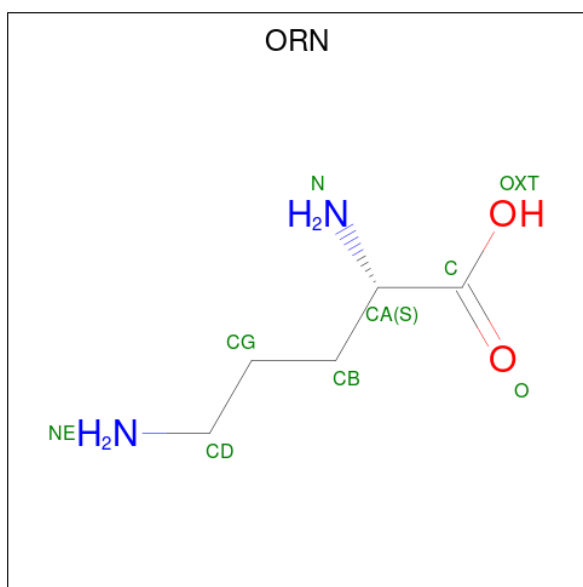
- Molecule 1 is a protein called Ornithine transcarbamylase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	10	0
			2431	1549	416	447	19			
1	B	304	Total	C	N	O	S	0	9	0
			2420	1542	412	448	18			
1	C	304	Total	C	N	O	S	0	10	0
			2425	1544	415	449	17			

There are 6 discrepancies between the modelled and reference sequences:

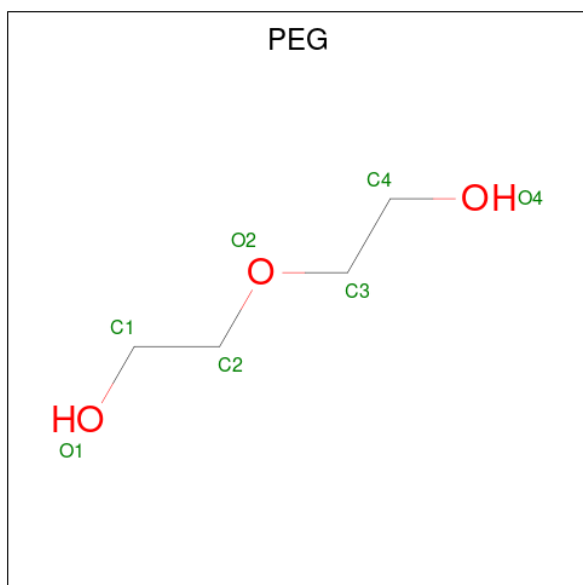
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	-	expression tag	UNP O50039
A	53	ASN	-	expression tag	UNP O50039
B	52	SER	-	expression tag	UNP O50039
B	53	ASN	-	expression tag	UNP O50039
C	52	SER	-	expression tag	UNP O50039
C	53	ASN	-	expression tag	UNP O50039

- Molecule 2 is L-ornithine (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



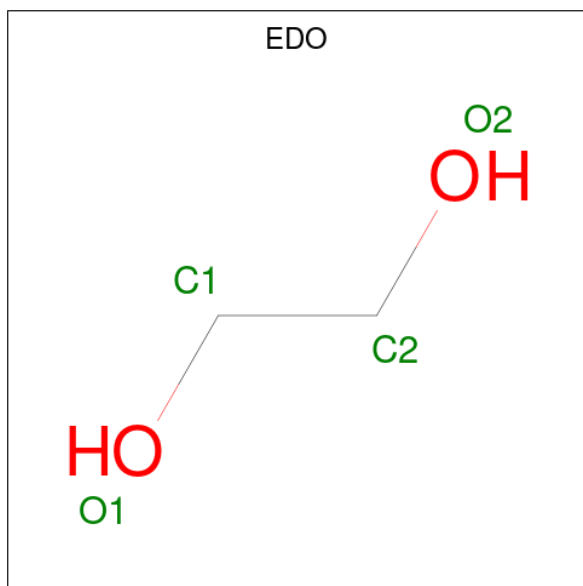
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	2	2		
2	B	1	Total	C	N	O	0	0
			9	5	2	2		
2	C	1	Total	C	N	O	0	0
			9	5	2	2		
2	C	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



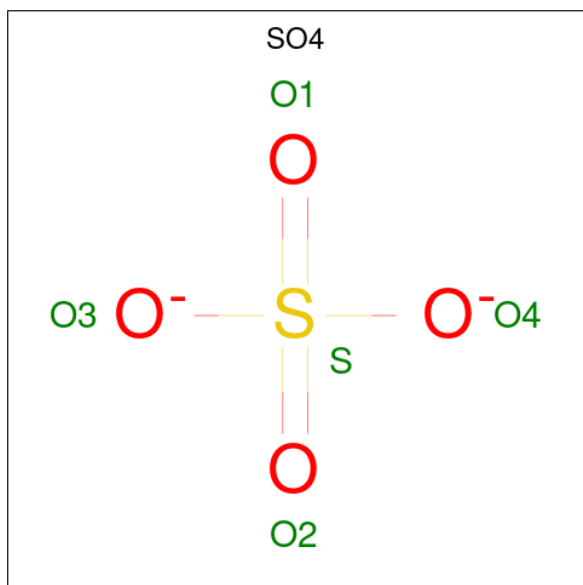
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Na 2	0	0
6	B	1	Total 1	Na 1	0	0
6	C	1	Total 1	Na 1	0	0

- Molecule 7 is water.

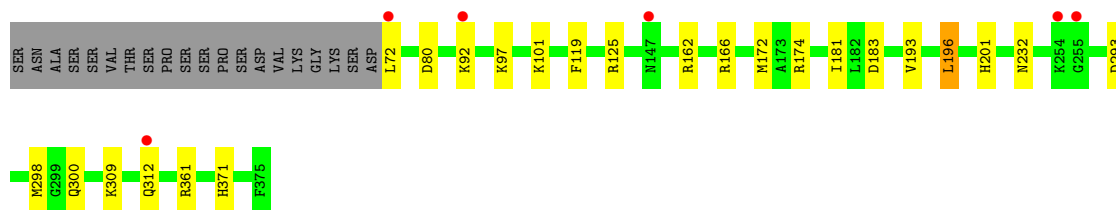
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	427	Total 429	O 429	0	2
7	B	426	Total 428	O 428	0	2
7	C	425	Total 428	O 428	0	3

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.

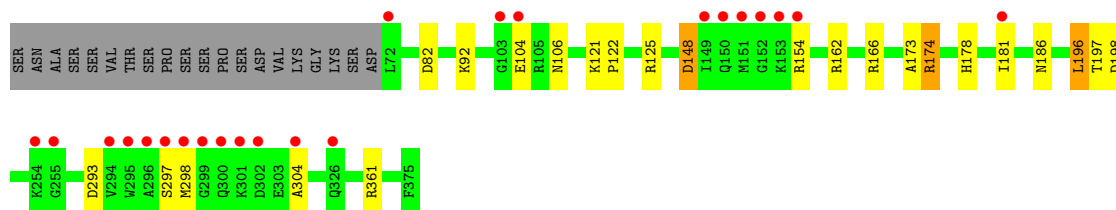
- Molecule 1: Ornithine transcarbamylase, chloroplastic

Chain A: 



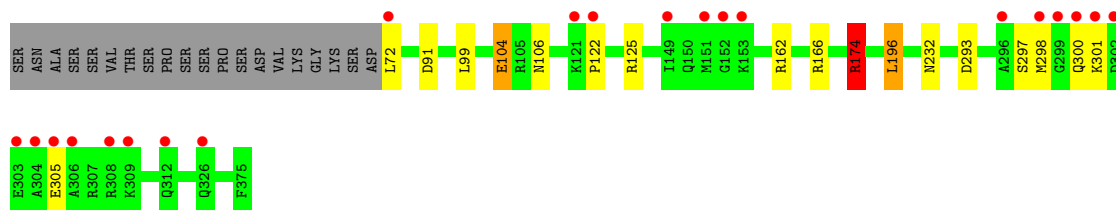
- Molecule 1: Ornithine transcarbamylase, chloroplastic

Chain B: 



- Molecule 1: Ornithine transcarbamylase, chloroplastic

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.31Å 155.38Å 189.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 1.50 49.02 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-1.50) 99.6 (49.02-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.119 , 0.156 0.168 , 0.190	Depositor DCC
R_{free} test set	1043 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.115 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.099 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8700	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: ORN, NA, EDO, PEG, SO4

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	0.76	0/2504	0.96	4/3377 (0.1%)
1	B	0.74	0/2493	0.99	5/3364 (0.1%)
1	C	0.78	2/2504 (0.1%)	1.00	5/3380 (0.1%)
All	All	0.76	2/7501 (0.0%)	0.98	14/10121 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174[A]	ARG	C-O	7.38	1.32	1.24
1	C	174[B]	ARG	C-O	7.38	1.32	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	GLU	CB-CA-C	6.66	121.72	109.46
1	C	293	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	293	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	174[A]	ARG	CA-C-O	6.08	126.96	120.46
1	C	174[B]	ARG	CA-C-O	6.08	126.96	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ASP	CA-C-N	-5.96	111.25	121.97
1	B	148	ASP	C-N-CA	-5.96	111.25	121.97
1	B	198	ASP	CA-CB-CG	5.83	118.42	112.60
1	A	293	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	91	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	183	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	300	GLN	CB-CA-C	-5.26	102.22	110.85
1	A	300	GLN	CG-CD-NE2	-5.08	108.79	116.40
1	B	82	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	174	ARG	Sidechain
1	A	361	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	361	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	174[A]	ARG	Sidechain
1	C	174[B]	ARG	Sidechain

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	2431	0	2447	18	0
1	B	2420	0	2430	23	0
1	C	2425	0	2435	21	0
2	A	9	0	11	0	0
2	B	9	0	11	0	0
2	C	18	0	22	11	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	30	7	0
4	B	12	0	18	6	0
4	C	16	0	24	6	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	C	15	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	429	0	0	2	0
7	B	428	0	0	4	0
7	C	428	0	0	7	0
All	All	8700	0	7458	65	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 4.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HA	7:C:529:HOH:O	1.54	1.06
1:B:104:GLU:OE2	1:B:106[A]:ASN:HB2	1.63	0.98
1:C:99:LEU:HD11	2:C:404:ORN:HD3	1.49	0.93
1:A:298:MET:HG2	7:A:799:HOH:O	1.70	0.89
1:C:104:GLU:HB3	2:C:404:ORN:C	2.05	0.86
1:B:104:GLU:OE2	1:B:106[A]:ASN:CB	2.30	0.79
1:C:166:ARG:HE	4:C:403:EDO:C2	2.03	0.72
1:A:166:ARG:HE	4:A:408:EDO:H11	1.57	0.70
1:C:162:ARG:HB3	4:C:403:EDO:H12	1.74	0.69
1:B:162:ARG:HB3	4:B:403:EDO:H12	1.73	0.69
1:A:162:ARG:HB3	4:A:408:EDO:H12	1.76	0.67
1:B:298:MET:HB2	1:B:304:ALA:HB2	1.78	0.65
1:B:297:SER:O	1:B:298:MET:HE2	1.96	0.65
1:B:92[B]:LYS:HG2	7:B:696:HOH:O	1.98	0.63
1:B:166:ARG:HE	4:B:403:EDO:C2	2.12	0.62
1:C:72:LEU:HB3	7:C:564:HOH:O	1.99	0.62
1:C:166:ARG:HE	4:C:403:EDO:H22	1.65	0.61
1:B:166:ARG:HE	4:B:403:EDO:H22	1.66	0.60
1:A:196[B]:LEU:HD11	1:A:232:ASN:ND2	2.16	0.60
2:C:404:ORN:NE	7:C:502:HOH:O	2.31	0.60
1:A:309:LYS:O	1:A:312[B]:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92[B]:LYS:HG2	7:A:683:HOH:O	2.03	0.58
1:C:72:LEU:HD13	7:C:564:HOH:O	2.04	0.58
1:C:166:ARG:HE	4:C:403:EDO:C1	2.17	0.57
1:A:92[A]:LYS:HZ1	1:A:371:HIS:N	2.03	0.56
1:C:298:MET:HA	1:C:301:LYS:HE3	1.86	0.56
1:B:173:ALA:HB3	1:B:181:ILE:CD1	2.36	0.56
1:A:166:ARG:HH21	4:A:408:EDO:H22	1.70	0.55
1:B:166:ARG:HE	4:B:403:EDO:H11	1.72	0.54
2:C:404:ORN:HB3	7:C:627:HOH:O	2.09	0.53
1:C:166:ARG:HE	4:C:403:EDO:H11	1.73	0.53
1:C:196[B]:LEU:CD1	2:C:401:ORN:HG3	2.40	0.52
1:B:178:HIS:O	1:B:181:ILE:HG22	2.11	0.51
1:C:104:GLU:HB3	2:C:404:ORN:CA	2.39	0.51
1:C:196[A]:LEU:HD11	1:C:232:ASN:ND2	2.26	0.51
1:B:166:ARG:HE	4:B:403:EDO:C1	2.23	0.51
1:A:166:ARG:HE	4:A:408:EDO:C1	2.25	0.49
1:A:97:LYS:O	1:A:101:LYS:HG2	2.12	0.49
1:B:104:GLU:OE2	1:B:106[A]:ASN:CG	2.55	0.49
1:A:172[B]:MET:HG2	1:A:193[B]:VAL:HG13	1.96	0.48
1:B:196[B]:LEU:HD23	1:B:197:THR:N	2.30	0.47
1:A:119:PHE:CE1	1:A:172[B]:MET:HE1	2.50	0.47
1:C:174[B]:ARG:HD3	7:C:506:HOH:O	2.14	0.47
1:B:186:ASN:HB3	7:B:754:HOH:O	2.14	0.46
1:B:104:GLU:OE1	7:B:501:HOH:O	2.21	0.46
1:B:298:MET:HB2	1:B:304:ALA:CB	2.46	0.45
1:C:106[A]:ASN:HB2	2:C:404:ORN:OXT	2.16	0.45
1:A:162:ARG:CB	4:A:408:EDO:H12	2.45	0.45
1:C:162:ARG:CB	4:C:403:EDO:H12	2.43	0.45
1:C:297:SER:O	1:C:300:GLN:HG2	2.18	0.44
1:B:162:ARG:CB	4:B:403:EDO:H12	2.43	0.44
1:A:166:ARG:HE	4:A:408:EDO:H22	1.82	0.43
1:C:106[A]:ASN:CB	2:C:404:ORN:OXT	2.66	0.43
1:C:104:GLU:CB	2:C:404:ORN:HB3	2.49	0.43
2:C:404:ORN:HG2	7:C:627:HOH:O	2.18	0.43
1:A:196[A]:LEU:HD12	1:A:201:HIS:CD2	2.55	0.42
1:B:154:ARG:O	1:B:154:ARG:HG2	2.20	0.42
1:A:72:LEU:HD11	1:A:80:ASP:O	2.20	0.42
1:B:121:LYS:HB3	1:B:122:PRO:HD2	2.01	0.41
1:A:166:ARG:NE	4:A:408:EDO:H11	2.31	0.41
1:B:154:ARG:NH1	7:B:520:HOH:O	2.53	0.41
1:B:148:ASP:HA	1:C:122:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CZ	1:A:172[B]:MET:HE1	2.56	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	312/324 (96%)	301 (96%)	9 (3%)	2 (1%)	21	6
1	B	311/324 (96%)	297 (96%)	12 (4%)	2 (1%)	21	6
1	C	312/324 (96%)	302 (97%)	8 (3%)	2 (1%)	21	6
All	All	935/972 (96%)	900 (96%)	29 (3%)	6 (1%)	36	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196[A]	LEU
1	A	196[B]	LEU
1	B	196[A]	LEU
1	B	196[B]	LEU
1	C	196[A]	LEU
1	C	196[B]	LEU

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	263/271 (97%)	262 (100%)	1 (0%)	84	71
1	B	262/271 (97%)	261 (100%)	1 (0%)	84	71
1	C	263/271 (97%)	262 (100%)	1 (0%)	84	71
All	All	788/813 (97%)	785 (100%)	3 (0%)	84	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ILE
1	B	174	ARG
1	C	305	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	278	ASN
1	A	315	GLN
1	C	278	ASN
1	C	300	GLN
1	C	315	GLN
1	C	326	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 for Mogul analysis.

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
4	EDO	B	403	-	3,3,3	0.69	0	2,2,2	1.27	0
4	EDO	C	409	-	3,3,3	0.10	0	2,2,2	0.19	0
5	SO4	C	407	-	4,4,4	0.35	0	6,6,6	0.09	0
5	SO4	C	406	-	4,4,4	0.37	0	6,6,6	0.07	0
3	PEG	B	402	-	6,6,6	0.23	0	5,5,5	0.24	0
2	ORN	A	401	-	7,8,8	1.03	1 (14%)	6,9,9	0.47	0
4	EDO	A	403	-	3,3,3	0.69	0	2,2,2	0.55	0
5	SO4	C	405	6	4,4,4	0.36	0	6,6,6	0.40	0
5	SO4	B	405	6	4,4,4	0.47	0	6,6,6	0.19	0
4	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	B	404	-	3,3,3	0.36	0	2,2,2	0.56	0
2	ORN	C	401	-	7,8,8	0.93	1 (14%)	6,9,9	0.44	0
4	EDO	C	403	-	3,3,3	0.64	0	2,2,2	1.49	0
4	EDO	A	408	-	3,3,3	0.15	0	2,2,2	0.41	0
2	ORN	C	404	-	7,8,8	1.63	2 (28%)	6,9,9	1.24	1 (16%)
4	EDO	C	408	-	3,3,3	0.23	0	2,2,2	0.19	0
5	SO4	A	404	-	4,4,4	0.49	0	6,6,6	0.63	0
4	EDO	A	406	-	3,3,3	0.06	0	2,2,2	0.17	0
3	PEG	C	402	-	6,6,6	0.25	0	5,5,5	0.31	0
5	SO4	A	405	6	4,4,4	0.56	0	6,6,6	0.22	0
4	EDO	A	409	-	3,3,3	0.41	0	2,2,2	0.38	0
3	PEG	A	402	-	6,6,6	0.17	0	5,5,5	0.23	0
4	EDO	B	406	-	3,3,3	0.06	0	2,2,2	0.21	0
2	ORN	B	401	-	7,8,8	0.96	1 (14%)	6,9,9	0.50	0
4	EDO	C	410	-	3,3,3	0.41	0	2,2,2	0.39	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
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	409	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	402	-	-	3/4/4/4	-
2	ORN	A	401	-	-	2/8/8/8	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	B	404	-	-	1/1/1/1	-
2	ORN	C	401	-	-	2/8/8/8	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	A	408	-	-	1/1/1/1	-
2	ORN	C	404	-	-	5/8/8/8	-
4	EDO	C	408	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
3	PEG	C	402	-	-	1/4/4/4	-
4	EDO	A	409	-	-	0/1/1/1	-
3	PEG	A	402	-	-	0/4/4/4	-
4	EDO	B	406	-	-	1/1/1/1	-
2	ORN	B	401	-	-	0/8/8/8	-
4	EDO	C	410	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	404	ORN	O-C	2.91	1.30	1.22
2	A	401	ORN	OXT-C	-2.63	1.22	1.30
2	C	404	ORN	OXT-C	-2.58	1.22	1.30
2	B	401	ORN	OXT-C	-2.51	1.22	1.30
2	C	401	ORN	OXT-C	-2.42	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	404	ORN	CB-CA-N	2.10	115.59	110.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	PEG	O1-C1-C2-O2
2	C	401	ORN	CA-CB-CG-CD
2	A	401	ORN	OXT-C-CA-N
3	B	402	PEG	O2-C3-C4-O4

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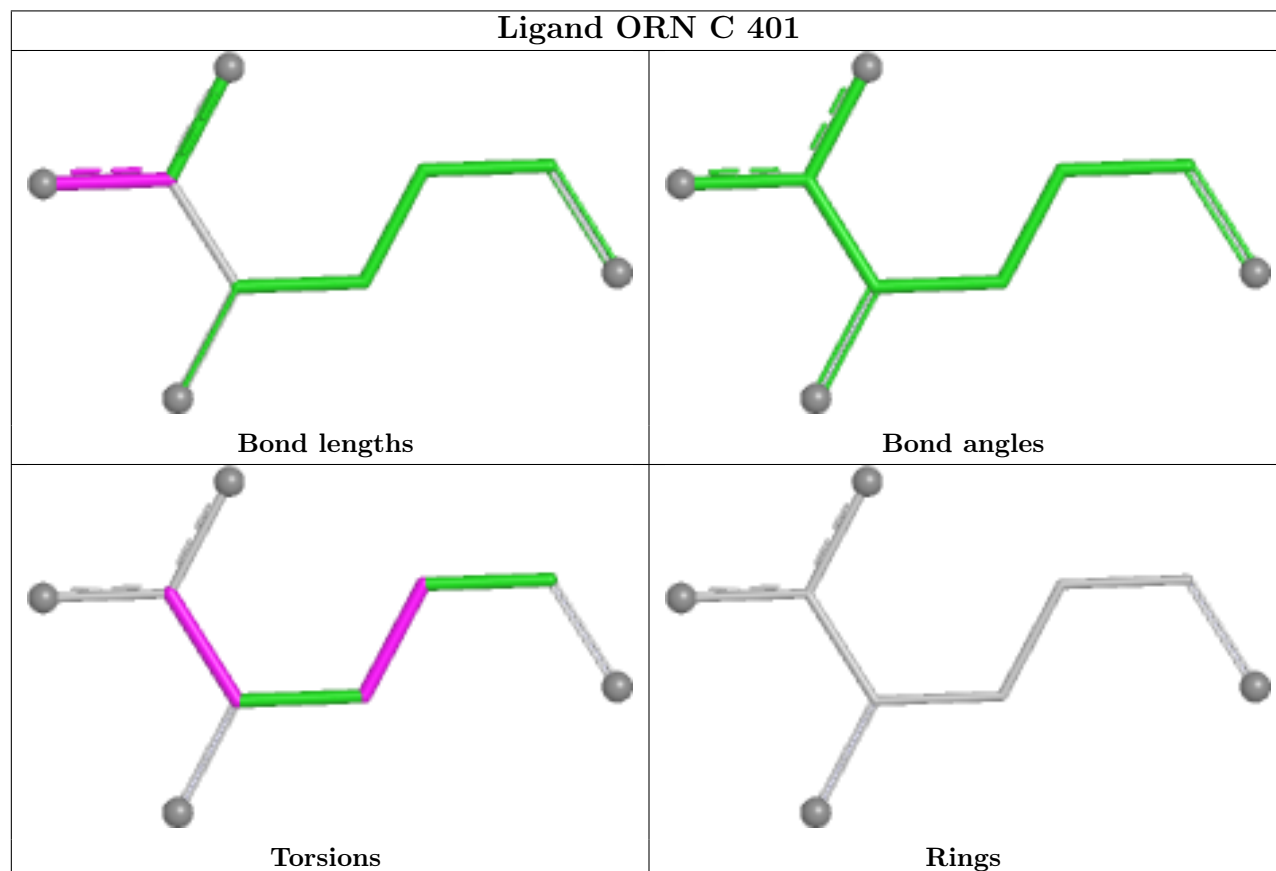
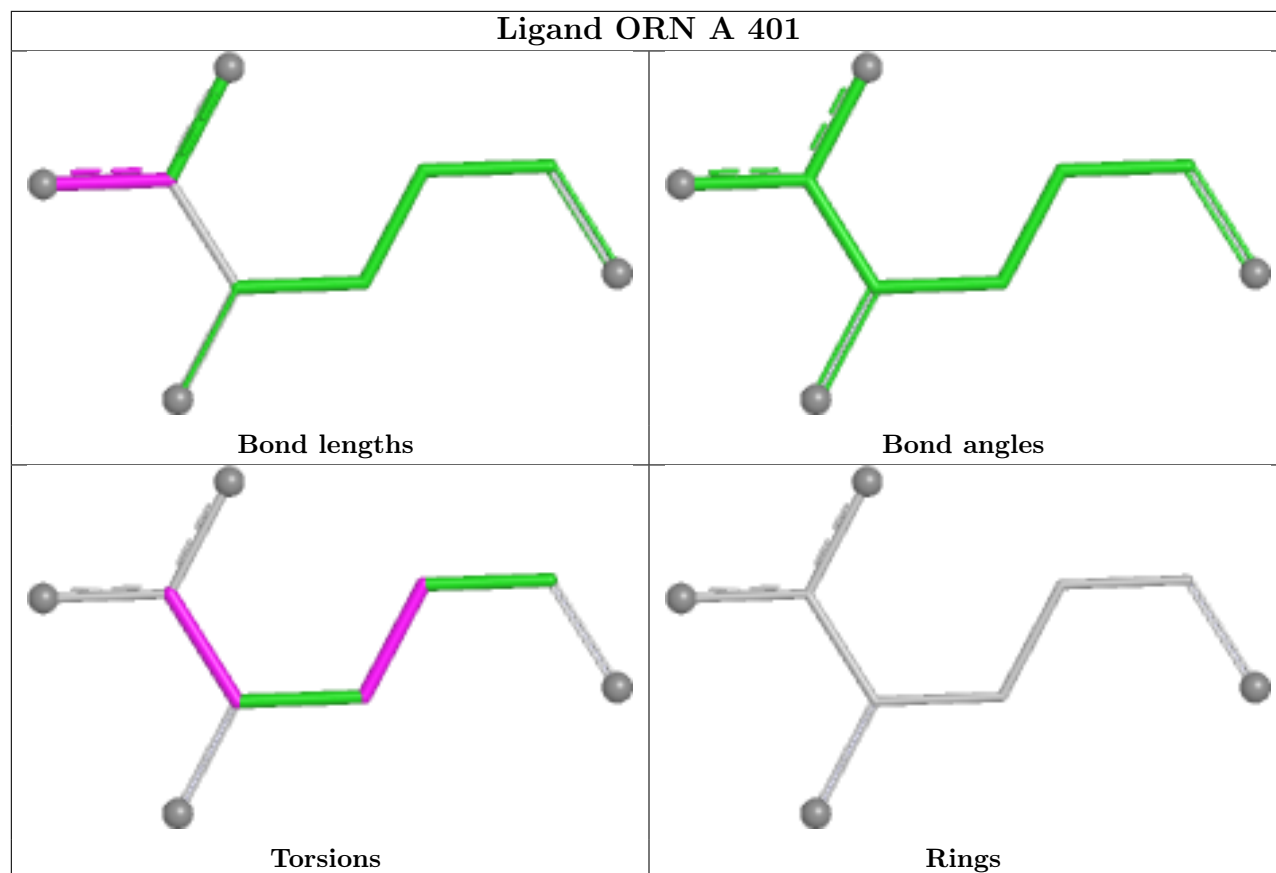
Mol	Chain	Res	Type	Atoms
4	A	408	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
2	C	401	ORN	OXT-C-CA-N
2	C	404	ORN	C-CA-CB-CG
4	C	403	EDO	O1-C1-C2-O2
2	C	404	ORN	O-C-CA-CB
2	A	401	ORN	CA-CB-CG-CD
4	B	406	EDO	O1-C1-C2-O2
3	B	402	PEG	C4-C3-O2-C2
3	C	402	PEG	O1-C1-C2-O2
4	A	406	EDO	O1-C1-C2-O2
2	C	404	ORN	CA-CB-CG-CD
2	C	404	ORN	OXT-C-CA-CB
2	C	404	ORN	OXT-C-CA-N
4	B	404	EDO	O1-C1-C2-O2

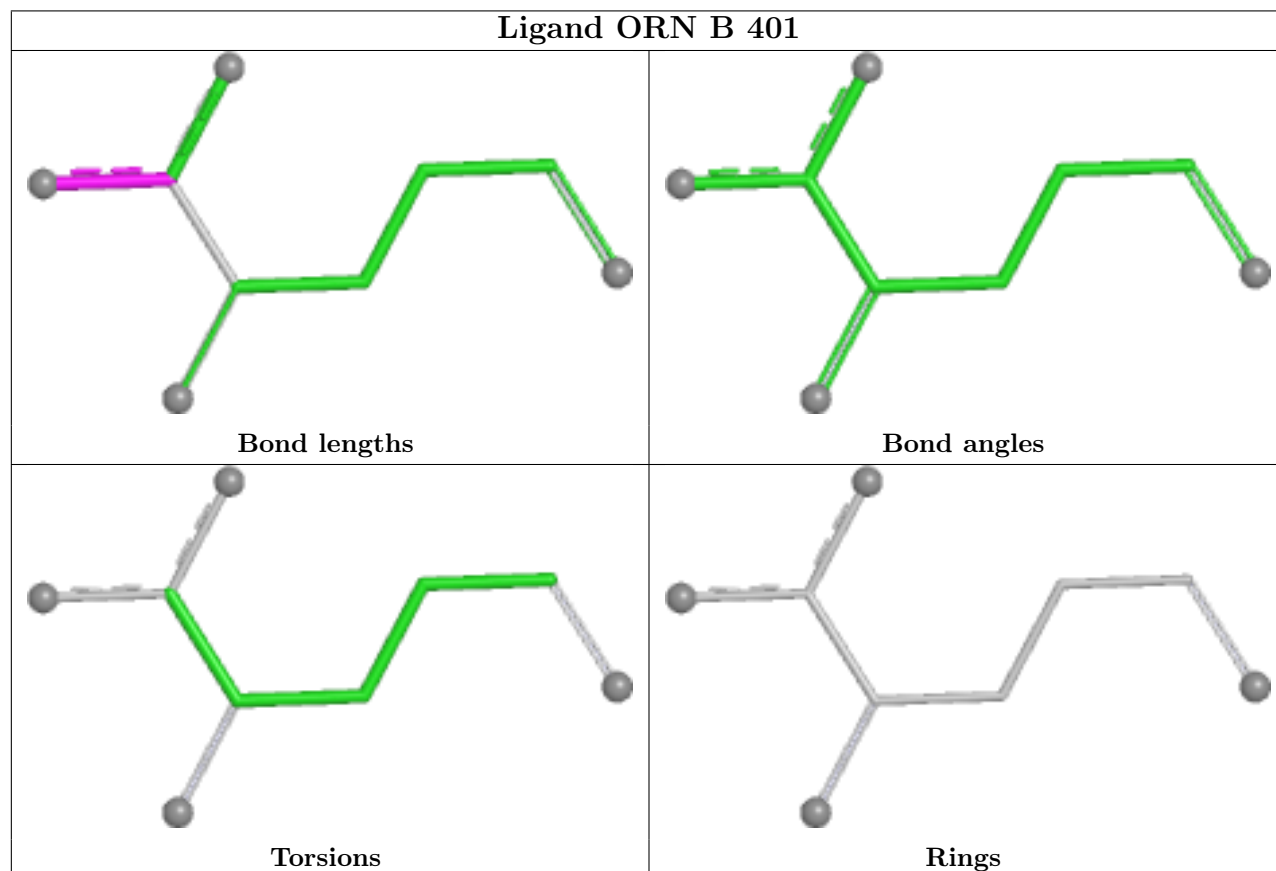
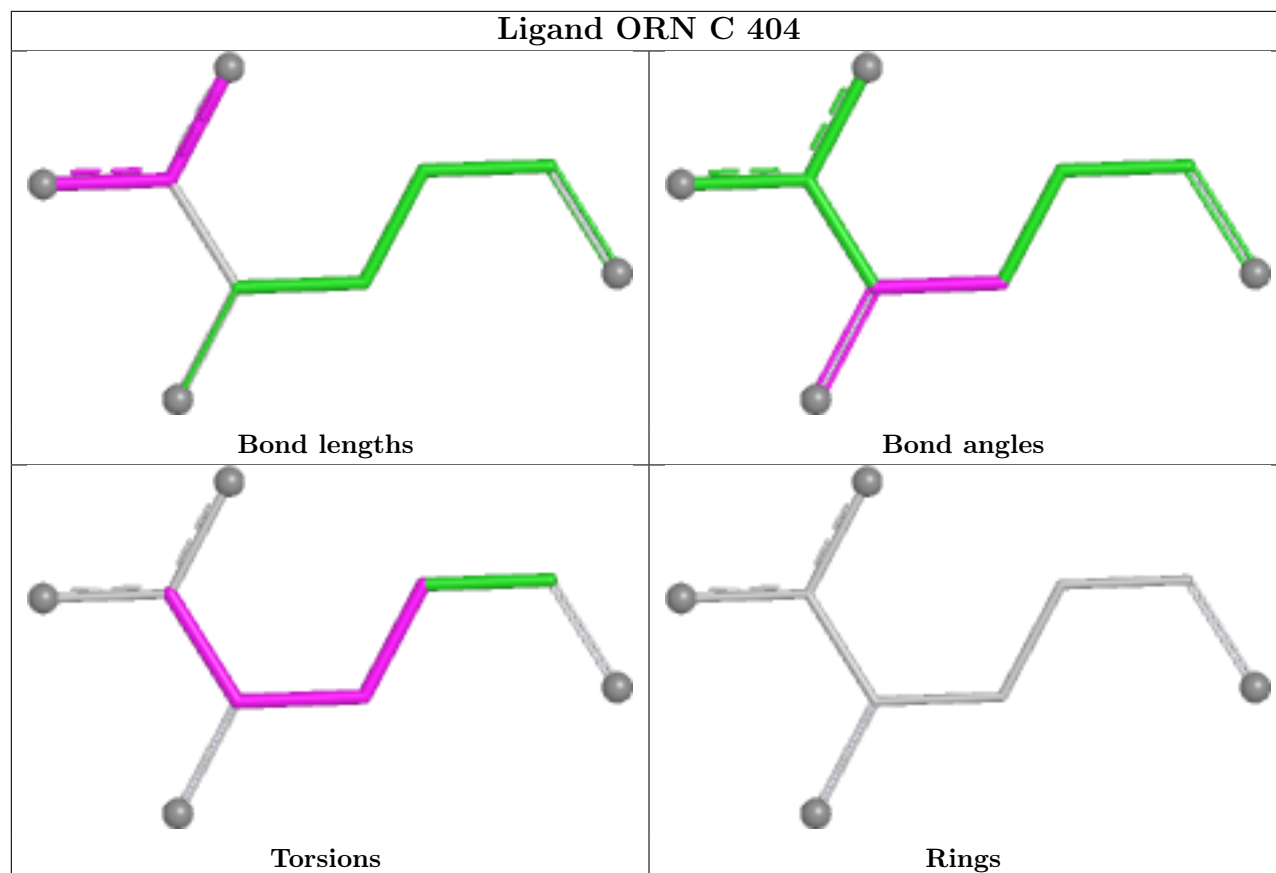
There are no ring outliers.

5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	EDO	6	0
2	C	401	ORN	1	0
4	C	403	EDO	6	0
4	A	408	EDO	7	0
2	C	404	ORN	10	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

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	304/324 (93%)	0.13	6 (1%) 65 68	9, 18, 29, 47	10 (3%)
1	B	304/324 (93%)	0.29	23 (7%) 20 21	7, 19, 42, 85	9 (2%)
1	C	304/324 (93%)	0.15	21 (6%) 23 25	9, 18, 36, 82	10 (3%)
All	All	912/972 (93%)	0.19	50 (5%) 30 33	7, 18, 35, 85	29 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	ALA	5.9
1	C	306	ALA	5.2
1	C	122	PRO	5.0
1	B	150	GLN	4.5
1	B	153	LYS	4.1
1	B	300	GLN	3.9
1	B	72	LEU	3.8
1	B	295	TRP	3.7
1	C	301	LYS	3.7
1	B	302	ASP	3.7
1	C	72	LEU	3.6
1	B	154	ARG	3.6
1	B	149	ILE	3.6
1	A	72	LEU	3.5
1	C	152	GLY	3.5
1	C	312	GLN	3.5
1	B	296	ALA	3.4
1	C	303	GLU	3.4
1	C	299	GLY	3.4
1	B	297	SER	3.3
1	C	326	GLN	3.3
1	C	151	MET	3.2
1	C	305	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	298	MET	3.1
1	B	299	GLY	3.1
1	B	152	GLY	3.0
1	A	254	LYS	2.8
1	C	309	LYS	2.8
1	C	302	ASP	2.7
1	C	300	GLN	2.6
1	B	103	GLY	2.5
1	B	255	GLY	2.5
1	B	151	MET	2.5
1	A	147	ASN	2.4
1	C	296	ALA	2.4
1	C	298	MET	2.4
1	A	92[A]	LYS	2.4
1	B	254	LYS	2.4
1	B	181	ILE	2.3
1	C	153	LYS	2.3
1	B	294	VAL	2.3
1	A	312[A]	GLN	2.2
1	C	308	ARG	2.2
1	B	104	GLU	2.2
1	A	255	GLY	2.2
1	C	149	ILE	2.2
1	B	326	GLN	2.2
1	B	304	ALA	2.1
1	B	301	LYS	2.0
1	C	121	LYS	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,

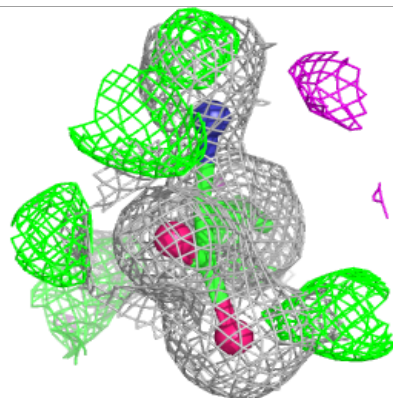
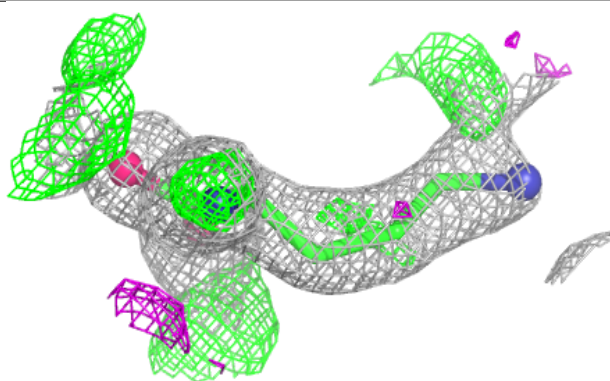
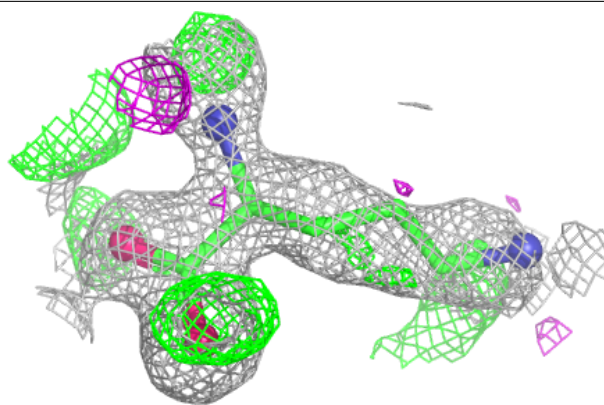
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	407	4/4	0.69	0.23	55,60,63,66	0
4	EDO	C	408	4/4	0.70	0.24	54,58,62,62	0
5	SO4	C	406	5/5	0.80	0.14	78,82,92,95	5
4	EDO	C	409	4/4	0.81	0.21	51,54,57,60	0
4	EDO	B	406	4/4	0.82	0.18	44,47,57,60	0
4	EDO	A	406	4/4	0.83	0.17	42,46,55,59	0
3	PEG	B	402	7/7	0.83	0.20	51,53,60,64	0
3	PEG	C	402	7/7	0.83	0.18	39,42,50,60	0
5	SO4	C	407	5/5	0.84	0.19	62,63,65,66	5
4	EDO	A	408	4/4	0.86	0.15	27,29,32,32	0
4	EDO	A	403	4/4	0.87	0.18	30,40,40,40	0
3	PEG	A	402	7/7	0.88	0.16	44,50,53,57	0
2	ORN	C	404	9/9	0.90	0.16	15,20,28,34	9
4	EDO	B	403	4/4	0.91	0.13	30,33,34,35	0
4	EDO	C	410	4/4	0.92	0.13	22,34,39,40	0
4	EDO	C	403	4/4	0.93	0.10	30,31,33,36	0
4	EDO	A	409	4/4	0.93	0.12	22,32,40,44	0
2	ORN	C	401	9/9	0.94	0.09	17,18,24,24	0
4	EDO	B	404	4/4	0.94	0.11	24,34,41,42	0
2	ORN	B	401	9/9	0.94	0.08	17,18,19,21	0
2	ORN	A	401	9/9	0.95	0.08	15,15,22,24	0
6	NA	A	410	1/1	0.95	0.08	33,33,33,33	0
6	NA	A	411	1/1	0.96	0.16	30,30,30,30	0
5	SO4	A	405	5/5	0.97	0.07	17,18,22,25	0
5	SO4	C	405	5/5	0.97	0.08	18,19,27,29	0
5	SO4	A	404	5/5	0.97	0.09	19,25,27,28	5
6	NA	B	407	1/1	0.98	0.05	23,23,23,23	0
6	NA	C	411	1/1	0.98	0.12	27,27,27,27	0
5	SO4	B	405	5/5	1.00	0.03	14,14,16,17	0

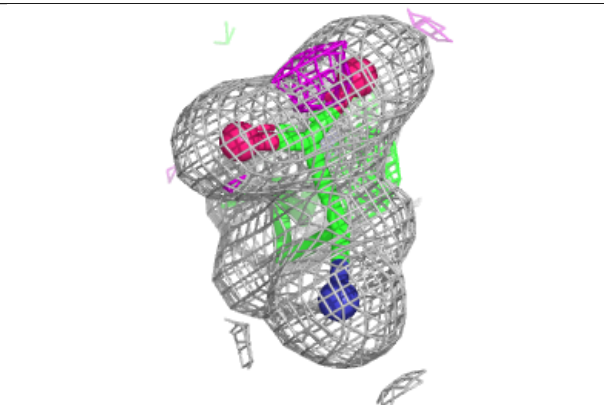
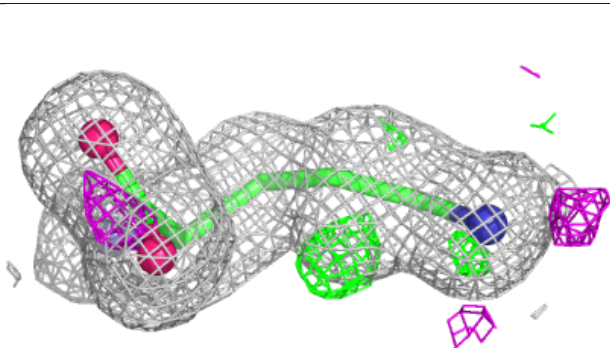
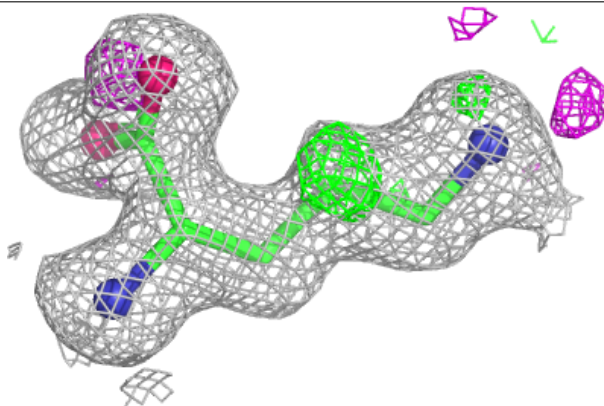
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ORN C 404:

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

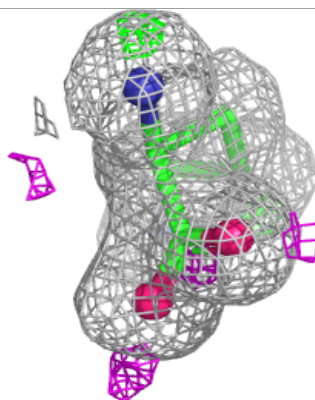
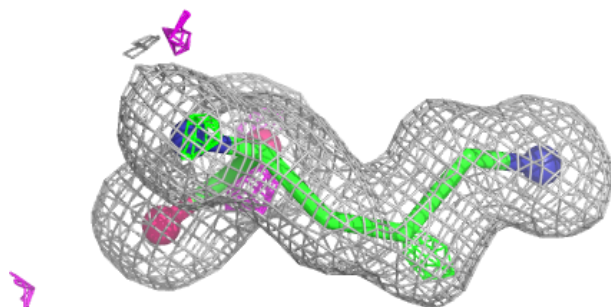
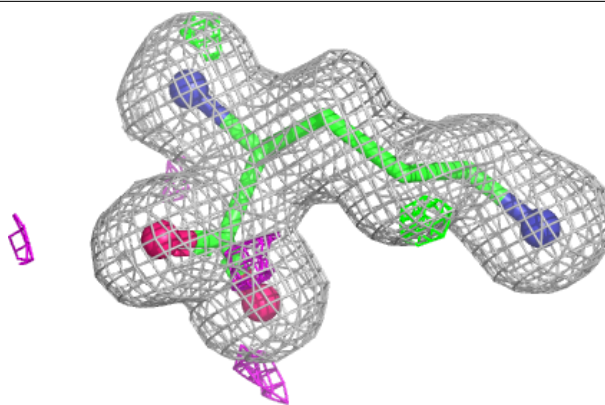
**Electron density around ORN C 401:**

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

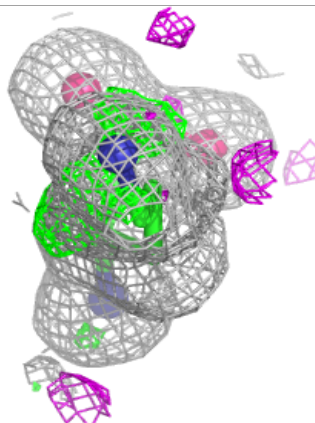
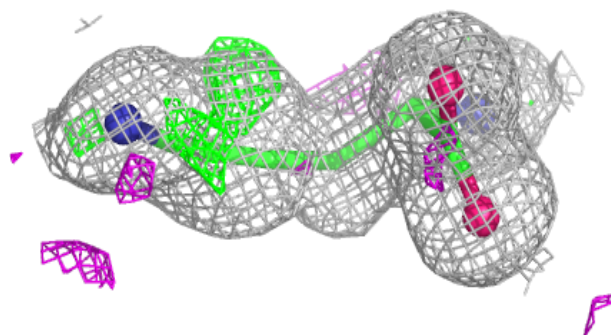
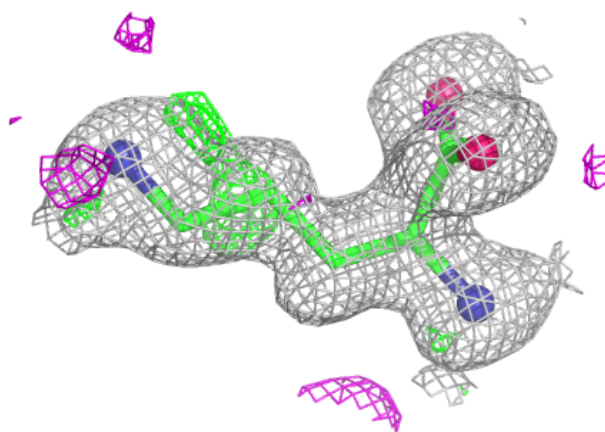


Electron density around ORN B 401:

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

**Electron density around ORN A 401:**

$2mF_o-DF_c$ (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.