



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 6TG3 / pdb_00006tg3
Title : Crystal Structure of the PBP/SBP MotA in complex with glucopinic acid from
A. tumefaciens B6/R10
Authors : Morera, S.; Vigouroux, S.
Deposited on : 2019-11-14
Resolution : 1.85 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

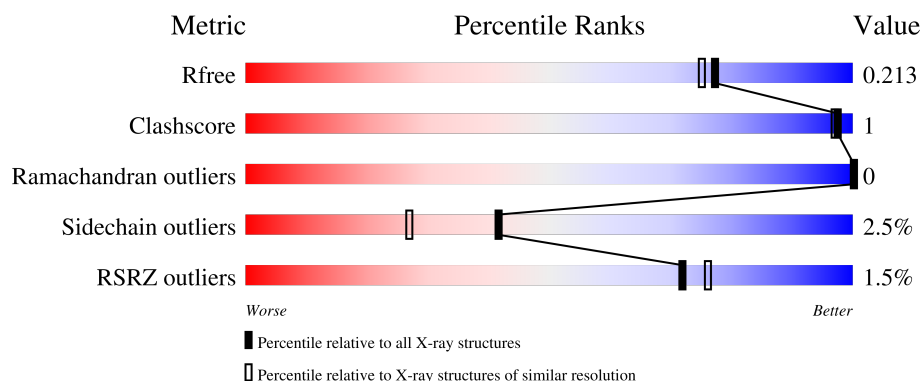
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	351	88% 5% 7%
1	B	351	89% 7%
1	C	351	88% 8%
1	D	351	89% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10449 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 MotA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	1	0
			2512	1595	423	485	9			
1	B	326	Total	C	N	O	S	0	0	0
			2509	1594	424	482	9			
1	C	323	Total	C	N	O	S	0	0	0
			2480	1577	416	479	8			
1	D	327	Total	C	N	O	S	0	0	0
			2515	1597	425	484	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP Q44384
A	11	GLY	-	expression tag	UNP Q44384
A	12	SER	-	expression tag	UNP Q44384
A	13	SER	-	expression tag	UNP Q44384
A	14	HIS	-	expression tag	UNP Q44384
A	15	HIS	-	expression tag	UNP Q44384
A	16	HIS	-	expression tag	UNP Q44384
A	17	HIS	-	expression tag	UNP Q44384
A	18	HIS	-	expression tag	UNP Q44384
A	19	HIS	-	expression tag	UNP Q44384
A	20	SER	-	expression tag	UNP Q44384
A	21	SER	-	expression tag	UNP Q44384
A	22	GLY	-	expression tag	UNP Q44384
A	23	LEU	-	expression tag	UNP Q44384
A	24	VAL	-	expression tag	UNP Q44384
A	25	PRO	-	expression tag	UNP Q44384
A	26	ARG	-	expression tag	UNP Q44384
A	27	GLY	-	expression tag	UNP Q44384
A	28	SER	-	expression tag	UNP Q44384
A	29	HIS	-	expression tag	UNP Q44384
A	30	MET	-	expression tag	UNP Q44384

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Chain	Residue	Modelled	Actual	Comment	Reference
A	355	HIS	-	expression tag	UNP Q44384
A	356	HIS	-	expression tag	UNP Q44384
A	357	HIS	-	expression tag	UNP Q44384
A	358	HIS	-	expression tag	UNP Q44384
A	359	HIS	-	expression tag	UNP Q44384
A	360	HIS	-	expression tag	UNP Q44384
B	10	MET	-	initiating methionine	UNP Q44384
B	11	GLY	-	expression tag	UNP Q44384
B	12	SER	-	expression tag	UNP Q44384
B	13	SER	-	expression tag	UNP Q44384
B	14	HIS	-	expression tag	UNP Q44384
B	15	HIS	-	expression tag	UNP Q44384
B	16	HIS	-	expression tag	UNP Q44384
B	17	HIS	-	expression tag	UNP Q44384
B	18	HIS	-	expression tag	UNP Q44384
B	19	HIS	-	expression tag	UNP Q44384
B	20	SER	-	expression tag	UNP Q44384
B	21	SER	-	expression tag	UNP Q44384
B	22	GLY	-	expression tag	UNP Q44384
B	23	LEU	-	expression tag	UNP Q44384
B	24	VAL	-	expression tag	UNP Q44384
B	25	PRO	-	expression tag	UNP Q44384
B	26	ARG	-	expression tag	UNP Q44384
B	27	GLY	-	expression tag	UNP Q44384
B	28	SER	-	expression tag	UNP Q44384
B	29	HIS	-	expression tag	UNP Q44384
B	30	MET	-	expression tag	UNP Q44384
B	355	HIS	-	expression tag	UNP Q44384
B	356	HIS	-	expression tag	UNP Q44384
B	357	HIS	-	expression tag	UNP Q44384
B	358	HIS	-	expression tag	UNP Q44384
B	359	HIS	-	expression tag	UNP Q44384
B	360	HIS	-	expression tag	UNP Q44384
C	10	MET	-	initiating methionine	UNP Q44384
C	11	GLY	-	expression tag	UNP Q44384
C	12	SER	-	expression tag	UNP Q44384
C	13	SER	-	expression tag	UNP Q44384
C	14	HIS	-	expression tag	UNP Q44384
C	15	HIS	-	expression tag	UNP Q44384
C	16	HIS	-	expression tag	UNP Q44384
C	17	HIS	-	expression tag	UNP Q44384
C	18	HIS	-	expression tag	UNP Q44384

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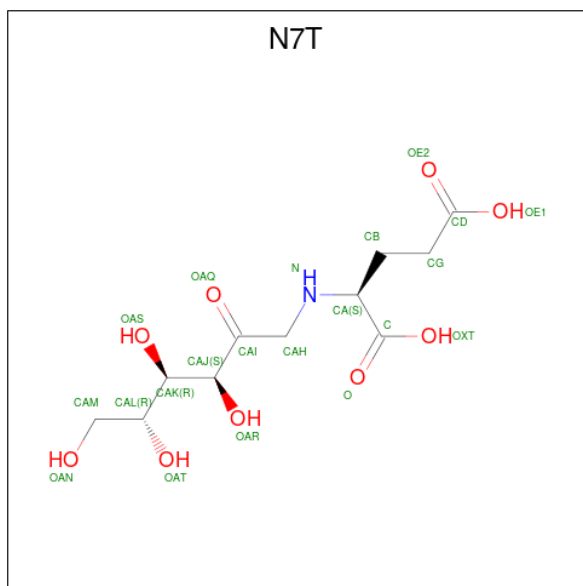
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	HIS	-	expression tag	UNP Q44384
C	20	SER	-	expression tag	UNP Q44384
C	21	SER	-	expression tag	UNP Q44384
C	22	GLY	-	expression tag	UNP Q44384
C	23	LEU	-	expression tag	UNP Q44384
C	24	VAL	-	expression tag	UNP Q44384
C	25	PRO	-	expression tag	UNP Q44384
C	26	ARG	-	expression tag	UNP Q44384
C	27	GLY	-	expression tag	UNP Q44384
C	28	SER	-	expression tag	UNP Q44384
C	29	HIS	-	expression tag	UNP Q44384
C	30	MET	-	expression tag	UNP Q44384
C	355	HIS	-	expression tag	UNP Q44384
C	356	HIS	-	expression tag	UNP Q44384
C	357	HIS	-	expression tag	UNP Q44384
C	358	HIS	-	expression tag	UNP Q44384
C	359	HIS	-	expression tag	UNP Q44384
C	360	HIS	-	expression tag	UNP Q44384
D	10	MET	-	initiating methionine	UNP Q44384
D	11	GLY	-	expression tag	UNP Q44384
D	12	SER	-	expression tag	UNP Q44384
D	13	SER	-	expression tag	UNP Q44384
D	14	HIS	-	expression tag	UNP Q44384
D	15	HIS	-	expression tag	UNP Q44384
D	16	HIS	-	expression tag	UNP Q44384
D	17	HIS	-	expression tag	UNP Q44384
D	18	HIS	-	expression tag	UNP Q44384
D	19	HIS	-	expression tag	UNP Q44384
D	20	SER	-	expression tag	UNP Q44384
D	21	SER	-	expression tag	UNP Q44384
D	22	GLY	-	expression tag	UNP Q44384
D	23	LEU	-	expression tag	UNP Q44384
D	24	VAL	-	expression tag	UNP Q44384
D	25	PRO	-	expression tag	UNP Q44384
D	26	ARG	-	expression tag	UNP Q44384
D	27	GLY	-	expression tag	UNP Q44384
D	28	SER	-	expression tag	UNP Q44384
D	29	HIS	-	expression tag	UNP Q44384
D	30	MET	-	expression tag	UNP Q44384
D	355	HIS	-	expression tag	UNP Q44384
D	356	HIS	-	expression tag	UNP Q44384
D	357	HIS	-	expression tag	UNP Q44384

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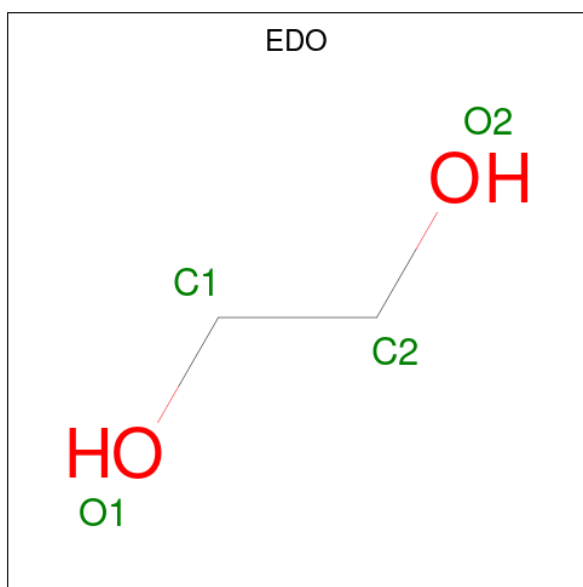
Chain	Residue	Modelled	Actual	Comment	Reference
D	358	HIS	-	expression tag	UNP Q44384
D	359	HIS	-	expression tag	UNP Q44384
D	360	HIS	-	expression tag	UNP Q44384

- Molecule 2 is (2 {S})-2-[[[(3 {S},4 {R},5 {R})-3,4,5,6-tetrakis(oxidanyl)-2-oxidanylidene-hexyl]amino]pentanedioic acid (CCD ID: N7T) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		
2	C	1	Total	C	N	O	0	0
			21	11	1	9		
2	D	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

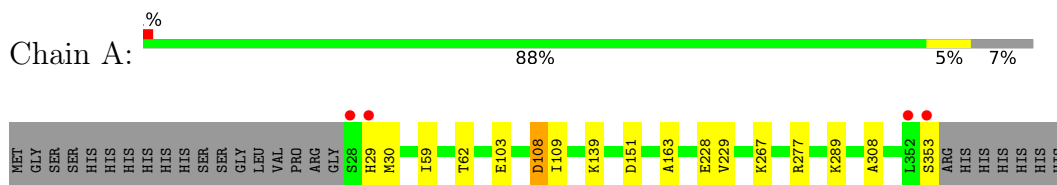
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	79	Total	O	0	0
			79	79		
4	C	66	Total	O	0	0
			66	66		
4	D	82	Total	O	0	0
			82	82		

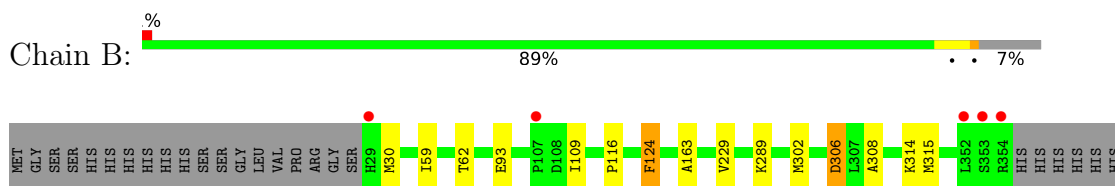
3 Residue-property plots

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.

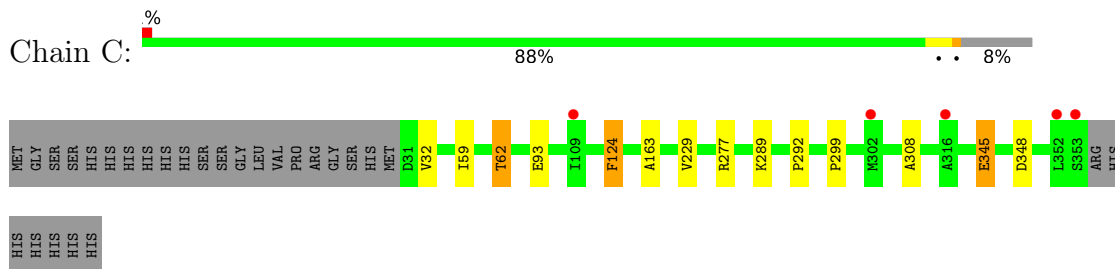
- Molecule 1: MotA



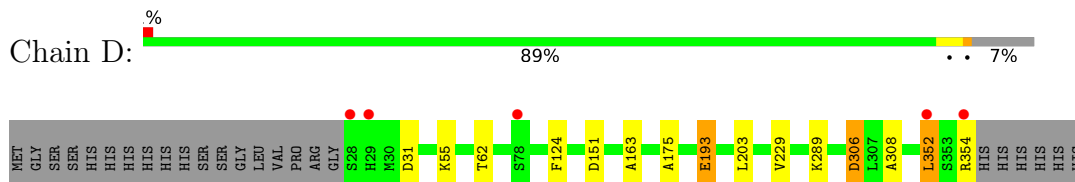
- Molecule 1: MotA



- Molecule 1: MotA



- Molecule 1: MotA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.63Å 131.93Å 70.38Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	48.12 – 1.85 48.12 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.12-1.85) 99.9 (48.12-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.179 , 0.199 0.186 , 0.213	Depositor DCC
R_{free} test set	5332 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.029 for h,-k,-l 0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10449	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, N7T

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	0.86	0/2575	1.11	2/3502 (0.1%)
1	B	0.86	1/2572 (0.0%)	1.11	2/3497 (0.1%)
1	C	0.81	0/2542	1.13	4/3458 (0.1%)
1	D	0.83	0/2578	1.17	8/3505 (0.2%)
All	All	0.84	1/10267 (0.0%)	1.13	16/13962 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	PRO	CA-C	5.20	1.54	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	352	LEU	CA-C-N	7.43	135.07	121.70
1	D	352	LEU	C-N-CA	7.43	135.07	121.70
1	D	193	GLU	CA-C-N	6.66	129.09	120.44
1	D	193	GLU	C-N-CA	6.66	129.09	120.44
1	B	124	PHE	CA-CB-CG	5.95	119.75	113.80
1	C	124	PHE	CA-CB-CG	5.95	119.75	113.80
1	B	306	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	32	VAL	N-CA-C	-5.85	101.99	109.30
1	D	306	ASP	CA-CB-CG	5.75	118.34	112.60
1	D	124	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	348	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	345	GLU	CB-CG-CD	5.29	121.59	112.60
1	D	31	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	151	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	108	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	151	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2512	0	2425	6	0
1	B	2509	0	2428	3	0
1	C	2480	0	2399	5	0
1	D	2515	0	2433	3	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	0	0
3	A	4	0	6	0	0
3	D	4	0	6	0	0
4	A	114	0	0	0	0
4	B	79	0	0	0	0
4	C	66	0	0	0	0
4	D	82	0	0	0	0
All	All	10449	0	9697	16	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 1.

All (16) 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:A:29:HIS:CG	1:A:30:MET:H	2.09	0.71
1:C:289:LYS:HB2	1:C:308:ALA:HB2	1.87	0.56
1:A:29:HIS:CG	1:A:30:MET:N	2.77	0.53
1:D:163:ALA:HB2	1:D:229:VAL:HG11	1.92	0.51
1:D:289:LYS:HB2	1:D:308:ALA:HB2	1.94	0.50
1:B:289:LYS:HB2	1:B:308:ALA:HB2	1.94	0.48
1:A:163:ALA:HB2	1:A:229:VAL:HG11	1.95	0.47
1:C:163:ALA:HB2	1:C:229:VAL:HG11	1.95	0.47
1:B:163:ALA:HB2	1:B:229:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLU:HG3	1:B:124:PHE:HB2	2.00	0.44
1:A:139:LYS:HE2	1:C:62:THR:HG23	2.00	0.42
1:A:289:LYS:HB2	1:A:308:ALA:HB2	2.02	0.41
1:A:103:GLU:HG2	1:A:267:LYS:HA	2.03	0.40
1:C:93:GLU:HG3	1:C:124:PHE:HB2	2.03	0.40
1:C:292:PRO:HG3	1:C:299:PRO:HD3	2.04	0.40
1:D:175:ALA:HB2	1:D:203:LEU:HG	2.03	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	325/351 (93%)	321 (99%)	4 (1%)	0	100	100
1	B	324/351 (92%)	321 (99%)	3 (1%)	0	100	100
1	C	321/351 (92%)	318 (99%)	3 (1%)	0	100	100
1	D	325/351 (93%)	321 (99%)	4 (1%)	0	100	100
All	All	1295/1404 (92%)	1281 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/274 (92%)	246 (97%)	7 (3%)	38	23
1	B	252/274 (92%)	244 (97%)	8 (3%)	34	19
1	C	249/274 (91%)	245 (98%)	4 (2%)	55	44
1	D	253/274 (92%)	247 (98%)	6 (2%)	43	28
All	All	1007/1096 (92%)	982 (98%)	25 (2%)	42	27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	62	THR
1	A	108	ASP
1	A	109	ILE
1	A	228	GLU
1	A	277	ARG
1	A	353	SER
1	B	30	MET
1	B	59	ILE
1	B	62	THR
1	B	109	ILE
1	B	302	MET
1	B	306	ASP
1	B	314	LYS
1	B	315	MET
1	C	59	ILE
1	C	62	THR
1	C	277	ARG
1	C	345	GLU
1	D	55	LYS
1	D	62	THR
1	D	193	GLU
1	D	306	ASP
1	D	352	LEU
1	D	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	166	ASN

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Mol	Chain	Res	Type
1	A	240	GLN
1	A	257	GLN
1	A	339	HIS
1	B	67	GLN
1	B	129	ASN
1	B	240	GLN
1	B	257	GLN
1	B	334	ASN
1	B	339	HIS
1	B	349	ASN
1	C	67	GLN
1	C	95	GLN
1	C	240	GLN
1	C	257	GLN
1	C	339	HIS
1	C	349	ASN
1	D	67	GLN
1	D	129	ASN
1	D	339	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	EDO	A	402	-	3,3,3	0.67	0	2,2,2	0.16	0
2	N7T	C	401	-	20,20,20	1.07	2 (10%)	20,26,26	1.25	1 (5%)
3	EDO	D	402	-	3,3,3	0.64	0	2,2,2	0.24	0
2	N7T	D	401	-	20,20,20	1.06	1 (5%)	20,26,26	1.44	4 (20%)
2	N7T	B	401	-	20,20,20	1.01	1 (5%)	20,26,26	1.53	4 (20%)
2	N7T	A	401	-	20,20,20	1.00	1 (5%)	20,26,26	1.36	1 (5%)

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
3	EDO	A	402	-	-	1/1/1/1	-
2	N7T	C	401	-	-	8/27/28/28	-
3	EDO	D	402	-	-	1/1/1/1	-
2	N7T	D	401	-	-	7/27/28/28	-
2	N7T	B	401	-	-	9/27/28/28	-
2	N7T	A	401	-	-	8/27/28/28	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	N7T	CAH-CAI	2.53	1.55	1.51
2	D	401	N7T	CAH-CAI	2.53	1.55	1.51
2	A	401	N7T	CAH-CAI	2.42	1.55	1.51
2	B	401	N7T	CAH-CAI	2.13	1.54	1.51
2	C	401	N7T	OE1-CD	-2.09	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	N7T	OAN-CAM-CAL	-3.38	104.06	111.16
2	D	401	N7T	OAN-CAM-CAL	-3.28	104.27	111.16
2	C	401	N7T	CAH-N-CA	-3.09	107.59	113.93
2	B	401	N7T	OAN-CAM-CAL	-2.81	105.25	111.16
2	B	401	N7T	OAR-CAJ-CAK	2.60	116.01	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	N7T	CAH-N-CA	-2.57	108.66	113.93
2	D	401	N7T	OAS-CAK-CAL	2.25	114.05	108.93
2	B	401	N7T	OE1-CD-CG	2.22	121.01	114.00
2	B	401	N7T	CAH-N-CA	-2.07	109.69	113.93
2	D	401	N7T	OE1-CD-CG	2.00	120.32	114.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	N7T	CAK-CAL-CAM-OAN
2	A	401	N7T	OAQ-CAI-CAJ-OAR
2	A	401	N7T	C-CA-N-CAH
2	A	401	N7T	CB-CA-N-CAH
2	B	401	N7T	OAQ-CAI-CAJ-OAR
2	B	401	N7T	C-CA-N-CAH
2	B	401	N7T	CB-CA-N-CAH
2	C	401	N7T	OAQ-CAI-CAJ-OAR
2	C	401	N7T	C-CA-N-CAH
2	C	401	N7T	CB-CA-N-CAH
2	D	401	N7T	OAQ-CAI-CAJ-OAR
2	D	401	N7T	C-CA-N-CAH
2	D	401	N7T	CB-CA-N-CAH
2	A	401	N7T	OAT-CAL-CAM-OAN
2	A	401	N7T	N-CAH-CAI-OAQ
2	D	401	N7T	N-CAH-CAI-OAQ
3	D	402	EDO	O1-C1-C2-O2
2	C	401	N7T	N-CAH-CAI-OAQ
2	B	401	N7T	N-CAH-CAI-OAQ
2	D	401	N7T	C-CA-CB-CG
2	C	401	N7T	O-C-CA-CB
2	B	401	N7T	OXT-C-CA-CB
2	C	401	N7T	OXT-C-CA-CB
2	B	401	N7T	C-CA-CB-CG
2	A	401	N7T	OE2-CD-CG-CB
2	C	401	N7T	OE1-CD-CG-CB
2	C	401	N7T	OE2-CD-CG-CB
2	A	401	N7T	OE1-CD-CG-CB
2	B	401	N7T	O-C-CA-CB
2	B	401	N7T	OE2-CD-CG-CB
2	D	401	N7T	OE2-CD-CG-CB
2	B	401	N7T	OE1-CD-CG-CB

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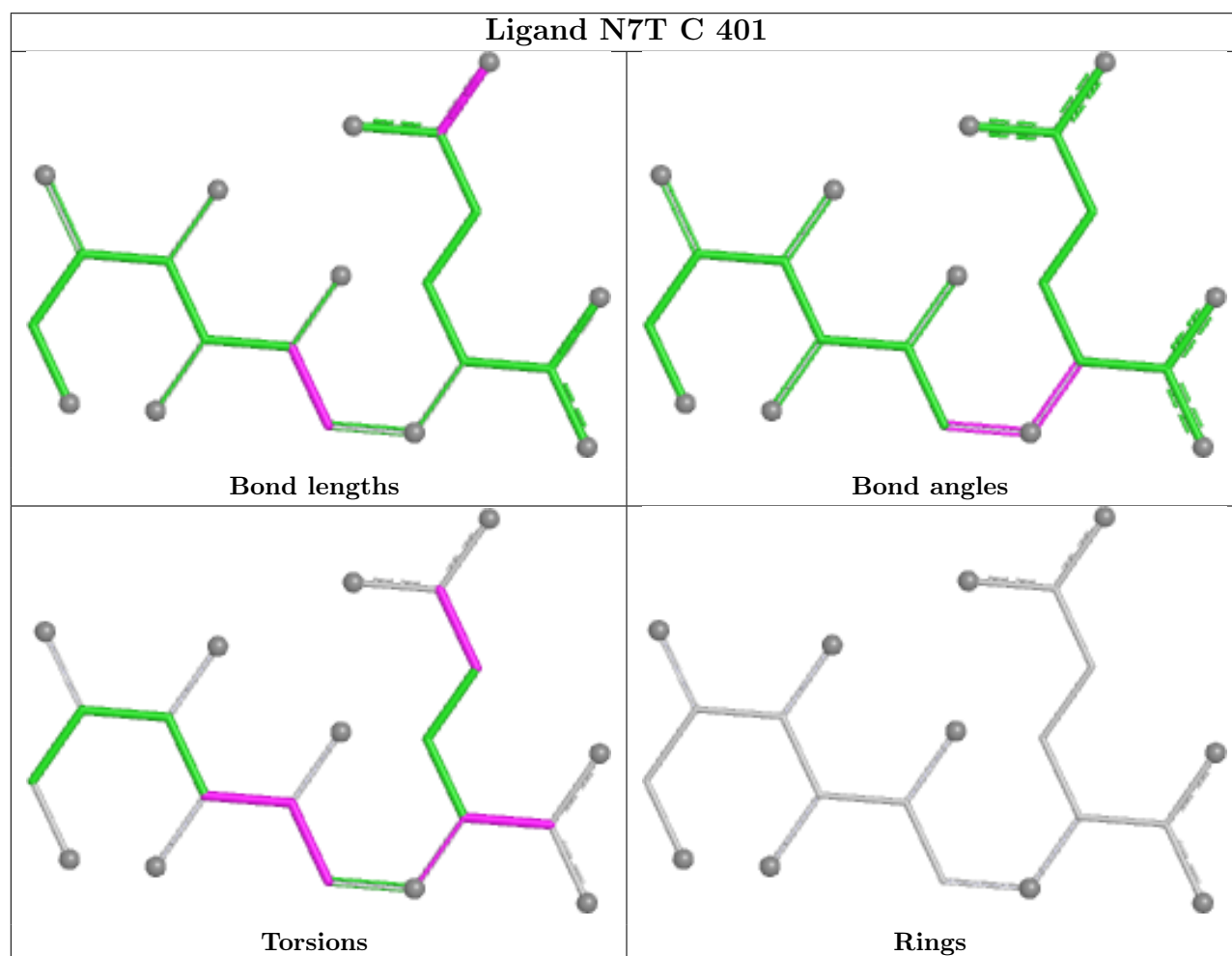
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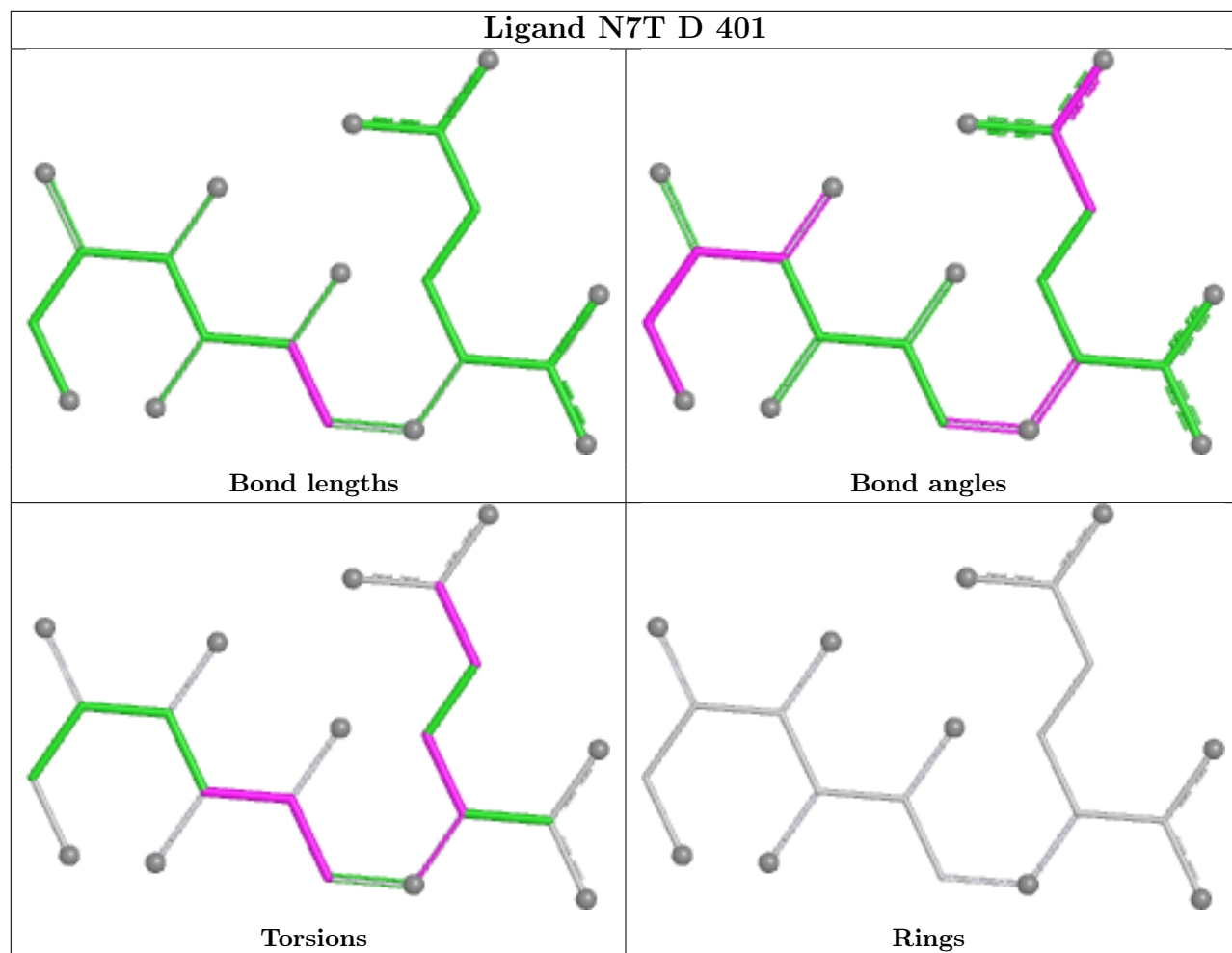
Mol	Chain	Res	Type	Atoms
2	D	401	N7T	OE1-CD-CG-CB
3	A	402	EDO	O1-C1-C2-O2

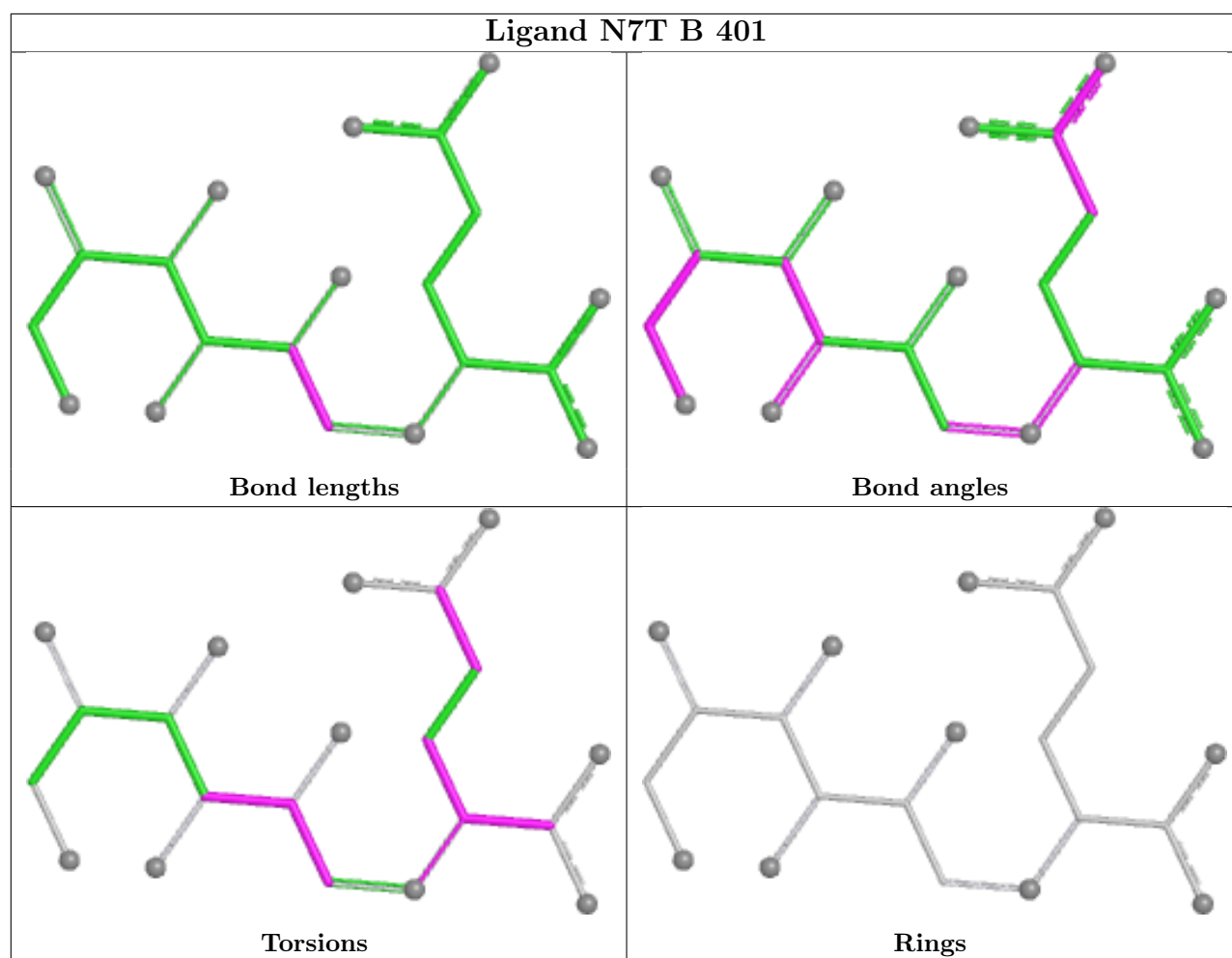
There are no ring outliers.

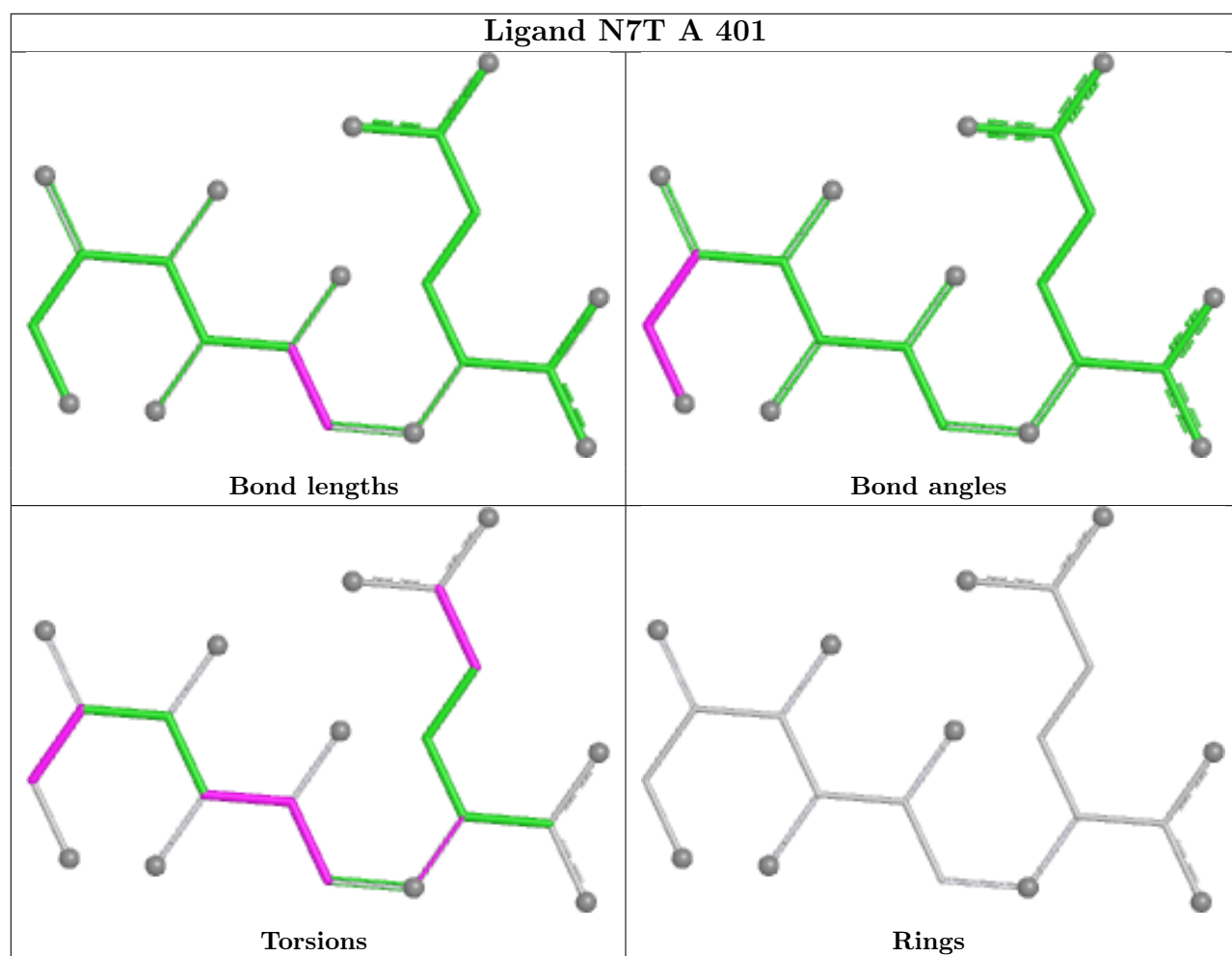
No monomer is involved in short contacts.

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	326/351 (92%)	-0.05	4 (1%) 76 80	22, 40, 67, 87	1 (0%)
1	B	326/351 (92%)	0.07	5 (1%) 72 76	24, 40, 67, 112	0
1	C	323/351 (92%)	0.09	5 (1%) 72 76	25, 46, 75, 116	0
1	D	327/351 (93%)	0.13	5 (1%) 72 76	25, 44, 80, 111	0
All	All	1302/1404 (92%)	0.06	19 (1%) 72 76	22, 42, 73, 116	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	SER	4.5
1	D	29	HIS	3.5
1	D	352	LEU	3.2
1	D	354	ARG	3.2
1	A	352	LEU	2.8
1	A	29	HIS	2.8
1	C	352	LEU	2.8
1	B	29	HIS	2.7
1	B	352	LEU	2.7
1	B	107	PRO	2.6
1	C	302	MET	2.5
1	D	78	SER	2.5
1	B	353	SER	2.4
1	B	354	ARG	2.4
1	D	28	SER	2.4
1	C	316	ALA	2.3
1	A	28	SER	2.2
1	C	109	ILE	2.1
1	C	353	SER	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](#)

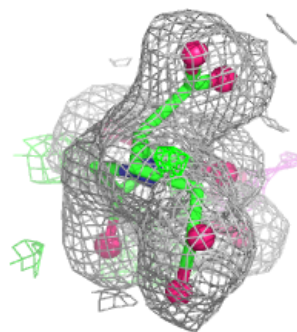
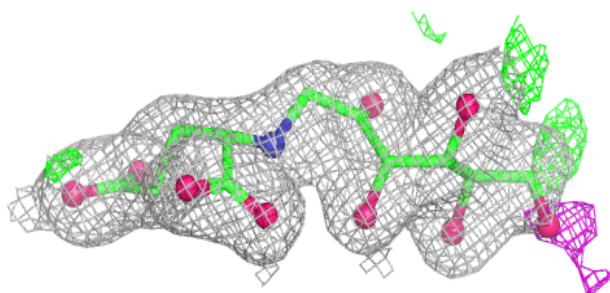
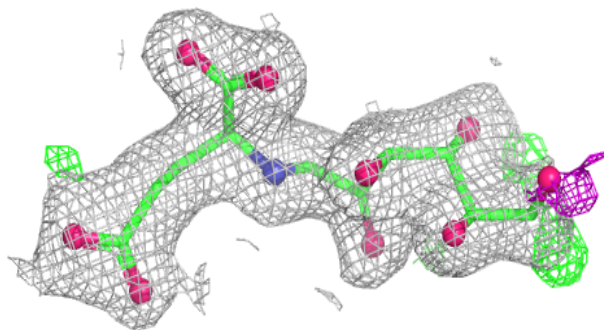
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	EDO	A	402	4/4	0.73	0.15	58,62,66,67	0
3	EDO	D	402	4/4	0.78	0.15	71,73,75,76	0
2	N7T	C	401	21/21	0.92	0.09	25,34,45,53	0
2	N7T	D	401	21/21	0.94	0.08	26,33,41,46	0
2	N7T	B	401	21/21	0.94	0.07	27,33,42,48	0
2	N7T	A	401	21/21	0.94	0.07	28,33,44,52	0

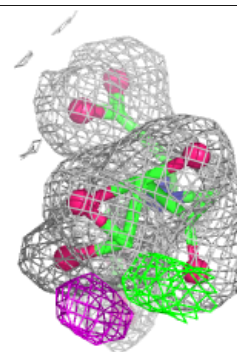
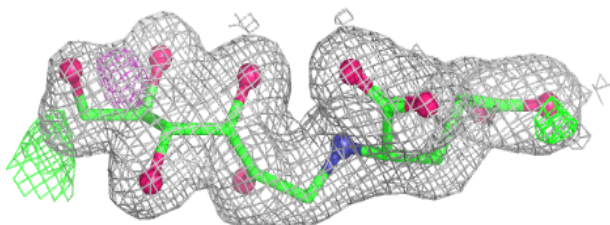
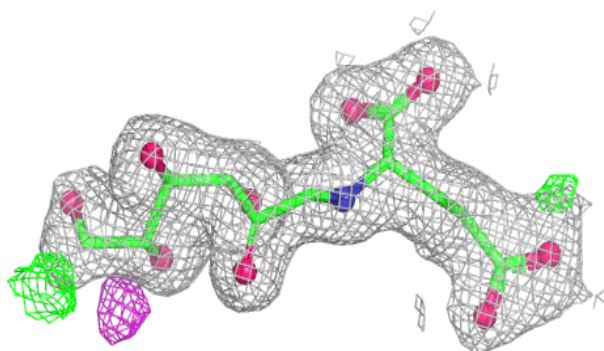
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N7T 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)

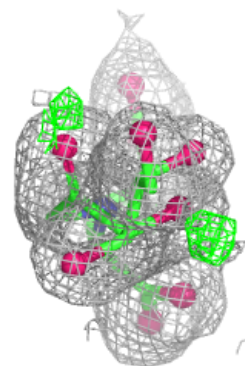
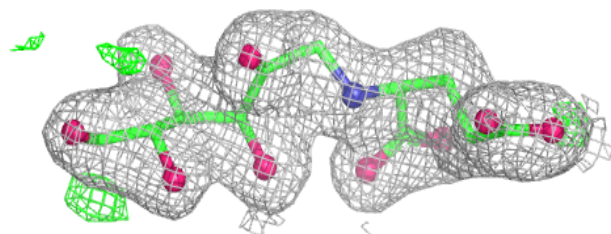
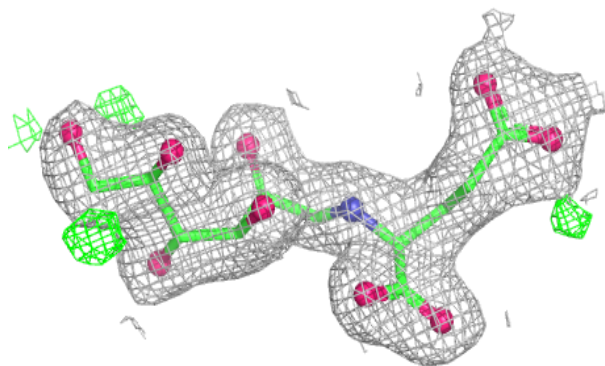
**Electron density around N7T D 401:**

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

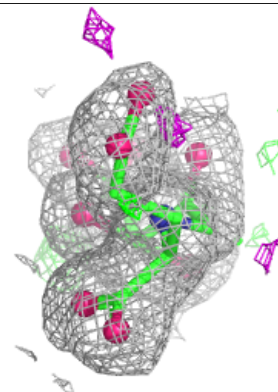
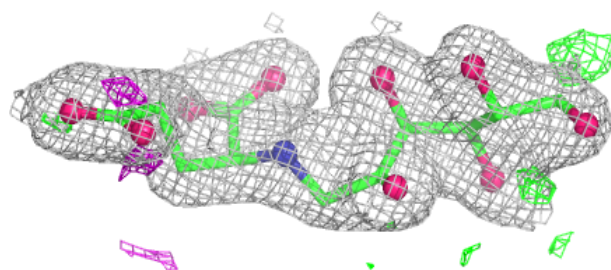
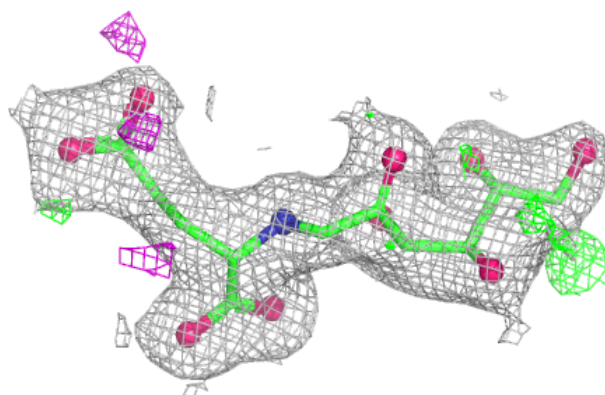


Electron density around N7T B 401:

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

**Electron density around N7T 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.