



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:17 AM EDT

PDB ID : 7VZN / pdb_00007vzn
Title : The structure of GdmN in complex with carbamoyl adenylate intermediate and 20-O-methyl-19-chloroproansamitocin
Authors : Wei, J.; Zheng, J.; Zhou, J.; Kang, Q.; Bai, L.
Deposited on : 2021-11-16
Resolution : 2.10 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

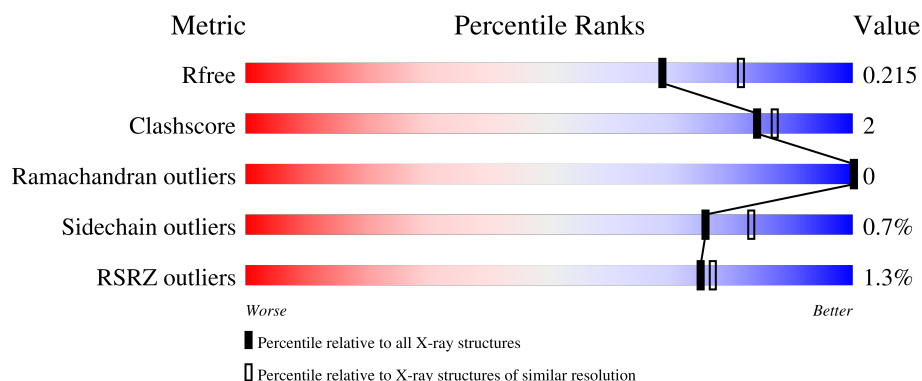
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

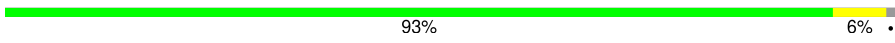
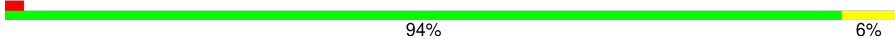
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	682	 93% 6% •
1	B	682	 94% 6%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10975 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.

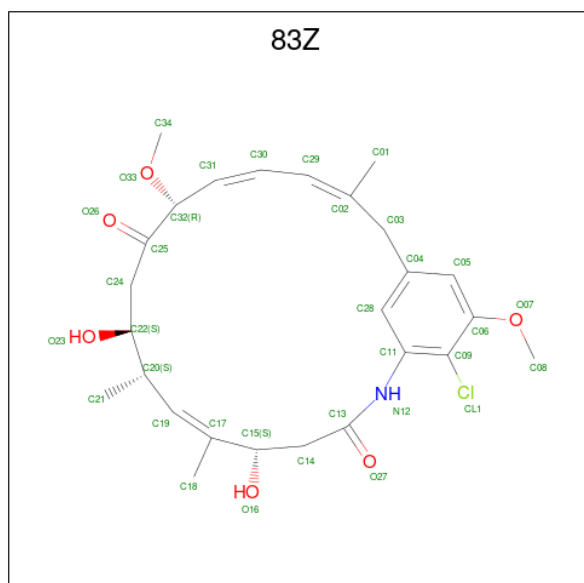
- Molecule 1 is a protein called GdmN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	1	0
			5197	3294	913	981	9			
1	B	679	Total	C	N	O	S	0	0	0
			5211	3299	916	987	9			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

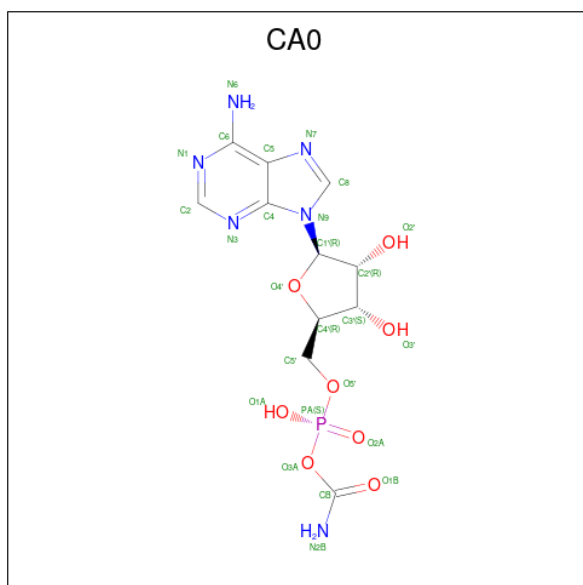
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is (5 {S},6 {E},8 {S},9 {S},12 {R},15 {E})-21-chloranyl-12,20-dimethoxy-6,8,16-trimethyl-5,9-bis(oxidanyl)-2-azabicyclo[16.3.1]docosa-1(21),6,15,18(22),19-pentaene-3,11-dione (CCD ID: 83Z) (formula: C₂₆H₃₄ClNO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			34	26	1	1	6		
3	B	1	Total	C	Cl	N	O	0	0
			34	26	1	1	6		

- Molecule 4 is 5'-O-[(S)-(carbamoyloxy)(hydroxy)phosphoryl]adenosine (CCD ID: CA0) (formula: C₁₁H₁₅N₆O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 26	C 11	N 6	O 8	P 1	0	0
4	B	1	Total 26	C 11	N 6	O 8	P 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

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



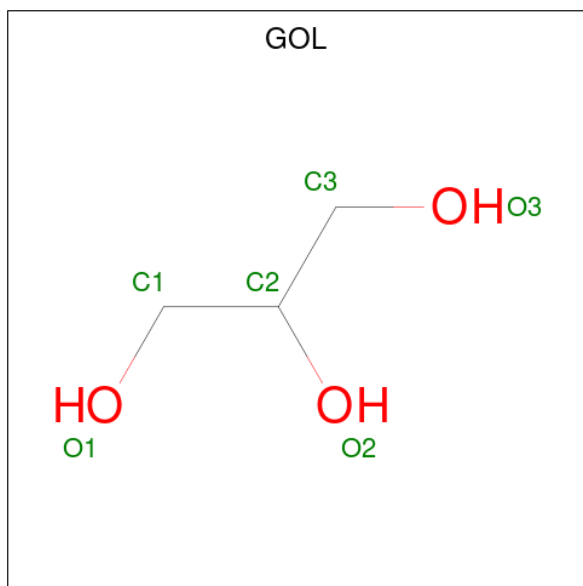
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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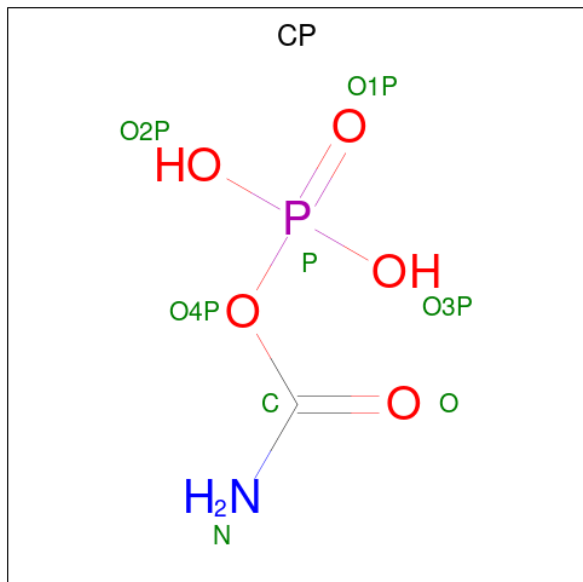
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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



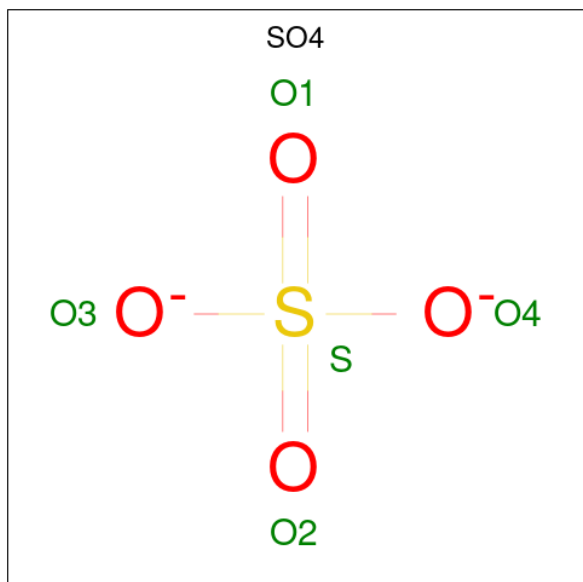
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (CCD ID: CP) (formula: $\text{CH}_4\text{NO}_5\text{P}$).



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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 10 is water.

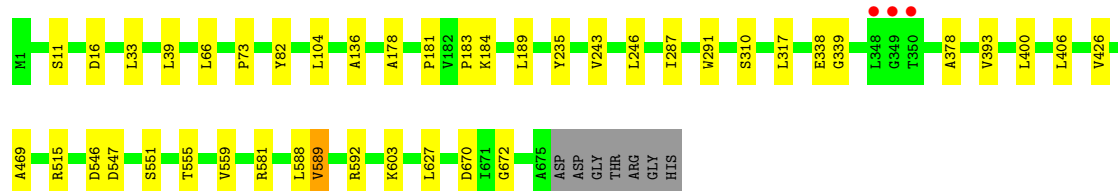
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	213	Total	O	0	0
			213	213		
10	B	142	Total	O	0	0
			142	142		

3 Residue-property plots [i](#)

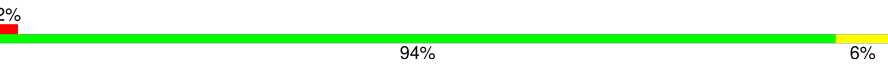
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

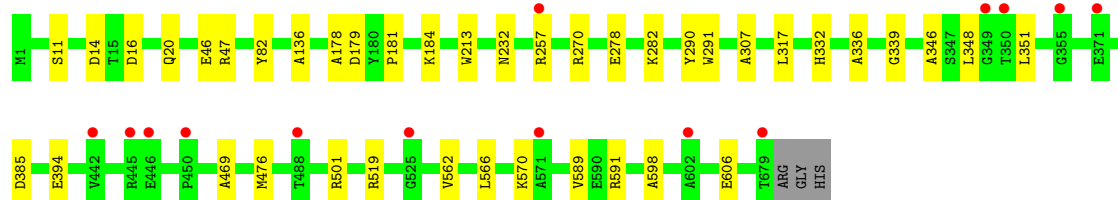
• Molecule 1: GdmN

Chain A: 



• Molecule 1: GdmN

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.39Å 111.39Å 230.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.62 – 2.10 28.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.62-2.10) 99.8 (28.62-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.214 0.183 , 0.215	Depositor DCC
R_{free} test set	4940 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10975	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GOL, EDO, SO4, 83Z, CP, FE, CA0, PEG

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	0.34	0/5318	0.50	0/7234
1	B	0.29	0/5332	0.48	0/7255
All	All	0.32	0/10650	0.49	0/14489

There are no bond length outliers.

There are no bond angle outliers.

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	5197	0	5098	27	0
1	B	5211	0	5093	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	0	0	0
3	B	34	0	0	1	0
4	A	26	0	14	0	0
4	B	26	0	14	0	0
5	A	7	0	10	2	0
6	A	32	0	48	3	0
6	B	16	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	0	0
7	B	6	0	8	1	0
8	A	8	0	2	0	0
9	A	10	0	0	0	0
9	B	5	0	0	0	0
10	A	213	0	0	0	0
10	B	142	0	0	0	0
All	All	10975	0	10319	48	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 2.

All (48) 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:393:VAL:HG11	1:A:515:ARG:HG2	1.75	0.68
1:A:378:ALA:HA	6:A:709:EDO:H21	1.77	0.64
1:A:181:PRO:HD2	1:A:184:LYS:HD2	1.78	0.64
1:B:181:PRO:HD2	1:B:184:LYS:HD2	1.80	0.63
1:B:11:SER:HB3	1:B:16:ASP:HA	1.82	0.62
1:B:179:ASP:H	6:B:705:EDO:H22	1.68	0.59
1:B:346:ALA:HB2	1:B:351:LEU:HD22	1.84	0.58
1:A:73:PRO:HG2	6:A:710:EDO:H21	1.87	0.57
1:A:547:ASP:OD1	5:A:704:PEG:H11	2.05	0.57
1:A:11:SER:HB3	1:A:16:ASP:HA	1.88	0.55
1:B:136:ALA:O	1:B:339:GLY:HA3	2.12	0.50
1:B:178:ALA:HB1	6:B:705:EDO:H22	1.93	0.50
1:A:136:ALA:O	1:A:339:GLY:HA3	2.12	0.50
1:B:476:MET:HB3	1:B:501:ARG:HG2	1.95	0.49
1:A:551:SER:O	1:A:555:THR:HG23	2.12	0.49
1:A:189:LEU:HD13	1:A:246:LEU:HD23	1.93	0.49
1:A:546:ASP:OD2	5:A:704:PEG:H42	2.12	0.49
1:A:588:LEU:HD11	1:A:627:LEU:HB2	1.95	0.48
1:B:178:ALA:HB2	1:B:291:TRP:CZ2	2.48	0.48
1:B:385:ASP:OD1	1:B:570:LYS:NZ	2.45	0.48
1:A:181:PRO:HB2	1:A:183:PRO:HD2	1.97	0.47
1:B:332:HIS:H	1:B:332:HIS:CD2	2.32	0.47
1:B:591:ARG:HH21	1:B:606:GLU:CD	2.24	0.46
1:A:547:ASP:HA	6:A:711:EDO:H12	1.98	0.45
1:A:592:ARG:CZ	1:A:603:LYS:HG2	2.47	0.44
1:A:581:ARG:HB3	1:B:598:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLN:HE22	7:B:708:GOL:H12	1.82	0.44
1:A:406:LEU:HG	1:A:559:VAL:HG13	2.00	0.44
1:A:178:ALA:HB2	1:A:291:TRP:CZ2	2.53	0.43
1:B:307:ALA:O	6:B:704:EDO:H22	2.17	0.43
1:A:104:LEU:HD13	1:B:257:ARG:HB3	2.00	0.43
1:B:213:TRP:HB3	1:B:270:ARG:HD2	2.00	0.43
1:A:589:VAL:HG23	1:B:589:VAL:HG13	2.01	0.43
1:B:317:LEU:HD12	1:B:469:ALA:HB3	2.00	0.43
1:A:243:VAL:HG12	3:B:702:83Z:CL1	2.56	0.42
1:B:232:ASN:HA	1:B:290:TYR:CE1	2.54	0.42
1:B:14:ASP:OD1	1:B:14:ASP:N	2.52	0.42
1:B:136:ALA:HB1	1:B:336:ALA:O	2.19	0.42
1:A:393:VAL:HB	1:A:515:ARG:NH1	2.35	0.42
1:A:400:LEU:HD21	1:A:426:VAL:HG23	2.01	0.41
1:B:278:GLU:HG2	1:B:282:LYS:HE2	2.01	0.41
1:B:394:GLU:OE1	1:B:519:ARG:NE	2.53	0.41
1:A:33:LEU:HD11	1:A:66:LEU:HD23	2.02	0.41
1:A:39:LEU:HD13	1:A:338:GLU:HG3	2.02	0.41
1:A:317:LEU:HD12	1:A:469:ALA:HB3	2.03	0.40
1:A:670:ASP:OD1	1:A:672:GLY:N	2.43	0.40
1:A:235:TYR:CE1	1:A:287:ILE:HD11	2.57	0.40
1:B:46:GLU:HG3	1:B:47:ARG:N	2.35	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	674/682 (99%)	655 (97%)	19 (3%)	0	100	100
1	B	677/682 (99%)	660 (98%)	17 (2%)	0	100	100
All	All	1351/1364 (99%)	1315 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/542 (99%)	533 (99%)	3 (1%)	78	86
1	B	536/542 (99%)	532 (99%)	4 (1%)	76	83
All	All	1072/1084 (99%)	1065 (99%)	7 (1%)	76	83

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

Mol	Chain	Res	Type
1	A	82	TYR
1	A	310	SER
1	A	589	VAL
1	B	82	TYR
1	B	348	LEU
1	B	562	VAL
1	B	566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	230	GLN
1	B	20	GLN
1	B	86	ASN
1	B	230	GLN
1	B	332	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](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	CA0	A	703	2	27,28,28	3.28	12 (44%)	39,42,42	1.98	12 (30%)
6	EDO	B	706	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	A	705	-	3,3,3	0.41	0	2,2,2	0.46	0
6	EDO	B	707	-	3,3,3	0.51	0	2,2,2	0.15	0
6	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.59	0
3	83Z	B	702	-	33,35,35	1.58	6 (18%)	37,48,48	2.24	8 (21%)
5	PEG	A	704	-	6,6,6	0.75	0	5,5,5	0.27	0
6	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	A	712	-	3,3,3	0.44	0	2,2,2	0.51	0
9	SO4	A	716	-	4,4,4	0.31	0	6,6,6	0.15	0
7	GOL	B	708	-	5,5,5	1.30	1 (20%)	5,5,5	1.15	0
9	SO4	A	715	-	4,4,4	0.19	0	6,6,6	0.27	0
6	EDO	B	704	-	3,3,3	0.35	0	2,2,2	0.26	0
7	GOL	A	713	-	5,5,5	1.05	0	5,5,5	0.98	0
8	CP	A	714	-	6,7,7	2.93	3 (50%)	7,10,10	2.20	2 (28%)
9	SO4	B	709	-	4,4,4	0.24	0	6,6,6	0.12	0
6	EDO	A	707	-	3,3,3	0.46	0	2,2,2	0.50	0
6	EDO	A	711	-	3,3,3	0.35	0	2,2,2	0.68	0
6	EDO	B	705	-	3,3,3	0.51	0	2,2,2	0.09	0
3	83Z	A	702	-	33,35,35	1.51	6 (18%)	37,48,48	2.37	13 (35%)
4	CA0	B	703	2	27,28,28	3.46	12 (44%)	39,42,42	2.12	14 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	710	-	3,3,3	0.43	0	2,2,2	0.34	0
6	EDO	A	709	-	3,3,3	0.40	0	2,2,2	0.42	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	CA0	A	703	2	-	2/13/31/31	0/3/3/3
6	EDO	B	706	-	-	1/1/1/1	-
6	EDO	A	705	-	-	1/1/1/1	-
6	EDO	B	707	-	-	0/1/1/1	-
6	EDO	A	706	-	-	1/1/1/1	-
3	83Z	B	702	-	-	7/42/42/42	0/1/2/2
5	PEG	A	704	-	-	1/4/4/4	-
6	EDO	A	708	-	-	1/1/1/1	-
6	EDO	A	712	-	-	0/1/1/1	-
7	GOL	B	708	-	-	2/4/4/4	-
6	EDO	B	704	-	-	0/1/1/1	-
7	GOL	A	713	-	-	2/4/4/4	-
8	CP	A	714	-	-	0/3/5/5	-
6	EDO	A	707	-	-	0/1/1/1	-
6	EDO	A	711	-	-	1/1/1/1	-
6	EDO	B	705	-	-	1/1/1/1	-
3	83Z	A	702	-	-	12/42/42/42	0/1/2/2
4	CA0	B	703	2	-	2/13/31/31	0/3/3/3
6	EDO	A	710	-	-	1/1/1/1	-
6	EDO	A	709	-	-	1/1/1/1	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	CA0	C3'-C2'	-9.21	1.28	1.53
4	A	703	CA0	C3'-C2'	-8.88	1.29	1.53
4	B	703	CA0	CB-N2B	8.51	1.48	1.33
4	A	703	CA0	CB-N2B	8.08	1.48	1.33
8	A	714	CP	C-N	5.66	1.43	1.33
4	B	703	CA0	O4'-C1'	-5.36	1.29	1.42
4	B	703	CA0	O4'-C4'	5.35	1.56	1.45
4	A	703	CA0	O4'-C1'	-5.34	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CA0	O4'-C4'	4.93	1.56	1.45
3	B	702	83Z	C13-N12	4.66	1.45	1.35
4	A	703	CA0	C6-N6	4.64	1.46	1.34
4	B	703	CA0	C6-N6	4.62	1.46	1.34
3	A	702	83Z	C13-N12	4.50	1.45	1.35
4	B	703	CA0	C2'-C1'	4.24	1.66	1.53
4	A	703	CA0	C2'-C1'	4.11	1.66	1.53
4	B	703	CA0	C5'-C4'	-4.09	1.39	1.51
4	A	703	CA0	C5'-C4'	-4.06	1.39	1.51
4	B	703	CA0	PA-O3A	3.80	1.67	1.60
8	A	714	CP	P-O4P	3.51	1.66	1.59
3	B	702	83Z	C30-C29	3.09	1.52	1.43
4	B	703	CA0	C8-N9	-2.94	1.32	1.37
3	A	702	83Z	C09-CL1	2.85	1.78	1.72
3	A	702	83Z	C30-C29	2.82	1.51	1.43
4	B	703	CA0	O3'-C3'	2.82	1.49	1.43
4	A	703	CA0	PA-O3A	2.77	1.65	1.60
3	A	702	83Z	C32-C31	2.73	1.53	1.50
4	A	703	CA0	O3'-C3'	2.65	1.49	1.43
3	B	702	83Z	C09-CL1	2.64	1.78	1.72
3	B	702	83Z	C32-C31	2.55	1.53	1.50
4	B	703	CA0	C5-N7	-2.47	1.34	1.39
3	B	702	83Z	O07-C06	2.44	1.41	1.37
8	A	714	CP	O-C	-2.34	1.18	1.22
3	A	702	83Z	O07-C06	2.24	1.40	1.37
4	A	703	CA0	C3'-C4'	2.12	1.58	1.53
4	A	703	CA0	C8-N9	-2.11	1.33	1.37
4	B	703	CA0	C3'-C4'	2.10	1.58	1.53
3	B	702	83Z	O26-C25	-2.07	1.18	1.21
3	A	702	83Z	O27-C13	-2.06	1.19	1.23
7	B	708	GOL	O2-C2	-2.06	1.37	1.43
4	A	703	CA0	C5-N7	-2.00	1.35	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	83Z	C30-C29-C02	-7.10	117.70	127.69
3	B	702	83Z	C14-C13-N12	6.06	122.12	114.62
3	A	702	83Z	C14-C13-N12	6.01	122.05	114.62
3	A	702	83Z	C01-C02-C03	5.48	120.12	115.53
3	B	702	83Z	C01-C02-C03	5.35	120.01	115.53
4	B	703	CA0	C5-C4-N3	-5.35	119.35	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	83Z	C30-C29-C02	-5.22	120.35	127.69
8	A	714	CP	O-C-N	-4.97	117.74	125.58
4	A	703	CA0	C5-C4-N3	-4.59	120.40	126.72
3	A	702	83Z	O07-C06-C09	4.35	120.21	115.44
4	A	703	CA0	N3-C2-N1	-4.33	122.03	128.58
3	A	702	83Z	C24-C22-C20	-4.07	105.83	114.23
4	B	703	CA0	N3-C2-N1	-3.75	122.91	128.58
4	B	703	CA0	N3-C4-N9	3.74	133.53	127.17
4	A	703	CA0	N3-C4-N9	3.58	133.25	127.17
4	B	703	CA0	C4-C5-N7	-3.57	106.50	110.58
4	B	703	CA0	C5-N7-C8	3.48	108.93	103.45
3	B	702	83Z	O27-C13-N12	-3.47	117.42	123.64
4	B	703	CA0	N9-C8-N7	-3.44	109.06	113.94
4	B	703	CA0	O1B-CB-N2B	-3.43	120.17	125.58
3	A	702	83Z	C14-C15-C17	-3.41	107.98	111.78
4	A	703	CA0	O3A-PA-O5'	3.38	113.16	103.00
4	B	703	CA0	C2-N3-C4	3.37	120.07	111.83
3	A	702	83Z	O16-C15-C14	3.37	118.08	109.96
4	A	703	CA0	O1A-PA-O3A	3.33	115.71	104.94
4	A	703	CA0	C2-N3-C4	3.22	119.70	111.83
3	B	702	83Z	O16-C15-C14	3.18	117.61	109.96
4	A	703	CA0	N9-C8-N7	-3.06	109.60	113.94
3	A	702	83Z	C34-O33-C32	-3.02	108.82	112.99
4	A	703	CA0	C5-N7-C8	2.97	108.12	103.45
4	B	703	CA0	O3A-PA-O5'	2.93	111.82	103.00
3	A	702	83Z	O27-C13-N12	-2.83	118.57	123.64
3	B	702	83Z	C34-O33-C32	-2.82	109.09	112.99
4	A	703	CA0	C4-C5-N7	-2.75	107.44	110.58
4	A	703	CA0	C4-N9-C8	2.62	108.49	105.74
3	A	702	83Z	C08-O07-C06	-2.61	113.69	117.51
4	B	703	CA0	O4'-C1'-N9	2.60	113.08	108.09
8	A	714	CP	O3P-P-O4P	2.54	112.72	105.32
4	B	703	CA0	C4-N9-C8	2.54	108.40	105.74
4	B	703	CA0	O1A-PA-O3A	2.49	113.00	104.94
3	B	702	83Z	C24-C22-C20	-2.39	109.30	114.23
4	B	703	CA0	C4'-O4'-C1'	-2.37	104.23	109.47
3	A	702	83Z	O07-C06-C05	-2.36	120.02	124.08
3	B	702	83Z	O07-C06-C09	2.19	117.84	115.44
3	A	702	83Z	C20-C19-C17	-2.12	123.10	128.00
4	A	703	CA0	O1B-CB-N2B	-2.08	122.30	125.58
4	B	703	CA0	C2'-C1'-N9	-2.05	108.21	113.30
3	A	702	83Z	C28-C11-C09	2.03	120.42	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CA0	C4'-O4'-C1'	-2.02	105.02	109.47

There are no chirality outliers.

All (36) torsion outliers are listed below:

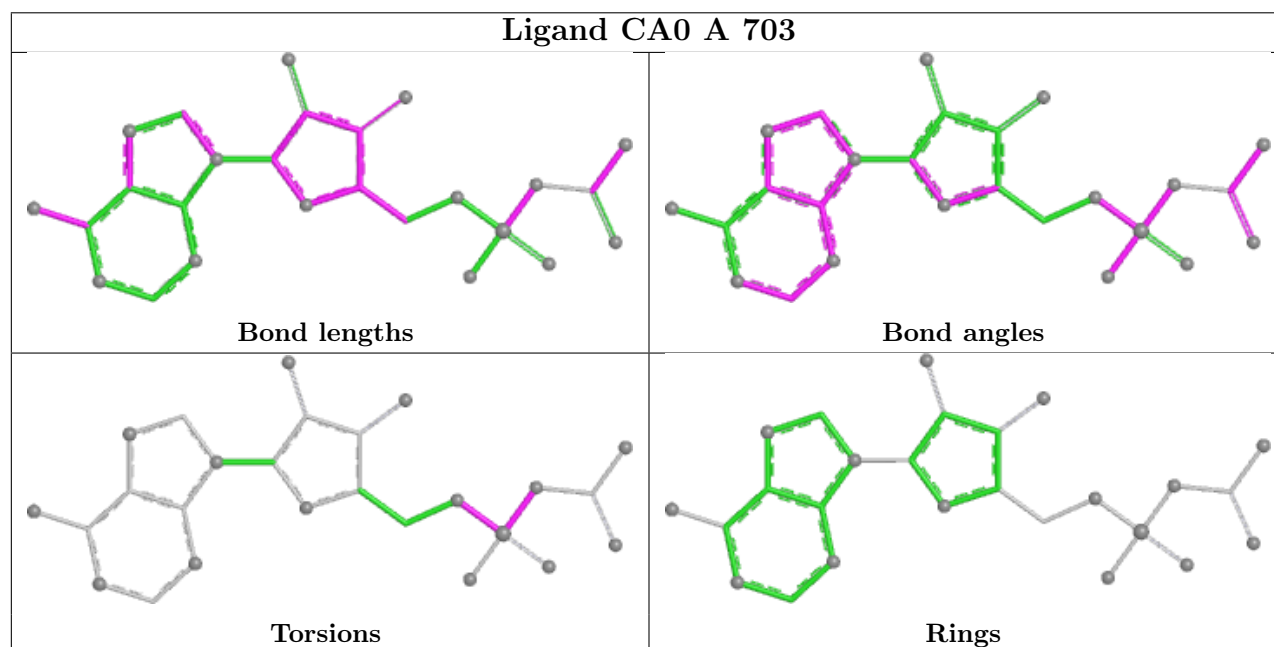
Mol	Chain	Res	Type	Atoms
3	A	702	83Z	C21-C20-C22-O23
3	A	702	83Z	C24-C25-C32-O33
3	A	702	83Z	O26-C25-C32-O33
3	B	702	83Z	C24-C25-C32-O33
3	B	702	83Z	O26-C25-C32-O33
4	A	703	CA0	C5'-O5'-PA-O2A
3	A	702	83Z	O27-C13-N12-C11
3	B	702	83Z	O27-C13-N12-C11
3	A	702	83Z	C14-C13-N12-C11
3	B	702	83Z	C14-C13-N12-C11
7	B	708	GOL	O1-C1-C2-C3
7	B	708	GOL	O1-C1-C2-O2
3	A	702	83Z	C21-C20-C22-C24
6	A	705	EDO	O1-C1-C2-O2
3	B	702	83Z	C21-C20-C22-O23
3	A	702	83Z	C31-C32-O33-C34
3	B	702	83Z	C21-C20-C22-C24
3	A	702	83Z	C19-C20-C22-O23
6	A	706	EDO	O1-C1-C2-O2
3	B	702	83Z	C31-C32-O33-C34
3	A	702	83Z	C02-C29-C30-C31
4	B	703	CA0	C5'-O5'-PA-O2A
5	A	704	PEG	C1-C2-O2-C3
6	A	711	EDO	O1-C1-C2-O2
6	B	705	EDO	O1-C1-C2-O2
6	B	706	EDO	O1-C1-C2-O2
3	A	702	83Z	C28-C11-N12-C13
4	A	703	CA0	CB-O3A-PA-O2A
3	A	702	83Z	O16-C15-C17-C19
7	A	713	GOL	O2-C2-C3-O3
6	A	709	EDO	O1-C1-C2-O2
6	A	708	EDO	O1-C1-C2-O2
4	B	703	CA0	CB-O3A-PA-O2A
7	A	713	GOL	C1-C2-C3-O3
3	A	702	83Z	C25-C32-O33-C34
6	A	710	EDO	O1-C1-C2-O2

There are no ring outliers.

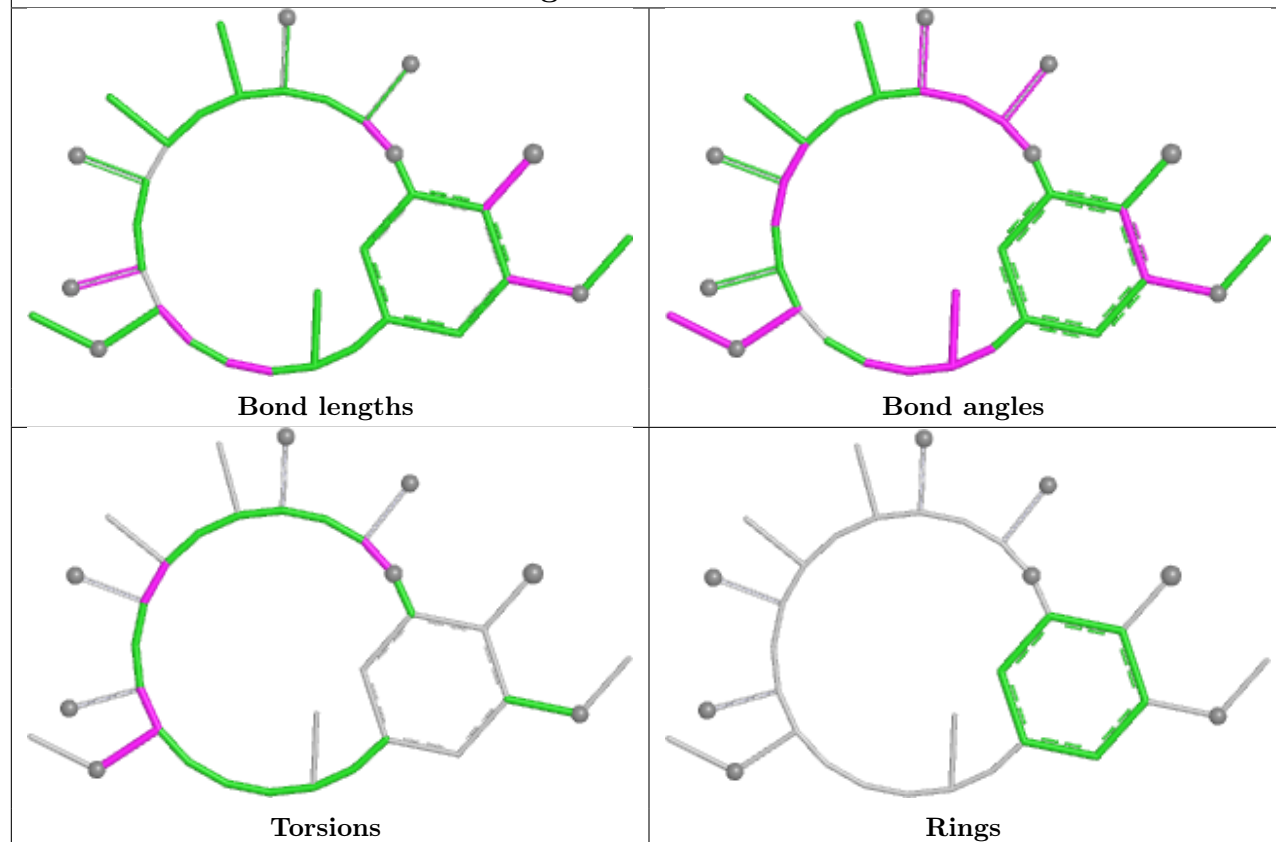
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	83Z	1	0
5	A	704	PEG	2	0
7	B	708	GOL	1	0
6	B	704	EDO	1	0
6	A	711	EDO	1	0
6	B	705	EDO	2	0
6	A	710	EDO	1	0
6	A	709	EDO	1	0

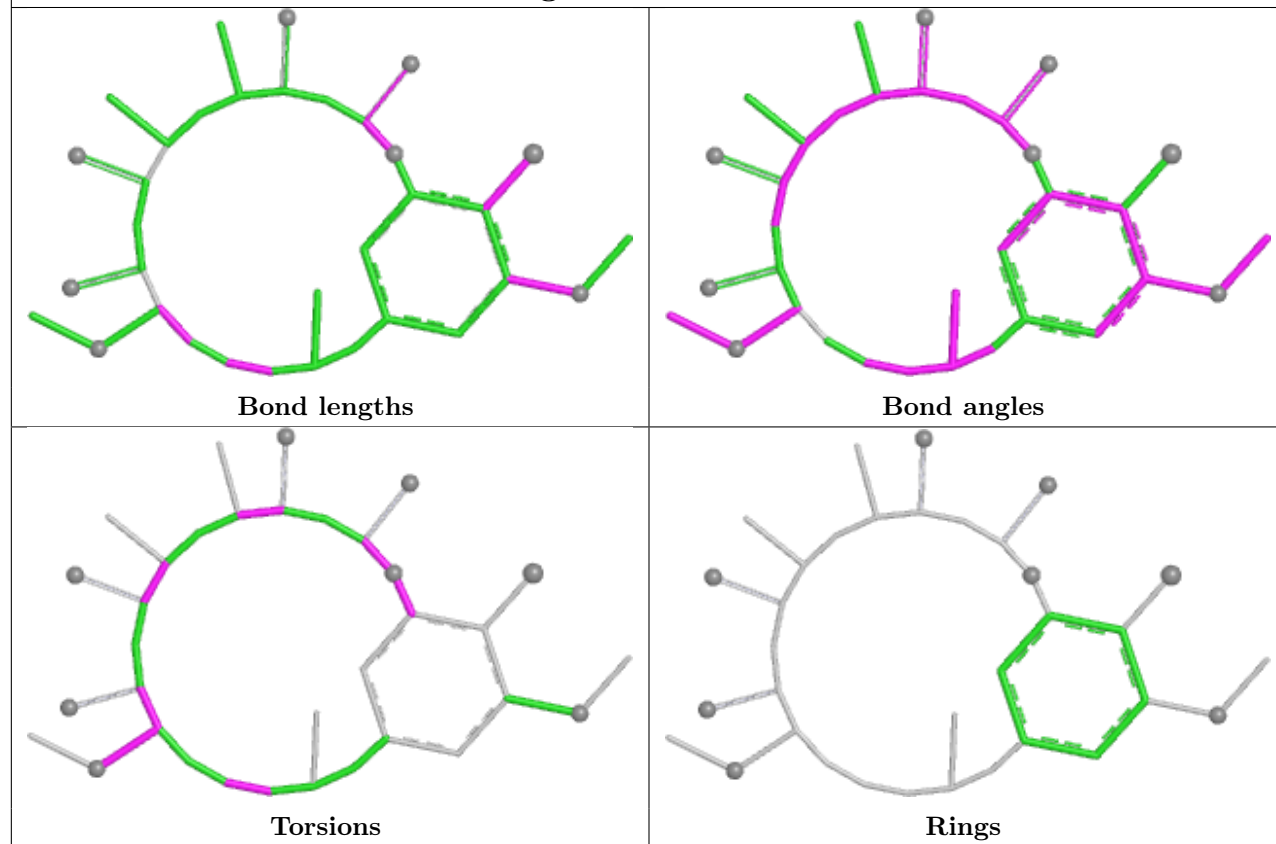
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

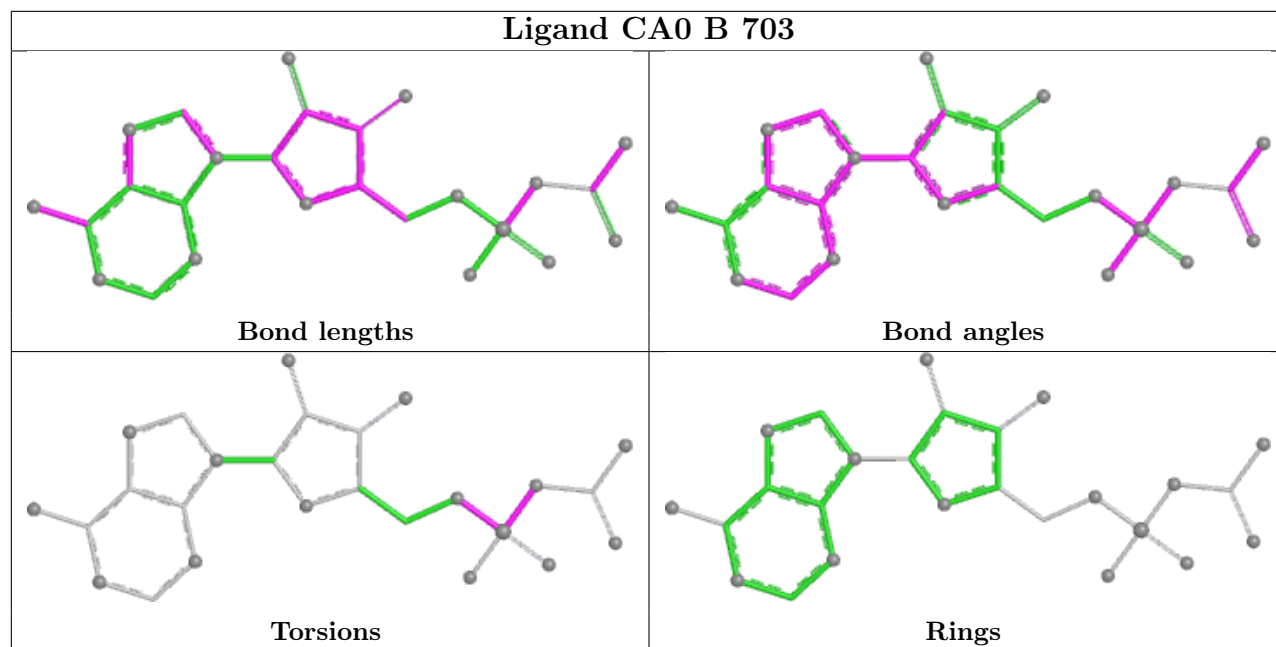


Ligand 83Z B 702



Ligand 83Z A 702





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	675/682 (98%)	-0.40	3 (0%) 88 90	13, 21, 36, 57	1 (0%)
1	B	679/682 (99%)	0.04	14 (2%) 63 66	17, 27, 47, 62	0
All	All	1354/1364 (99%)	-0.18	17 (1%) 75 77	13, 24, 43, 62	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	THR	4.7
1	A	348	LEU	4.2
1	B	679	THR	3.6
1	B	602	ALA	3.2
1	B	446	GLU	3.0
1	A	349	GLY	3.0
1	A	350	THR	2.6
1	B	445	ARG	2.5
1	B	488	THR	2.5
1	B	571	ALA	2.4
1	B	450	PRO	2.4
1	B	371	GLU	2.3
1	B	525	GLY	2.3
1	B	355	GLY	2.3
1	B	349	GLY	2.2
1	B	442	VAL	2.2
1	B	257	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

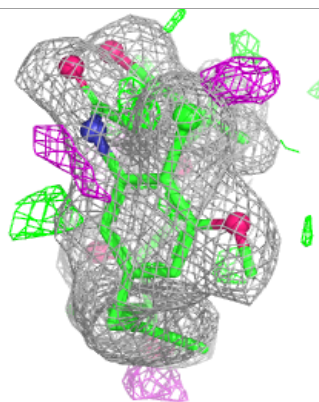
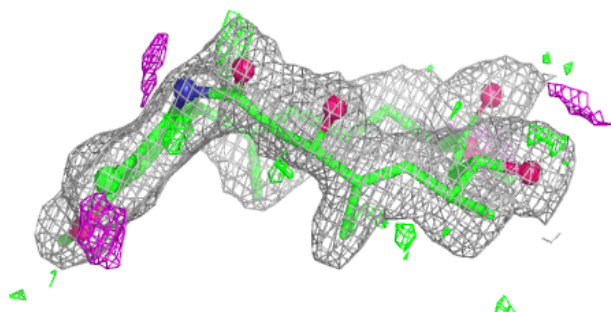
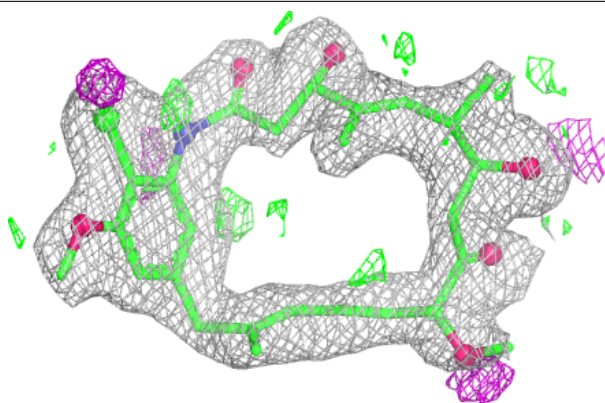
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	713	6/6	0.71	0.16	46,48,52,53	0
5	PEG	A	704	7/7	0.73	0.20	28,31,37,38	0
6	EDO	A	705	4/4	0.74	0.19	32,42,47,58	0
6	EDO	A	707	4/4	0.75	0.17	39,40,40,41	0
6	EDO	A	706	4/4	0.77	0.25	36,45,45,49	0
6	EDO	A	709	4/4	0.78	0.26	28,30,40,48	0
7	GOL	B	708	6/6	0.82	0.17	27,36,40,43	0
9	SO4	A	716	5/5	0.82	0.17	49,55,59,60	0
6	EDO	A	710	4/4	0.85	0.17	32,37,37,37	0
6	EDO	A	708	4/4	0.86	0.11	36,38,39,47	0
3	83Z	A	702	34/34	0.86	0.13	21,31,38,42	34
8	CP	A	714	8/8	0.87	0.16	26,42,47,50	0
6	EDO	B	706	4/4	0.87	0.12	43,44,47,52	0
3	83Z	B	702	34/34	0.89	0.12	19,29,40,51	34
6	EDO	B	705	4/4	0.90	0.21	21,30,38,41	0
6	EDO	B	707	4/4	0.91	0.12	32,33,35,37	0
6	EDO	B	704	4/4	0.92	0.23	21,22,32,37	0
6	EDO	A	711	4/4	0.93	0.23	20,21,23,24	0
6	EDO	A	712	4/4	0.94	0.10	17,24,27,29	0
4	CA0	B	703	26/26	0.95	0.07	19,22,26,31	0
4	CA0	A	703	26/26	0.96	0.07	13,18,23,33	26
9	SO4	B	709	5/5	0.96	0.12	36,39,41,42	0
2	FE	B	701	1/1	0.99	0.02	20,20,20,20	0
9	SO4	A	715	5/5	0.99	0.05	23,23,25,25	0
2	FE	A	701	1/1	1.00	0.01	17,17,17,17	0

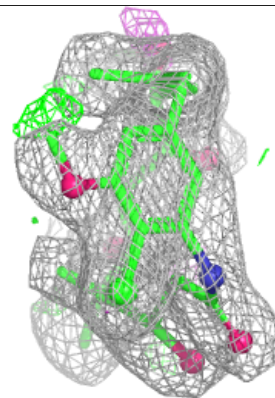
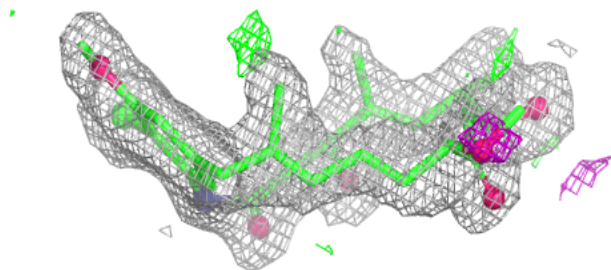
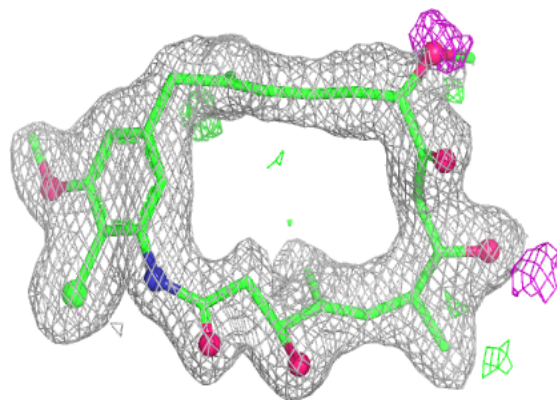
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 83Z A 702:

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

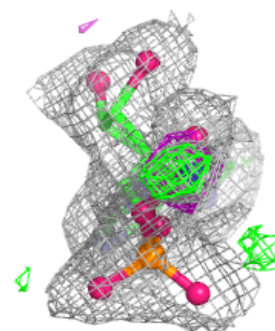
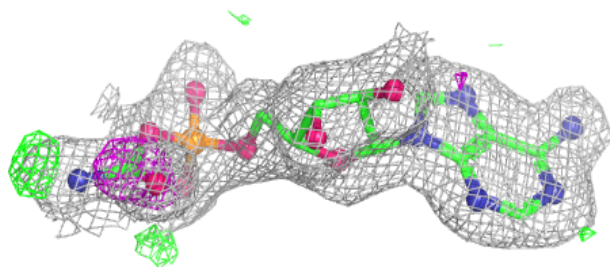
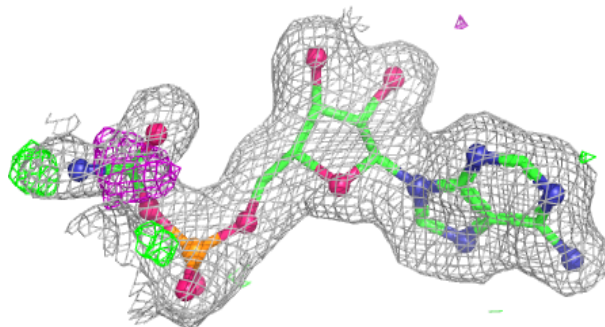
**Electron density around 83Z B 702:**

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

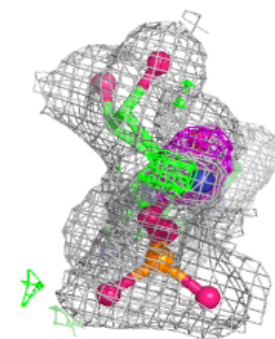
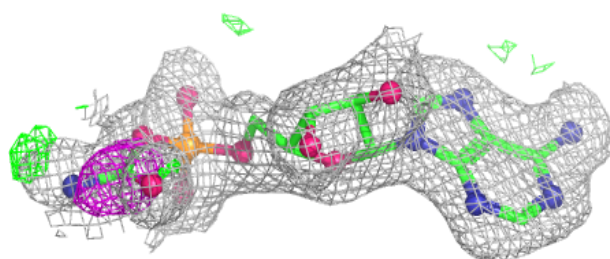
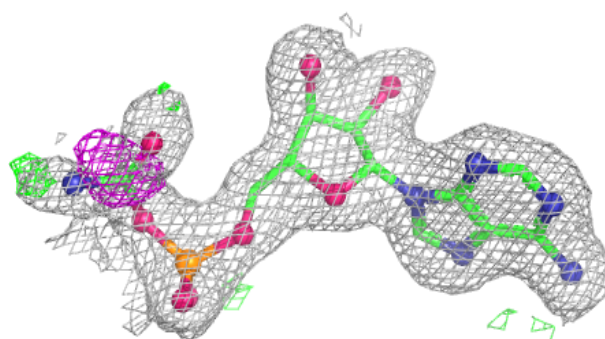


Electron density around CA0 B 703:

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

**Electron density around CA0 A 703:**

$2mF_o-DF_c$ (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.