



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:07 AM UTC

PDB ID : 1YLS / pdb_00001yls
Title : Crystal structure of selenium-modified Diels-Alder ribozyme complexed with the product of the reaction between N-pentylmaleimide and covalently attached 9-hydroxymethylantracene
Authors : Serganov, A.; Keiper, S.; Malinina, L.; Tereshko, V.; Skripkin, E.; Hobartner, C.; Polonskaia, A.; Phan, A.T.; Wombacher, R.; Micura, R.; Dauter, Z.; Jaschke, A.; Patel, D.J.
Deposited on : 2005-01-19
Resolution : 3.00 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)

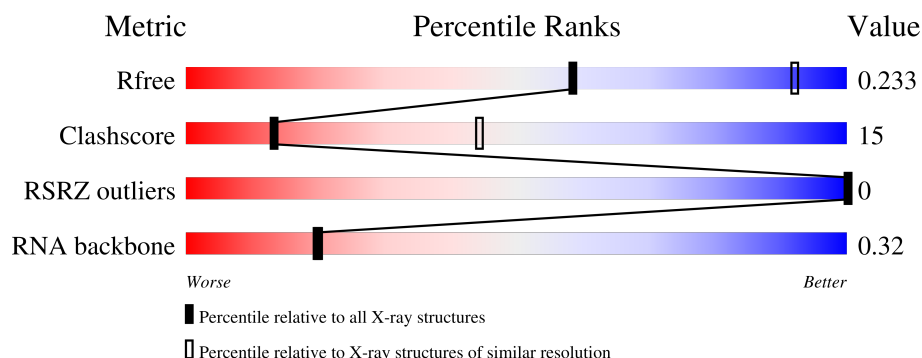
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	11	45% 45% 9%
1	C	11	36% 45% 18%
2	B	38	34% 45% 16% 5%
2	D	38	34% 50% 13% •

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2258 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.

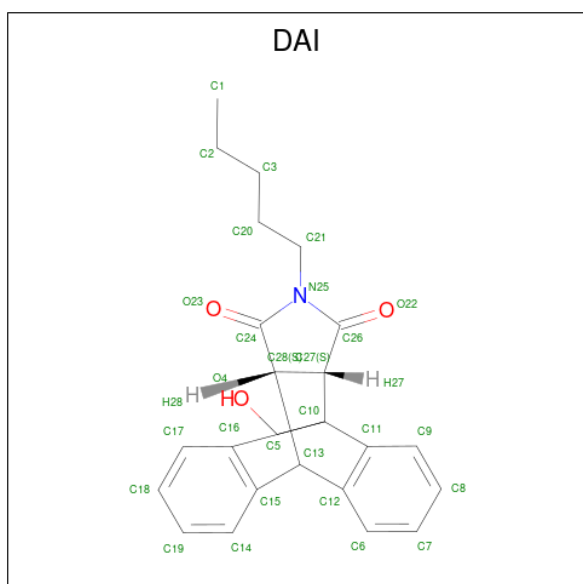
- Molecule 1 is a RNA chain called RNA Diels-Alder ribozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	P	Se	0	0	0
			237	106	42	76	11	2			
1	C	11	Total	C	N	O	P	Se	0	0	0
			237	106	42	76	11	2			

- Molecule 2 is a RNA chain called RNA Diels-Alder ribozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	38	Total	C	N	O	P	Se	0	0	0
			816	366	148	261	37	4			
2	D	38	Total	C	N	O	P	Se	0	0	0
			816	366	148	261	37	4			

- Molecule 3 is (3AS,9AS)-2-PENTYL-4-HYDROXYMETHYL-3A,4,9,9A-TETRAHYDRO-4,9[1',2']-BENZENO-1H-BENZ[F]ISOINDOLE-1,3(2H)-DIONE (CCD ID: DAI) (formula: C₂₄H₂₅NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	24	1	3		
3	C	1	Total	C	N	O	0	0
			28	24	1	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total	Mg	0	0
			7	7		
4	D	6	Total	Mg	0	0
			6	6		

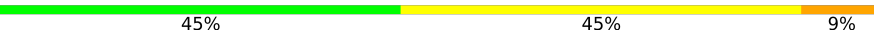
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	41	Total	O	0	0
			41	41		
5	C	3	Total	O	0	0
			3	3		
5	D	36	Total	O	0	0
			36	36		

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: RNA Diels-Alder ribozyme

Chain A: 

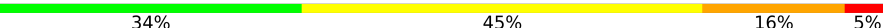


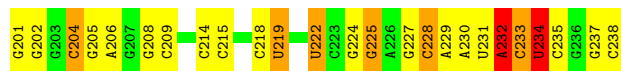
- Molecule 1: RNA Diels-Alder ribozyme

Chain C: 



- Molecule 2: RNA Diels-Alder ribozyme

Chain B: 



- Molecule 2: RNA Diels-Alder ribozyme

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.87Å 43.27Å 79.93Å 90.00° 106.19° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.00) 92.2 (20.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.209 , 0.234 0.211 , 0.233	Depositor DCC
R_{free} test set	502 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.126 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2258	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 6.87% 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: DAI, CSL, MG, UMS

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	0.90	0/217	0.93	0/335
1	C	0.85	1/217 (0.5%)	0.95	0/335
2	B	1.00	2/819 (0.2%)	1.07	0/1278
2	D	0.96	1/819 (0.1%)	1.06	0/1278
All	All	0.96	4/2072 (0.2%)	1.04	0/3226

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	232	A	O5'-C5'	-6.01	1.33	1.42
1	C	110	CSL	O3'-P	5.90	1.62	1.56
2	D	233	C	C3'-O3'	-5.82	1.33	1.42
2	B	234	U	C3'-O3'	-5.24	1.35	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	237	0	125	1	0
1	C	237	0	125	8	0
2	B	816	0	422	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	816	0	422	22	0
3	A	28	0	25	0	0
3	C	28	0	25	1	0
4	B	7	0	0	0	0
4	D	6	0	0	0	0
5	A	3	0	0	0	0
5	B	41	0	0	0	0
5	C	3	0	0	0	0
5	D	36	0	0	0	0
All	All	2258	0	1144	49	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 15.

All (49) 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:106:UMS:HA'3	1:C:107:C:H5'	1.67	0.76
1:A:106:UMS:HA'3	1:A:107:C:H5'	1.69	0.75
2:B:224:G:H2'	2:B:225:G:O4'	1.95	0.66
2:B:201:G:H2'	2:B:202:G:C8	2.33	0.64
1:C:106:UMS:HA'3	1:C:107:C:C5'	2.32	0.60
2:B:237:G:O2'	2:B:238:C:H5'	2.05	0.56
2:D:207:G:H5''	2:D:208:G:H5'	1.88	0.56
2:D:204:CSL:O2P	2:D:204:CSL:H6	2.06	0.55
1:C:101:G:C8	1:C:101:G:H5'	2.44	0.53
2:D:214:C:H2'	2:D:215:C:C6	2.43	0.53
2:D:233:C:H2'	2:D:233:C:O2	2.12	0.50
1:C:106:UMS:H2'	1:C:107:C:C6	2.48	0.49
2:B:229:A:H2'	2:B:230:A:O4'	2.12	0.49
2:B:204:CSL:H6	2:B:204:CSL:O2P	2.13	0.48
1:C:101:G:H5'	1:C:101:G:H8	1.77	0.48
2:D:201:G:H2'	2:D:202:G:C8	2.48	0.48
2:B:218:C:H2'	2:B:219:UMS:H6	1.96	0.47
2:B:237:G:C2'	2:B:238:C:H5'	2.45	0.47
2:D:217:G:C4	2:D:218:C:C5	3.02	0.47
2:D:215:C:H2'	2:D:216:G:O4'	2.14	0.47
2:D:201:G:H2'	2:D:202:G:H8	1.79	0.47
2:B:201:G:H2'	2:B:202:G:H8	1.80	0.46
2:B:233:C:O2	2:B:233:C:C2'	2.62	0.46
2:B:202:G:H8	2:B:202:G:O5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:G:C6	2:D:218:C:C4	3.03	0.46
2:D:214:C:N4	2:D:215:C:N4	2.63	0.46
2:B:227:G:C2'	2:B:228:C:O5'	2.64	0.45
2:D:204:CSL:H2'	2:D:205:G:O5'	2.17	0.45
2:B:214:C:H2'	2:B:215:C:C6	2.52	0.45
2:D:230:A:H2'	2:D:231:U:O4'	2.17	0.44
2:D:214:C:H2'	2:D:215:C:H6	1.82	0.43
2:D:218:C:H2'	2:D:219:UMS:H6	2.00	0.43
2:D:209:CSL:H6	2:D:209:CSL:O5'	2.19	0.43
2:D:209:CSL:H4'	2:D:209:CSL:HA'3	2.01	0.42
2:B:222:UMS:O2	2:B:222:UMS:HA'2	2.19	0.42
1:C:109:C:H2'	1:C:110:CSL:H6	2.01	0.42
2:B:204:CSL:SE2'	2:B:205:G:H5'	2.70	0.42
2:B:219:UMS:HA'2	2:B:219:UMS:H4'	2.01	0.42
1:C:106:UMS:HA'3	1:C:107:C:C4'	2.50	0.42
2:B:232:A:O2'	2:B:234:U:OP2	2.37	0.42
2:B:233:C:O2	2:B:233:C:H2'	2.20	0.41
2:D:217:G:C5	2:D:218:C:C5	3.08	0.41
2:D:233:C:O2	2:D:233:C:C2'	2.68	0.41
2:D:214:C:C4	2:D:215:C:N4	2.88	0.41
1:C:106:UMS:CA'	1:C:107:C:H5'	2.45	0.41
2:D:210:C:O2'	2:D:211:G:H5'	2.20	0.41
2:D:232:A:N3	2:D:234:U:O2'	2.49	0.40
3:C:100:DAI:H8	2:D:234:U:C2	2.55	0.40
2:B:205:G:H2'	2:B:206:A:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	6/11 (54%)	3 (50%)	0
1	C	6/11 (54%)	2 (33%)	0
2	B	29/38 (76%)	7 (24%)	2 (6%)
2	D	29/38 (76%)	7 (24%)	1 (3%)
All	All	70/98 (71%)	19 (27%)	3 (4%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	103	A
1	A	108	G
1	A	109	C
2	B	208	G
2	B	225	G
2	B	228	C
2	B	231	U
2	B	233	C
2	B	234	U
2	B	235	C
1	C	105	C
1	C	108	G
2	D	217	G
2	D	225	G
2	D	226	A
2	D	233	C
2	D	234	U
2	D	235	C
2	D	236	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	232	A
2	B	233	C
2	D	233	C

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

12 non-standard protein/DNA/RNA residues 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
2	CSL	B	209	2	17,22,23	1.17	1 (5%)	22,31,34	1.15	3 (13%)
2	CSL	D	209	2	17,22,23	1.21	1 (5%)	22,31,34	1.16	2 (9%)
2	CSL	D	204	1,2	17,22,23	0.88	1 (5%)	22,31,34	1.22	2 (9%)
1	UMS	A	106	1,2	17,22,23	0.83	1 (5%)	22,31,34	0.80	1 (4%)
1	CSL	C	110	1,2	17,22,23	0.68	0	22,31,34	1.07	2 (9%)
1	CSL	A	110	1,2	17,22,23	0.55	0	22,31,34	0.94	1 (4%)
2	UMS	B	219	2	17,22,23	1.14	1 (5%)	22,31,34	1.11	3 (13%)
2	UMS	D	219	2	17,22,23	1.03	0	22,31,34	0.97	2 (9%)
2	UMS	B	222	2	17,22,23	0.72	0	22,31,34	1.12	3 (13%)
1	UMS	C	106	1,2	17,22,23	0.71	0	22,31,34	0.90	1 (4%)
2	CSL	B	204	1,2	17,22,23	0.74	0	22,31,34	0.96	2 (9%)
2	UMS	D	222	2	17,22,23	0.56	0	22,31,34	0.91	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
2	CSL	B	209	2	-	0/7/27/28	0/2/2/2
2	CSL	D	209	2	-	0/7/27/28	0/2/2/2
2	CSL	D	204	1,2	-	3/7/27/28	0/2/2/2
1	UMS	A	106	1,2	-	0/7/27/28	0/2/2/2
1	CSL	C	110	1,2	-	0/7/27/28	0/2/2/2
1	CSL	A	110	1,2	-	0/7/27/28	0/2/2/2
2	UMS	B	219	2	-	0/7/27/28	0/2/2/2
2	UMS	D	219	2	-	0/7/27/28	0/2/2/2
2	UMS	B	222	2	-	0/7/27/28	0/2/2/2
1	UMS	C	106	1,2	-	0/7/27/28	0/2/2/2
2	CSL	B	204	1,2	-	3/7/27/28	0/2/2/2
2	UMS	D	222	2	-	0/7/27/28	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	CSL	C1'-N1	-3.30	1.38	1.47
2	D	209	CSL	O5'-C5'	-3.29	1.34	1.44
2	D	204	CSL	C1'-N1	2.35	1.54	1.47
2	B	219	UMS	O5'-C5'	-2.29	1.37	1.44
1	A	106	UMS	O5'-C5'	-2.03	1.38	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	CSL	O3'-C3'-C2'	3.56	116.29	110.64
2	D	204	CSL	C2'-C3'-C4'	-3.47	97.11	106.97
2	B	222	UMS	O4'-C1'-N1	3.31	115.86	108.36
1	C	110	CSL	C3'-C2'-C1'	-3.27	99.02	103.53
2	B	209	CSL	O3'-C3'-C2'	3.17	115.67	110.64
2	B	219	UMS	C2'-C3'-C4'	-3.10	98.18	106.97
2	B	209	CSL	C3'-C2'-C1'	-2.75	99.74	103.53
1	C	106	UMS	C2'-C3'-C4'	-2.74	99.18	106.97
2	D	204	CSL	C3'-C2'-C1'	-2.66	99.87	103.53
2	D	222	UMS	C3'-C2'-C1'	-2.65	99.87	103.53
2	B	219	UMS	O3'-C3'-C2'	2.63	114.81	110.64
1	C	110	CSL	C2'-C3'-C4'	-2.54	99.75	106.97
2	D	219	UMS	C2'-C3'-C4'	-2.43	100.06	106.97
2	D	209	CSL	C2'-C3'-C4'	-2.39	100.17	106.97
1	A	110	CSL	C3'-C2'-C1'	-2.36	100.28	103.53
1	A	106	UMS	C2'-C3'-C4'	-2.33	100.37	106.97
2	B	204	CSL	O3'-C3'-C2'	2.28	114.26	110.64
2	B	209	CSL	C2'-C3'-C4'	-2.23	100.63	106.97
2	B	222	UMS	C3'-C2'-C1'	-2.21	100.48	103.53
2	D	219	UMS	O3'-C3'-C2'	2.19	114.12	110.64
2	B	204	CSL	C3'-C2'-C1'	-2.12	100.61	103.53
2	B	222	UMS	C2'-C3'-C4'	-2.06	101.12	106.97
2	B	219	UMS	C3'-C2'-C1'	-2.03	100.73	103.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	204	CSL	O4'-C4'-C5'-O5'
2	D	204	CSL	C3'-C4'-C5'-O5'
2	B	204	CSL	O4'-C4'-C5'-O5'
2	B	204	CSL	C3'-C4'-C5'-O5'
2	D	204	CSL	C4'-C5'-O5'-P
2	B	204	CSL	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	209	CSL	2	0
2	D	204	CSL	2	0
1	A	106	UMS	1	0
1	C	110	CSL	1	0
2	B	219	UMS	2	0
2	D	219	UMS	1	0
2	B	222	UMS	1	0
1	C	106	UMS	5	0
2	B	204	CSL	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 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
3	DAI	A	100	-	32,32,32	2.63	7 (21%)	44,49,49	1.86	8 (18%)
3	DAI	C	100	-	32,32,32	2.22	7 (21%)	44,49,49	1.84	7 (15%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAI	A	100	-	-	2/8/58/58	0/6/5/5
3	DAI	C	100	-	-	1/8/58/58	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	100	DAI	C26-N25	-8.94	1.26	1.38
3	C	100	DAI	C26-N25	-7.83	1.28	1.38
3	A	100	DAI	C24-N25	-7.78	1.28	1.38
3	C	100	DAI	C24-N25	-6.66	1.29	1.38
3	A	100	DAI	C12-C13	-4.54	1.45	1.51
3	A	100	DAI	C15-C13	-4.41	1.45	1.51
3	C	100	DAI	C12-C13	-3.34	1.47	1.51
3	C	100	DAI	C15-C13	-2.72	1.48	1.51
3	C	100	DAI	C15-C16	-2.72	1.37	1.40
3	A	100	DAI	C10-C11	-2.64	1.49	1.53
3	A	100	DAI	C15-C16	-2.58	1.37	1.40
3	A	100	DAI	C12-C11	-2.33	1.37	1.40
3	C	100	DAI	C27-C26	-2.27	1.48	1.51
3	C	100	DAI	C12-C11	-2.05	1.38	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	100	DAI	C28-C27-C26	-5.24	100.62	104.55
3	C	100	DAI	C27-C26-N25	5.16	113.45	108.38
3	C	100	DAI	O22-C26-C27	-5.15	121.60	127.50
3	A	100	DAI	C27-C26-N25	4.82	113.13	108.38
3	C	100	DAI	C28-C27-C26	-4.75	101.00	104.55
3	A	100	DAI	O23-C24-C28	-4.37	121.93	127.51
3	A	100	DAI	C28-C24-N25	4.13	111.93	108.46
3	A	100	DAI	O22-C26-C27	-4.12	122.78	127.50
3	C	100	DAI	O23-C24-C28	-4.11	122.26	127.51
3	A	100	DAI	C27-C28-C24	-4.07	101.77	104.85
3	C	100	DAI	C27-C28-C24	-3.58	102.14	104.85
3	C	100	DAI	C28-C24-N25	3.51	111.41	108.46
3	A	100	DAI	C20-C21-N25	-2.33	106.85	112.36
3	C	100	DAI	C20-C21-N25	-2.29	106.93	112.36
3	A	100	DAI	C27-C28-C13	2.14	111.31	109.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

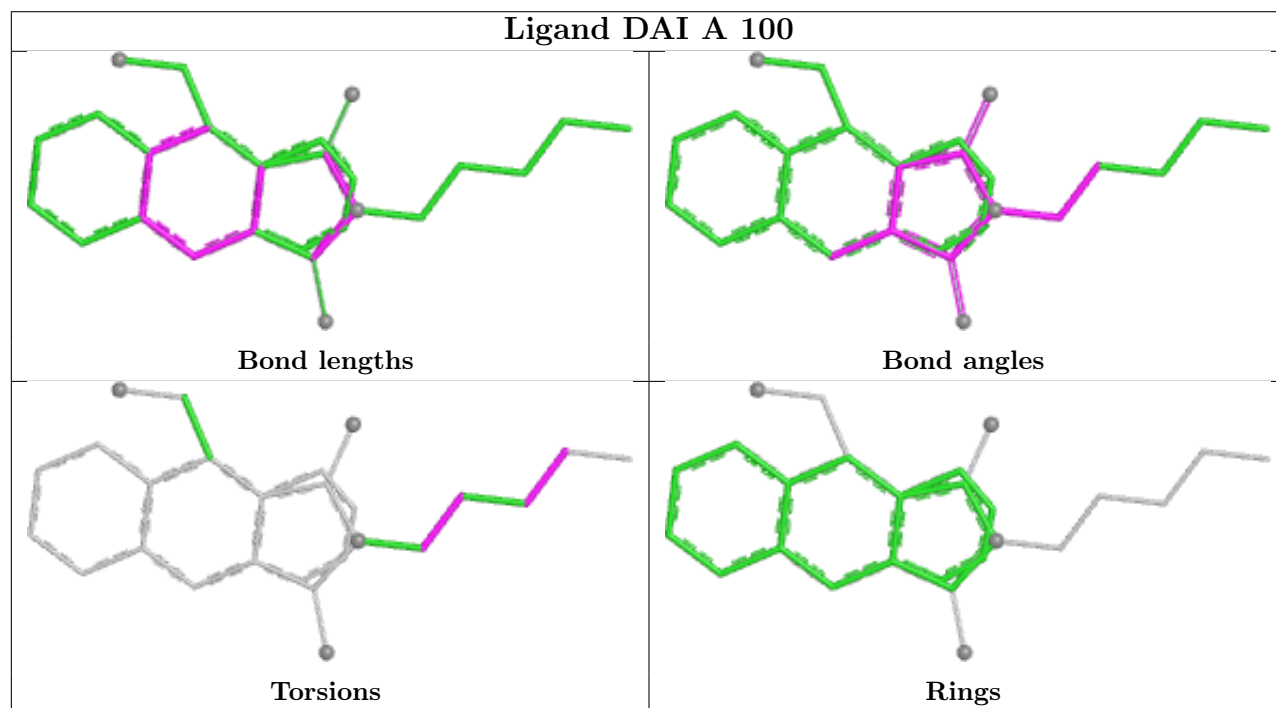
Mol	Chain	Res	Type	Atoms
3	C	100	DAI	C21-C20-C3-C2
3	A	100	DAI	C1-C2-C3-C20
3	A	100	DAI	C3-C20-C21-N25

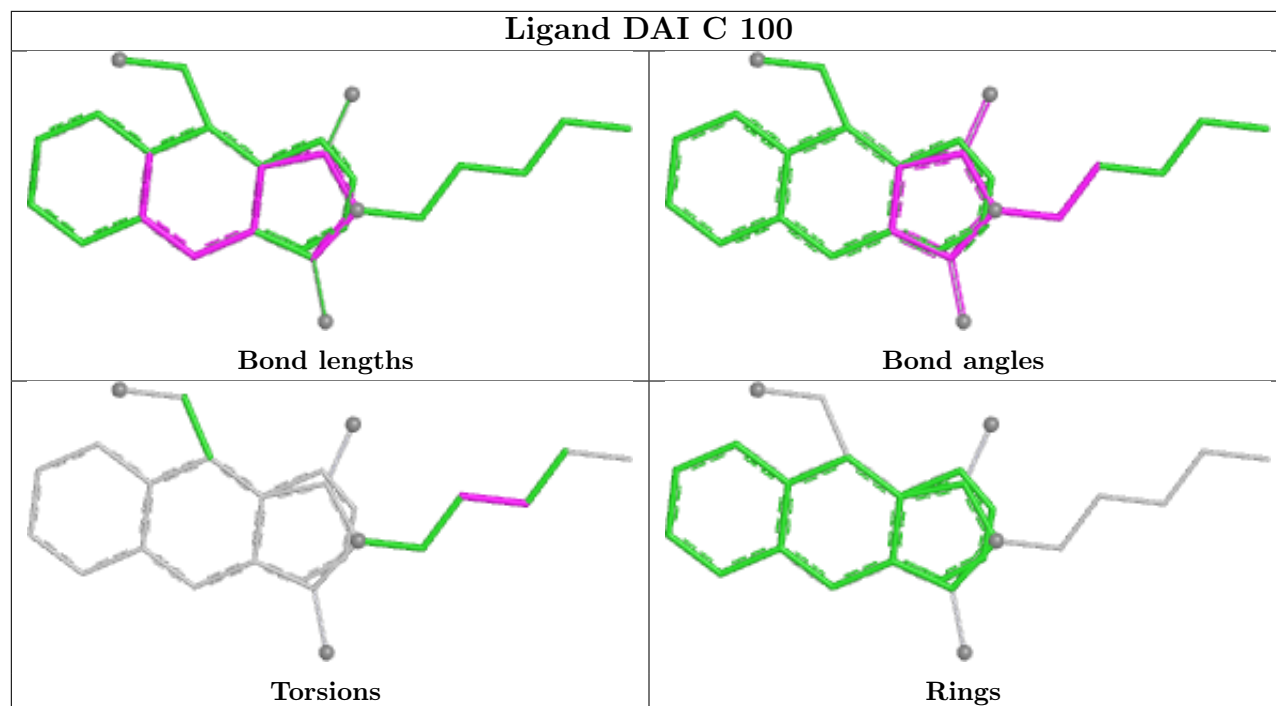
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	100	DAI	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.





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	9/11 (81%)	-1.48	0 100 100	13, 20, 24, 29	0
1	C	9/11 (81%)	-1.28	0 100 100	24, 25, 34, 36	0
2	B	34/38 (89%)	-1.36	0 100 100	13, 22, 30, 34	0
2	D	34/38 (89%)	-1.22	0 100 100	12, 25, 34, 37	0
All	All	86/98 (87%)	-1.31	0 100 100	12, 24, 34, 37	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSL	D	204	21/22	0.93	0.12	36,38,42,53	0
2	UMS	D	219	21/22	0.97	0.07	23,26,32,42	0
2	UMS	B	222	21/22	0.98	0.08	23,37,41,51	0
1	UMS	C	106	21/22	0.98	0.07	24,33,35,44	0
1	CSL	C	110	21/22	0.98	0.07	31,35,38,45	0
1	CSL	A	110	21/22	0.98	0.07	19,23,30,37	0
2	CSL	B	204	21/22	0.98	0.06	24,35,41,55	0
2	UMS	D	222	21/22	0.98	0.06	10,19,26,35	0
2	CSL	D	209	21/22	0.99	0.05	22,23,30,44	0
1	UMS	A	106	21/22	0.99	0.05	23,28,34,45	0
2	UMS	B	219	21/22	0.99	0.05	18,23,29,41	0
2	CSL	B	209	21/22	1.00	0.04	16,20,29,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

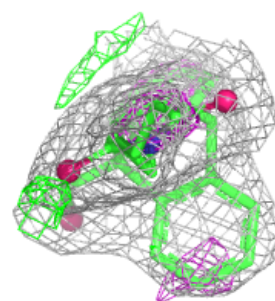
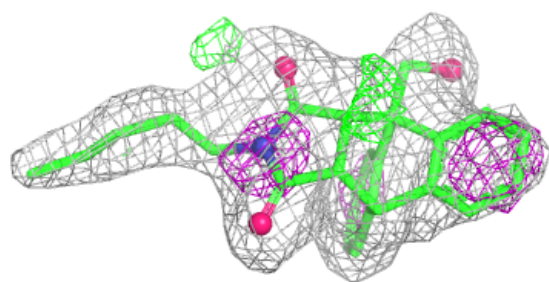
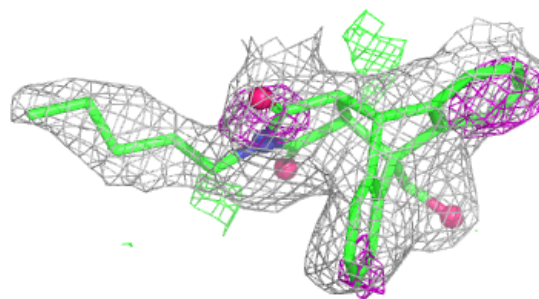
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	D	342	1/1	0.93	0.12	59,59,59,59	0
4	MG	D	344	1/1	0.95	0.18	87,87,87,87	0
4	MG	B	243	1/1	0.96	0.08	57,57,57,57	0
4	MG	D	343	1/1	0.96	0.15	55,55,55,55	0
4	MG	B	245	1/1	0.96	0.11	72,72,72,72	0
3	DAI	C	100	28/28	0.97	0.07	21,26,28,28	0
4	MG	B	244	1/1	0.97	0.07	92,92,92,92	0
4	MG	D	247	1/1	0.99	0.11	37,37,37,37	0
4	MG	D	341	1/1	0.99	0.06	25,25,25,25	0
4	MG	B	242	1/1	0.99	0.04	51,51,51,51	0
3	DAI	A	100	28/28	0.99	0.06	22,25,27,28	0
4	MG	B	246	1/1	0.99	0.05	41,41,41,41	0
4	MG	B	241	1/1	1.00	0.03	34,34,34,34	0
4	MG	D	340	1/1	1.00	0.01	28,28,28,28	0
4	MG	B	240	1/1	1.00	0.02	21,21,21,21	0

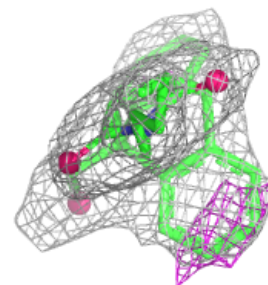
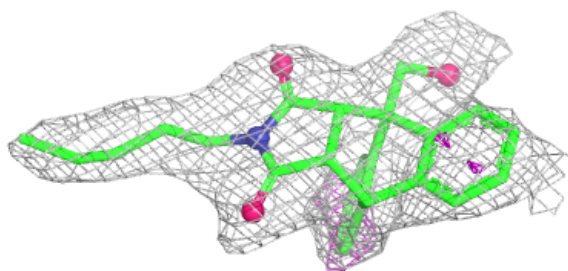
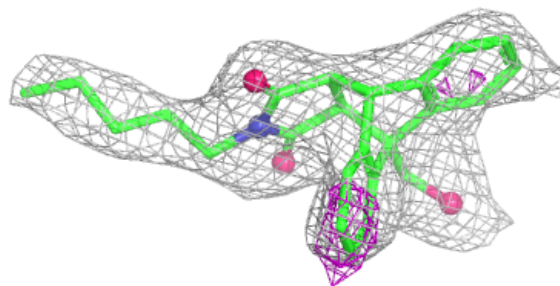
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DAI C 100:

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

**Electron density around DAI A 100:**

$2mF_o-DF_c$ (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.