



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:39 PM EDT

PDB ID : 1PN4  
Title : Crystal structure of 2-enoyl-CoA hydratase 2 domain of *Candida tropicalis* multifunctional enzyme type 2 complexed with (3R)-hydroxydecanoyl-CoA.  
Authors : Koski, M.K.; Haapalainen, A.M.; Hiltunen, J.K.; Glumoff, T.  
Deposited on : 2003-06-12  
Resolution : 2.35 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

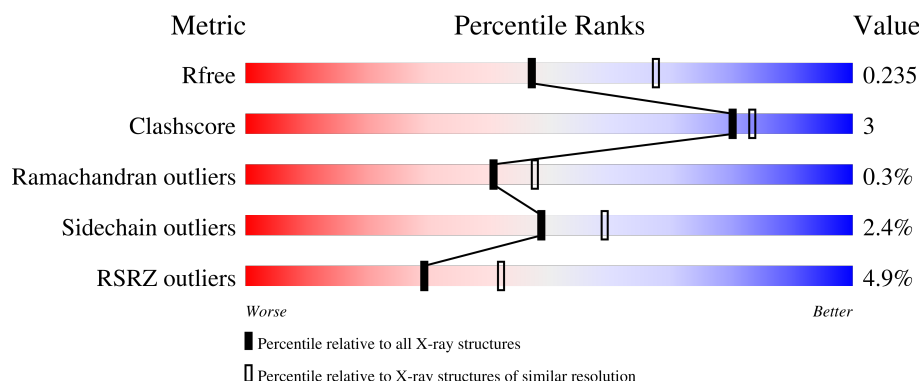
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	280	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 89%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">89%</span> </div> <div style="width: 8%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">8%</span> </div> <div style="width: 3%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">.</span> </div> </div>
1	B	280	<div> <div style="width: 5%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">5%</span> </div> <div style="width: 87%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">87%</span> </div> <div style="width: 9%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">9%</span> </div> <div style="width: 1%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">..</span> </div> </div>
1	C	280	<div> <div style="width: 7%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">7%</span> </div> <div style="width: 76%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">76%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">10%</span> </div> <div style="width: 12%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">12%</span> </div> </div>
1	D	280	<div> <div style="width: 6%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="width: 88%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">88%</span> </div> <div style="width: 9%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">9%</span> </div> <div style="width: 1%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">..</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9087 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.

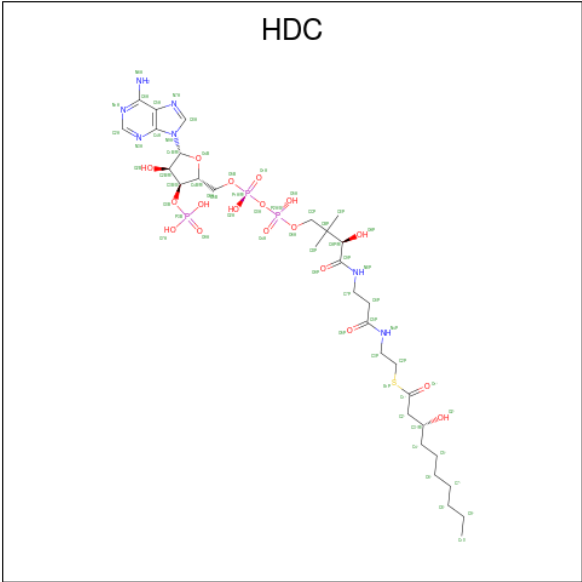
- Molecule 1 is a protein called Peroxisomal hydratase-dehydrogenase-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	15	0	0
			2152	1385	366	396	5			
1	B	272	Total	C	N	O	S	29	0	0
			2152	1385	366	396	5			
1	C	247	Total	C	N	O	S	51	0	0
			1962	1266	330	362	4			
1	D	273	Total	C	N	O	S	24	0	0
			2160	1389	367	399	5			

There are 8 discrepancies between the modelled and reference sequences:

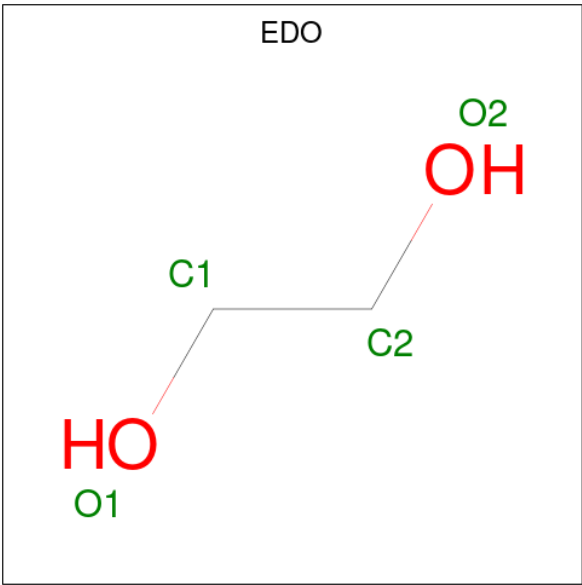
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	GLU	engineered mutation	UNP P22414
A	187	GLN	HIS	engineered mutation	UNP P22414
B	1	MET	GLU	engineered mutation	UNP P22414
B	187	GLN	HIS	engineered mutation	UNP P22414
C	1	MET	GLU	engineered mutation	UNP P22414
C	187	GLN	HIS	engineered mutation	UNP P22414
D	1	MET	GLU	engineered mutation	UNP P22414
D	187	GLN	HIS	engineered mutation	UNP P22414

- Molecule 2 is 3R-HYDROXYDECANOYL-COENZYME A (three-letter code: HDC) (formula: C<sub>31</sub>H<sub>54</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		
2	D	1	Total	C	N	O	P	S	5	0
			60	31	7	18	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

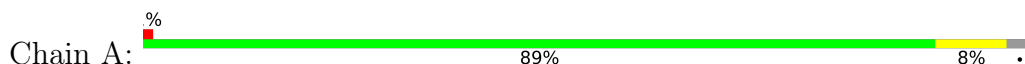
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	149	Total	O	0	0
			149	149		
4	C	89	Total	O	0	0
			89	89		
4	D	86	Total	O	0	0
			86	86		

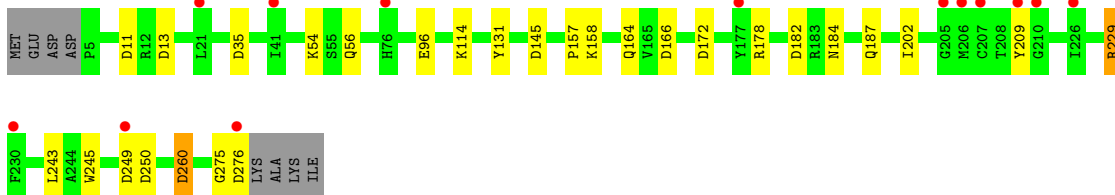
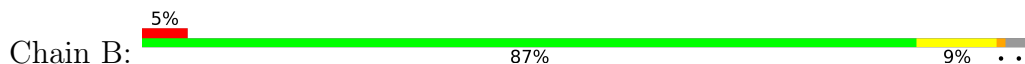
### 3 Residue-property plots [i](#)

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.

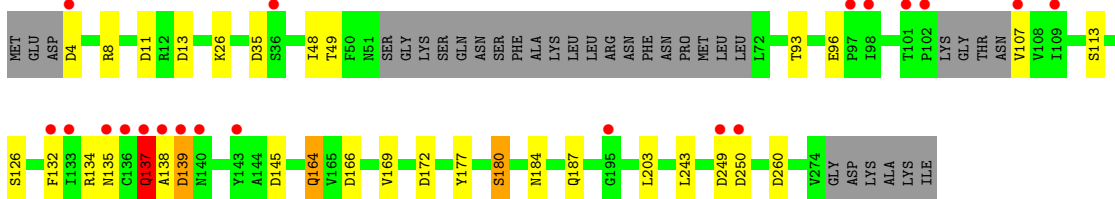
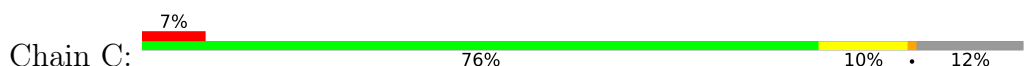
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



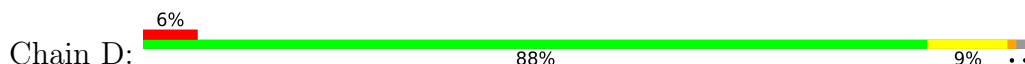
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase

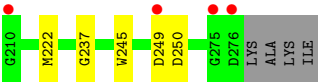


- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.64Å 151.29Å 81.62Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	35.00 – 2.35 34.32 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.00-2.35) 97.4 (34.32-2.36)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.1, CNS	Depositor
R, $R_{free}$	0.171 , 0.225 0.193 , 0.235	Depositor DCC
$R_{free}$ test set	2363 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, HDC

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	0.69	0/2208	0.82	4/3001 (0.1%)
1	B	0.75	3/2208 (0.1%)	0.95	13/3001 (0.4%)
1	C	0.72	4/2013 (0.2%)	0.97	15/2739 (0.5%)
1	D	0.76	4/2216 (0.2%)	0.88	7/3013 (0.2%)
All	All	0.73	11/8645 (0.1%)	0.91	39/11754 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	LYS	CB-CG	-9.61	1.26	1.52
1	D	250	ASP	CB-CG	-8.79	1.33	1.51
1	C	8	ARG	CG-CD	-8.12	1.31	1.51
1	C	26	LYS	CD-CE	-7.06	1.33	1.51
1	B	54	LYS	CB-CG	-6.95	1.33	1.52
1	B	114	LYS	CD-CE	-6.81	1.34	1.51
1	D	119	LYS	CB-CG	-6.58	1.34	1.52
1	B	158	LYS	CG-CD	-6.52	1.30	1.52
1	C	135	ASN	CB-CG	6.46	1.66	1.51
1	D	114	LYS	CE-NZ	-6.21	1.33	1.49
1	C	132	PHE	CB-CG	6.06	1.61	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASP	CB-CG-OD2	12.10	129.19	118.30
1	B	54	LYS	CA-CB-CG	9.41	134.11	113.40
1	B	229	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	C	139	ASP	N-CA-C	8.86	134.93	111.00
1	B	11	ASP	CB-CG-OD2	8.85	126.27	118.30
1	C	137	GLN	CB-CA-C	7.86	126.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	GLN	N-CA-CB	-7.74	96.67	110.60
1	C	13	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	172	ASP	CB-CG-OD2	6.85	124.46	118.30
1	C	250	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	229	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	172	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	249	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	C	145	ASP	CB-CG-OD2	6.32	123.98	118.30
1	D	194	LYS	CB-CG-CD	6.27	127.90	111.60
1	B	172	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	145	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	249	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	249	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	13	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	11	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	4	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	35	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	13	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	260	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	11	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	35	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	250	ASP	CB-CG-OD2	5.54	123.28	118.30
1	D	249	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	135	ASN	CA-CB-CG	-5.35	101.64	113.40
1	B	166	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	209	TYR	N-CA-CB	-5.22	101.21	110.60
1	B	158	LYS	CB-CG-CD	5.21	125.16	111.60
1	A	117	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	166	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	172	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	132	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	D	209	TYR	N-CA-CB	-5.04	101.53	110.60
1	D	145	ASP	CB-CG-OD2	5.02	122.82	118.30

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	2152	0	2135	10	0
1	B	2152	0	2135	8	0
1	C	1962	0	1934	8	0
1	D	2160	0	2138	11	0
2	A	60	0	50	4	0
2	B	60	0	50	7	0
2	D	60	0	50	2	0
3	A	4	0	6	0	0
3	B	12	0	18	0	0
4	A	141	0	0	2	0
4	B	149	0	0	2	0
4	C	89	0	0	0	0
4	D	86	0	0	0	0
All	All	9087	0	8516	45	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 3.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2277:HDC:O9P	2:B:2277:HDC:C9P	1.73	1.34
2:B:2277:HDC:OAP	2:B:2277:HDC:CAP	1.77	1.33
2:D:3277:HDC:O9P	2:D:3277:HDC:C9P	1.76	1.32
2:A:1277:HDC:O9P	2:A:1277:HDC:C9P	1.76	1.31
2:A:1277:HDC:OAP	2:A:1277:HDC:CAP	1.79	1.31
2:D:3277:HDC:CAP	2:D:3277:HDC:OAP	1.79	1.30
1:D:134:ARG:HH11	1:D:134:ARG:HG3	1.41	0.82
1:C:184:ASN:HB3	1:C:187:GLN:HE22	1.53	0.72
1:D:32:TYR:CZ	1:D:34:ASN:HB2	2.31	0.66
1:C:184:ASN:HB3	1:C:187:GLN:NE2	2.12	0.65
1:B:56:GLN:HG3	2:B:2277:HDC:H101	1.77	0.65
1:B:157:PRO:HG2	1:B:245:TRP:CD1	2.34	0.62
2:B:2277:HDC:C9P	2:B:2277:HDC:OAP	2.51	0.56
1:A:152:ASN:HB3	1:A:154:PHE:CE2	2.41	0.55
1:D:157:PRO:HG2	1:D:245:TRP:CD1	2.44	0.53
1:D:98:ILE:HG21	1:D:146:ARG:HD3	1.89	0.53
1:D:185:PRO:HB2	1:D:192:PHE:CG	2.48	0.49
1:A:184:ASN:HB3	1:A:187:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HD13	1:C:93:THR:HG21	1.95	0.47
1:D:75:GLU:HB2	1:D:130:THR:HB	1.97	0.46
1:A:164:GLN:HG2	4:A:1412:HOH:O	2.16	0.45
2:B:2277:HDC:H103	4:B:2406:HOH:O	2.16	0.45
1:C:177:TYR:O	1:C:180:SER:HB2	2.16	0.45
1:D:43:THR:HA	1:D:78:LEU:CD2	2.47	0.45
1:D:134:ARG:HH11	1:D:134:ARG:CG	2.19	0.45
1:A:81:HIS:NE2	1:A:126:SER:HB2	2.32	0.45
1:A:114:LYS:NZ	4:A:1398:HOH:O	2.49	0.45
1:A:83:TRP:CG	1:A:84:PRO:HA	2.53	0.44
1:C:164:GLN:HG3	1:C:243:LEU:HD12	1.99	0.44
1:C:48:ILE:HD12	1:C:49:THR:N	2.33	0.44
1:B:229:ARG:NH2	4:B:2351:HOH:O	2.47	0.43
1:C:107:VAL:HG21	1:C:138:ALA:H	1.83	0.43
1:B:178:ARG:HB2	1:B:182:ASP:O	2.19	0.43
1:A:183:ARG:O	1:A:184:ASN:C	2.57	0.43
1:D:194:LYS:HA	1:D:198:PHE:O	2.19	0.42
1:A:184:ASN:HD22	2:A:1277:HDC:H4'2	1.84	0.42
1:A:197:LYS:HA	1:A:197:LYS:HD3	1.84	0.42
1:B:184:ASN:HB3	1:B:187:GLN:OE1	2.19	0.41
1:D:169:VAL:O	1:D:237:GLY:HA2	2.20	0.41
1:A:71:LEU:CD2	2:A:1277:HDC:H5'2	2.50	0.41
1:B:131:TYR:CE1	2:B:2277:HDC:H6'2	2.55	0.41
1:D:134:ARG:HG3	1:D:134:ARG:NH1	2.21	0.41
1:C:169:VAL:HG11	1:C:203:LEU:HD22	2.02	0.41
1:B:202:ILE:HD12	2:B:2277:HDC:H22	2.03	0.40
1:B:164:GLN:HG3	1:B:243:LEU:HD12	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	270/280 (96%)	261 (97%)	9 (3%)	0	100	100
1	B	270/280 (96%)	263 (97%)	6 (2%)	1 (0%)	34	38
1	C	241/280 (86%)	235 (98%)	4 (2%)	2 (1%)	19	20
1	D	271/280 (97%)	267 (98%)	4 (2%)	0	100	100
All	All	1052/1120 (94%)	1026 (98%)	23 (2%)	3 (0%)	41	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	139	ASP
1	C	137	GLN
1	B	275	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/240 (97%)	227 (97%)	6 (3%)	46	56
1	B	233/240 (97%)	229 (98%)	4 (2%)	60	72
1	C	212/240 (88%)	204 (96%)	8 (4%)	33	41
1	D	234/240 (98%)	230 (98%)	4 (2%)	60	72
All	All	912/960 (95%)	890 (98%)	22 (2%)	49	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLU
1	A	126	SER
1	A	140	ASN
1	A	171	GLU
1	A	243	LEU
1	A	250	ASP
1	B	96	GLU
1	B	250	ASP

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Mol	Chain	Res	Type
1	B	260	ASP
1	B	276	ASP
1	C	96	GLU
1	C	113	SER
1	C	126	SER
1	C	134	ARG
1	C	137	GLN
1	C	164	GLN
1	C	180	SER
1	C	260	ASP
1	D	69	MET
1	D	96	GLU
1	D	134	ARG
1	D	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	140	ASN
1	B	152	ASN
1	C	140	ASN
1	C	187	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
2	HDC	B	2277	-	53,62,62	4.51	7 (13%)	65,89,89	1.66	13 (20%)
3	EDO	B	503	-	3,3,3	0.38	0	2,2,2	0.21	0
3	EDO	A	504	-	3,3,3	0.39	0	2,2,2	0.36	0
3	EDO	B	502	-	3,3,3	0.34	0	2,2,2	0.14	0
2	HDC	A	1277	-	53,62,62	4.73	5 (9%)	65,89,89	1.67	12 (18%)
3	EDO	B	501	-	3,3,3	0.33	0	2,2,2	0.65	0
2	HDC	D	3277	-	53,62,62	4.76	7 (13%)	65,89,89	1.79	13 (20%)

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	HDC	B	2277	-	-	8/58/78/78	0/3/3/3
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
2	HDC	A	1277	-	-	4/58/78/78	0/3/3/3
3	EDO	B	501	-	-	0/1/1/1	-
2	HDC	D	3277	-	-	4/58/78/78	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3277	HDC	O9P-C9P	26.85	1.76	1.23
2	A	1277	HDC	O9P-C9P	26.83	1.76	1.23
2	B	2277	HDC	O9P-C9P	25.39	1.73	1.23
2	A	1277	HDC	OAP-CAP	20.44	1.79	1.42
2	D	3277	HDC	OAP-CAP	20.20	1.79	1.42
2	B	2277	HDC	OAP-CAP	19.04	1.77	1.42
2	B	2277	HDC	C2A-N3A	4.51	1.39	1.32
2	D	3277	HDC	C2A-N3A	4.43	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2277	HDC	C2A-N1A	3.19	1.39	1.33
2	D	3277	HDC	C2A-N1A	3.10	1.39	1.33
2	A	1277	HDC	C2A-N3A	2.84	1.36	1.32
2	A	1277	HDC	C2A-N1A	2.59	1.38	1.33
2	A	1277	HDC	P1A-O1A	2.53	1.59	1.50
2	D	3277	HDC	P1A-O1A	2.43	1.59	1.50
2	B	2277	HDC	P2A-O4A	2.40	1.59	1.50
2	B	2277	HDC	O5P-C5P	-2.40	1.18	1.23
2	B	2277	HDC	P1A-O1A	2.26	1.58	1.50
2	D	3277	HDC	C6'-C5'	-2.25	1.38	1.51
2	D	3277	HDC	P2A-O4A	2.24	1.58	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3277	HDC	N3A-C2A-N1A	-5.64	119.86	128.68
2	D	3277	HDC	C3'-C2'-C1'	5.14	125.63	113.89
2	A	1277	HDC	N3A-C2A-N1A	-4.79	121.18	128.68
2	B	2277	HDC	N3A-C2A-N1A	-4.78	121.21	128.68
2	A	1277	HDC	O2'-C3'-C4'	-4.60	96.05	109.21
2	D	3277	HDC	P1A-O3A-P2A	-4.33	117.97	132.83
2	B	2277	HDC	C6P-C7P-N8P	-4.16	103.50	111.90
2	A	1277	HDC	C4'-C3'-C2'	4.14	127.70	112.78
2	B	2277	HDC	C3'-C2'-C1'	4.11	123.27	113.89
2	A	1277	HDC	P1A-O3A-P2A	-4.08	118.82	132.83
2	D	3277	HDC	C6P-C7P-N8P	-3.91	104.01	111.90
2	A	1277	HDC	C3'-C2'-C1'	3.90	122.80	113.89
2	A	1277	HDC	C6P-C7P-N8P	-3.80	104.22	111.90
2	B	2277	HDC	P1A-O3A-P2A	-3.78	119.86	132.83
2	D	3277	HDC	O9P-C9P-N8P	-3.59	115.29	122.99
2	D	3277	HDC	CAP-C9P-N8P	3.45	123.45	116.58
2	B	2277	HDC	O5P-C5P-N4P	-3.35	116.69	123.01
2	B	2277	HDC	CAP-C9P-N8P	3.28	123.12	116.58
2	D	3277	HDC	O5P-C5P-N4P	-3.27	116.85	123.01
2	B	2277	HDC	O1'-C1'-S1P	3.02	126.54	122.61
2	D	3277	HDC	C2B-C3B-C4B	2.96	108.47	103.22
2	D	3277	HDC	C4'-C3'-C2'	2.88	123.17	112.78
2	A	1277	HDC	O5P-C5P-N4P	-2.68	117.95	123.01
2	D	3277	HDC	O3B-C3B-C2B	-2.54	102.48	111.68
2	B	2277	HDC	C2P-S1P-C1'	2.53	109.74	101.87
2	A	1277	HDC	C2B-C3B-C4B	2.45	107.56	103.22
2	B	2277	HDC	C2P-C3P-N4P	2.42	117.50	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3277	HDC	C2'-C1'-S1P	2.41	116.61	113.63
2	A	1277	HDC	O3B-C3B-C2B	-2.36	103.13	111.68
2	A	1277	HDC	C7'-C6'-C5'	-2.35	102.48	114.42
2	A	1277	HDC	C2P-S1P-C1'	2.35	109.19	101.87
2	A	1277	HDC	CDP-CBP-CAP	2.33	112.86	108.82
2	B	2277	HDC	OAP-CAP-CBP	2.32	115.72	110.25
2	B	2277	HDC	O3B-C3B-C2B	-2.27	103.44	111.68
2	D	3277	HDC	N6A-C6A-N1A	2.19	123.12	118.57
2	B	2277	HDC	O7A-P3B-O8A	2.15	115.86	107.64
2	D	3277	HDC	C2P-C3P-N4P	2.14	116.91	112.42
2	B	2277	HDC	O6A-CCP-CBP	2.06	113.86	110.55

There are no chirality outliers.

All (17) torsion outliers are listed below:

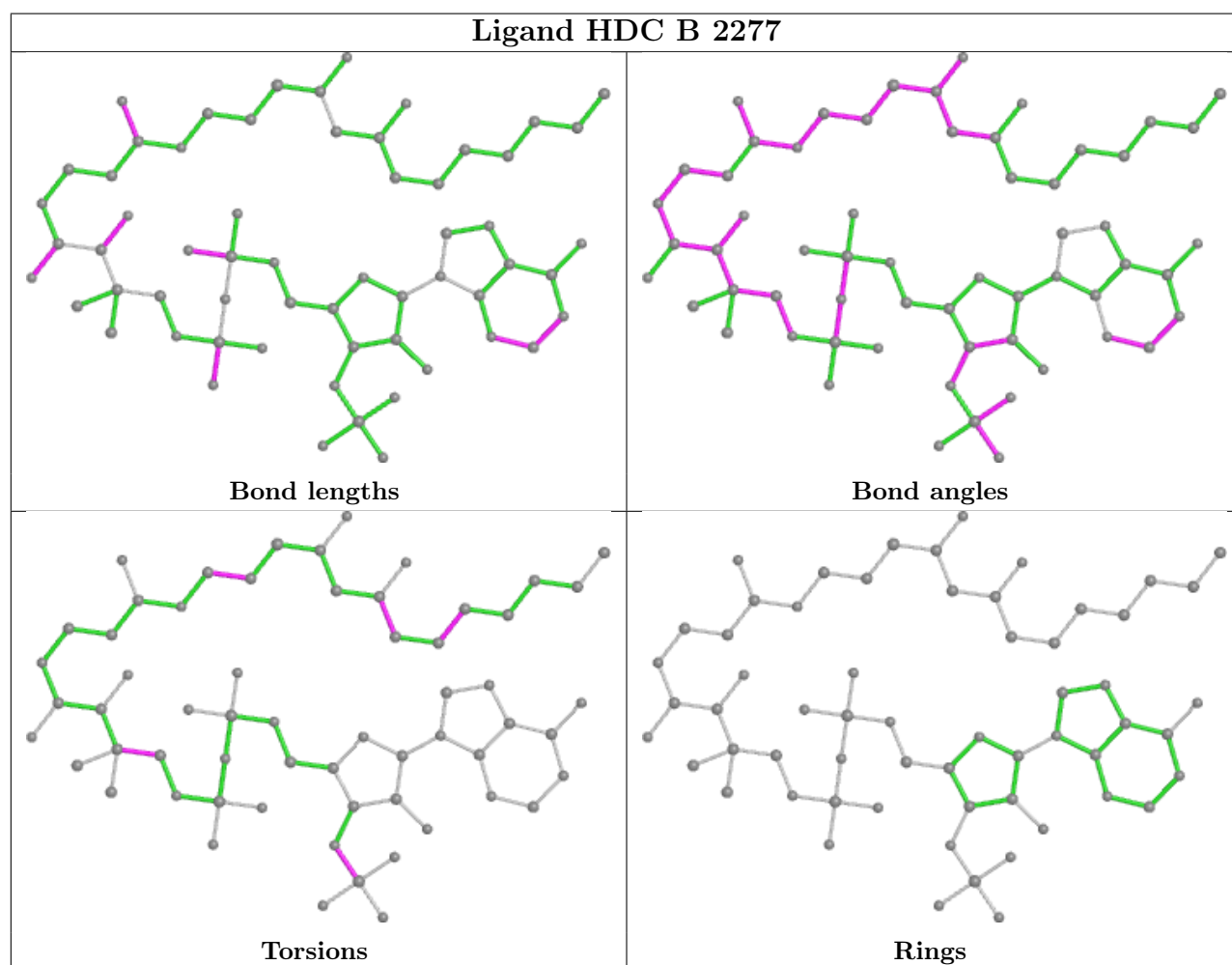
Mol	Chain	Res	Type	Atoms
2	B	2277	HDC	C3B-O3B-P3B-O7A
2	B	2277	HDC	C4'-C5'-C6'-C7'
2	A	1277	HDC	C6'-C7'-C8'-C9'
2	B	2277	HDC	C3B-O3B-P3B-O9A
2	D	3277	HDC	P1A-O3A-P2A-O5A
2	A	1277	HDC	C4'-C5'-C6'-C7'
2	D	3277	HDC	C6'-C7'-C8'-C9'
2	B	2277	HDC	CAP-CBP-CCP-O6A
2	B	2277	HDC	CEP-CBP-CCP-O6A
3	B	503	EDO	O1-C1-C2-O2
2	A	1277	HDC	P1A-O3A-P2A-O4A
2	B	2277	HDC	CDP-CBP-CCP-O6A
2	B	2277	HDC	S1P-C2P-C3P-N4P
2	A	1277	HDC	P1A-O3A-P2A-O5A
2	D	3277	HDC	P1A-O3A-P2A-O4A
2	B	2277	HDC	C2'-C3'-C4'-C5'
2	D	3277	HDC	C7'-C8'-C9'-C10

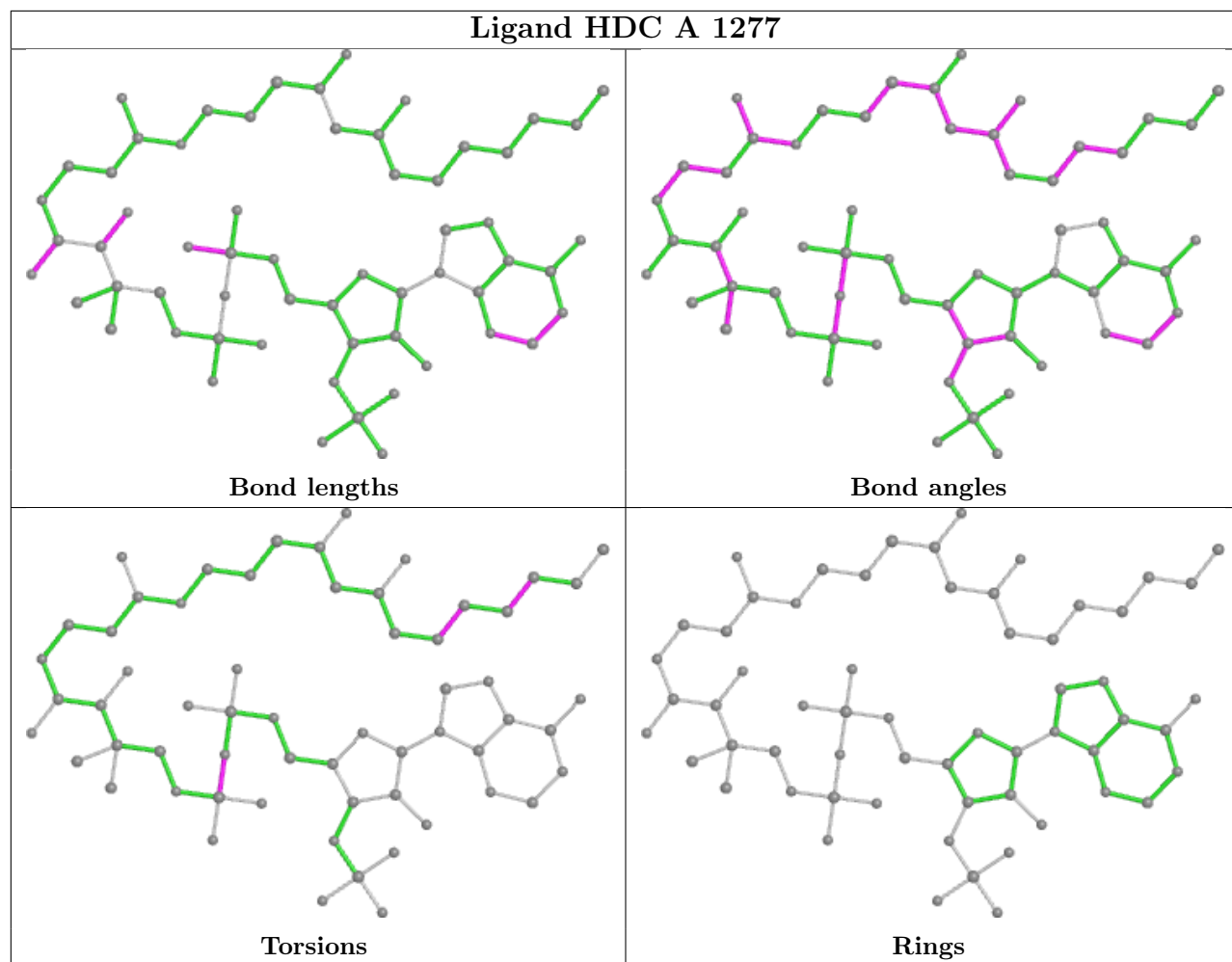
There are no ring outliers.

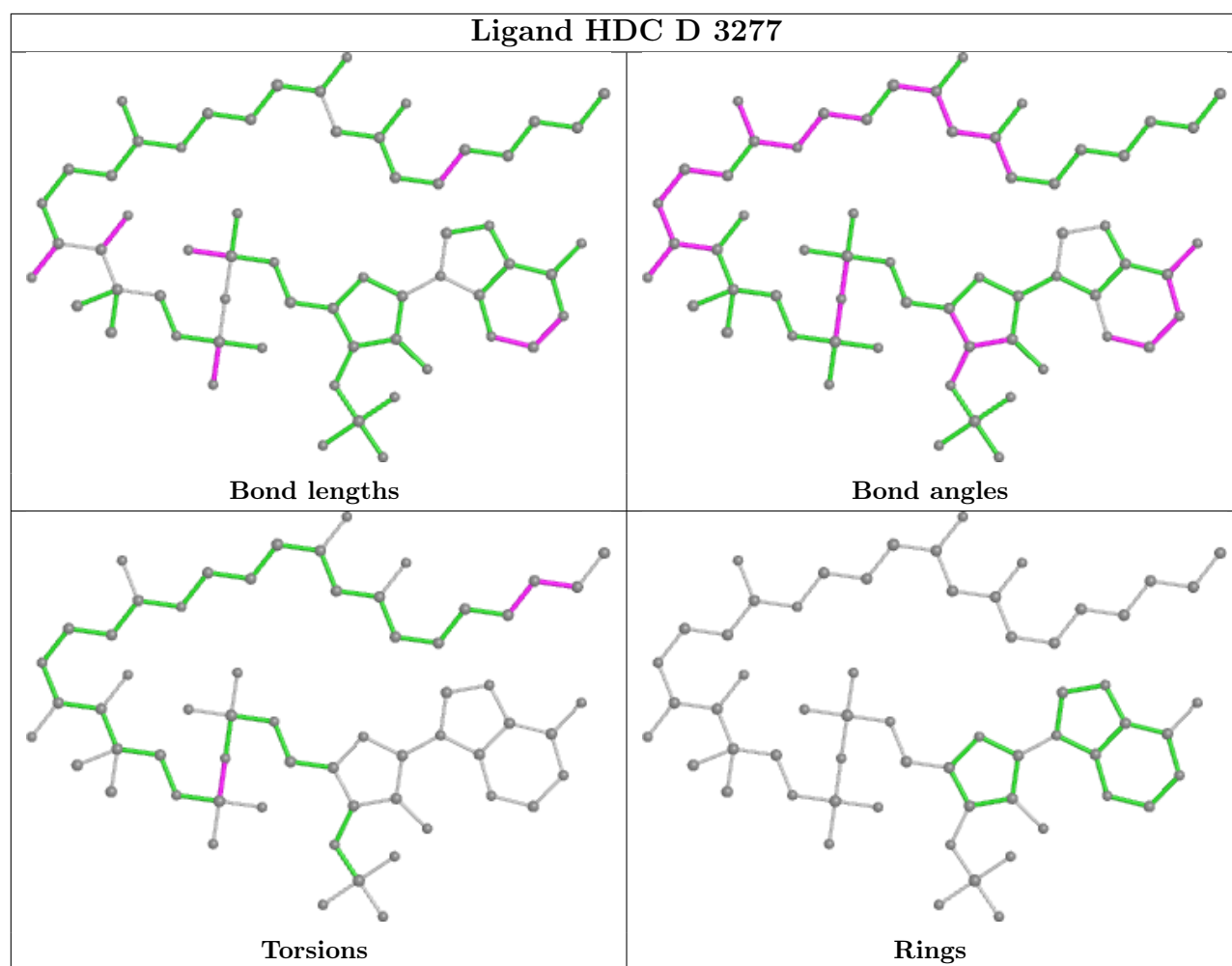
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2277	HDC	7	0
2	A	1277	HDC	4	0
2	D	3277	HDC	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	272/280 (97%)	0.05	3 (1%) 80 87	5, 14, 24, 41	5 (1%)
1	B	272/280 (97%)	0.19	13 (4%) 30 43	7, 14, 20, 38	11 (4%)
1	C	247/280 (88%)	0.30	20 (8%) 12 17	4, 14, 29, 37	14 (5%)
1	D	273/280 (97%)	0.27	16 (5%) 22 33	6, 13, 24, 37	9 (3%)
All	All	1064/1120 (95%)	0.20	52 (4%) 29 42	4, 14, 24, 41	39 (3%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	5.5
1	C	136	CYS	5.3
1	C	135	ASN	4.8
1	C	139	ASP	4.5
1	C	107	VAL	4.2
1	A	275	GLY	4.2
1	C	138	ALA	4.1
1	B	276	ASP	3.8
1	C	102	PRO	3.7
1	C	132	PHE	3.7
1	C	109	ILE	3.4
1	C	133	ILE	3.3
1	D	275	GLY	3.3
1	D	158	LYS	3.2
1	A	276	ASP	3.2
1	B	206	MET	3.2
1	C	140	ASN	3.2
1	B	249	ASP	3.1
1	D	4	ASP	3.0
1	B	205	GLY	2.9
1	D	249	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	250	ASP	2.9
1	B	209	TYR	2.8
1	C	137	GLN	2.8
1	C	143	TYR	2.6
1	D	209	TYR	2.6
1	B	207	CYS	2.5
1	C	101	THR	2.5
1	C	98	ILE	2.5
1	D	276	ASP	2.4
1	D	118	ASN	2.4
1	B	226	ILE	2.4
1	C	97	PRO	2.3
1	D	5	PRO	2.3
1	D	191	ASN	2.3
1	D	145	ASP	2.3
1	B	210	GLY	2.3
1	B	230	PHE	2.3
1	B	41	ILE	2.3
1	B	177	TYR	2.3
1	D	104	GLY	2.3
1	D	94	THR	2.2
1	A	249	ASP	2.2
1	B	76	HIS	2.2
1	C	4	ASP	2.2
1	B	21	LEU	2.2
1	D	135	ASN	2.1
1	D	210	GLY	2.1
1	D	53	GLY	2.1
1	D	105	THR	2.1
1	C	36	SER	2.1
1	C	195	GLY	2.1

## 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

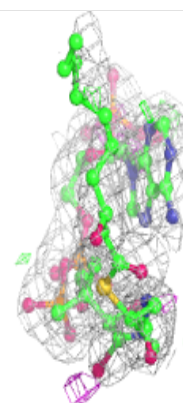
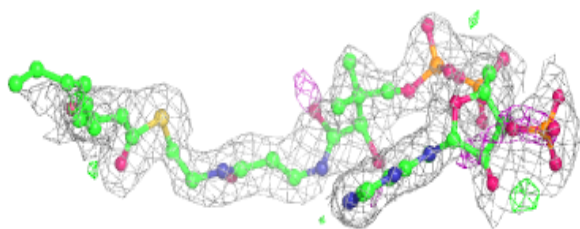
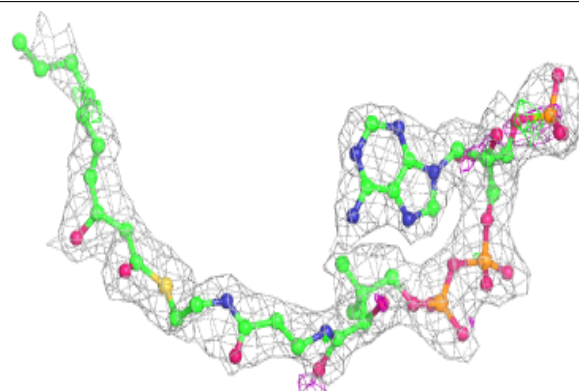
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	HDC	D	3277	60/60	0.82	0.20	11,20,33,34	5
3	EDO	B	503	4/4	0.82	0.21	45,45,46,47	0
2	HDC	A	1277	60/60	0.86	0.17	12,23,34,38	0
2	HDC	B	2277	60/60	0.88	0.17	13,20,27,28	0
3	EDO	B	502	4/4	0.91	0.26	23,25,27,29	0
3	EDO	A	504	4/4	0.91	0.21	37,37,37,39	0
3	EDO	B	501	4/4	0.94	0.24	30,30,31,33	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.

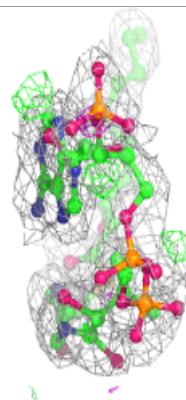
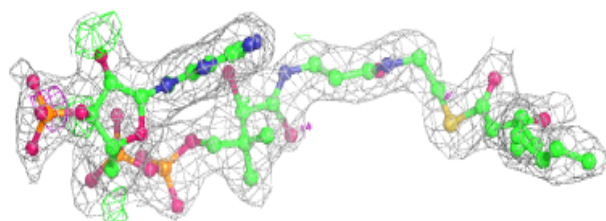
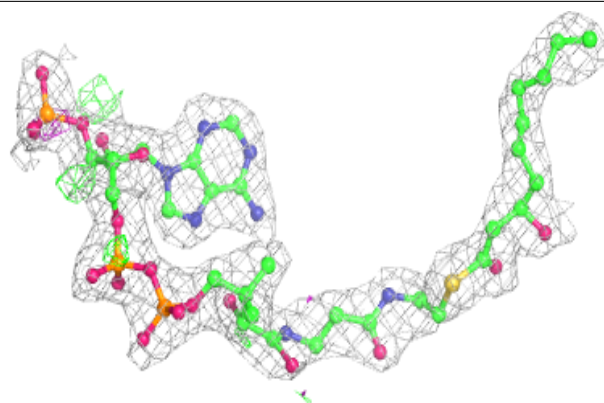
### Electron density around HDC D 3277:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

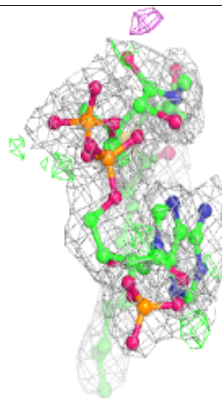
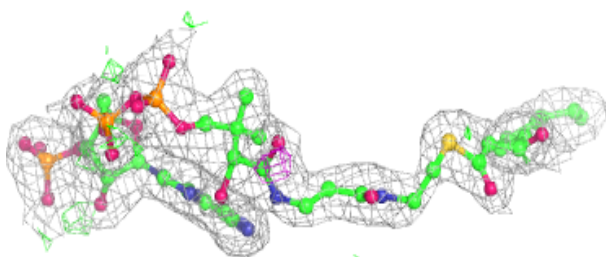
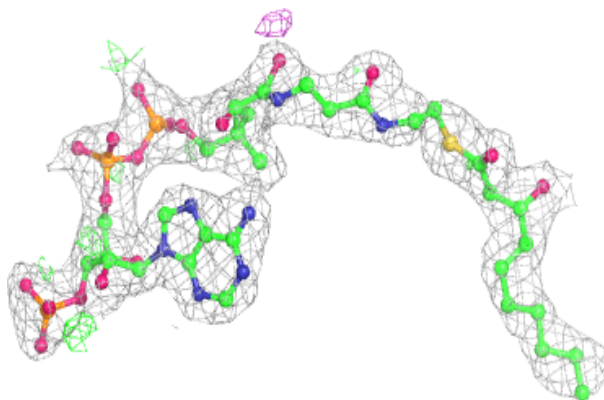


**Electron density around HDC A 1277:**

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

**Electron density around HDC B 2277:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.