



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:26 PM UTC

PDB ID : 1PN4 / pdb_00001pn4
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

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

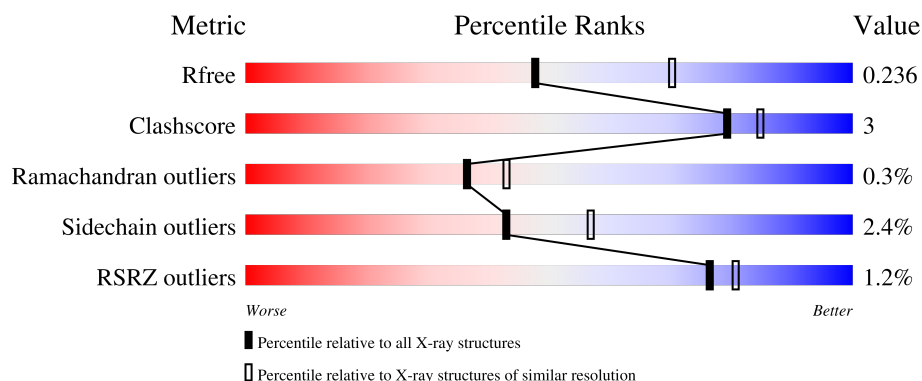
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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	
1	B	280	
1	C	280	
1	D	280	

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.

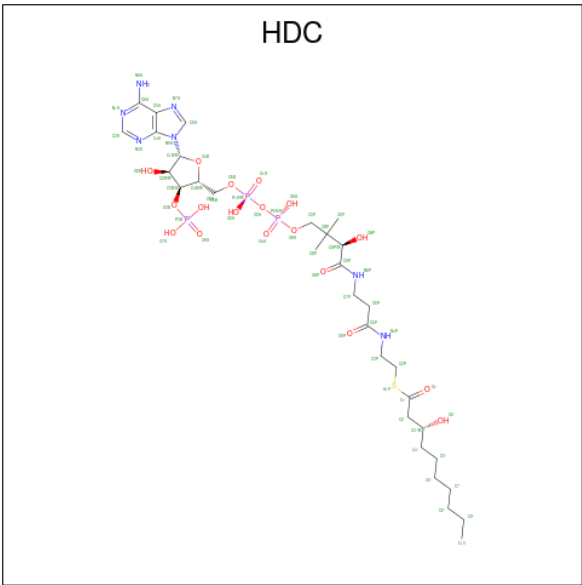
- Molecule 1 is a protein called Peroxisomal hydratase-dehydrogenase-epimerase.

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:

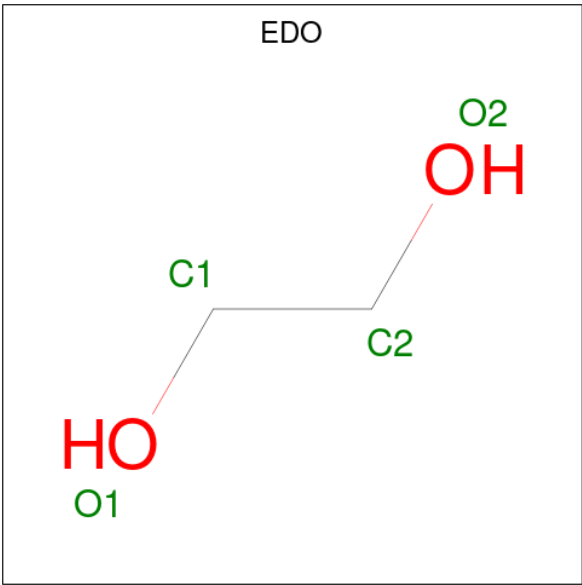
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	GLU	engineered mutation	UNP P22414
A	187	GLN	HIS	engineered mutation	UNP P22414
B	1	MET	GLU	engineered mutation	UNP P22414
B	187	GLN	HIS	engineered mutation	UNP P22414
C	1	MET	GLU	engineered mutation	UNP P22414
C	187	GLN	HIS	engineered mutation	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 (CCD ID: HDC) (formula: $C_{31}H_{54}N_7O_{18}P_3S$).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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		

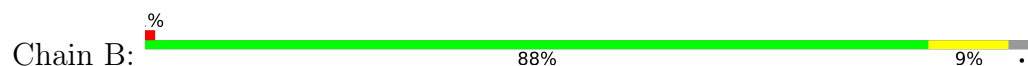
3 Residue-property plots [i](#)

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.

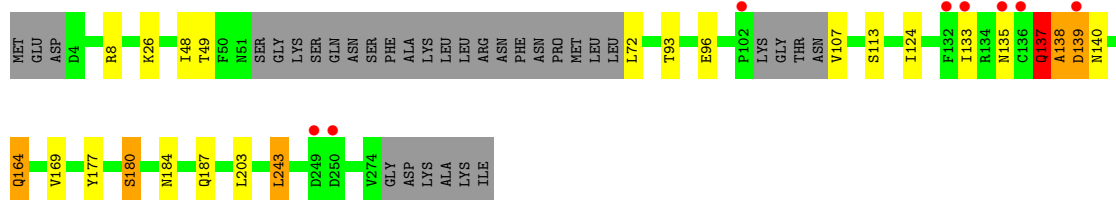
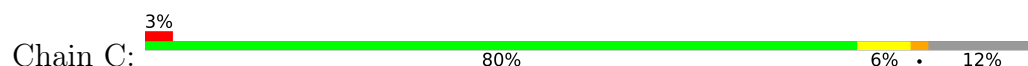
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



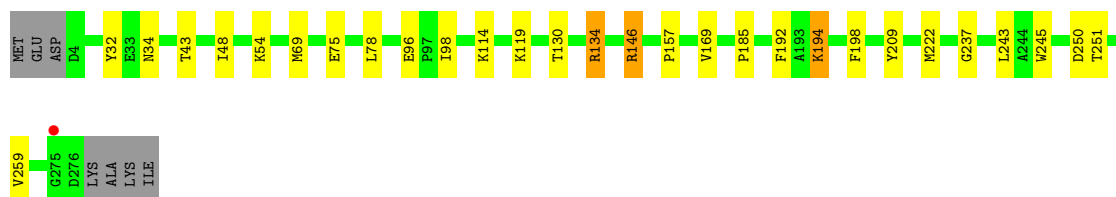
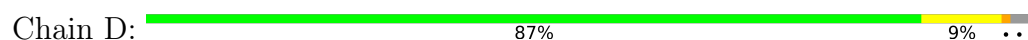
- Molecule 1: Peroxisomal hydratase-dehydrogenase-epimerase



- 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, α , β , γ	48.64Å 151.29Å 81.62Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	35.00 – 2.35 35.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.00-2.35) 97.4 (35.00-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.1, CNS	Depositor
R, R_{free}	0.171 , 0.225 0.194 , 0.236	Depositor DCC
R_{free} test set	2363 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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, 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	0.87	0/2208	0.95	0/3001
1	B	0.92	5/2208 (0.2%)	1.02	5/3001 (0.2%)
1	C	0.91	4/2013 (0.2%)	1.13	13/2739 (0.5%)
1	D	0.91	4/2216 (0.2%)	1.01	5/3013 (0.2%)
All	All	0.90	13/8645 (0.2%)	1.03	23/11754 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	LYS	CB-CG	-8.62	1.26	1.52
1	C	133	ILE	CA-CB	-7.60	1.44	1.53
1	D	250	ASP	CB-CG	-7.50	1.33	1.52
1	B	158	LYS	CG-CD	-7.39	1.30	1.52
1	C	8	ARG	CG-CD	-6.93	1.31	1.52
1	C	26	LYS	CD-CE	-6.28	1.33	1.52
1	B	54	LYS	CB-CG	-6.22	1.33	1.52
1	B	114	LYS	CD-CE	-6.07	1.34	1.52
1	D	119	LYS	CB-CG	-5.88	1.34	1.52
1	C	135	ASN	CB-CG	5.54	1.66	1.52
1	B	69	MET	SD-CE	-5.51	1.65	1.79
1	D	114	LYS	CE-NZ	-5.27	1.33	1.49
1	B	119	LYS	CG-CD	-5.06	1.37	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ASP	N-CA-C	11.33	134.93	110.80
1	C	135	ASN	CA-CB-CG	-10.96	101.64	112.60
1	B	54	LYS	CA-CB-CG	10.01	134.11	114.10
1	C	137	GLN	OE1-CD-NE2	-9.26	113.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ASN	N-CA-C	8.95	122.75	109.59
1	C	137	GLN	N-CA-CB	-8.18	96.67	110.49
1	C	137	GLN	CB-CA-C	7.89	126.12	110.42
1	D	250	ASP	CA-CB-CG	7.76	120.36	112.60
1	D	194	LYS	CB-CG-CD	7.22	127.90	111.30
1	C	137	GLN	CG-CD-NE2	6.68	126.43	116.40
1	C	139	ASP	CA-C-N	6.65	130.81	121.24
1	C	139	ASP	C-N-CA	6.65	130.81	121.24
1	C	124	ILE	CB-CA-C	-6.23	106.41	111.71
1	B	209	TYR	N-CA-CB	-6.11	101.21	110.07
1	D	251	THR	N-CA-C	6.07	118.80	108.90
1	B	158	LYS	CB-CG-CD	6.03	125.16	111.30
1	D	209	TYR	N-CA-CB	-5.89	101.53	110.07
1	C	138	ALA	CA-C-N	5.72	132.47	121.54
1	C	138	ALA	C-N-CA	5.72	132.47	121.54
1	C	139	ASP	CA-CB-CG	-5.47	107.13	112.60
1	D	259	VAL	N-CA-C	5.19	115.63	110.23
1	B	208	THR	CA-C-N	5.07	127.33	120.44
1	B	208	THR	C-N-CA	5.07	127.33	120.44

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	2152	0	2135	9	0
1	B	2152	0	2135	9	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
1:A:183:ARG:O	1:A:184:ASN:C	2.57	0.47
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:B:46:HIS:CG	1:B:206:MET:HE2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

5.3.1 Protein backbone

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%)	30	34
1	C	241/280 (86%)	235 (98%)	4 (2%)	2 (1%)	16	17
1	D	271/280 (97%)	267 (98%)	4 (2%)	0	100	100
All	All	1052/1120 (94%)	1026 (98%)	23 (2%)	3 (0%)	36	43

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%)	229 (98%)	4 (2%)	53	68
1	B	233/240 (97%)	229 (98%)	4 (2%)	53	68
1	C	212/240 (88%)	205 (97%)	7 (3%)	33	44
1	D	234/240 (98%)	227 (97%)	7 (3%)	36	48
All	All	912/960 (95%)	890 (98%)	22 (2%)	43	57

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

Mol	Chain	Res	Type
1	A	126	SER
1	A	171	GLU
1	A	243	LEU
1	A	250	ASP
1	B	96	GLU
1	B	243	LEU
1	B	250	ASP
1	B	276	ASP
1	C	72	LEU
1	C	96	GLU
1	C	113	SER
1	C	137	GLN
1	C	164	GLN
1	C	180	SER
1	C	243	LEU
1	D	48	ILE
1	D	69	MET
1	D	96	GLU
1	D	134	ARG

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Mol	Chain	Res	Type
1	D	146	ARG
1	D	222	MET
1	D	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	140	ASN
1	A	268	ASN
1	B	152	ASN
1	B	164	GLN
1	B	268	ASN
1	C	140	ASN
1	C	187	GLN
1	D	140	ASN
1	D	164	GLN
1	D	268	ASN

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](#)

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	A	1277	-	60,62,62	4.62	5 (8%)	83,89,89	1.75	18 (21%)
2	HDC	B	2277	-	60,62,62	4.40	8 (13%)	83,89,89	1.79	23 (27%)
3	EDO	B	503	-	3,3,3	0.35	0	2,2,2	0.21	0
3	EDO	B	502	-	3,3,3	0.31	0	2,2,2	0.08	0
3	EDO	A	504	-	3,3,3	0.36	0	2,2,2	0.40	0
2	HDC	D	3277	-	60,62,62	4.64	8 (13%)	83,89,89	1.81	20 (24%)
3	EDO	B	501	-	3,3,3	0.31	0	2,2,2	0.68	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
2	HDC	A	1277	-	-	5/62/78/78	0/3/3/3
2	HDC	B	2277	-	-	6/62/78/78	0/3/3/3
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
2	HDC	D	3277	-	-	5/62/78/78	0/3/3/3
3	EDO	B	501	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3277	HDC	O9P-C9P	27.81	1.76	1.23
2	A	1277	HDC	O9P-C9P	27.79	1.76	1.23
2	B	2277	HDC	O9P-C9P	26.29	1.73	1.23
2	A	1277	HDC	OAP-CAP	21.25	1.79	1.42
2	D	3277	HDC	OAP-CAP	21.00	1.79	1.42
2	B	2277	HDC	OAP-CAP	19.79	1.77	1.42
2	B	2277	HDC	C2A-N1A	3.33	1.39	1.33
2	D	3277	HDC	C2A-N1A	3.23	1.39	1.33
2	B	2277	HDC	C2A-N3A	3.06	1.39	1.33
2	D	3277	HDC	C2A-N3A	2.99	1.39	1.33
2	B	2277	HDC	C2'-C1'	-2.90	1.45	1.51
2	A	1277	HDC	C2A-N1A	2.70	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1277	HDC	P1A-O1A	2.61	1.59	1.50
2	D	3277	HDC	C6'-C5'	-2.58	1.38	1.51
2	D	3277	HDC	P1A-O1A	2.51	1.59	1.50
2	B	2277	HDC	P2A-O4A	2.48	1.59	1.50
2	B	2277	HDC	O5P-C5P	-2.45	1.18	1.23
2	B	2277	HDC	P1A-O1A	2.34	1.58	1.50
2	D	3277	HDC	P2A-O4A	2.32	1.58	1.50
2	D	3277	HDC	C5A-N7A	-2.26	1.35	1.39
2	A	1277	HDC	C5A-N7A	-2.14	1.35	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3277	HDC	N1A-C2A-N3A	-5.76	119.86	128.58
2	D	3277	HDC	C3'-C2'-C1'	5.28	125.63	113.86
2	A	1277	HDC	O2'-C3'-C4'	-4.99	96.05	109.35
2	A	1277	HDC	N1A-C2A-N3A	-4.89	121.18	128.58
2	B	2277	HDC	N1A-C2A-N3A	-4.87	121.21	128.58
2	A	1277	HDC	C4'-C3'-C2'	4.40	127.70	112.88
2	B	2277	HDC	C5A-C4A-N3A	-4.34	120.74	126.72
2	B	2277	HDC	C3'-C2'-C1'	4.22	123.27	113.86
2	D	3277	HDC	C5A-C4A-N3A	-4.09	121.08	126.72
2	A	1277	HDC	C3'-C2'-C1'	4.01	122.80	113.86
2	B	2277	HDC	C6P-C7P-N8P	-4.00	103.50	112.00
2	D	3277	HDC	C6P-C7P-N8P	-3.75	104.01	112.00
2	A	1277	HDC	C5A-C4A-N3A	-3.68	121.64	126.72
2	D	3277	HDC	CAP-C9P-N8P	3.67	123.45	116.48
2	A	1277	HDC	C6P-C7P-N8P	-3.66	104.22	112.00
2	D	3277	HDC	O9P-C9P-N8P	-3.63	115.29	122.98
2	B	2277	HDC	O3A-P2A-O4A	-3.63	99.79	110.70
2	B	2277	HDC	CAP-C9P-N8P	3.50	123.12	116.48
2	A	1277	HDC	N9A-C8A-N7A	-3.46	109.03	113.94
2	A	1277	HDC	O5A-P2A-O3A	3.45	116.59	107.27
2	B	2277	HDC	N9A-C8A-N7A	-3.32	109.22	113.94
2	D	3277	HDC	N3A-C4A-N9A	3.32	132.82	127.17
2	B	2277	HDC	O5P-C5P-N4P	-3.23	116.69	123.03
2	D	3277	HDC	C2A-N3A-C4A	3.22	119.70	111.83
2	B	2277	HDC	N3A-C4A-N9A	3.18	132.57	127.17
2	D	3277	HDC	O5P-C5P-N4P	-3.15	116.85	123.03
2	D	3277	HDC	C4'-C3'-C2'	3.06	123.17	112.88
2	B	2277	HDC	O1'-C1'-S1P	3.03	126.54	122.68
2	D	3277	HDC	C2B-C3B-C4B	2.99	108.47	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2277	HDC	C2A-N3A-C4A	2.92	118.97	111.83
2	A	1277	HDC	C5A-N7A-C8A	2.87	107.95	103.45
2	A	1277	HDC	C2A-N3A-C4A	2.82	118.71	111.83
2	D	3277	HDC	N9A-C8A-N7A	-2.80	109.96	113.94
2	B	2277	HDC	O5A-P2A-O3A	2.77	114.76	107.27
2	A	1277	HDC	O3A-P2A-O4A	-2.77	102.39	110.70
2	B	2277	HDC	C5A-N7A-C8A	2.69	107.68	103.45
2	B	2277	HDC	C2P-S1P-C1'	2.67	109.74	101.84
2	A	1277	HDC	O5P-C5P-N4P	-2.59	117.95	123.03
2	D	3277	HDC	O3B-C3B-C2B	-2.56	102.48	111.68
2	A	1277	HDC	N3A-C4A-N9A	2.54	131.49	127.17
2	D	3277	HDC	O5A-P2A-O3A	2.53	114.10	107.27
2	A	1277	HDC	C2P-S1P-C1'	2.49	109.19	101.84
2	A	1277	HDC	C2B-C3B-C4B	2.47	107.56	103.24
2	B	2277	HDC	C2P-C3P-N4P	2.44	117.50	112.41
2	D	3277	HDC	C5A-N7A-C8A	2.42	107.25	103.45
2	D	3277	HDC	C2'-C1'-S1P	2.42	116.61	113.56
2	A	1277	HDC	CDP-CBP-CAP	2.40	112.86	108.77
2	B	2277	HDC	OAP-CAP-CBP	2.39	115.72	110.18
2	A	1277	HDC	O3B-C3B-C2B	-2.38	103.13	111.68
2	A	1277	HDC	C7'-C6'-C5'	-2.35	102.48	114.37
2	D	3277	HDC	P3B-O3B-C3B	-2.35	117.16	123.43
2	B	2277	HDC	O3B-C3B-C2B	-2.30	103.44	111.68
2	B	2277	HDC	C6A-C5A-C4A	2.27	120.28	117.18
2	D	3277	HDC	C5A-C6A-N6A	-2.24	117.75	123.29
2	B	2277	HDC	OAP-CAP-C9P	-2.18	100.28	109.38
2	D	3277	HDC	C2P-C3P-N4P	2.15	116.91	112.41
2	B	2277	HDC	O7A-P3B-O8A	2.15	115.86	107.80
2	D	3277	HDC	N6A-C6A-N1A	2.13	123.12	118.38
2	B	2277	HDC	C4'-C3'-C2'	2.09	119.91	112.88
2	B	2277	HDC	O6A-CCP-CBP	2.06	113.86	110.55
2	B	2277	HDC	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2277	HDC	C4'-C5'-C6'-C7'
2	A	1277	HDC	C6'-C7'-C8'-C9'
2	D	3277	HDC	P1A-O3A-P2A-O5A
2	B	2277	HDC	CEP-CBP-CCP-O6A
2	A	1277	HDC	C4'-C5'-C6'-C7'

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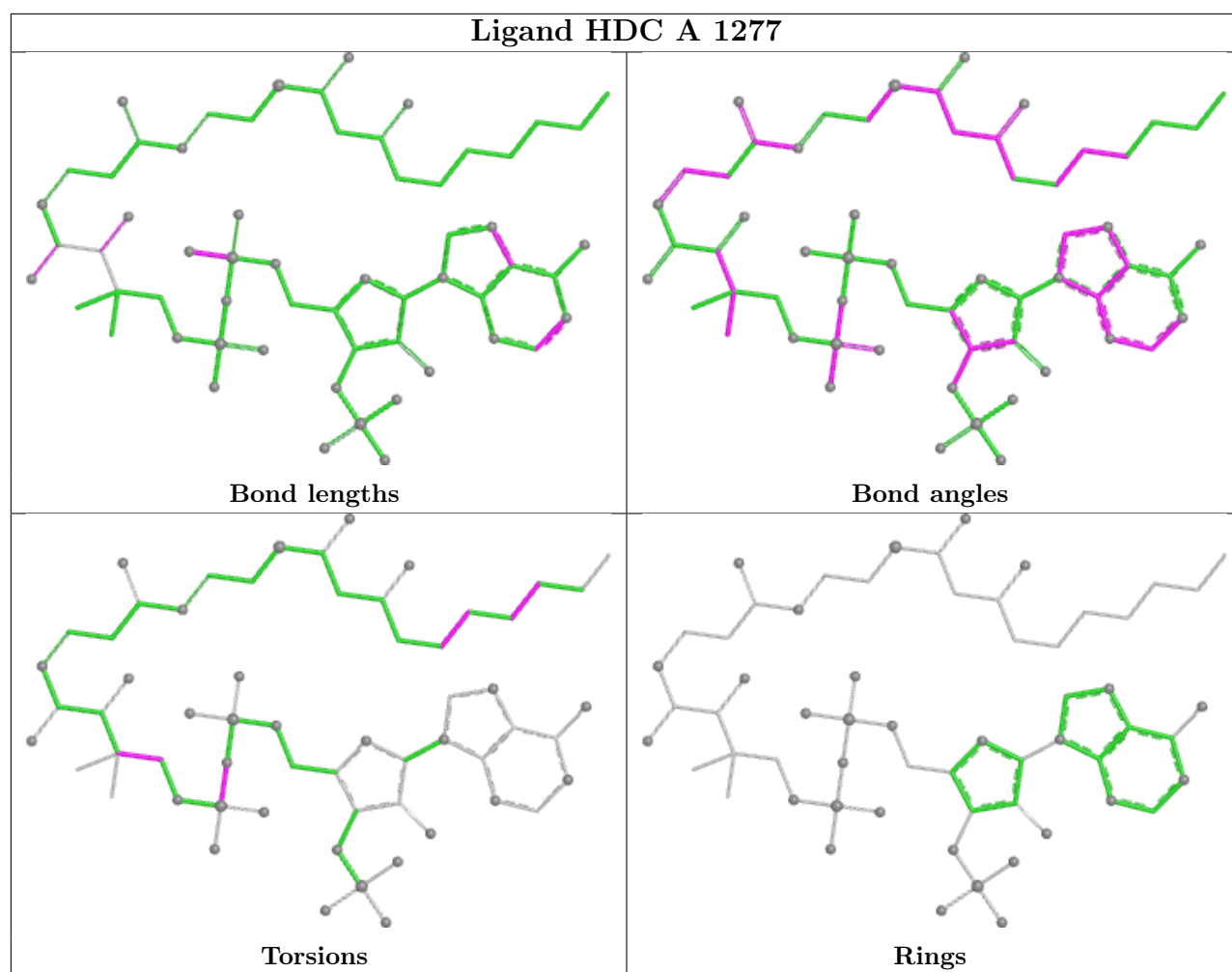
Mol	Chain	Res	Type	Atoms
2	B	2277	HDC	CAP-CBP-CCP-O6A
2	D	3277	HDC	C6'-C7'-C8'-C9'
2	A	1277	HDC	P1A-O3A-P2A-O4A
2	B	2277	HDC	C3B-O3B-P3B-O7A
3	B	503	EDO	O1-C1-C2-O2
2	A	1277	HDC	P1A-O3A-P2A-O5A
2	D	3277	HDC	P1A-O3A-P2A-O4A
2	A	1277	HDC	CDP-CBP-CCP-O6A
2	B	2277	HDC	CDP-CBP-CCP-O6A
2	D	3277	HDC	CEP-CBP-CCP-O6A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

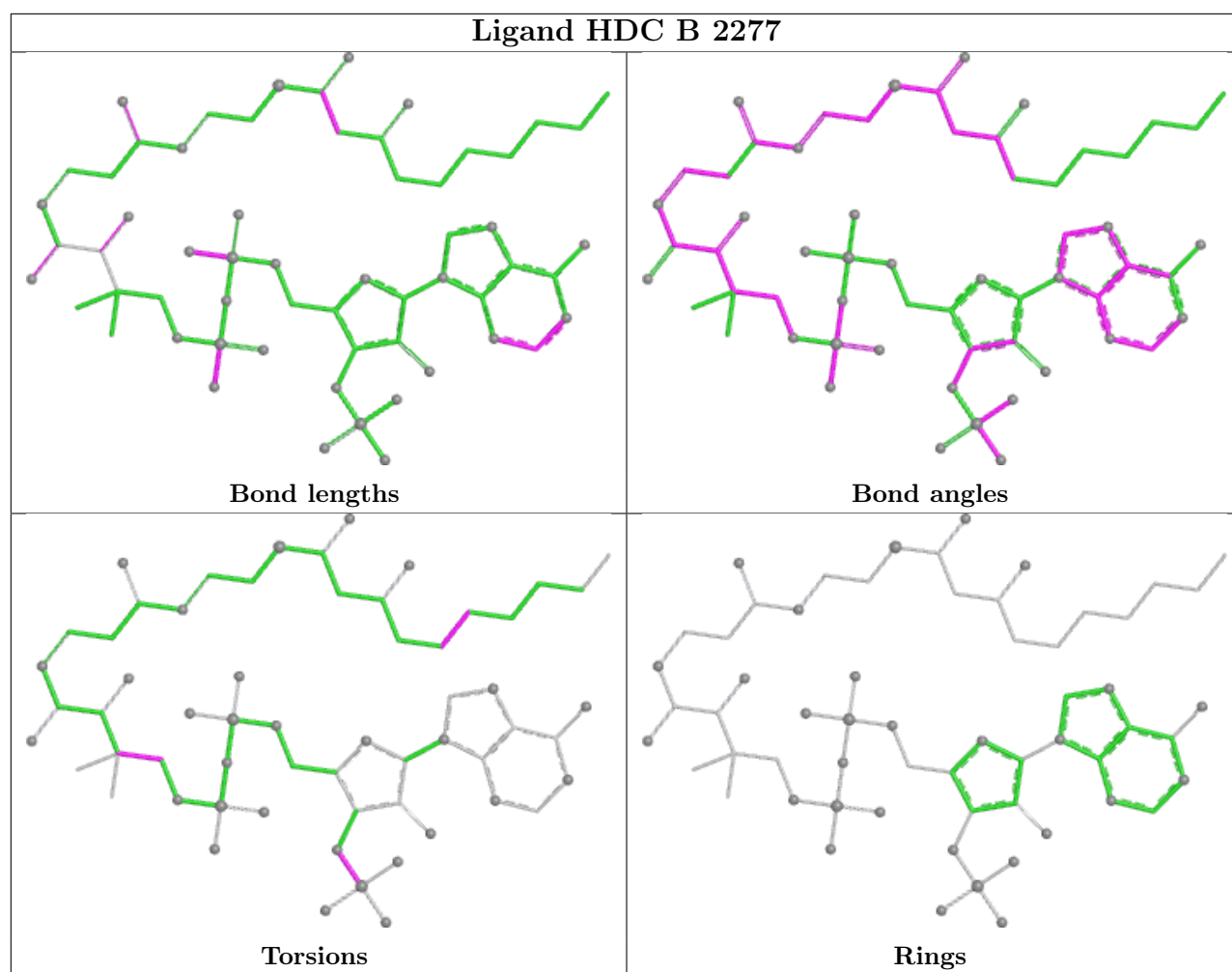
There are no ring outliers.

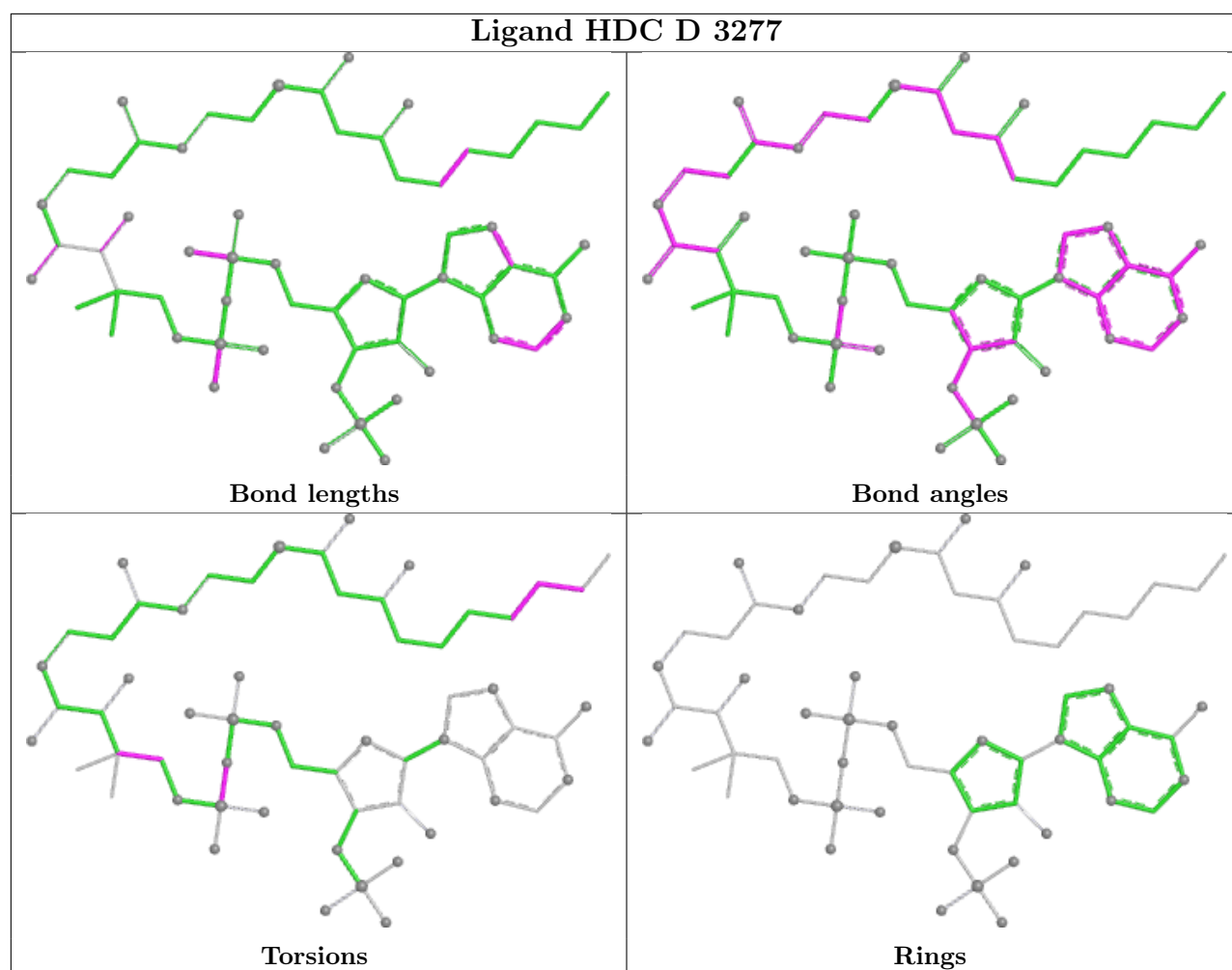
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1277	HDC	4	0
2	B	2277	HDC	7	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, 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	272/280 (97%)	-0.33	2 (0%) 84 87	5, 14, 23, 37	5 (1%)
1	B	272/280 (97%)	-0.33	2 (0%) 84 87	7, 14, 20, 38	11 (4%)
1	C	247/280 (88%)	-0.04	8 (3%) 50 57	4, 14, 26, 37	14 (5%)
1	D	273/280 (97%)	-0.17	1 (0%) 88 91	6, 13, 24, 37	9 (3%)
All	All	1064/1120 (95%)	-0.22	13 (1%) 76 81	4, 14, 23, 38	39 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	ASN	3.5
1	C	249	ASP	3.3
1	B	276	ASP	3.0
1	C	132	PHE	2.9
1	C	250	ASP	2.8
1	A	275	GLY	2.8
1	C	133	ILE	2.8
1	A	276	ASP	2.8
1	B	250	ASP	2.6
1	C	136	CYS	2.6
1	C	102	PRO	2.3
1	D	275	GLY	2.3
1	C	139	ASP	2.3

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

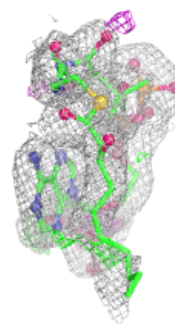
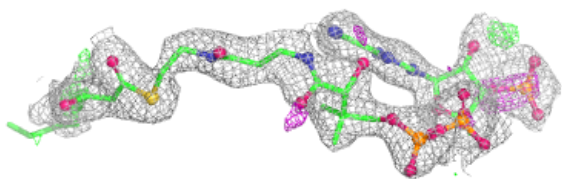
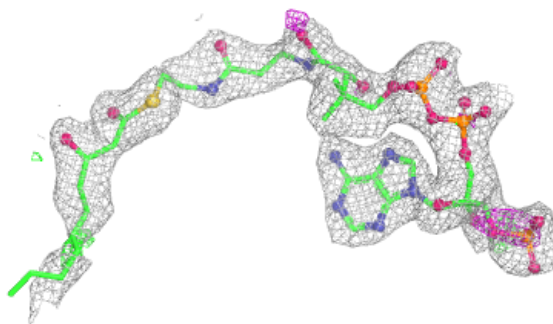
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	503	4/4	0.88	0.14	45,45,46,47	0
2	HDC	D	3277	60/60	0.89	0.10	11,20,33,34	5
2	HDC	A	1277	60/60	0.90	0.10	12,23,34,38	0
3	EDO	A	504	4/4	0.92	0.14	37,37,37,39	0
3	EDO	B	502	4/4	0.93	0.13	23,25,27,29	0
2	HDC	B	2277	60/60	0.93	0.09	13,20,27,28	0
3	EDO	B	501	4/4	0.94	0.10	30,30,31,33	0

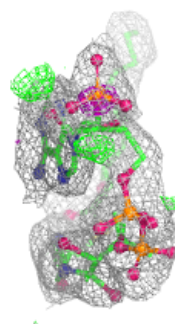
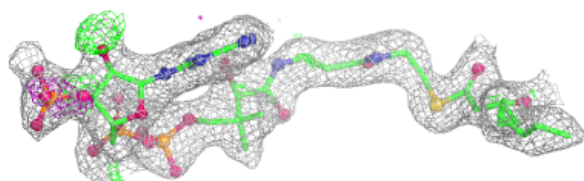
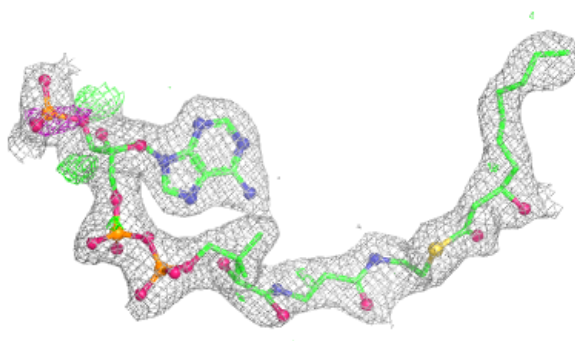
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDC D 3277:

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

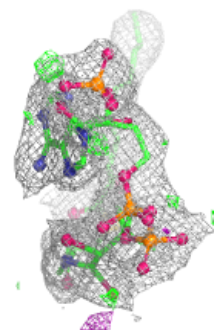
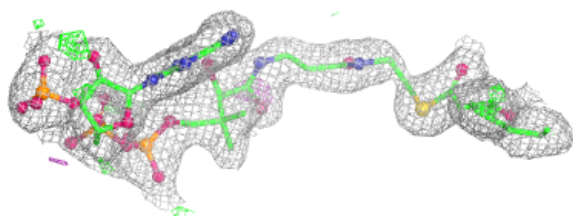
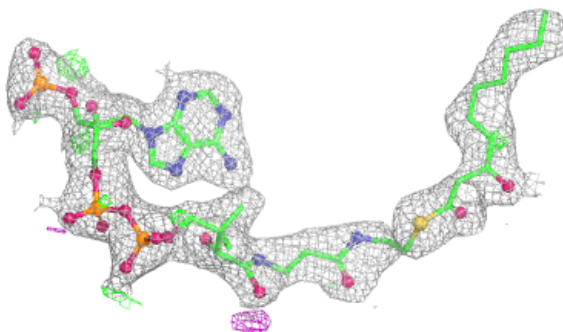
**Electron density around HDC A 1277:**

$2mF_o-DF_c$ (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.