



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:07 am BST

PDB ID : 6BAD
Title : Lactate Dehydrogenase in complex with inhibitor (R)-3-((2-chlorophenyl)thio)-6-(3-((4-fluorophenyl)amino)phenyl)-4-hydroxy-6-(thiophen-3-yl)-5,6-dihydro-2H-pyran-2-one
Authors : Ultsch, M.; Eigenbrot, C.
Deposited on : 2017-10-12
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 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 : 2.11
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) : 2.11

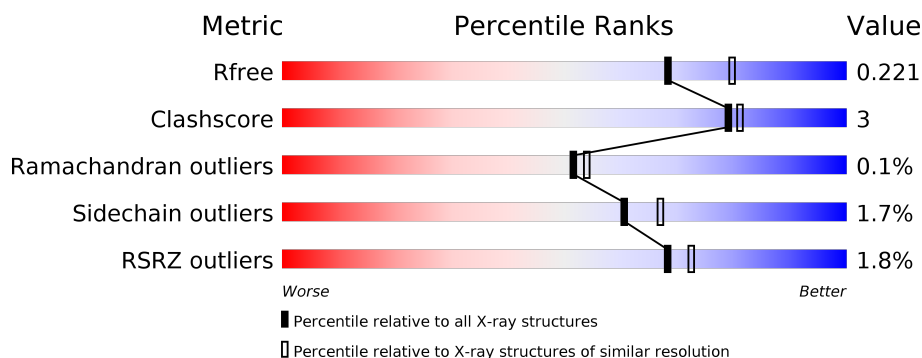
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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.

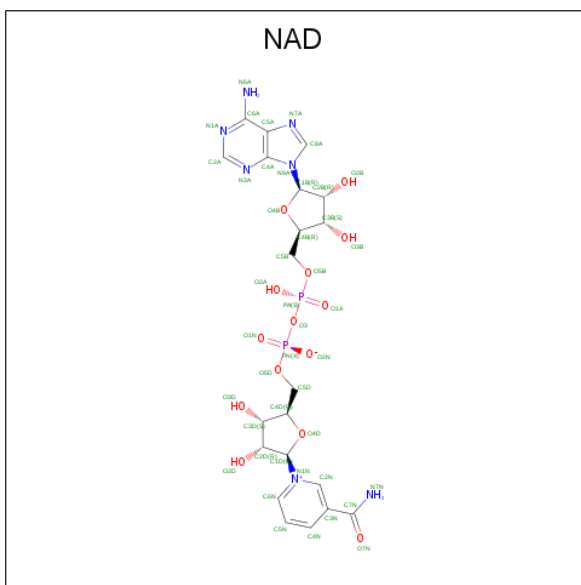
Mol	Chain	Length	Quality of chain
1	A	331	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	331	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	C	331	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	D	331	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total 2598	C 1661	N 443	O 480	S 14	0	4	0
1	B	331	Total 2576	C 1644	N 442	O 477	S 13	0	1	0
1	C	331	Total 2574	C 1644	N 440	O 477	S 13	0	1	0
1	D	331	Total 2582	C 1654	N 439	O 475	S 14	0	3	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



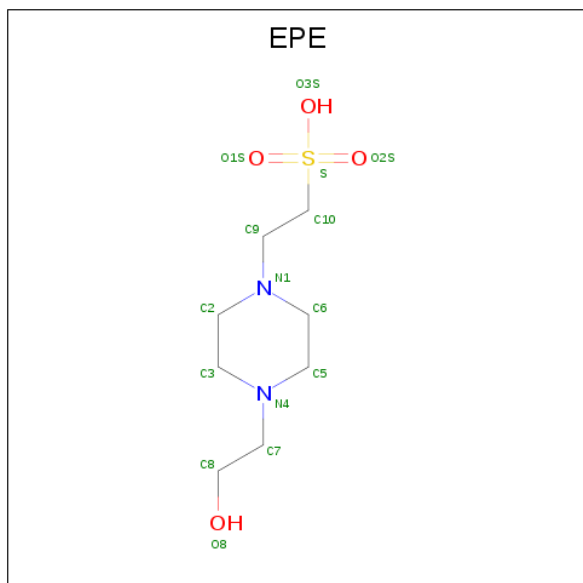
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



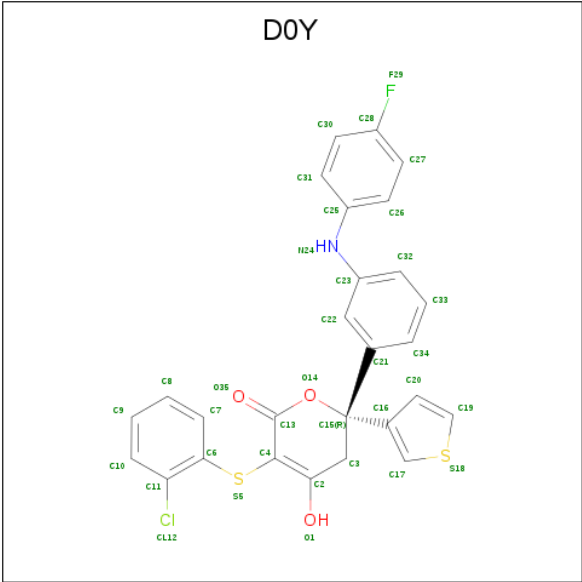
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is (6R)-3-[(2-chlorophenyl)sulfanyl]-6-{3-[(4-fluorophenyl)amino]phenyl}-4-hydroxy-6-(thiophen-3-yl)-5,6-dihydro-2H-pyran-2-one (three-letter code: D0Y) (formula: C₂₇H₁₉ClFNO₃S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	N	O	S	0	0
			35	27	1	1	1	3	2		
5	B	1	Total	C	Cl	F	N	O	S	0	0
			35	27	1	1	1	3	2		
5	C	1	Total	C	Cl	F	N	O	S	0	0
			35	27	1	1	1	3	2		
5	D	1	Total	C	Cl	F	N	O	S	0	0
			35	27	1	1	1	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total	O	0	0
			192	192		
6	B	180	Total	O	0	0
			180	180		
6	C	192	Total	O	0	0
			192	192		
6	D	187	Total	O	0	0
			187	187		

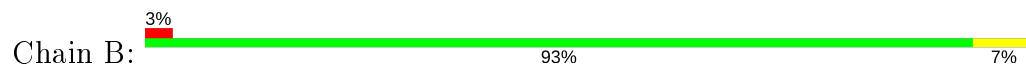
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.40 Å 80.71 Å 102.43 Å 90.00° 96.81° 90.00°	Depositor
Resolution (Å)	46.64 – 2.10 46.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.64-2.10) 97.3 (46.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.08 Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.194 , 0.230 0.189 , 0.221	Depositor DCC
R_{free} test set	1452 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11527	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: EPE, SO4, NAD, D0Y

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	0.48	0/2652	0.62	0/3584
1	B	0.49	0/2623	0.63	0/3546
1	C	0.48	0/2621	0.61	0/3543
1	D	0.50	0/2636	0.61	0/3564
All	All	0.49	0/10532	0.62	0/14237

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 [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	2598	0	2692	16	0
1	B	2576	0	2669	17	0
1	C	2574	0	2669	16	0
1	D	2582	0	2681	13	0
2	A	44	0	25	0	0
2	B	44	0	25	0	0
2	C	44	0	25	1	0
2	D	44	0	25	1	0
3	A	30	0	34	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	34	4	0
3	C	45	0	51	4	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	35	0	0	0	0
5	B	35	0	0	0	0
5	C	35	0	0	0	0
5	D	35	0	0	1	0
6	A	192	0	0	2	0
6	B	180	0	0	1	0
6	C	192	0	0	1	0
6	D	187	0	0	0	0
All	All	11527	0	10930	61	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 (61) 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:B:276:ILE:HD13	1:B:282:ILE:HD13	1.64	0.79
1:C:151:GLY:O	3:C:802:EPE:H72	1.86	0.76
1:D:104:SER:HB3	1:D:107:ASN:HD22	1.52	0.74
1:B:153:PRO:HA	3:B:802:EPE:H91	1.76	0.67
1:C:276:ILE:HD13	1:C:282:ILE:HD13	1.77	0.66
1:C:276:ILE:HD11	1:C:286:VAL:HG23	1.77	0.66
1:B:276:ILE:HD11	1:B:286:VAL:HG23	1.80	0.63
1:A:109:VAL:HG11	1:A:141:ILE:HG21	1.79	0.63
1:C:276:ILE:HG12	1:C:288:LEU:HB2	1.82	0.60
1:B:276:ILE:HG12	1:B:288:LEU:HB2	1.84	0.60
1:D:200:TRP:CE3	1:D:203[B]:MET:SD	2.96	0.59
1:D:293[A]:ILE:HD12	1:D:301:ASP:HB2	1.85	0.56
1:D:247:THR:HG23	2:D:801:NAD:H5N	1.86	0.56
1:A:231:LYS:O	1:A:234:VAL:HG22	2.08	0.54
1:A:109:VAL:HG22	1:A:138:PRO:HG2	1.89	0.54
1:C:293:ILE:HD12	1:C:301:ASP:HB2	1.90	0.53
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.90	0.53
1:B:168:ARG:HH12	1:B:247:THR:HG21	1.74	0.53
1:C:247:THR:HG23	2:C:801:NAD:H5N	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LEU:HD13	1:D:214:HIS:HB2	1.91	0.52
1:A:168:ARG:HH12	1:A:247:THR:HG21	1.75	0.51
1:A:293:ILE:HD12	1:A:301:ASP:HB2	1.91	0.51
1:B:115:ILE:HG23	1:B:119:ILE:HD12	1.91	0.51
1:C:231:LYS:O	1:C:234:VAL:HG22	2.11	0.50
1:B:240:VAL:HG11	1:B:247:THR:HG22	1.94	0.50
1:A:99:GLN:HE22	3:A:803:EPE:H61	1.77	0.49
1:A:240:VAL:HG11	1:A:247:THR:HG22	1.95	0.49
1:D:99:GLN:HA	1:D:108:LEU:HD11	1.93	0.49
1:C:238:TYR:CE2	3:C:806:EPE:H21	2.47	0.49
1:A:3:LEU:HD13	1:B:214:HIS:HB2	1.93	0.48
1:D:203[A]:MET:HG2	1:D:210:LEU:HD22	1.95	0.48
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.96	0.48
1:B:240:VAL:CG1	1:B:247:THR:HG22	2.44	0.48
1:B:109:VAL:HG22	1:B:138:PRO:HG2	1.96	0.47
1:A:240:VAL:CG1	1:A:247:THR:HG22	2.45	0.47
1:B:114:ASN:HA	1:B:117:LYS:HD3	1.97	0.46
1:B:99:GLN:HE22	3:B:803:EPE:H62	1.80	0.46
5:D:803:D0Y:C26	5:D:803:D0Y:C22	2.93	0.46
3:C:806:EPE:H61	3:C:806:EPE:H101	1.65	0.46
1:C:232:GLN:HG2	6:C:1073:HOH:O	2.16	0.45
1:B:115:ILE:HG23	1:B:119:ILE:CD1	2.46	0.45
1:D:200:TRP:HE3	1:D:203[B]:MET:SD	2.39	0.45
1:A:238:TYR:OH	3:A:803:EPE:H51	2.17	0.45
3:B:802:EPE:H21	6:B:945:HOH:O	2.16	0.45
1:A:234:VAL:HG21	6:A:1091:HOH:O	2.16	0.45
1:A:327:LYS:HE3	6:A:914:HOH:O	2.17	0.44
1:C:109:VAL:CG2	1:C:138:PRO:HG2	2.47	0.43
1:A:190:GLY:HA3	1:A:315:LEU:HD21	1.99	0.43
1:B:105:ARG:O	1:B:109:VAL:HG23	2.18	0.43
1:D:276:ILE:HD11	1:D:290:VAL:HG11	2.01	0.43
3:B:802:EPE:H22	3:B:802:EPE:H102	1.63	0.42
1:A:55:ASP:O	1:B:243:LEU:HB3	2.19	0.42
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.55	0.41
1:B:109:VAL:CG2	1:B:138:PRO:HG2	2.51	0.41
1:A:190:GLY:HA3	1:A:315:LEU:CD2	2.51	0.41
1:D:225:GLN:HB3	1:D:228:GLU:HG2	2.03	0.41
1:C:113:VAL:HG22	1:C:145:VAL:HG21	2.03	0.40
1:C:141:ILE:HG13	1:C:322:LEU:HD22	2.03	0.40
1:C:276:ILE:CD1	1:C:286:VAL:HG23	2.49	0.40
1:A:20:ASN:HD21	1:D:20:ASN:HD21	1.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:PRO:HG3	3:C:803:EPE:O3S	2.21	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	333/331 (101%)	326 (98%)	7 (2%)	0	100	100
1	B	330/331 (100%)	321 (97%)	9 (3%)	0	100	100
1	C	330/331 (100%)	323 (98%)	6 (2%)	1 (0%)	41	41
1	D	332/331 (100%)	323 (97%)	9 (3%)	0	100	100
All	All	1325/1324 (100%)	1293 (98%)	31 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLU

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	291/287 (101%)	286 (98%)	5 (2%)	60	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	288/287 (100%)	284 (99%)	4 (1%)	67	73
1	C	288/287 (100%)	281 (98%)	7 (2%)	49	53
1	D	289/287 (101%)	285 (99%)	4 (1%)	67	73
All	All	1156/1148 (101%)	1136 (98%)	20 (2%)	60	67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	109	VAL
1	A	165	ASP
1	A	275	MET
1	A	315	LEU
1	B	12	LEU
1	B	19	GLN
1	B	165	ASP
1	B	275	MET
1	C	12	LEU
1	C	148	LYS
1	C	165	ASP
1	C	176	ARG
1	C	228	GLU
1	C	275	MET
1	C	310	GLU
1	D	6	GLN
1	D	12	LEU
1	D	165	ASP
1	D	275	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	107	ASN
1	A	163	ASN
1	B	225	GLN
1	B	297	ASN
1	C	16	GLN
1	C	19	GLN
1	C	296	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	297	ASN
1	D	99	GLN
1	D	107	ASN
1	D	330	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 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$
5	D0Y	B	805	-	37,39,39	1.03	2 (5%)	40,56,56	1.17	2 (5%)
3	EPE	A	803	-	15,15,15	1.10	1 (6%)	18,20,20	0.60	1 (5%)
4	SO4	C	805	-	4,4,4	0.44	0	6,6,6	0.15	0
5	D0Y	C	807	-	37,39,39	1.07	2 (5%)	40,56,56	1.15	4 (10%)
2	NAD	C	801	-	42,48,48	1.84	9 (21%)	50,73,73	1.27	5 (10%)
2	NAD	A	801	-	42,48,48	1.78	7 (16%)	50,73,73	1.38	6 (12%)
2	NAD	D	801	-	42,48,48	1.76	8 (19%)	50,73,73	1.30	7 (14%)
3	EPE	B	803	-	15,15,15	0.90	1 (6%)	18,20,20	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	C	803	-	15,15,15	1.24	1 (6%)	18,20,20	0.57	1 (5%)
4	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.22	0
3	EPE	C	806	-	15,15,15	0.86	1 (6%)	18,20,20	0.51	0
5	D0Y	D	803	-	37,39,39	1.26	2 (5%)	40,56,56	1.14	4 (10%)
3	EPE	C	802	-	15,15,15	1.60	1 (6%)	18,20,20	0.67	0
4	SO4	C	804	-	4,4,4	0.18	0	6,6,6	0.11	0
5	D0Y	A	805	-	37,39,39	1.17	3 (8%)	40,56,56	1.25	4 (10%)
4	SO4	B	804	-	4,4,4	0.27	0	6,6,6	0.11	0
3	EPE	A	802	-	15,15,15	1.14	1 (6%)	18,20,20	0.38	0
3	EPE	B	802	-	15,15,15	0.89	1 (6%)	18,20,20	0.46	0
4	SO4	D	802	-	4,4,4	0.38	0	6,6,6	0.22	0
2	NAD	B	801	-	42,48,48	1.81	9 (21%)	50,73,73	1.31	5 (10%)

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
5	D0Y	B	805	-	-	2/14/38/38	0/5/5/5
3	EPE	B	802	-	-	5/9/19/19	0/1/1/1
5	D0Y	C	807	-	-	2/14/38/38	0/5/5/5
2	NAD	C	801	-	-	4/26/62/62	0/5/5/5
2	NAD	A	801	-	-	6/26/62/62	0/5/5/5
2	NAD	D	801	-	-	4/26/62/62	0/5/5/5
3	EPE	B	803	-	-	4/9/19/19	0/1/1/1
3	EPE	C	803	-	-	2/9/19/19	0/1/1/1
3	EPE	C	806	-	-	6/9/19/19	0/1/1/1
5	D0Y	D	803	-	-	2/14/38/38	0/5/5/5
3	EPE	C	802	-	-	4/9/19/19	0/1/1/1
2	NAD	B	801	-	-	5/26/62/62	0/5/5/5
5	D0Y	A	805	-	-	2/14/38/38	0/5/5/5
3	EPE	A	802	-	-	5/9/19/19	0/1/1/1
3	EPE	A	803	-	-	5/9/19/19	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	EPE	C10-S	-6.07	1.68	1.77
2	C	801	NAD	C7N-N7N	5.61	1.43	1.33
2	A	801	NAD	C7N-N7N	5.16	1.42	1.33
2	D	801	NAD	C7N-N7N	4.99	1.42	1.33
3	C	803	EPE	C10-S	-4.75	1.70	1.77
2	B	801	NAD	C7N-N7N	4.72	1.42	1.33
2	A	801	NAD	C2B-C3B	-4.58	1.40	1.53
2	C	801	NAD	C2B-C3B	-4.38	1.41	1.53
5	D	803	D0Y	C17-C16	-4.30	1.34	1.37
3	A	802	EPE	C10-S	-4.24	1.71	1.77
3	A	803	EPE	C10-S	-4.16	1.71	1.77
2	D	801	NAD	C2B-C3B	-4.14	1.42	1.53
2	B	801	NAD	C2B-C3B	-4.12	1.42	1.53
5	D	803	D0Y	C17-S18	4.05	1.76	1.70
5	B	805	D0Y	C17-S18	3.63	1.75	1.70
5	C	807	D0Y	C17-S18	3.62	1.75	1.70
2	A	801	NAD	O2D-C2D	-3.55	1.34	1.43
5	A	805	D0Y	C17-S18	3.33	1.75	1.70
2	A	801	NAD	C6A-N6A	3.31	1.46	1.34
3	B	802	EPE	C10-S	-3.29	1.72	1.77
2	B	801	NAD	C6A-N6A	3.27	1.46	1.34
2	D	801	NAD	O2D-C2D	-3.25	1.35	1.43
3	B	803	EPE	C10-S	-3.24	1.72	1.77
2	C	801	NAD	C6A-N6A	3.24	1.45	1.34
2	B	801	NAD	O2D-C2D	-3.09	1.35	1.43
3	C	806	EPE	C10-S	-3.07	1.73	1.77
2	B	801	NAD	C2D-C1D	-3.03	1.49	1.53
2	C	801	NAD	O2D-C2D	-3.01	1.35	1.43
2	D	801	NAD	C6A-N6A	2.98	1.44	1.34
2	C	801	NAD	C2B-C1B	-2.75	1.49	1.53
2	D	801	NAD	C2B-C1B	-2.73	1.49	1.53
5	A	805	D0Y	C17-C16	-2.72	1.35	1.37
2	B	801	NAD	C2N-N1N	2.67	1.38	1.35
2	B	801	NAD	C2B-C1B	-2.63	1.49	1.53
5	B	805	D0Y	C17-C16	-2.60	1.35	1.37
2	D	801	NAD	C2D-C1D	-2.41	1.50	1.53
2	A	801	NAD	C2D-C1D	-2.38	1.50	1.53
5	A	805	D0Y	C6-S5	2.37	1.80	1.77
2	C	801	NAD	C5D-C4D	-2.34	1.44	1.51
2	B	801	NAD	C5D-C4D	-2.28	1.44	1.51
2	D	801	NAD	C5D-C4D	-2.28	1.44	1.51
2	C	801	NAD	C2D-C1D	-2.22	1.50	1.53
5	C	807	D0Y	C17-C16	-2.22	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	NAD	C5B-C4B	-2.22	1.44	1.51
2	B	801	NAD	C5B-C4B	-2.16	1.44	1.51
2	D	801	NAD	C5B-C4B	-2.12	1.45	1.51
2	A	801	NAD	C5B-C4B	-2.10	1.45	1.51
2	C	801	NAD	O4B-C4B	-2.07	1.40	1.45
2	A	801	NAD	O4B-C4B	-2.02	1.40	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	D0Y	C16-C17-S18	-5.04	109.05	112.29
2	C	801	NAD	N3A-C2A-N1A	-4.98	120.90	128.68
2	D	801	NAD	N3A-C2A-N1A	-4.79	121.20	128.68
2	A	801	NAD	N3A-C2A-N1A	-4.78	121.21	128.68
2	B	801	NAD	N3A-C2A-N1A	-4.75	121.26	128.68
5	B	805	D0Y	C16-C17-S18	-4.52	109.38	112.29
5	D	803	D0Y	C16-C17-S18	-4.04	109.69	112.29
3	B	803	EPE	O2S-S-C10	-3.51	102.69	106.92
2	A	801	NAD	O4B-C1B-C2B	-3.28	102.13	106.93
2	A	801	NAD	C3N-C7N-N7N	3.14	121.52	117.75
2	B	801	NAD	C3N-C7N-N7N	3.13	121.51	117.75
2	D	801	NAD	PN-O3-PA	-3.06	122.31	132.83
5	C	807	D0Y	C16-C17-S18	-3.03	110.34	112.29
2	B	801	NAD	O4B-C1B-C2B	-2.95	102.62	106.93
5	A	805	D0Y	O14-C13-O35	2.93	121.30	117.58
2	C	801	NAD	PN-O3-PA	-2.90	122.86	132.83
2	A	801	NAD	PN-O3-PA	-2.86	123.01	132.83
2	C	801	NAD	C3N-C7N-N7N	2.83	121.15	117.75
2	D	801	NAD	C3N-C7N-N7N	2.75	121.05	117.75
2	B	801	NAD	PN-O3-PA	-2.75	123.40	132.83
5	C	807	D0Y	C6-S5-C4	2.49	105.97	102.81
5	A	805	D0Y	C6-S5-C4	2.46	105.93	102.81
2	B	801	NAD	O7N-C7N-N7N	-2.43	119.12	122.58
5	C	807	D0Y	O14-C13-O35	2.34	120.55	117.58
5	D	803	D0Y	O14-C13-O35	2.32	120.52	117.58
5	C	807	D0Y	O14-C15-C16	2.29	111.95	106.98
2	D	801	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
2	C	801	NAD	O7N-C7N-N7N	-2.25	119.38	122.58
2	D	801	NAD	O4B-C1B-C2B	-2.23	103.66	106.93
2	D	801	NAD	O7N-C7N-N7N	-2.23	119.41	122.58
2	C	801	NAD	C4A-C5A-N7A	-2.19	107.12	109.40
2	A	801	NAD	O4D-C1D-C2D	-2.18	103.74	106.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	EPE	O3S-S-C10	-2.14	102.30	105.77
3	A	803	EPE	O1S-S-C10	-2.11	104.37	106.92
2	A	801	NAD	O7N-C7N-N7N	-2.11	119.58	122.58
5	A	805	D0Y	O14-C15-C16	2.10	111.54	106.98
2	D	801	NAD	C4A-C5A-N7A	-2.10	107.21	109.40
5	D	803	D0Y	C30-C28-C27	-2.09	120.04	122.83
5	D	803	D0Y	C31-C30-C28	2.07	120.51	118.36
5	B	805	D0Y	O14-C15-C16	2.02	111.37	106.98

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	EPE	C10-C9-N1-C2
2	C	801	NAD	O4D-C1D-N1N-C2N
2	C	801	NAD	O4D-C1D-N1N-C6N
2	C	801	NAD	C2D-C1D-N1N-C2N
2	A	801	NAD	O4D-C1D-N1N-C2N
2	A	801	NAD	O4D-C1D-N1N-C6N
2	A	801	NAD	C2D-C1D-N1N-C2N
2	D	801	NAD	O4D-C1D-N1N-C2N
2	D	801	NAD	O4D-C1D-N1N-C6N
2	D	801	NAD	C2D-C1D-N1N-C2N
3	C	806	EPE	C10-C9-N1-C6
3	C	802	EPE	C10-C9-N1-C6
2	B	801	NAD	O4D-C1D-N1N-C2N
2	B	801	NAD	O4D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C2N
3	A	802	EPE	C9-C10-S-O1S
3	A	802	EPE	C9-C10-S-O2S
3	A	802	EPE	C9-C10-S-O3S
3	C	803	EPE	N4-C7-C8-O8
3	B	803	EPE	N4-C7-C8-O8
3	C	806	EPE	C9-C10-S-O3S
3	A	803	EPE	C9-C10-S-O3S
3	B	803	EPE	C8-C7-N4-C5
3	C	806	EPE	N4-C7-C8-O8
3	B	802	EPE	C10-C9-N1-C6
3	B	803	EPE	C10-C9-N1-C2
3	C	802	EPE	C10-C9-N1-C2
3	C	802	EPE	N4-C7-C8-O8
3	B	802	EPE	C8-C7-N4-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	802	EPE	C8-C7-N4-C5
3	C	806	EPE	C9-C10-S-O1S
3	C	806	EPE	C9-C10-S-O2S
3	A	803	EPE	C9-C10-S-O1S
3	A	803	EPE	C9-C10-S-O2S
3	B	803	EPE	C10-C9-N1-C6
3	C	806	EPE	C10-C9-N1-C2
5	C	807	D0Y	C16-C15-C21-C22
5	B	805	D0Y	C16-C15-C21-C22
2	A	801	NAD	PN-O3-PA-O1A
2	B	801	NAD	PN-O3-PA-O1A
5	C	807	D0Y	C16-C15-C21-C34
5	A	805	D0Y	C16-C15-C21-C22
5	A	805	D0Y	C16-C15-C21-C34
5	D	803	D0Y	C16-C15-C21-C22
3	A	803	EPE	C8-C7-N4-C5
5	B	805	D0Y	C16-C15-C21-C34
5	D	803	D0Y	C16-C15-C21-C34
2	A	801	NAD	C2D-C1D-N1N-C6N
2	A	801	NAD	O4B-C4B-C5B-O5B
3	A	802	EPE	C8-C7-N4-C3
3	A	802	EPE	C8-C7-N4-C5
2	C	801	NAD	O4B-C4B-C5B-O5B
2	D	801	NAD	O4B-C4B-C5B-O5B
2	B	801	NAD	O4B-C4B-C5B-O5B
3	B	802	EPE	S-C10-C9-N1
3	C	802	EPE	S-C10-C9-N1
3	A	803	EPE	C8-C7-N4-C3
3	C	803	EPE	C10-C9-N1-C2

There are no ring outliers.

9 monomers are involved in 13 short contacts:

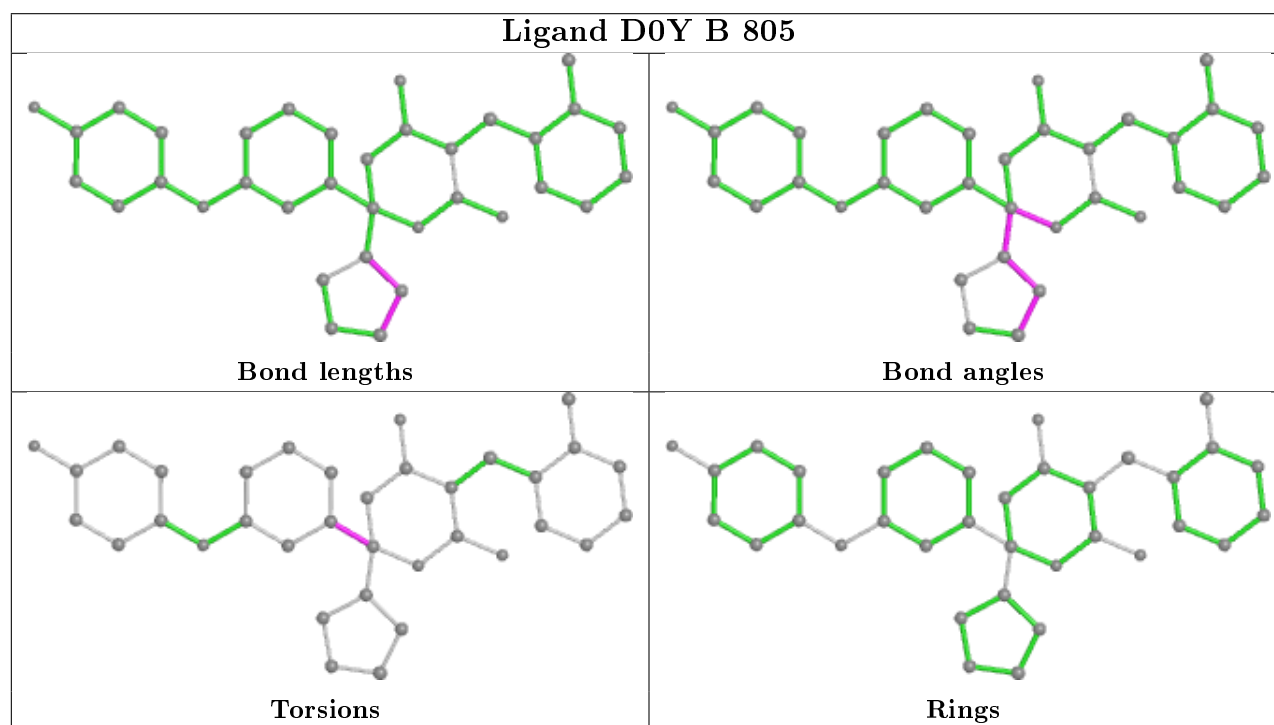
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	EPE	2	0
2	C	801	NAD	1	0
2	D	801	NAD	1	0
3	B	803	EPE	1	0
3	C	803	EPE	1	0
3	C	806	EPE	2	0
5	D	803	D0Y	1	0
3	C	802	EPE	1	0

Continued on next page...

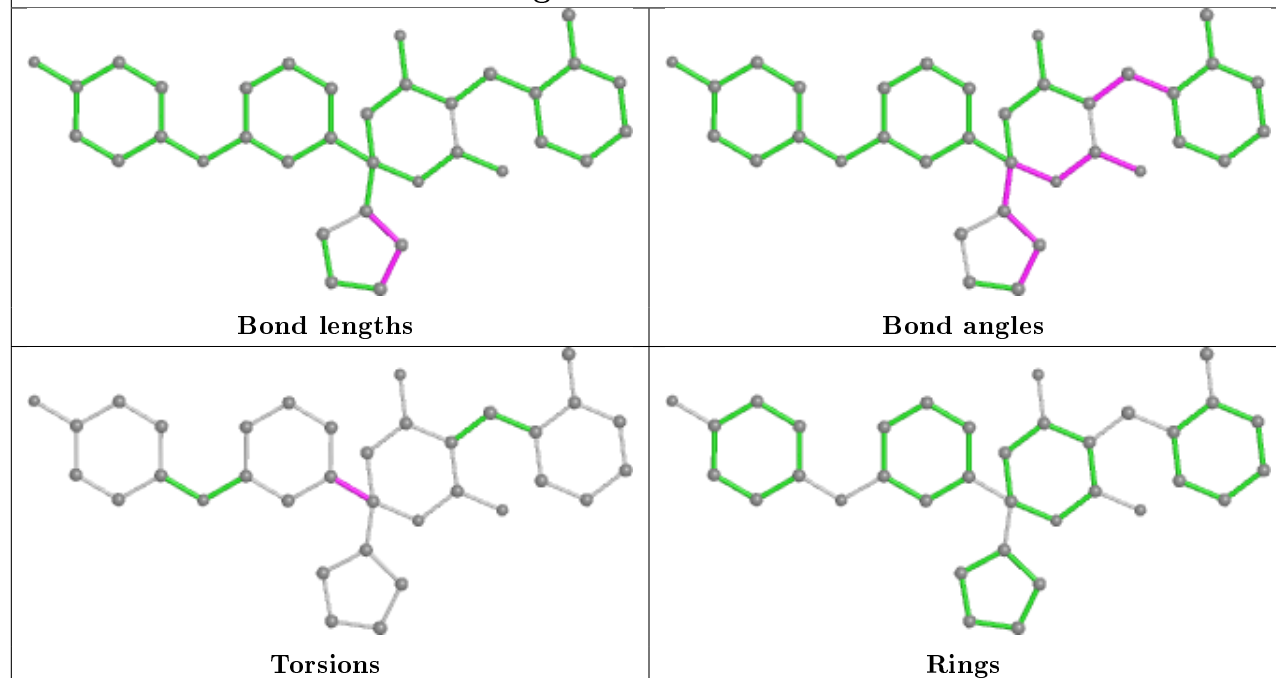
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	EPE	3	0

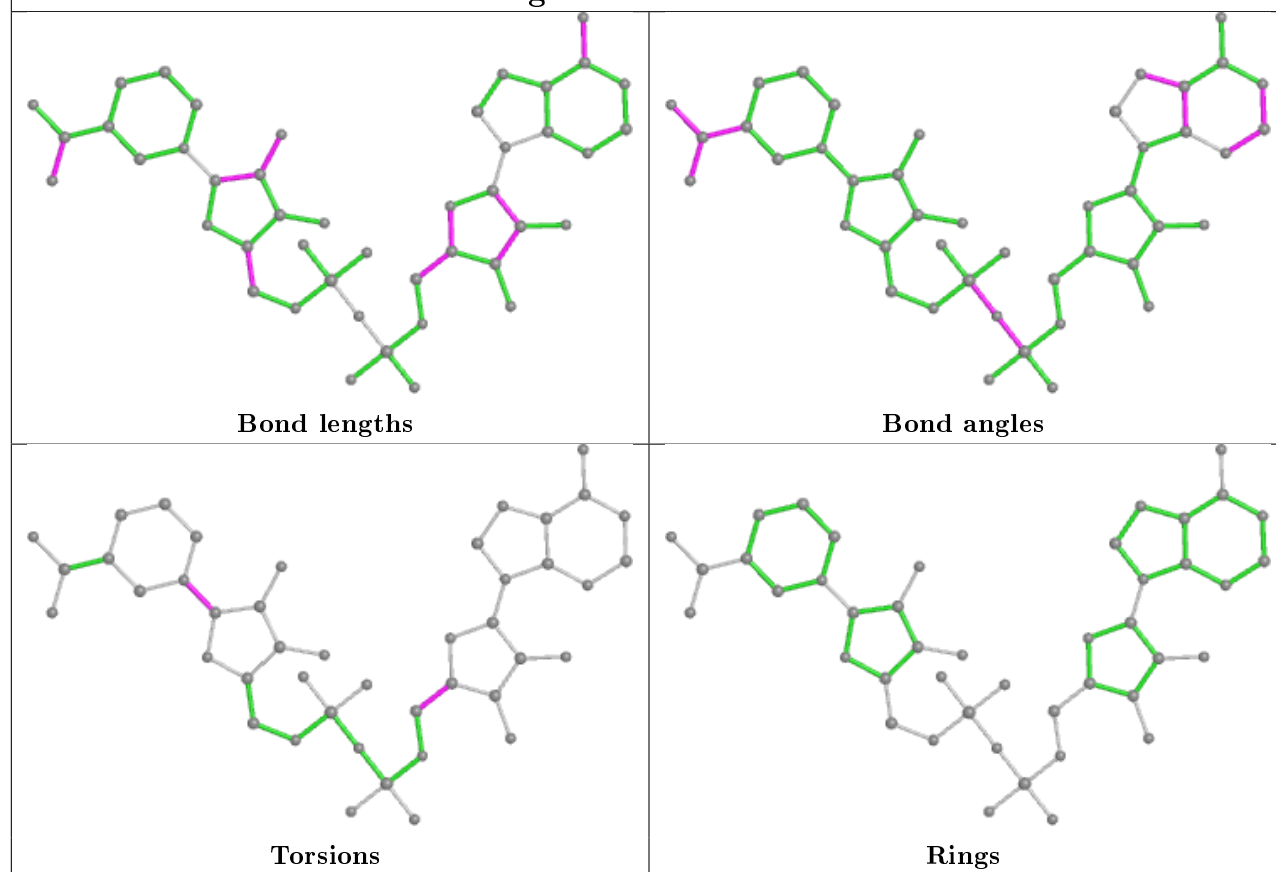
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

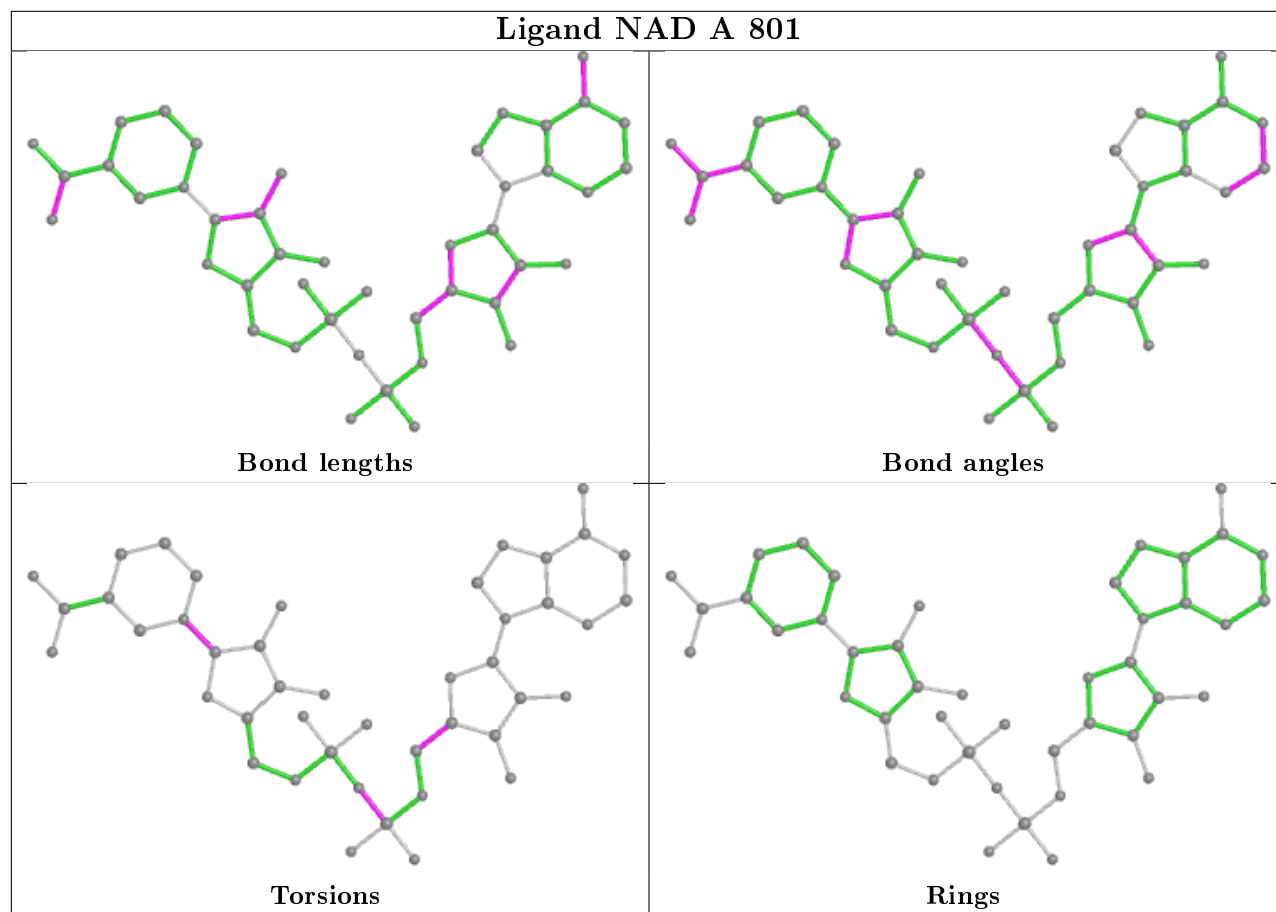


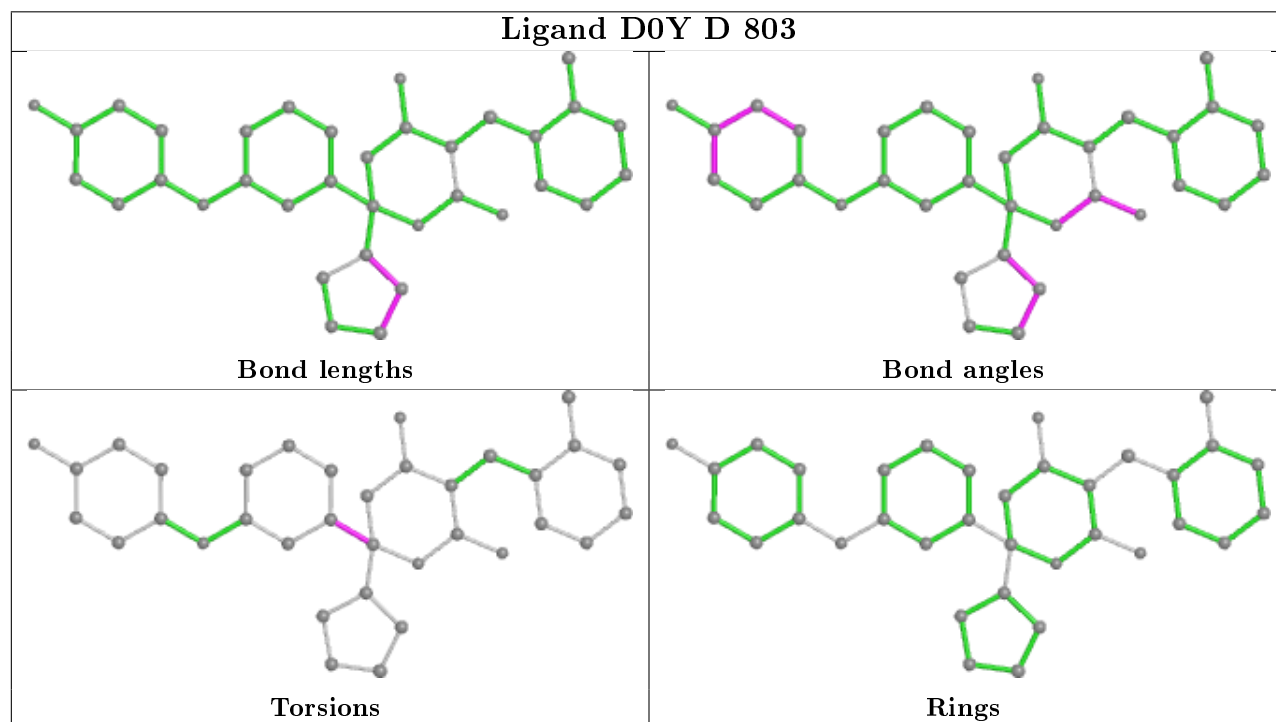
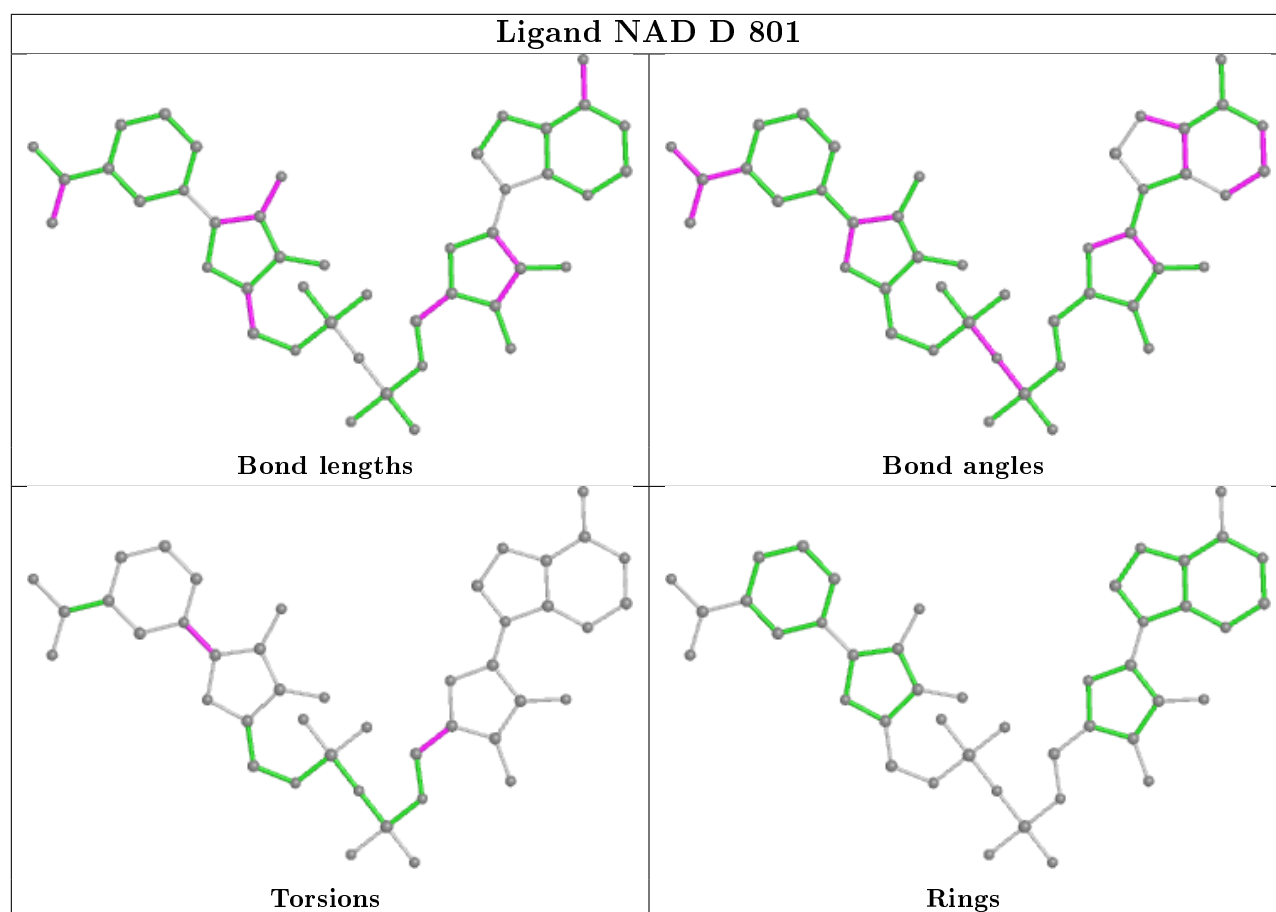
Ligand D0Y C 807



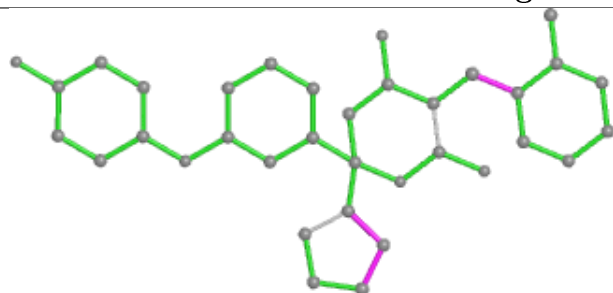
Ligand NAD C 801



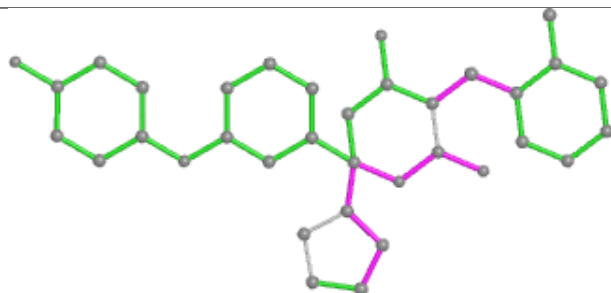




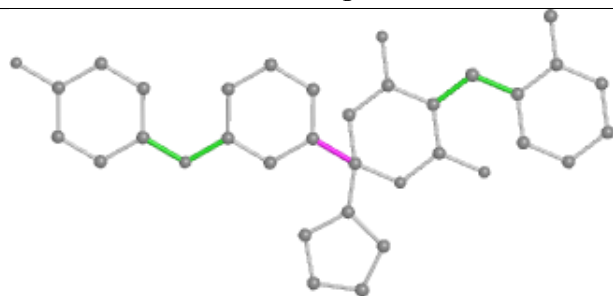
Ligand D0Y A 805



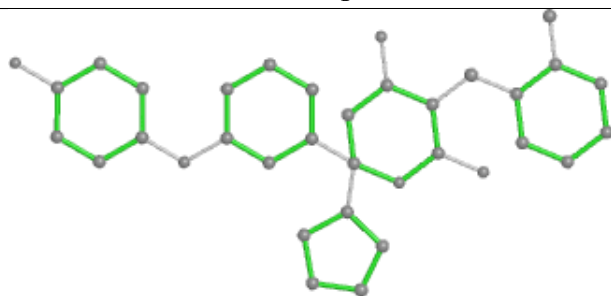
Bond lengths



Bond angles

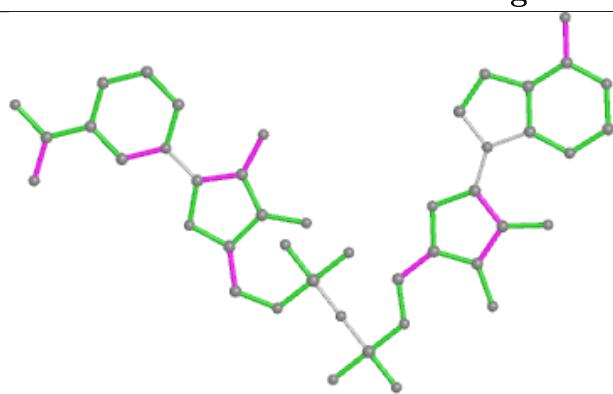


Torsions

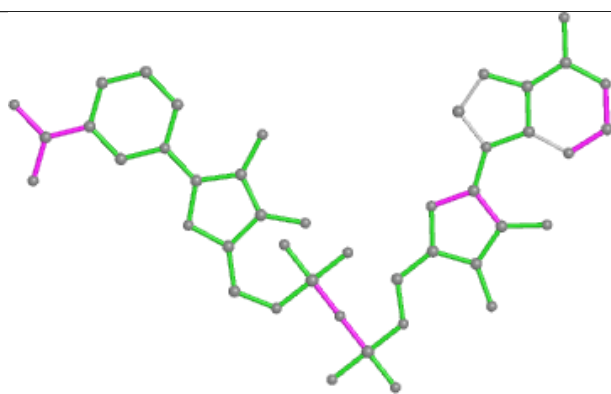


Rings

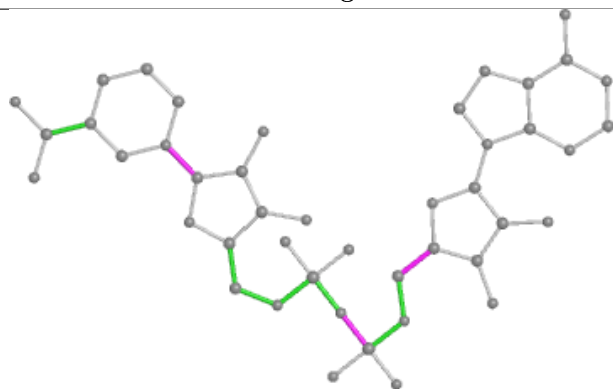
Ligand NAD B 801



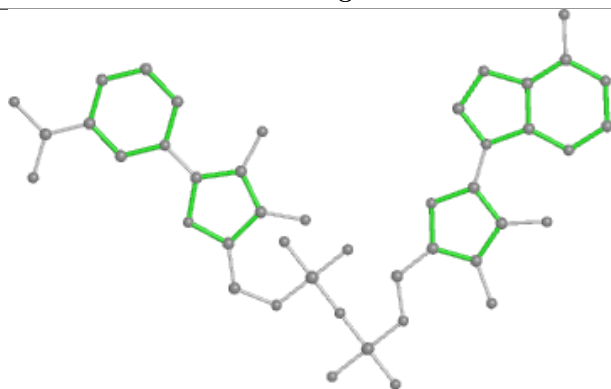
Bond lengths



Bond angles



Torsions



Rings

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	331/331 (100%)	-0.31	3 (0%) 84 86	10, 21, 44, 68	0
1	B	331/331 (100%)	-0.26	9 (2%) 54 60	12, 21, 45, 81	0
1	C	331/331 (100%)	-0.14	6 (1%) 68 72	11, 21, 45, 82	0
1	D	331/331 (100%)	-0.16	6 (1%) 68 72	10, 20, 48, 85	0
All	All	1324/1324 (100%)	-0.22	24 (1%) 68 72	10, 21, 46, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	GLU	5.9
1	D	1	ALA	5.5
1	D	16	GLN	4.0
1	C	331	PHE	3.9
1	C	1	ALA	3.8
1	D	105	ARG	3.6
1	C	330	GLN	3.5
1	C	13	LYS	3.2
1	C	14	GLU	3.2
1	B	331	PHE	3.1
1	B	15	GLU	2.7
1	B	14	GLU	2.6
1	B	101	GLU	2.6
1	B	72[A]	ARG	2.6
1	B	100	GLN	2.6
1	D	13	LYS	2.5
1	B	221	LYS	2.5
1	C	106	LEU	2.5
1	B	16	GLN	2.4
1	A	229	VAL	2.2
1	A	101	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118[A]	PHE	2.2
1	D	331	PHE	2.2
1	B	13	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

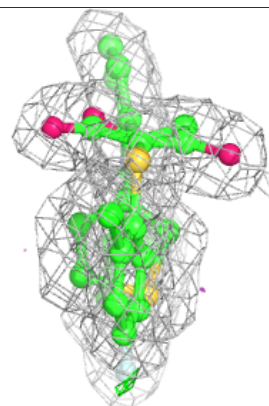
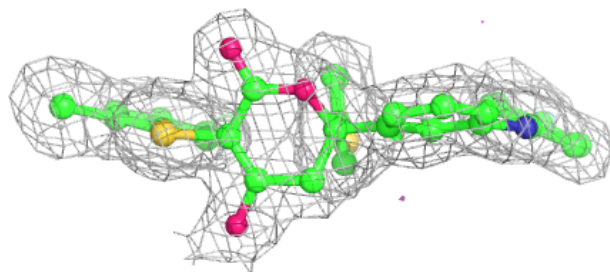
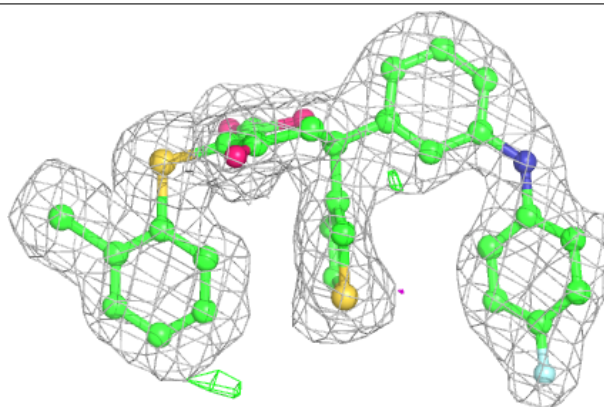
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EPE	C	806	15/15	0.80	0.20	65,67,73,74	0
4	SO4	C	805	5/5	0.81	0.24	51,51,54,57	0
3	EPE	B	802	15/15	0.86	0.28	57,69,81,81	0
3	EPE	B	803	15/15	0.86	0.20	38,43,48,48	15
3	EPE	A	802	15/15	0.87	0.21	56,62,65,65	15
3	EPE	C	802	15/15	0.87	0.18	51,57,59,60	0
4	SO4	C	804	5/5	0.89	0.16	29,32,33,36	5
4	SO4	A	804	5/5	0.93	0.18	43,49,51,52	0
4	SO4	B	804	5/5	0.93	0.18	58,60,62,62	0
3	EPE	C	803	15/15	0.94	0.16	29,34,51,52	0
5	D0Y	C	807	35/35	0.95	0.09	14,19,24,26	0
5	D0Y	D	803	35/35	0.95	0.10	17,20,47,51	0
4	SO4	D	802	5/5	0.95	0.15	25,32,37,39	0
3	EPE	A	803	15/15	0.95	0.18	39,46,56,58	0
5	D0Y	A	805	35/35	0.96	0.10	15,22,25,27	0
5	D0Y	B	805	35/35	0.96	0.09	13,19,31,36	0
2	NAD	D	801	44/44	0.97	0.08	13,16,19,21	0
2	NAD	B	801	44/44	0.97	0.09	12,18,23,24	0
2	NAD	C	801	44/44	0.97	0.08	15,19,22,25	0
2	NAD	A	801	44/44	0.97	0.08	12,17,21,23	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.

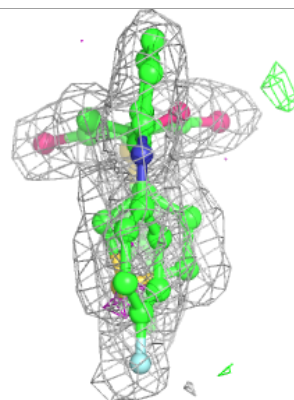
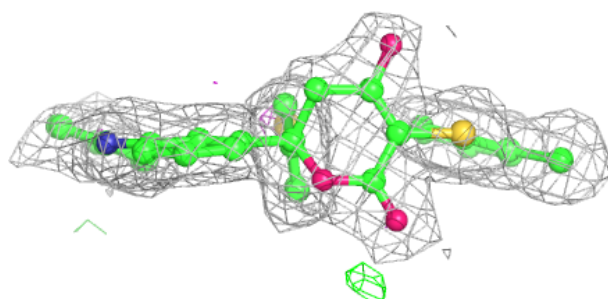
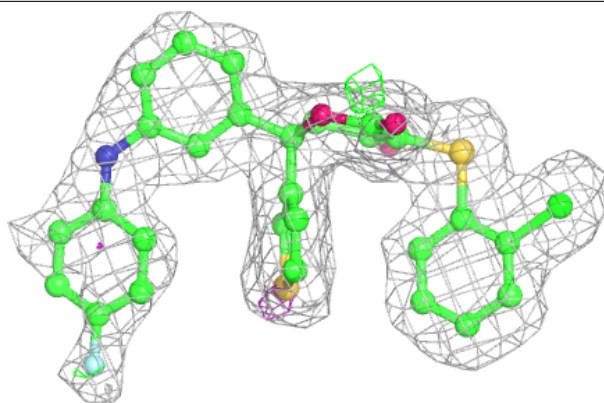
Electron density around D0Y C 807:

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

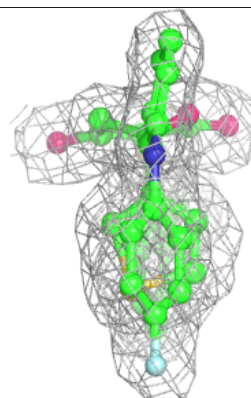
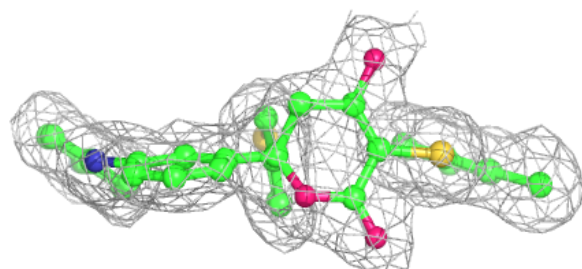
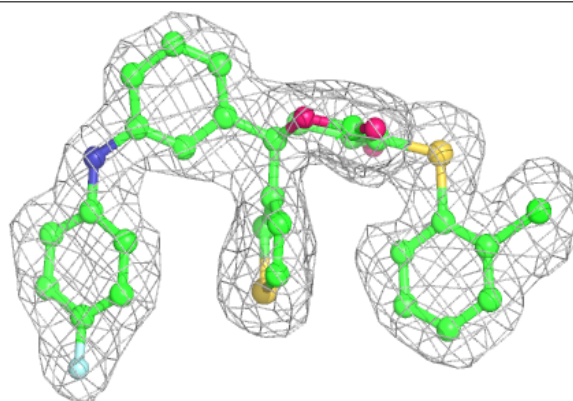


Electron density around D0Y D 803:

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

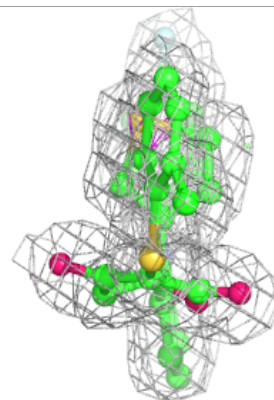
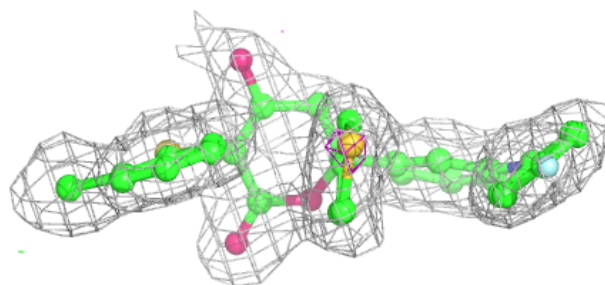
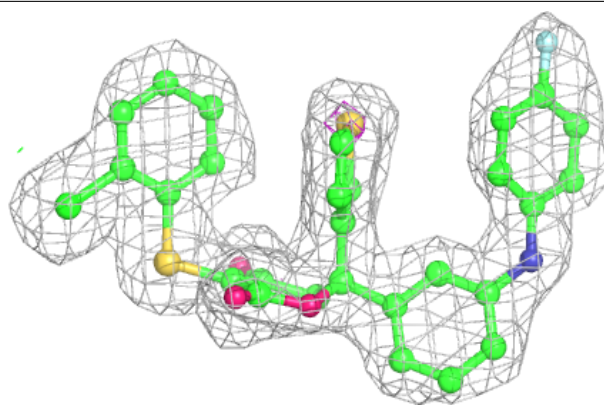
**Electron density around D0Y A 805:**

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

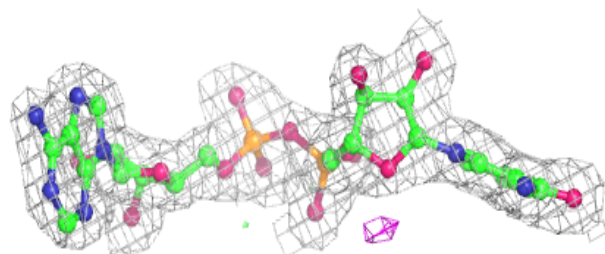
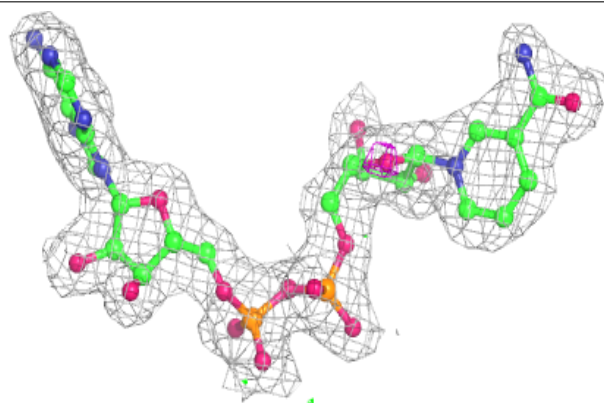


Electron density around D0Y B 805:

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

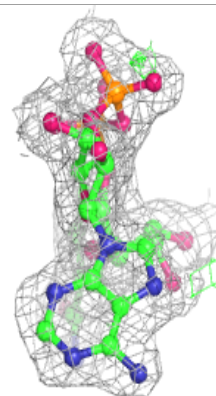
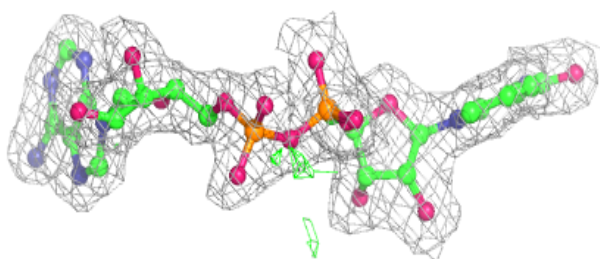
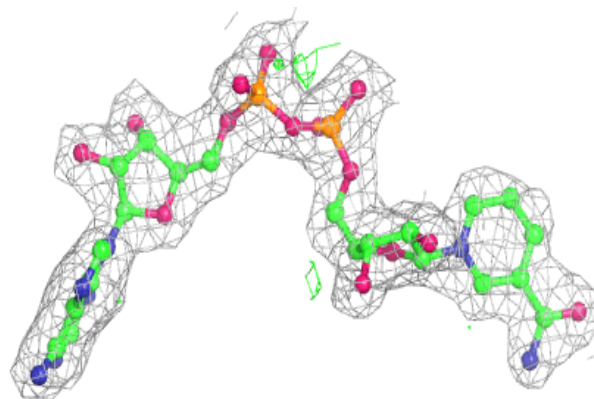
**Electron density around NAD D 801:**

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

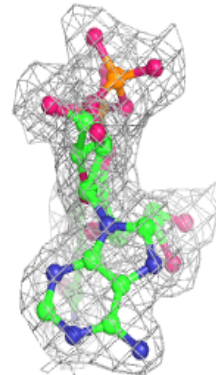
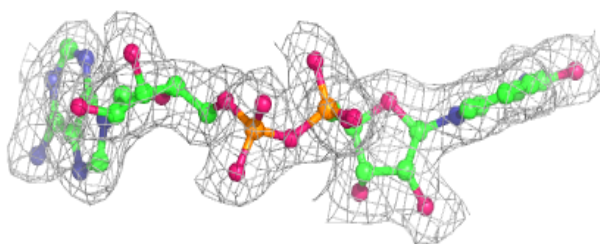
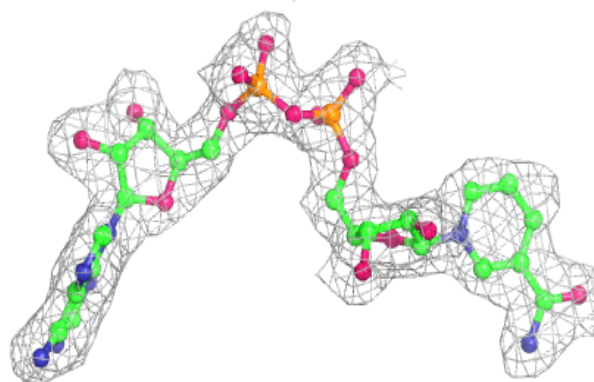


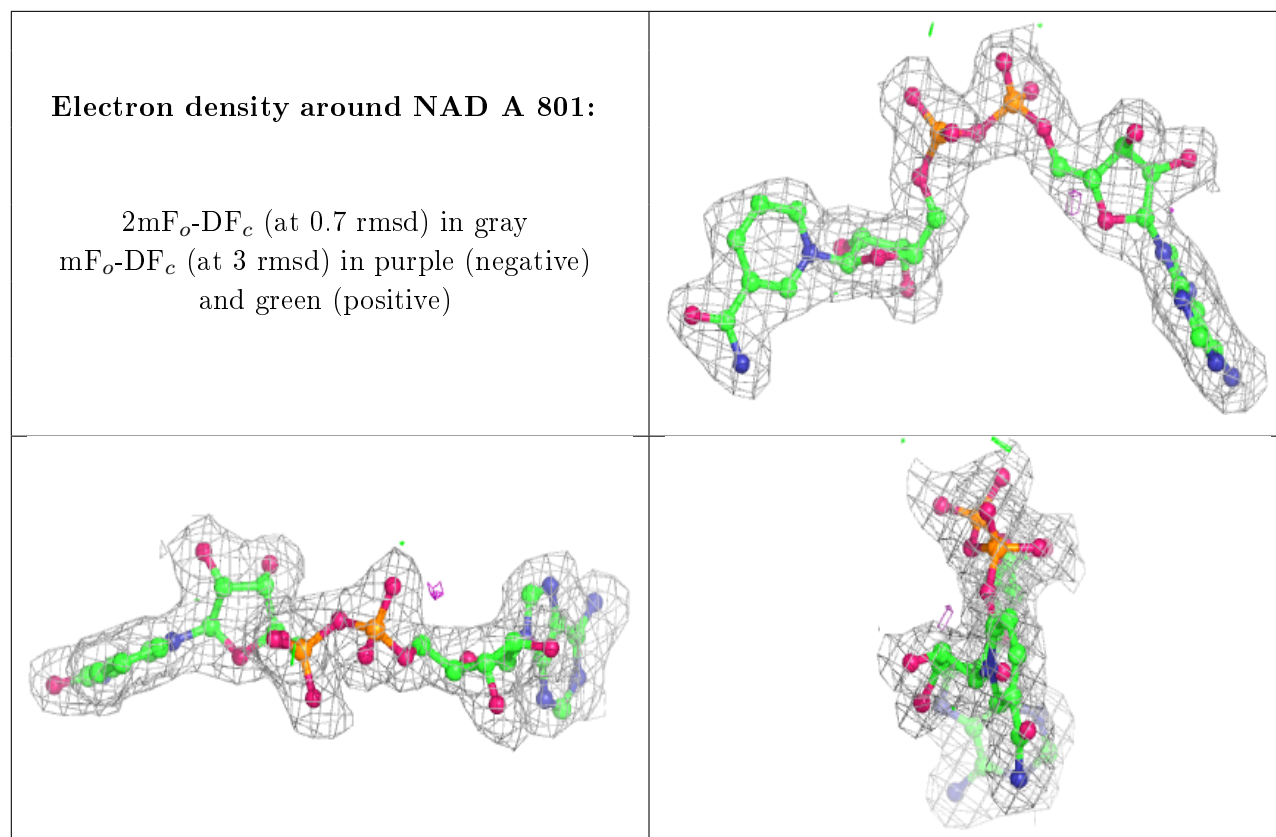
Electron density around NAD B 801:

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

**Electron density around NAD C 801:**

$2mF_o-DF_c$ (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.