Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 05:33 pm GMT

PDB ID	:	6TBC
Title	:	Crystal structure of S. aureus FabI in complex with NADPH and kalimantacin B
Authors	:	Fage, C.D.; Masschelein, J.
Deposited on	:	2019-11-01
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

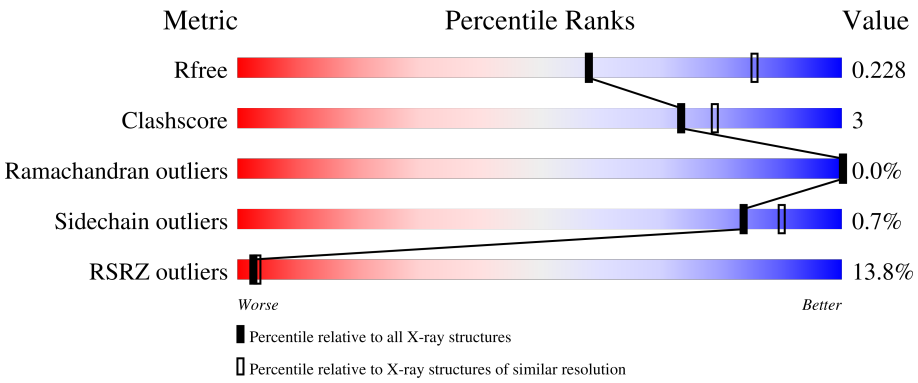
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	261	14% 92% 8%
1	B	261	11% 93% 7%
1	C	261	9% 92% 7% ••
1	D	261	16% 90% 8% •
1	E	261	13% 90% 8% •

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Mol	Chain	Length	Quality of chain
1	F	261	11% 92% 7%
1	G	261	20% 92% 8%
1	H	261	15% 90% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16627 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 Enoyl-[acyl-carrier-protein] reductase [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1998	1258	346	389	5	0	0	0
1	B	260	1998	1258	346	389	5	0	0	0
1	C	259	1992	1255	345	387	5	2	0	0
1	D	258	1982	1249	342	386	5	0	0	0
1	E	258	1982	1249	342	386	5	0	0	0
1	F	258	1982	1249	342	386	5	0	0	0
1	G	259	1992	1255	345	387	5	0	0	0
1	H	258	1982	1249	342	386	5	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A0J9X1X7
A	-3	SER	-	expression tag	UNP A0A0J9X1X7
A	-2	HIS	-	expression tag	UNP A0A0J9X1X7
A	-1	MET	-	expression tag	UNP A0A0J9X1X7
A	0	ALA	-	expression tag	UNP A0A0J9X1X7
A	1	SER	-	expression tag	UNP A0A0J9X1X7
A	2	LEU	-	expression tag	UNP A0A0J9X1X7
B	-4	GLY	-	expression tag	UNP A0A0J9X1X7
B	-3	SER	-	expression tag	UNP A0A0J9X1X7
B	-2	HIS	-	expression tag	UNP A0A0J9X1X7
B	-1	MET	-	expression tag	UNP A0A0J9X1X7
B	0	ALA	-	expression tag	UNP A0A0J9X1X7
B	1	SER	-	expression tag	UNP A0A0J9X1X7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	LEU	-	expression tag	UNP A0A0J9X1X7
C	-4	GLY	-	expression tag	UNP A0A0J9X1X7
C	-3	SER	-	expression tag	UNP A0A0J9X1X7
C	-2	HIS	-	expression tag	UNP A0A0J9X1X7
C	-1	MET	-	expression tag	UNP A0A0J9X1X7
C	0	ALA	-	expression tag	UNP A0A0J9X1X7
C	1	SER	-	expression tag	UNP A0A0J9X1X7
C	2	LEU	-	expression tag	UNP A0A0J9X1X7
D	-4	GLY	-	expression tag	UNP A0A0J9X1X7
D	-3	SER	-	expression tag	UNP A0A0J9X1X7
D	-2	HIS	-	expression tag	UNP A0A0J9X1X7
D	-1	MET	-	expression tag	UNP A0A0J9X1X7
D	0	ALA	-	expression tag	UNP A0A0J9X1X7
D	1	SER	-	expression tag	UNP A0A0J9X1X7
D	2	LEU	-	expression tag	UNP A0A0J9X1X7
E	-4	GLY	-	expression tag	UNP A0A0J9X1X7
E	-3	SER	-	expression tag	UNP A0A0J9X1X7
E	-2	HIS	-	expression tag	UNP A0A0J9X1X7
E	-1	MET	-	expression tag	UNP A0A0J9X1X7
E	0	ALA	-	expression tag	UNP A0A0J9X1X7
E	1	SER	-	expression tag	UNP A0A0J9X1X7
E	2	LEU	-	expression tag	UNP A0A0J9X1X7
F	-4	GLY	-	expression tag	UNP A0A0J9X1X7
F	-3	SER	-	expression tag	UNP A0A0J9X1X7
F	-2	HIS	-	expression tag	UNP A0A0J9X1X7
F	-1	MET	-	expression tag	UNP A0A0J9X1X7
F	0	ALA	-	expression tag	UNP A0A0J9X1X7
F	1	SER	-	expression tag	UNP A0A0J9X1X7
F	2	LEU	-	expression tag	UNP A0A0J9X1X7
G	-4	GLY	-	expression tag	UNP A0A0J9X1X7
G	-3	SER	-	expression tag	UNP A0A0J9X1X7
G	-2	HIS	-	expression tag	UNP A0A0J9X1X7
G	-1	MET	-	expression tag	UNP A0A0J9X1X7
G	0	ALA	-	expression tag	UNP A0A0J9X1X7
G	1	SER	-	expression tag	UNP A0A0J9X1X7
G	2	LEU	-	expression tag	UNP A0A0J9X1X7
H	-4	GLY	-	expression tag	UNP A0A0J9X1X7
H	-3	SER	-	expression tag	UNP A0A0J9X1X7
H	-2	HIS	-	expression tag	UNP A0A0J9X1X7
H	-1	MET	-	expression tag	UNP A0A0J9X1X7
H	0	ALA	-	expression tag	UNP A0A0J9X1X7
H	1	SER	-	expression tag	UNP A0A0J9X1X7

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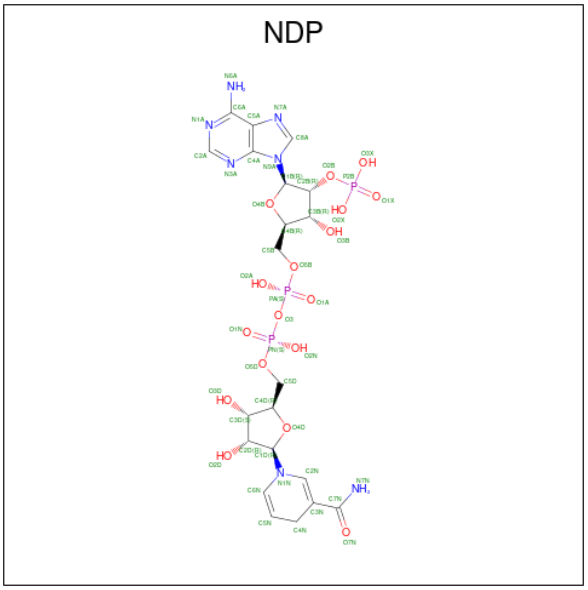
Chain	Residue	Modelled	Actual	Comment	Reference
H	2	LEU	-	expression tag	UNP A0A0J9X1X7

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0
2	C	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0
2	E	1	48	21	7	17	3	0	0
2	F	1	48	21	7	17	3	0	0
2	G	1	48	21	7	17	3	0	0
2	H	1	48	21	7	17	3	0	0

- Molecule 3 is (2 {E},5 {R},10 {E},12 {E},15 {S},19 {R})-20-[[(2 {R},3 {R})-3-aminocarbonyloxy-2-methyl-butanoyl]amino]-3,5,15-trimethyl-7-methylidene-19-oxidanyl-17-oxidanylidene-icosa-2,10,12-trienoic acid (three-letter code: N5H) (formula: $C_{30}H_{48}N_2O_7$) (labeled as "Ligand of Interest" by depositor).

N5H

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	39	30	2	7	0	0
3	B	1	39	30	2	7	0	0
3	C	1	39	30	2	7	0	0
3	D	1	39	30	2	7	0	0
3	E	1	39	30	2	7	0	0
3	F	1	39	30	2	7	0	0
3	G	1	39	30	2	7	0	0
3	H	1	39	30	2	7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	4	4	4	0	0
4	B	3	3	3	0	0
4	C	6	6	6	0	0
4	D	1	1	1	0	0

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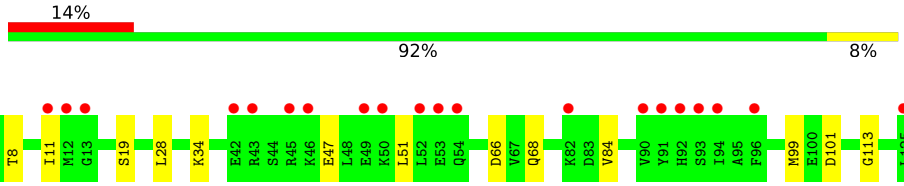
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	4	4	4	0	0
			Total	O		
4	F	1	1	1	0	0
			Total	O		
4	G	3	3	3	0	0
			Total	O		
4	H	1	1	1	0	0

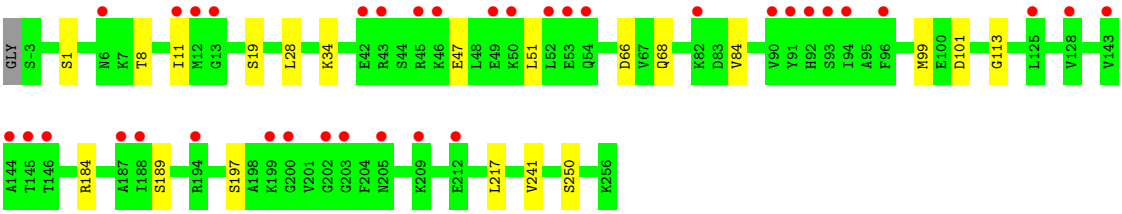
3 Residue-property plots (i)

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: Enoyl-[acyl-carrier-protein] reductase [NADPH]

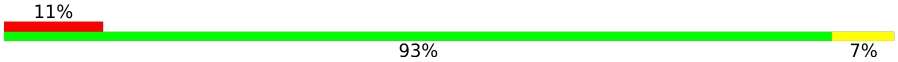
Chain A:

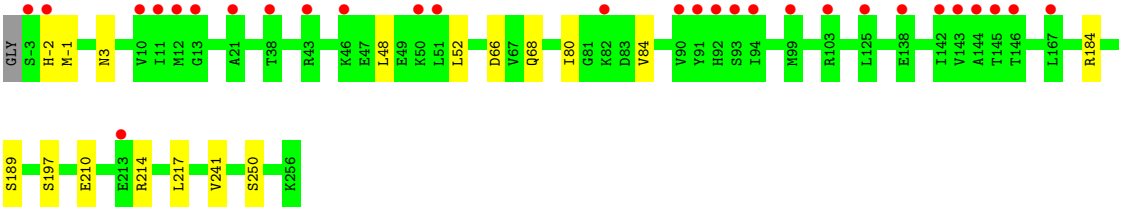




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

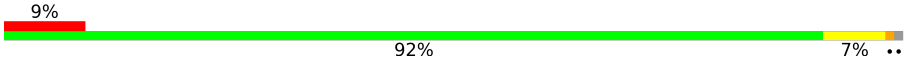
Chain B:

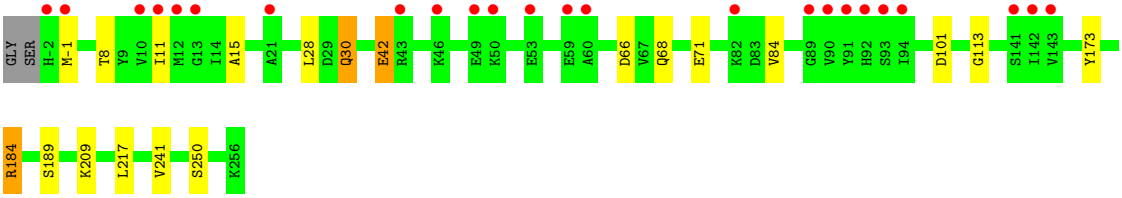




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

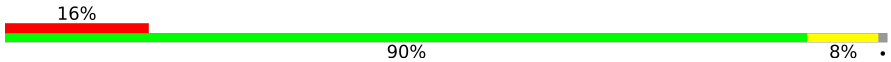
Chain C:

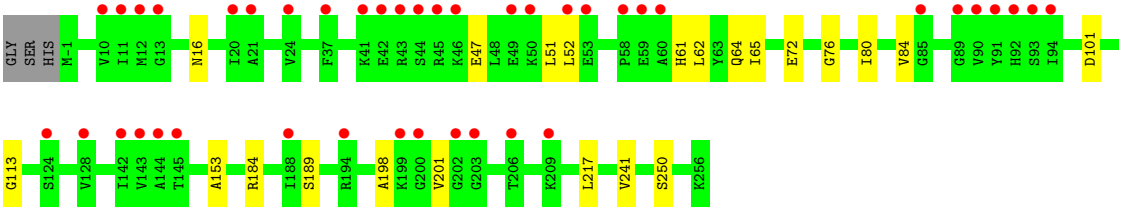




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

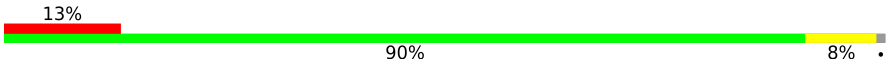
Chain D:

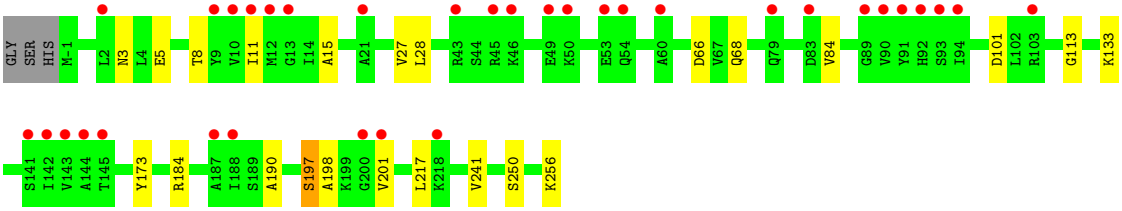




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

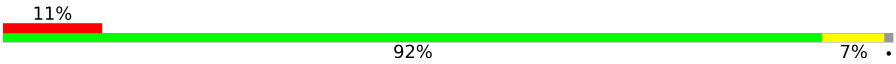
Chain E:

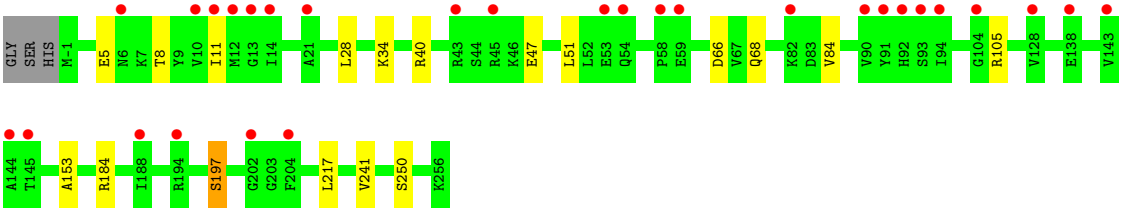




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

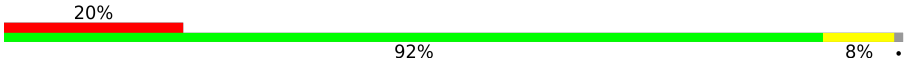
Chain F:

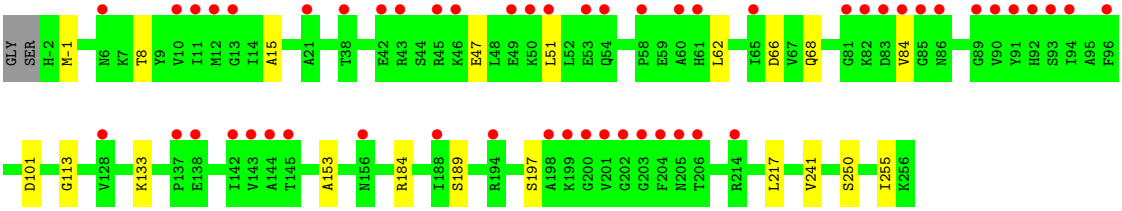




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

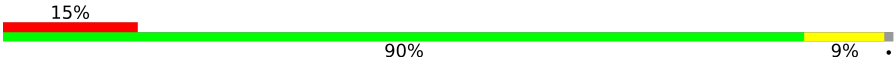
Chain G:

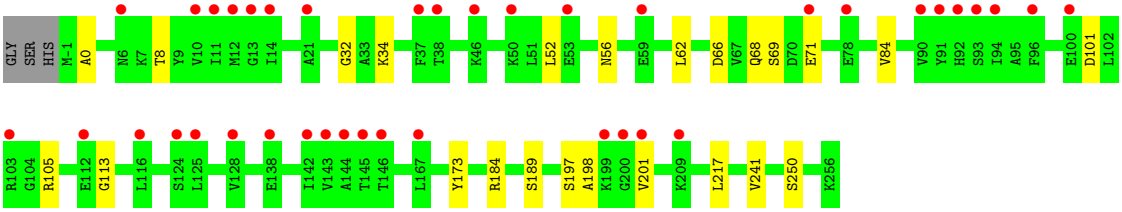




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.32Å 108.56Å 296.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 2.55 29.62 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.64-2.55) 100.0 (29.62-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.190 , 0.237 0.189 , 0.228	Depositor DCC
R_{free} test set	3452 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	87.9	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16627	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, N5H

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	0/2026	0.76	0/2730
1	B	0.68	0/2026	0.79	0/2730
1	C	0.73	2/2020 (0.1%)	0.78	1/2722 (0.0%)
1	D	0.69	0/2009	0.77	0/2707
1	E	0.69	0/2009	0.76	0/2707
1	F	0.69	0/2009	0.77	0/2707
1	G	0.68	0/2020	0.76	0/2722
1	H	0.69	0/2009	0.79	0/2707
All	All	0.69	2/16128 (0.0%)	0.77	1/21732 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLU	CD-OE2	-6.86	1.18	1.25
1	C	71	GLU	CB-CG	5.55	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	ARG	NE-CZ-NH2	5.93	123.27	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	42	GLU	Sidechain

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	1998	0	2013	10	1
1	B	1998	0	2013	15	0
1	C	1992	0	2008	14	0
1	D	1982	0	2001	15	0
1	E	1982	0	2001	20	0
1	F	1982	0	2001	14	1
1	G	1992	0	2008	15	0
1	H	1982	0	2001	20	0
2	A	48	0	26	1	0
2	B	48	0	26	0	0
2	C	48	0	26	1	0
2	D	48	0	26	0	0
2	E	48	0	26	3	0
2	F	48	0	26	1	0
2	G	48	0	26	2	0
2	H	48	0	26	1	0
3	A	39	0	0	0	0
3	B	39	0	0	1	0
3	C	39	0	0	0	0
3	D	39	0	0	0	0
3	E	39	0	0	4	0
3	F	39	0	0	1	0
3	G	39	0	0	0	0
3	H	39	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	4	0	0	0	0
4	F	1	0	0	0	0
4	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
All	All	16627	0	16254	107	1

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 (107) 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:F:34:LYS:NZ	1:F:84:VAL:HG13	1.92	0.83
1:D:65:ILE:HD12	1:D:72:GLU:O	1.78	0.83
1:H:197:SER:HB2	2:H:301:NDP:O1A	1.82	0.79
1:G:133:LYS:HE3	1:H:105:ARG:HH12	1.55	0.72
1:B:48:LEU:O	1:B:52:LEU:HD13	1.93	0.69
1:B:-2:HIS:ND1	1:E:5:GLU:OE2	2.27	0.68
1:H:34:LYS:CE	1:H:84:VAL:HG13	2.24	0.68
1:C:-1:MET:SD	1:H:56:ASN:ND2	2.66	0.68
1:B:48:LEU:O	1:B:52:LEU:CD1	2.42	0.67
1:H:69:SER:OG	1:H:71:GLU:HG2	1.96	0.66
1:F:40:ARG:HB3	2:F:301:NDP:O1X	1.98	0.63
1:D:65:ILE:HD11	1:D:76:GLY:HA3	1.80	0.63
1:F:34:LYS:HZ3	1:F:84:VAL:HG13	1.65	0.61
1:B:3:ASN:HD22	1:E:3:ASN:CG	2.04	0.61
1:H:34:LYS:HE3	1:H:84:VAL:HG13	1.83	0.59
1:B:-2:HIS:HA	1:C:30:GLN:NE2	2.20	0.56
1:D:64:GLN:O	1:D:65:ILE:HD13	2.06	0.56
1:E:201:VAL:HG21	3:E:302:N5H:C05	2.36	0.56
1:E:197:SER:OG	3:E:302:N5H:N28	2.39	0.55
1:A:34:LYS:HE3	1:A:84:VAL:HG13	1.89	0.55
1:A:19:SER:OG	2:A:301:NDP:O1A	2.20	0.54
1:B:197:SER:OG	3:B:302:N5H:N28	2.41	0.53
1:D:16:ASN:HA	1:D:47:GLU:HG2	1.91	0.52
1:E:133:LYS:HE3	1:F:105:ARG:HH12	1.75	0.52
1:H:69:SER:HG	1:H:71:GLU:HG2	1.74	0.52
1:G:15:ALA:HB2	2:G:301:NDP:H3B	1.93	0.51
1:H:8:THR:HG21	1:H:84:VAL:HG11	1.92	0.51
1:E:15:ALA:HB2	2:E:301:NDP:H3B	1.92	0.51
1:G:133:LYS:HE3	1:H:105:ARG:NH1	2.23	0.50
1:D:80:ILE:O	1:D:84:VAL:HG22	2.11	0.50
1:B:48:LEU:O	1:B:52:LEU:HD12	2.12	0.50
1:E:27:VAL:HG13	1:H:0:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ASP:OD1	1:G:68:GLN:HB2	2.12	0.50
1:B:80:ILE:O	1:B:84:VAL:HG12	2.12	0.50
1:F:66:ASP:OD1	1:F:68:GLN:HB2	2.12	0.49
1:F:8:THR:HG21	1:F:84:VAL:HG11	1.94	0.49
1:A:8:THR:HG21	1:A:84:VAL:HG11	1.94	0.49
1:E:256:LYS:HE2	1:G:255:ILE:O	2.12	0.49
1:H:66:ASP:OD1	1:H:68:GLN:HB2	2.12	0.49
1:A:66:ASP:OD1	1:A:68:GLN:HB2	2.12	0.49
1:B:66:ASP:OD1	1:B:68:GLN:HB2	2.12	0.49
1:C:66:ASP:OD1	1:C:68:GLN:HB2	2.12	0.49
1:G:8:THR:HG21	1:G:84:VAL:HG11	1.95	0.49
1:C:173:TYR:CZ	1:D:153:ALA:HA	2.48	0.48
1:B:3:ASN:HB2	1:E:3:ASN:ND2	2.28	0.48
1:G:47:GLU:O	1:G:51:LEU:HD13	2.14	0.47
1:B:-1:MET:H	1:C:30:GLN:HE22	1.62	0.47
1:C:8:THR:HG21	1:C:84:VAL:HG11	1.96	0.47
1:D:52:LEU:HD11	1:D:62:LEU:HD11	1.96	0.47
1:E:101:ASP:OD2	1:E:113:GLY:HA3	2.15	0.47
1:C:217:LEU:HB2	1:C:250:SER:HB3	1.97	0.46
1:E:66:ASP:OD1	1:E:68:GLN:HB2	2.15	0.46
1:F:217:LEU:HB2	1:F:250:SER:HB3	1.98	0.46
1:H:101:ASP:OD2	1:H:113:GLY:HA3	2.16	0.46
1:A:217:LEU:HB2	1:A:250:SER:HB3	1.97	0.46
1:D:62:LEU:N	1:D:62:LEU:HD12	2.31	0.46
1:D:101:ASP:OD2	1:D:113:GLY:HA3	2.16	0.46
2:E:301:NDP:C2N	3:E:302:N5H:O38	2.63	0.46
1:G:153:ALA:HA	1:H:173:TYR:CZ	2.50	0.46
1:A:47:GLU:O	1:A:51:LEU:HD13	2.16	0.46
1:G:101:ASP:OD2	1:G:113:GLY:HA3	2.17	0.45
1:D:217:LEU:HB2	1:D:250:SER:HB3	1.98	0.45
1:G:133:LYS:CE	1:H:105:ARG:HH12	2.27	0.45
1:D:47:GLU:O	1:D:51:LEU:HG	2.16	0.45
1:F:47:GLU:O	1:F:51:LEU:HD13	2.16	0.45
1:D:65:ILE:CD1	1:D:76:GLY:HA3	2.46	0.45
1:H:217:LEU:HB2	1:H:250:SER:HB3	1.99	0.45
1:C:84:VAL:HG12	1:C:84:VAL:O	2.17	0.45
1:A:101:ASP:OD2	1:A:113:GLY:HA3	2.17	0.45
1:G:62:LEU:N	1:G:62:LEU:HD12	2.32	0.44
1:B:217:LEU:HB2	1:B:250:SER:HB3	2.00	0.44
1:C:101:ASP:OD2	1:C:113:GLY:HA3	2.17	0.44
1:E:8:THR:HG21	1:E:84:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:VAL:HG12	1:G:84:VAL:O	2.18	0.44
1:G:197:SER:HB2	2:G:301:NDP:O1A	2.17	0.44
1:G:217:LEU:HB2	1:G:250:SER:HB3	2.00	0.44
1:F:197:SER:OG	3:F:302:N5H:N28	2.50	0.43
1:C:-1:MET:HE1	1:H:32:GLY:HA2	2.00	0.43
1:H:84:VAL:HG12	1:H:84:VAL:O	2.18	0.43
1:E:217:LEU:HB2	1:E:250:SER:HB3	1.99	0.43
1:E:11:ILE:HD11	1:E:28:LEU:HD12	2.00	0.43
1:A:84:VAL:O	1:A:84:VAL:HG12	2.18	0.43
1:C:11:ILE:HD11	1:C:28:LEU:HD12	2.00	0.43
1:D:61:HIS:C	1:D:62:LEU:HD12	2.39	0.43
1:C:184:ARG:HD2	1:C:241:VAL:O	2.19	0.42
1:B:210:GLU:OE2	1:B:214:ARG:NH2	2.52	0.42
1:F:34:LYS:NZ	1:F:84:VAL:CG1	2.74	0.42
1:H:52:LEU:HD11	1:H:62:LEU:HD11	2.01	0.42
1:E:84:VAL:O	1:E:84:VAL:HG12	2.20	0.41
1:F:84:VAL:HG12	1:F:84:VAL:O	2.19	0.41
1:F:11:ILE:HD11	1:F:28:LEU:HD12	2.02	0.41
1:G:184:ARG:HD2	1:G:241:VAL:O	2.20	0.41
1:H:184:ARG:HD2	1:H:241:VAL:O	2.21	0.41
1:A:11:ILE:HD11	1:A:28:LEU:HD12	2.02	0.41
1:A:184:ARG:HD2	1:A:241:VAL:O	2.21	0.41
1:D:184:ARG:HD2	1:D:241:VAL:O	2.20	0.41
1:D:198:ALA:O	1:D:201:VAL:HG22	2.20	0.41
1:B:-2:HIS:HD2	1:C:30:GLN:HG3	1.86	0.41
1:B:184:ARG:HD2	1:B:241:VAL:O	2.20	0.41
1:E:198:ALA:O	1:E:201:VAL:HG22	2.21	0.41
1:E:197:SER:OG	3:E:302:N5H:C27	2.69	0.41
1:E:173:TYR:CZ	1:F:153:ALA:HA	2.56	0.40
1:E:184:ARG:HD2	1:E:241:VAL:O	2.21	0.40
1:F:184:ARG:HD2	1:F:241:VAL:O	2.21	0.40
1:H:198:ALA:O	1:H:201:VAL:HG22	2.21	0.40
1:C:15:ALA:HB2	2:C:301:NDP:O3B	2.20	0.40
1:E:190:ALA:HB3	2:E:301:NDP:C5N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:SER:OG	1:F:5:GLU:OE2[2_555]	2.15	0.05

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	258/261 (99%)	247 (96%)	11 (4%)	0	100	100
1	B	258/261 (99%)	247 (96%)	11 (4%)	0	100	100
1	C	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	D	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
1	E	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
1	F	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
1	G	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	34	46
1	H	256/261 (98%)	247 (96%)	9 (4%)	0	100	100
All	All	2054/2088 (98%)	1976 (96%)	77 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	-1	MET

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	213/213 (100%)	210 (99%)	3 (1%)	67	79
1	B	213/213 (100%)	212 (100%)	1 (0%)	88	93
1	C	212/213 (100%)	209 (99%)	3 (1%)	67	79
1	D	211/213 (99%)	210 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	211/213 (99%)	210 (100%)	1 (0%)	88	93
1	F	211/213 (99%)	210 (100%)	1 (0%)	88	93
1	G	212/213 (100%)	211 (100%)	1 (0%)	88	93
1	H	211/213 (99%)	210 (100%)	1 (0%)	88	93
All	All	1694/1704 (99%)	1682 (99%)	12 (1%)	84	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	MET
1	A	189	SER
1	A	197	SER
1	B	189	SER
1	C	30	GLN
1	C	189	SER
1	C	209	LYS
1	D	189	SER
1	E	197	SER
1	F	197	SER
1	G	189	SER
1	H	189	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

16 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	$\#\|Z\| > 2$
3	N5H	B	302	-	38,38,38	1.94	6 (15%)	42,48,48	1.75	8 (19%)
3	N5H	D	302	-	38,38,38	1.81	8 (21%)	42,48,48	1.85	11 (26%)
3	N5H	F	302	-	38,38,38	1.83	8 (21%)	42,48,48	1.73	10 (23%)
2	NDP	E	301	-	45,52,52	1.46	7 (15%)	53,80,80	1.43	8 (15%)
2	NDP	H	301	-	45,52,52	1.33	5 (11%)	53,80,80	1.48	9 (16%)
3	N5H	A	302	-	38,38,38	1.93	6 (15%)	42,48,48	2.12	14 (33%)
3	N5H	G	302	-	38,38,38	1.79	5 (13%)	42,48,48	1.72	8 (19%)
2	NDP	A	301	-	45,52,52	1.37	5 (11%)	53,80,80	1.27	7 (13%)
3	N5H	E	302	-	38,38,38	2.06	8 (21%)	42,48,48	1.57	8 (19%)
2	NDP	C	301	-	45,52,52	1.43	3 (6%)	53,80,80	1.38	9 (16%)
2	NDP	D	301	-	45,52,52	1.36	3 (6%)	53,80,80	1.48	6 (11%)
2	NDP	G	301	-	45,52,52	1.32	4 (8%)	53,80,80	1.48	11 (20%)
3	N5H	H	302	-	38,38,38	1.89	5 (13%)	42,48,48	1.67	8 (19%)
2	NDP	B	301	-	45,52,52	1.40	5 (11%)	53,80,80	1.42	7 (13%)
3	N5H	C	302	-	38,38,38	1.87	6 (15%)	42,48,48	1.98	11 (26%)
2	NDP	F	301	-	45,52,52	1.30	3 (6%)	53,80,80	1.61	10 (18%)

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
3	N5H	B	302	-	-	3/47/47/47	-
3	N5H	D	302	-	-	6/47/47/47	-
3	N5H	F	302	-	-	6/47/47/47	-
2	NDP	E	301	-	-	9/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	H	301	-	-	6/30/77/77	0/5/5/5
3	N5H	A	302	-	-	12/47/47/47	-
3	N5H	G	302	-	-	12/47/47/47	-
2	NDP	A	301	-	-	6/30/77/77	0/5/5/5
3	N5H	E	302	-	-	2/47/47/47	-
2	NDP	C	301	-	-	5/30/77/77	0/5/5/5
2	NDP	D	301	-	-	11/30/77/77	0/5/5/5
2	NDP	G	301	-	-	5/30/77/77	0/5/5/5
3	N5H	H	302	-	-	4/47/47/47	-
2	NDP	B	301	-	-	8/30/77/77	0/5/5/5
3	N5H	C	302	-	-	14/47/47/47	-
2	NDP	F	301	-	-	4/30/77/77	0/5/5/5

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	N5H	C27-N28	7.01	1.46	1.33
3	H	302	N5H	C27-N28	6.97	1.46	1.33
3	B	302	N5H	C27-N28	6.87	1.46	1.33
3	A	302	N5H	C27-N28	6.74	1.46	1.33
3	D	302	N5H	C27-N28	6.34	1.45	1.33
3	C	302	N5H	C20-N19	6.21	1.47	1.33
3	C	302	N5H	C27-N28	6.11	1.44	1.33
3	F	302	N5H	C27-N28	6.07	1.44	1.33
3	H	302	N5H	C20-N19	6.07	1.46	1.33
3	G	302	N5H	C27-N28	5.98	1.44	1.33
3	E	302	N5H	C20-N19	5.82	1.46	1.33
2	C	301	NDP	C4N-C3N	-5.82	1.38	1.49
3	B	302	N5H	C20-N19	5.64	1.45	1.33
3	F	302	N5H	C20-N19	5.51	1.45	1.33
3	G	302	N5H	C20-N19	5.37	1.45	1.33
2	D	301	NDP	C4N-C3N	-5.26	1.39	1.49
2	E	301	NDP	C4N-C3N	-5.22	1.39	1.49
2	F	301	NDP	C4N-C3N	-5.19	1.39	1.49
3	A	302	N5H	C20-N19	5.14	1.44	1.33
2	A	301	NDP	C4N-C3N	-5.11	1.39	1.49
2	B	301	NDP	C4N-C3N	-5.11	1.39	1.49
2	G	301	NDP	C4N-C3N	-5.05	1.40	1.49
2	H	301	NDP	C4N-C3N	-4.71	1.40	1.49
3	E	302	N5H	O26-C24	-4.59	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NDP	C4N-C5N	-4.56	1.37	1.48
3	D	302	N5H	C20-N19	4.37	1.43	1.33
2	B	301	NDP	C4N-C5N	-4.15	1.38	1.48
3	G	302	N5H	O26-C24	-3.96	1.40	1.46
2	F	301	NDP	C4N-C5N	-3.86	1.38	1.48
2	H	301	NDP	C4N-C5N	-3.81	1.38	1.48
2	A	301	NDP	C4N-C5N	-3.80	1.39	1.48
3	B	302	N5H	O26-C24	-3.78	1.40	1.46
2	G	301	NDP	C4N-C5N	-3.77	1.39	1.48
3	A	302	N5H	O26-C24	-3.75	1.40	1.46
2	E	301	NDP	C4N-C5N	-3.74	1.39	1.48
2	D	301	NDP	C4N-C5N	-3.73	1.39	1.48
3	D	302	N5H	O26-C24	-3.71	1.40	1.46
2	D	301	NDP	C6N-C5N	3.71	1.40	1.33
3	E	302	N5H	C15-C13	3.47	1.56	1.51
2	B	301	NDP	C6N-C5N	3.36	1.39	1.33
2	A	301	NDP	C6N-C5N	3.30	1.39	1.33
3	H	302	N5H	C07-C06	3.29	1.53	1.44
3	B	302	N5H	C07-C06	3.26	1.53	1.44
3	F	302	N5H	O26-C24	-3.24	1.41	1.46
3	A	302	N5H	C07-C06	3.22	1.53	1.44
3	H	302	N5H	O26-C24	-3.19	1.41	1.46
3	C	302	N5H	O26-C24	-3.16	1.41	1.46
2	E	301	NDP	C6N-C5N	3.13	1.38	1.33
3	E	302	N5H	C07-C06	3.09	1.53	1.44
3	C	302	N5H	C07-C06	3.03	1.52	1.44
2	G	301	NDP	C6N-C5N	2.98	1.38	1.33
3	G	302	N5H	C07-C06	2.84	1.52	1.44
2	C	301	NDP	C6N-C5N	2.82	1.38	1.33
3	F	302	N5H	O21-C20	-2.82	1.17	1.23
3	A	302	N5H	O29-C27	-2.81	1.18	1.21
2	H	301	NDP	C6N-C5N	2.78	1.38	1.33
3	B	302	N5H	C15-C13	2.75	1.55	1.51
3	F	302	N5H	C07-C06	2.74	1.52	1.44
3	D	302	N5H	C07-C06	2.69	1.52	1.44
3	F	302	N5H	C36-C37	2.68	1.55	1.47
3	E	302	N5H	C36-C37	2.60	1.54	1.47
3	D	302	N5H	O21-C20	-2.55	1.18	1.23
2	F	301	NDP	C6N-C5N	2.55	1.37	1.33
3	C	302	N5H	O26-C27	2.52	1.41	1.35
3	F	302	N5H	O29-C27	-2.49	1.18	1.21
3	H	302	N5H	O21-C20	-2.45	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	N5H	O29-C27	-2.44	1.18	1.21
3	G	302	N5H	O21-C20	-2.39	1.18	1.23
3	A	302	N5H	C15-C13	2.32	1.54	1.51
2	E	301	NDP	O4B-C1B	2.32	1.44	1.41
2	H	301	NDP	C2N-C3N	2.30	1.41	1.34
3	D	302	N5H	O26-C27	2.24	1.40	1.35
3	F	302	N5H	C15-C13	2.21	1.54	1.51
2	G	301	NDP	C2N-C3N	2.20	1.41	1.34
3	D	302	N5H	C15-C13	2.19	1.54	1.51
2	E	301	NDP	P2B-O2B	2.16	1.63	1.59
2	E	301	NDP	C2N-C3N	2.16	1.41	1.34
2	A	301	NDP	C5A-C4A	2.14	1.46	1.40
3	B	302	N5H	O29-C27	-2.13	1.19	1.21
2	B	301	NDP	C5A-C4A	2.08	1.46	1.40
2	B	301	NDP	C2A-N3A	2.08	1.35	1.32
3	E	302	N5H	O26-C27	2.07	1.40	1.35
3	C	302	N5H	C36-C37	2.05	1.53	1.47
2	E	301	NDP	C7N-C3N	2.04	1.53	1.48
2	A	301	NDP	C2A-N3A	2.03	1.35	1.32
3	E	302	N5H	O38-C37	-2.01	1.25	1.30
2	H	301	NDP	C5A-C4A	2.01	1.46	1.40

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	N5H	O26-C27-N28	6.97	121.42	110.58
3	C	302	N5H	O26-C27-N28	6.19	120.21	110.58
3	D	302	N5H	C09-C08-C07	-5.93	117.76	125.41
3	A	302	N5H	O26-C27-O29	-5.23	118.40	123.69
3	E	302	N5H	C09-C08-C07	-5.23	118.66	125.41
3	B	302	N5H	O26-C27-N28	5.19	118.65	110.58
3	D	302	N5H	O26-C27-N28	4.79	118.03	110.58
3	G	302	N5H	C09-C08-C07	-4.76	119.27	125.41
3	F	302	N5H	O26-C27-N28	4.62	117.76	110.58
3	C	302	N5H	O29-C27-N28	-4.55	118.00	125.51
3	B	302	N5H	C09-C08-C07	-4.41	119.71	125.41
2	D	301	NDP	O5B-C5B-C4B	-4.40	93.85	108.99
2	D	301	NDP	N3A-C2A-N1A	-4.15	122.19	128.68
3	C	302	N5H	C03-C04-C05	-4.03	103.89	112.59
3	F	302	N5H	C09-C08-C07	-4.00	120.25	125.41
3	B	302	N5H	O26-C27-O29	-3.99	119.66	123.69
3	D	302	N5H	O29-C27-N28	-3.98	118.95	125.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	302	N5H	C03-C04-C05	-3.94	104.08	112.59
2	F	301	NDP	N3A-C2A-N1A	-3.89	122.60	128.68
2	G	301	NDP	N3A-C2A-N1A	-3.80	122.74	128.68
2	B	301	NDP	N3A-C2A-N1A	-3.74	122.83	128.68
3	H	302	N5H	C09-C08-C07	-3.72	120.61	125.41
3	G	302	N5H	O26-C27-N28	3.72	116.36	110.58
3	F	302	N5H	C03-C04-C05	-3.66	104.68	112.59
2	E	301	NDP	O2B-P2B-O1X	-3.66	95.26	109.39
2	A	301	NDP	N3A-C2A-N1A	-3.64	122.99	128.68
2	H	301	NDP	N3A-C2A-N1A	-3.62	123.02	128.68
2	G	301	NDP	O2B-P2B-O1X	-3.59	95.52	109.39
3	A	302	N5H	C09-C08-C07	-3.53	120.85	125.41
2	E	301	NDP	N3A-C2A-N1A	-3.49	123.22	128.68
2	F	301	NDP	C3N-C2N-N1N	-3.48	118.14	123.10
3	A	302	N5H	C22-C20-N19	3.47	121.64	116.44
2	F	301	NDP	C1B-N9A-C4A	-3.34	120.77	126.64
2	E	301	NDP	C1B-N9A-C4A	-3.33	120.78	126.64
3	H	302	N5H	C23-C22-C24	-3.30	108.29	111.79
2	C	301	NDP	N3A-C2A-N1A	-3.29	123.54	128.68
2	C	301	NDP	O2N-PN-O1N	3.25	128.32	112.24
3	E	302	N5H	C03-C04-C05	-3.25	105.57	112.59
3	F	302	N5H	O29-C27-N28	-3.25	120.15	125.51
3	H	302	N5H	O26-C27-N28	3.24	115.62	110.58
3	A	302	N5H	O29-C27-N28	-3.23	120.18	125.51
3	E	302	N5H	O38-C37-O39	-3.21	116.01	122.67
3	H	302	N5H	O26-C27-O29	-3.18	120.48	123.69
3	B	302	N5H	C03-C04-C05	-3.16	105.77	112.59
3	G	302	N5H	O38-C37-C36	3.14	123.26	113.50
3	C	302	N5H	C09-C08-C07	-3.14	121.36	125.41
2	H	301	NDP	O5B-C5B-C4B	-3.07	98.43	108.99
2	G	301	NDP	O5B-C5B-C4B	-3.05	98.48	108.99
3	H	302	N5H	C03-C04-C05	-3.05	106.00	112.59
3	F	302	N5H	O38-C37-C36	3.05	122.96	113.50
2	F	301	NDP	O5B-C5B-C4B	-3.05	98.50	108.99
2	F	301	NDP	O3X-P2B-O2X	3.03	119.22	107.64
3	D	302	N5H	C03-C04-C05	-3.02	106.07	112.59
3	A	302	N5H	O38-C37-C36	3.01	122.83	113.50
2	F	301	NDP	O2N-PN-O1N	2.98	126.97	112.24
3	H	302	N5H	C22-C20-N19	2.96	120.88	116.44
3	C	302	N5H	C09-C10-C12	2.96	114.70	110.80
3	A	302	N5H	C23-C22-C24	-2.95	108.67	111.79
3	G	302	N5H	C31-C30-C02	-2.92	108.97	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	NDP	O2N-PN-O1N	2.92	126.65	112.24
3	G	302	N5H	C22-C20-N19	2.86	120.72	116.44
3	E	302	N5H	O26-C27-N28	2.85	115.01	110.58
2	A	301	NDP	O2B-P2B-O1X	-2.84	98.44	109.39
3	C	302	N5H	C10-C12-C13	-2.82	109.57	115.94
3	H	302	N5H	O38-C37-C36	2.81	122.22	113.50
2	D	301	NDP	C1B-N9A-C4A	-2.80	121.73	126.64
2	B	301	NDP	O5B-C5B-C4B	-2.79	99.37	108.99
3	C	302	N5H	C15-C13-C12	2.79	119.21	116.48
2	H	301	NDP	O4D-C1D-N1N	2.78	113.49	108.06
3	F	302	N5H	C22-C20-N19	2.71	120.49	116.44
2	E	301	NDP	O3X-P2B-O1X	2.70	121.24	110.68
3	A	302	N5H	O21-C20-N19	-2.68	117.24	122.99
3	A	302	N5H	C35-C34-C33	2.67	121.84	115.27
2	D	301	NDP	O2N-PN-O1N	2.63	125.26	112.24
2	C	301	NDP	O4B-C1B-C2B	-2.63	102.03	106.59
3	A	302	N5H	C03-C04-C05	-2.62	106.93	112.59
3	F	302	N5H	C09-C10-C12	-2.61	107.35	110.80
2	F	301	NDP	PN-O3-PA	-2.61	123.89	132.83
3	B	302	N5H	O38-C37-C36	2.59	121.54	113.50
2	B	301	NDP	O3X-P2B-O2B	-2.57	94.49	105.99
3	C	302	N5H	O21-C20-C22	-2.56	116.40	121.02
2	B	301	NDP	O3X-P2B-O2X	2.55	117.38	107.64
3	A	302	N5H	O26-C24-C22	2.55	111.33	106.40
2	G	301	NDP	C4A-C5A-N7A	-2.54	106.75	109.40
2	E	301	NDP	O2A-PA-O1A	2.54	124.80	112.24
2	A	301	NDP	C4A-C5A-N7A	-2.51	106.78	109.40
2	C	301	NDP	O5B-C5B-C4B	-2.51	100.36	108.99
2	H	301	NDP	C3N-C2N-N1N	-2.50	119.52	123.10
2	B	301	NDP	C3D-C2D-C1D	-2.50	96.67	101.43
3	E	302	N5H	C15-C13-C12	2.50	118.93	116.48
3	E	302	N5H	O38-C37-C36	2.50	121.26	113.50
2	D	301	NDP	O7N-C7N-C3N	-2.49	116.20	120.90
3	E	302	N5H	O14-C13-C12	-2.47	118.03	121.55
3	D	302	N5H	C15-C13-C12	2.46	118.89	116.48
2	F	301	NDP	C2A-N1A-C6A	2.46	122.96	118.75
2	C	301	NDP	PN-O3-PA	-2.46	124.40	132.83
2	E	301	NDP	O5D-C5D-C4D	2.43	117.34	108.99
2	D	301	NDP	C3N-C2N-N1N	-2.42	119.64	123.10
3	G	302	N5H	O29-C27-N28	-2.42	121.51	125.51
2	A	301	NDP	C1B-N9A-C4A	-2.37	122.47	126.64
2	H	301	NDP	O4B-C4B-C3B	2.37	109.81	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	N5H	C31-C30-C02	-2.36	110.45	116.69
2	F	301	NDP	O4B-C4B-C3B	2.36	109.79	105.11
2	E	301	NDP	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	301	NDP	C3N-C7N-N7N	2.36	121.85	117.67
3	A	302	N5H	O39-C37-C36	-2.35	116.41	123.89
3	B	302	N5H	C15-C13-C12	2.35	118.78	116.48
2	H	301	NDP	C1D-N1N-C6N	-2.32	115.84	120.83
3	B	302	N5H	O29-C27-N28	-2.31	121.69	125.51
3	C	302	N5H	O38-C37-C36	2.30	120.64	113.50
3	C	302	N5H	C22-C20-N19	2.29	119.87	116.44
2	G	301	NDP	C3B-C2B-C1B	-2.28	98.60	102.89
2	A	301	NDP	O2X-P2B-O1X	2.28	119.59	110.68
2	H	301	NDP	C2A-N1A-C6A	2.26	122.62	118.75
2	G	301	NDP	O2X-P2B-O1X	2.25	119.48	110.68
3	H	302	N5H	O39-C37-C36	-2.25	116.75	123.89
3	D	302	N5H	O38-C37-C36	2.25	120.47	113.50
3	F	302	N5H	C07-C06-C05	-2.24	112.61	125.51
3	E	302	N5H	O29-C27-N28	-2.22	121.84	125.51
2	B	301	NDP	C3N-C2N-N1N	-2.22	119.93	123.10
2	F	301	NDP	O5D-PN-O1N	-2.20	100.47	109.07
2	G	301	NDP	C5B-C4B-C3B	-2.18	107.01	115.18
2	A	301	NDP	O4B-C1B-C2B	-2.16	102.84	106.59
3	B	302	N5H	C03-C02-C30	2.16	122.73	115.88
3	D	302	N5H	C31-C30-C02	-2.15	111.01	116.69
3	D	302	N5H	O26-C24-C25	2.15	112.48	108.21
2	A	301	NDP	O4D-C1D-N1N	2.13	112.22	108.06
3	A	302	N5H	C34-C36-C37	-2.12	123.11	127.11
2	C	301	NDP	C4A-C5A-N7A	-2.12	107.19	109.40
2	G	301	NDP	C2A-N1A-C6A	2.10	122.34	118.75
3	F	302	N5H	O39-C37-C36	-2.10	117.23	123.89
2	G	301	NDP	O2N-PN-O1N	2.09	122.58	112.24
2	H	301	NDP	N6A-C6A-N1A	2.09	122.92	118.57
2	G	301	NDP	C3N-C2N-N1N	-2.09	120.11	123.10
2	C	301	NDP	O2X-P2B-O2B	-2.08	96.65	105.99
2	H	301	NDP	C1B-N9A-C4A	-2.08	122.99	126.64
3	D	302	N5H	C07-C06-C05	-2.08	113.57	125.51
2	C	301	NDP	C3N-C2N-N1N	-2.07	120.14	123.10
3	D	302	N5H	C22-C20-N19	2.05	119.52	116.44
3	G	302	N5H	O21-C20-N19	-2.04	118.62	122.99
2	C	301	NDP	O2B-P2B-O1X	-2.03	101.55	109.39
3	D	302	N5H	C03-C02-C30	2.02	122.28	115.88
3	F	302	N5H	C31-C30-C02	-2.02	111.37	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	NDP	C1B-N9A-C4A	-2.01	123.11	126.64
3	A	302	N5H	C03-C02-C30	2.00	122.23	115.88

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NDP	C2B-O2B-P2B-O2X
2	B	301	NDP	C5D-O5D-PN-O2N
2	D	301	NDP	C2B-O2B-P2B-O1X
2	D	301	NDP	C5D-O5D-PN-O2N
2	E	301	NDP	O4B-C4B-C5B-O5B
2	E	301	NDP	C3B-C4B-C5B-O5B
2	E	301	NDP	C5D-O5D-PN-O1N
2	E	301	NDP	C5D-O5D-PN-O2N
2	H	301	NDP	C2B-O2B-P2B-O1X
3	A	302	N5H	C08-C09-C10-C11
3	A	302	N5H	C08-C09-C10-C12
3	A	302	N5H	C11-C10-C12-C13
3	A	302	N5H	C13-C15-C16-C18
3	A	302	N5H	C02-C30-C31-C32
3	A	302	N5H	C34-C36-C37-O38
3	A	302	N5H	C34-C36-C37-O39
3	C	302	N5H	C08-C09-C10-C11
3	C	302	N5H	C08-C09-C10-C12
3	C	302	N5H	C13-C15-C16-O17
3	D	302	N5H	C13-C15-C16-O17
3	D	302	N5H	C13-C15-C16-C18
3	G	302	N5H	C13-C15-C16-C18
3	G	302	N5H	N28-C27-O26-C24
3	G	302	N5H	C02-C30-C31-C32
3	F	302	N5H	C05-C06-C07-C08
3	H	302	N5H	C05-C06-C07-C08
3	C	302	N5H	C34-C36-C37-O38
3	C	302	N5H	C34-C36-C37-O39
3	E	302	N5H	C34-C36-C37-O39
3	H	302	N5H	C34-C36-C37-O38
2	B	301	NDP	O4B-C4B-C5B-O5B
3	D	302	N5H	C05-C06-C07-C08
3	C	302	N5H	C05-C06-C07-C08
3	G	302	N5H	C05-C06-C07-C08
3	D	302	N5H	C34-C36-C37-O38

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Mol	Chain	Res	Type	Atoms
3	D	302	N5H	C34-C36-C37-O39
3	E	302	N5H	C34-C36-C37-O38
3	F	302	N5H	C34-C36-C37-O38
3	F	302	N5H	C34-C36-C37-O39
3	G	302	N5H	C34-C36-C37-O38
3	G	302	N5H	C34-C36-C37-O39
3	H	302	N5H	C34-C36-C37-O39
3	G	302	N5H	O29-C27-O26-C24
3	C	302	N5H	C07-C08-C09-C10
2	D	301	NDP	O4B-C4B-C5B-O5B
2	G	301	NDP	O4D-C4D-C5D-O5D
2	E	301	NDP	C4B-C5B-O5B-PA
2	A	301	NDP	C2B-O2B-P2B-O1X
3	C	302	N5H	C11-C10-C12-C13
3	C	302	N5H	C13-C15-C16-C18
2	B	301	NDP	C5D-O5D-PN-O3
2	D	301	NDP	C2B-O2B-P2B-O2X
2	F	301	NDP	C2B-O2B-P2B-O3X
2	H	301	NDP	C5D-O5D-PN-O3
2	A	301	NDP	O4D-C4D-C5D-O5D
2	G	301	NDP	O4D-C1D-N1N-C6N
2	H	301	NDP	O4D-C1D-N1N-C6N
2	D	301	NDP	C5D-O5D-PN-O1N
2	H	301	NDP	C5D-O5D-PN-O2N
3	B	302	N5H	C09-C10-C12-C13
3	G	302	N5H	C08-C09-C10-C12
2	C	301	NDP	O4D-C1D-N1N-C6N
3	A	302	N5H	C13-C15-C16-O17
3	G	302	N5H	C13-C15-C16-O17
3	B	302	N5H	C34-C36-C37-O38
3	B	302	N5H	C34-C36-C37-O39
2	H	301	NDP	O4B-C4B-C5B-O5B
2	D	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	O4D-C1D-N1N-C6N
2	F	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	PN-O3-PA-O2A
2	D	301	NDP	PA-O3-PN-O2N
2	F	301	NDP	PN-O3-PA-O2A
2	G	301	NDP	PN-O3-PA-O2A
2	H	301	NDP	PA-O3-PN-O2N
2	G	301	NDP	C3D-C4D-C5D-O5D
2	B	301	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	E	301	NDP	O4D-C1D-N1N-C6N
3	A	302	N5H	C15-C16-C18-N19
3	C	302	N5H	C15-C16-C18-N19
3	G	302	N5H	C23-C22-C24-C25
2	B	301	NDP	PN-O3-PA-O1A
2	D	301	NDP	PN-O3-PA-O1A
3	F	302	N5H	C07-C08-C09-C10
3	H	302	N5H	C03-C04-C05-C06
3	A	302	N5H	C02-C03-C04-C05
2	B	301	NDP	C3B-C4B-C5B-O5B
2	C	301	NDP	O4B-C4B-C5B-O5B
2	E	301	NDP	C2D-C1D-N1N-C6N
3	F	302	N5H	C03-C04-C05-C06
3	C	302	N5H	C01-C02-C03-C04
3	D	302	N5H	C03-C04-C05-C06
2	C	301	NDP	C2B-O2B-P2B-O2X
2	D	301	NDP	C5D-O5D-PN-O3
2	E	301	NDP	C5B-O5B-PA-O3
2	E	301	NDP	C5D-O5D-PN-O3
3	G	302	N5H	C23-C22-C24-O26
3	C	302	N5H	C03-C04-C05-C06
2	F	301	NDP	O4B-C4B-C5B-O5B
2	B	301	NDP	PN-O3-PA-O2A
2	B	301	NDP	PA-O3-PN-O1N
2	C	301	NDP	PN-O3-PA-O1A
2	D	301	NDP	PN-O3-PA-O2A
2	D	301	NDP	PA-O3-PN-O1N
3	A	302	N5H	C10-C12-C13-C15
3	C	302	N5H	C10-C12-C13-C15
2	A	301	NDP	C5D-O5D-PN-O1N
3	C	302	N5H	C09-C10-C12-C13
3	F	302	N5H	C09-C10-C12-C13
3	G	302	N5H	C08-C09-C10-C11
2	A	301	NDP	O4B-C4B-C5B-O5B
2	G	301	NDP	O4B-C4B-C5B-O5B
3	A	302	N5H	O29-C27-O26-C24

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	N5H	1	0

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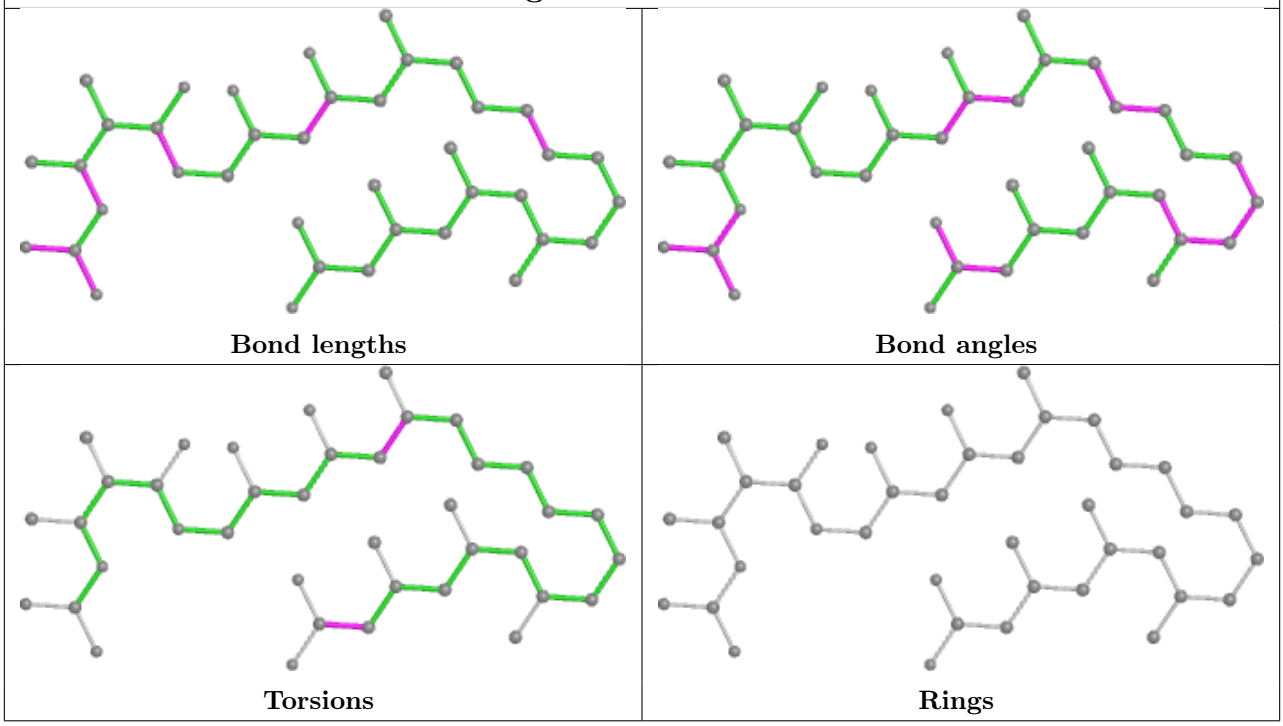
Continued from previous page...

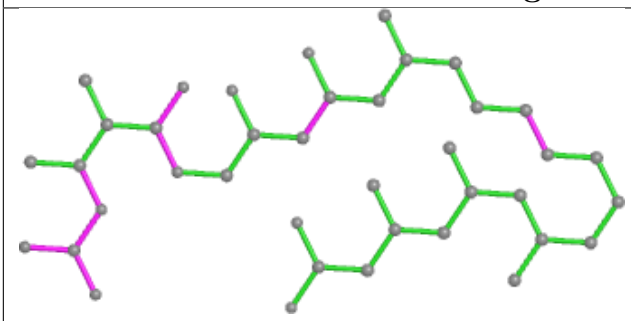
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	N5H	1	0
2	E	301	NDP	3	0
2	H	301	NDP	1	0
2	A	301	NDP	1	0
3	E	302	N5H	4	0
2	C	301	NDP	1	0
2	G	301	NDP	2	0
2	F	301	NDP	1	0

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

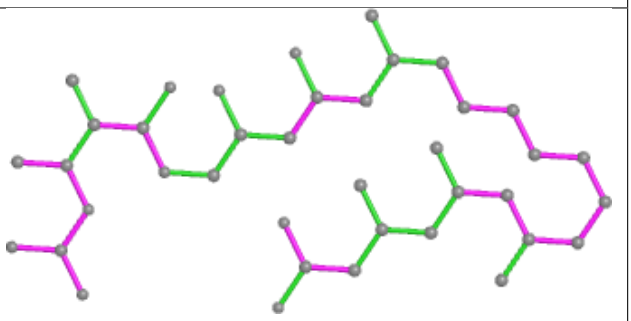
Ligand N5H B 302



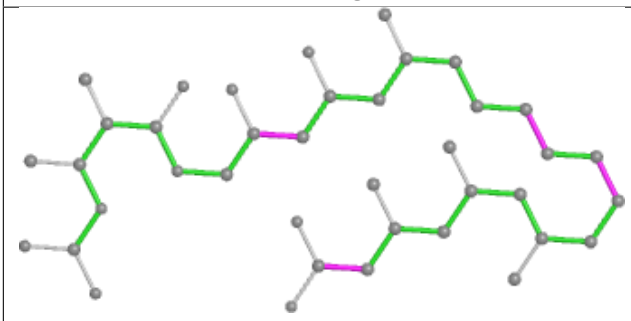
Ligand N5H D 302



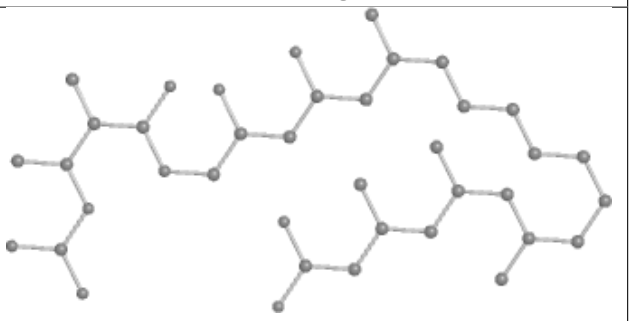
Bond lengths



Bond angles

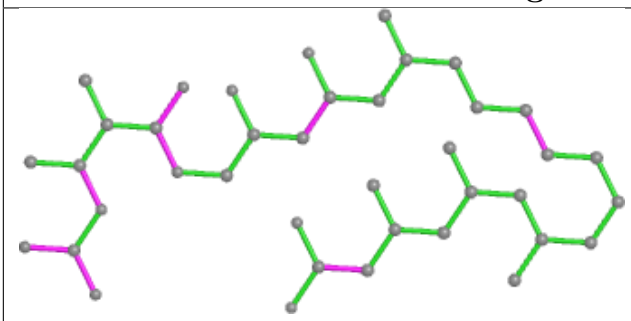


Torsions

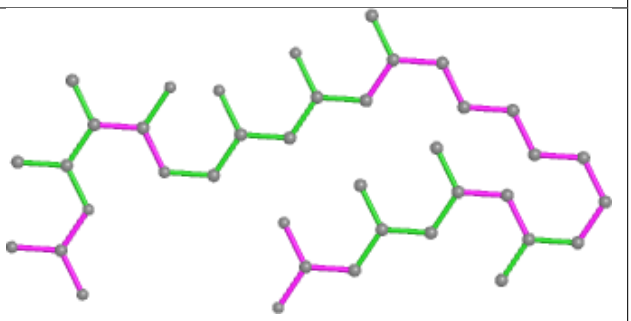


Rings

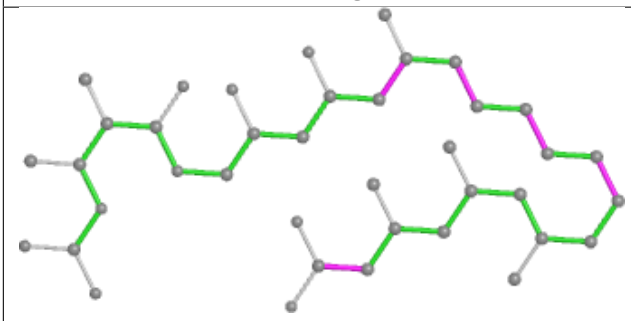
Ligand N5H F 302



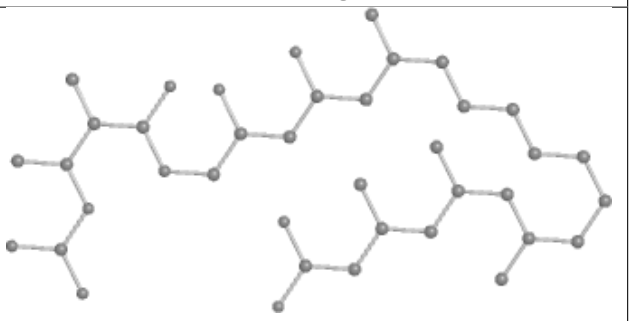
Bond lengths



Bond angles

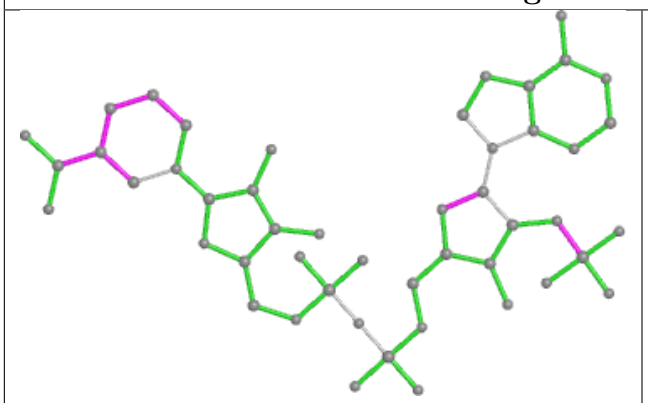


Torsions

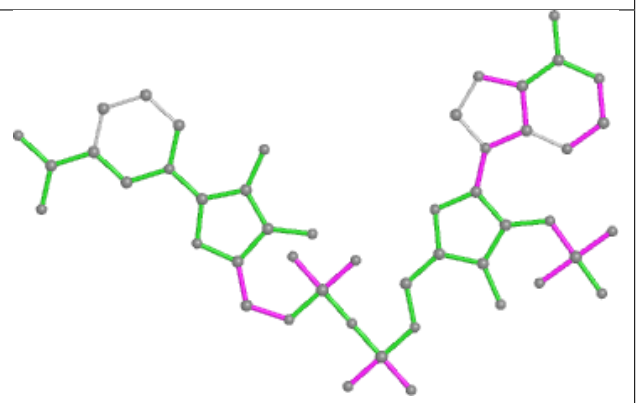


Rings

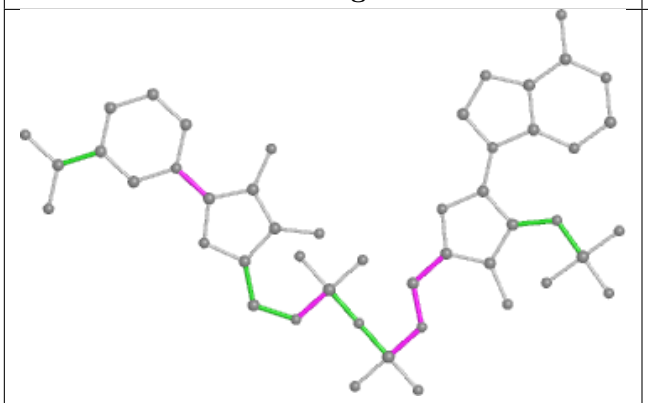
Ligand NDP E 301



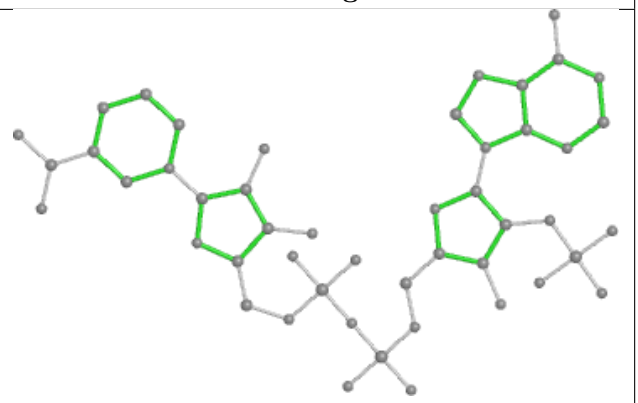
Bond lengths



Bond angles

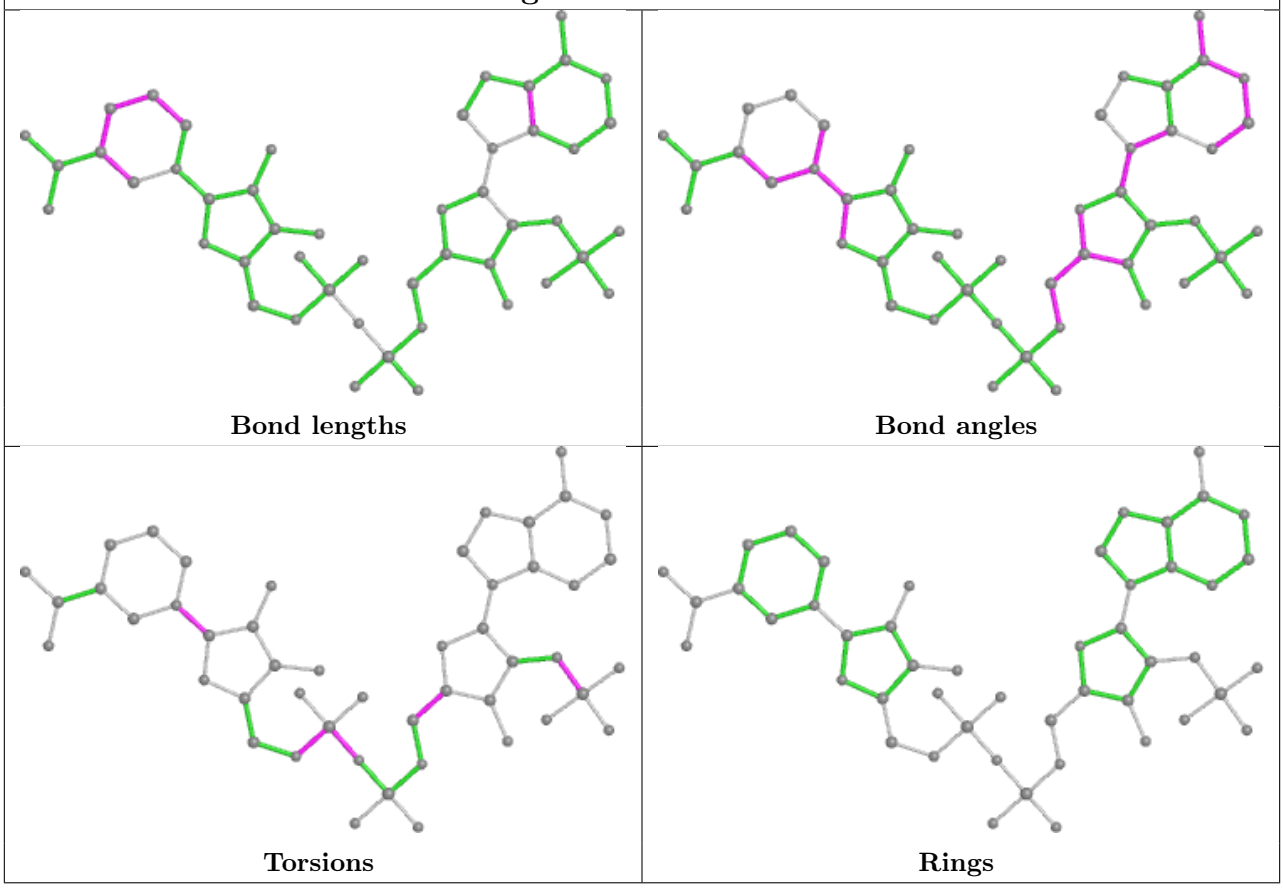


Torsions

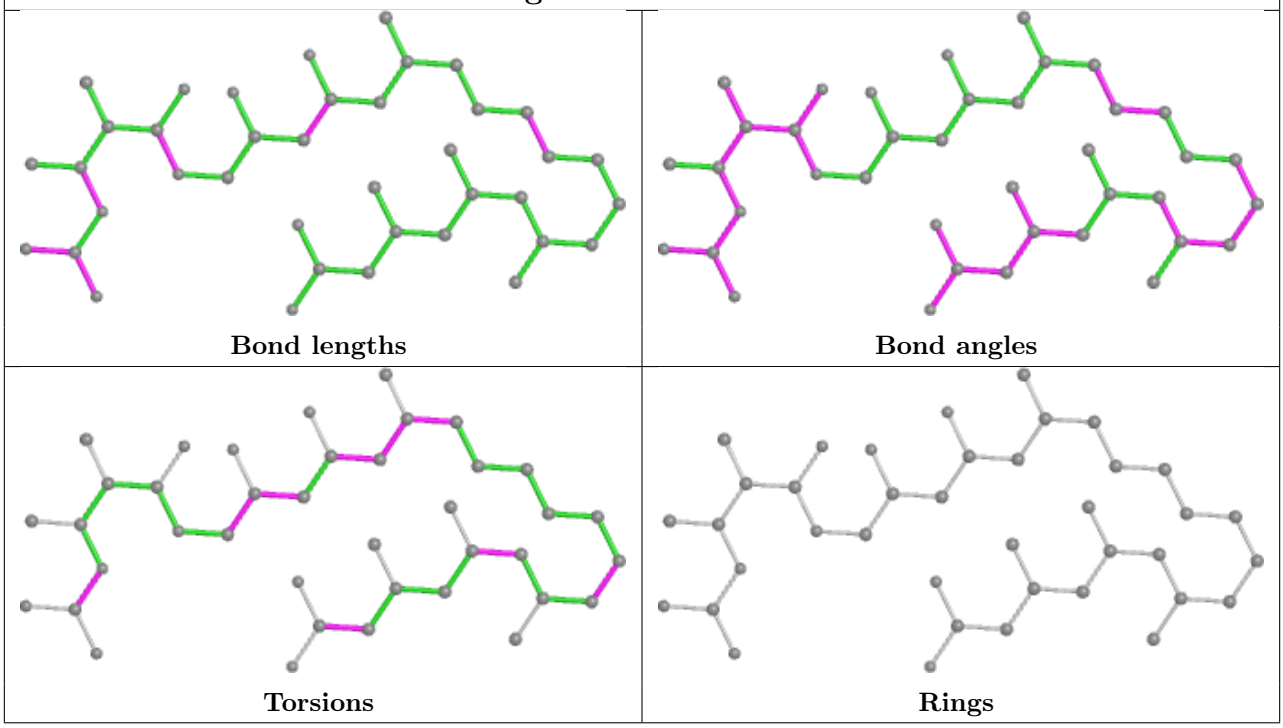


Rings

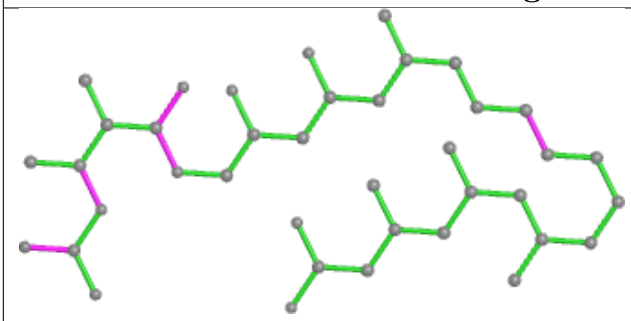
Ligand NDP H 301



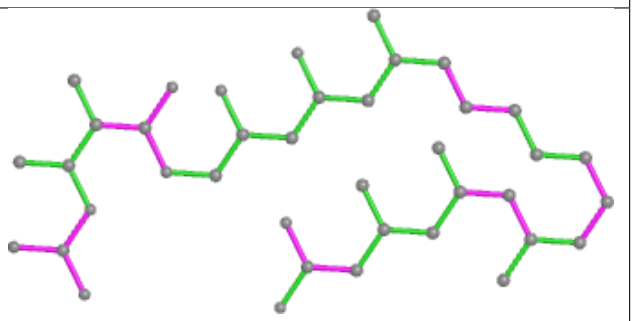
Ligand N5H A 302



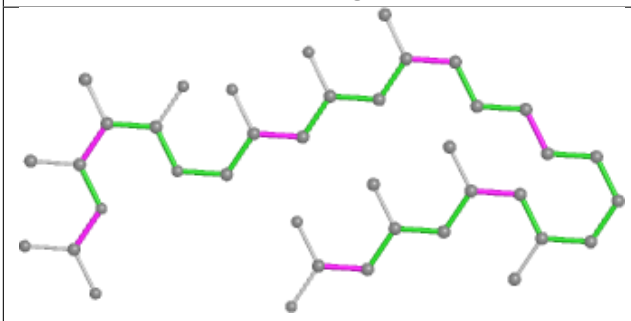
Ligand N5H G 302



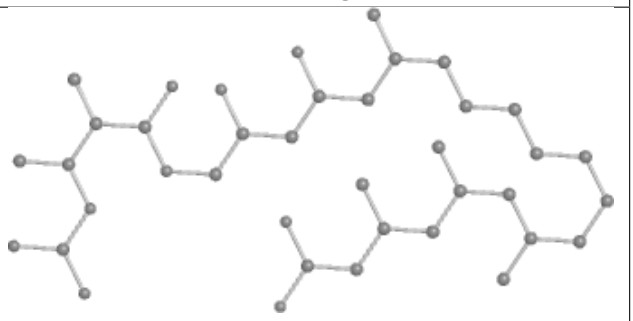
Bond lengths



Bond angles

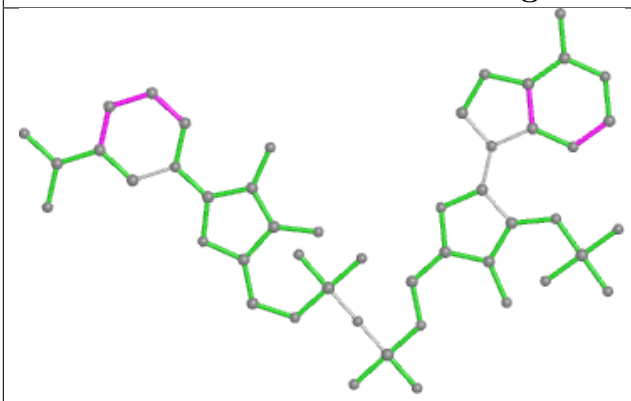


Torsions

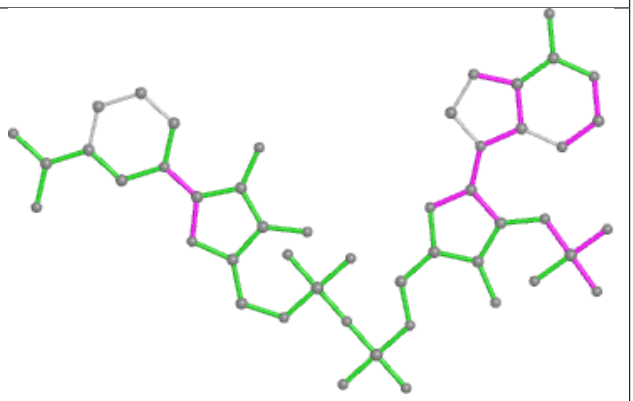


Rings

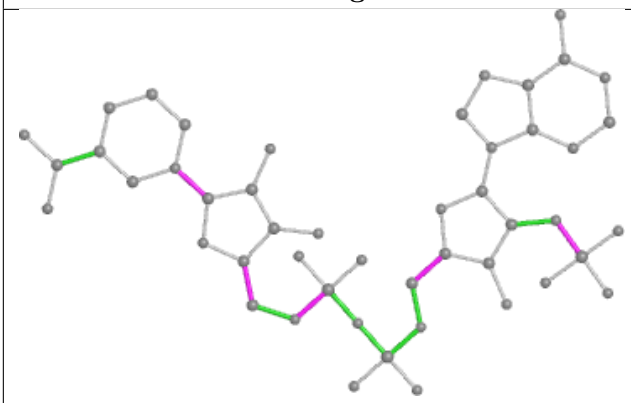
Ligand NDP A 301



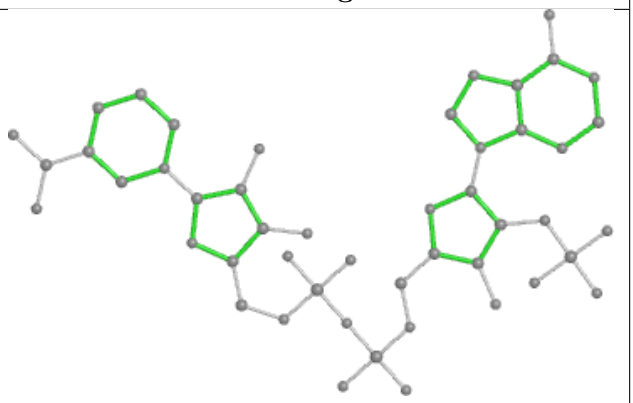
Bond lengths



Bond angles

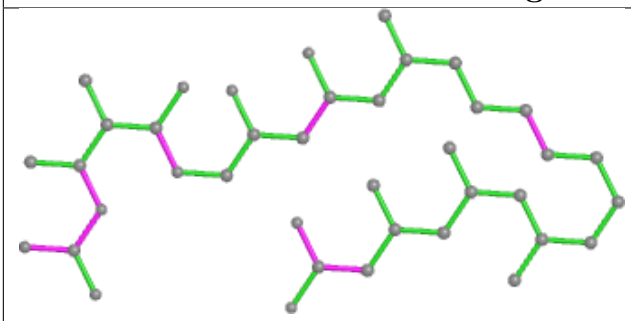


Torsions

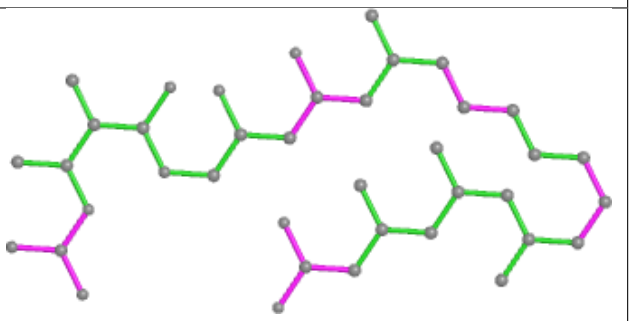


Rings

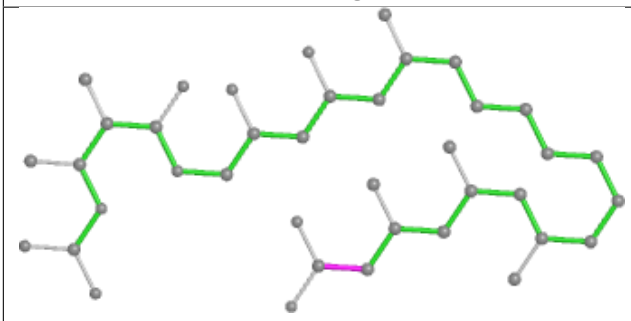
Ligand N5H E 302



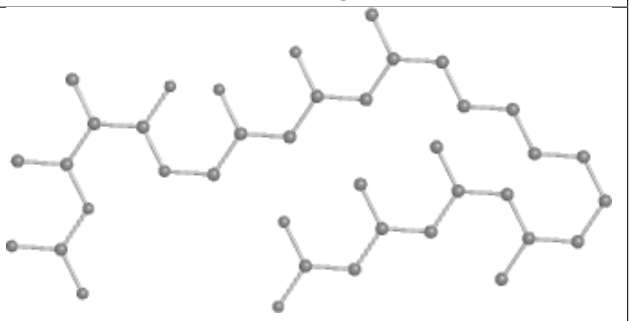
Bond lengths



Bond angles

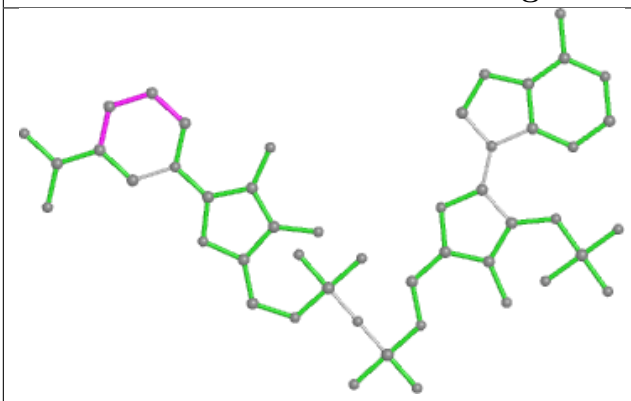


Torsions

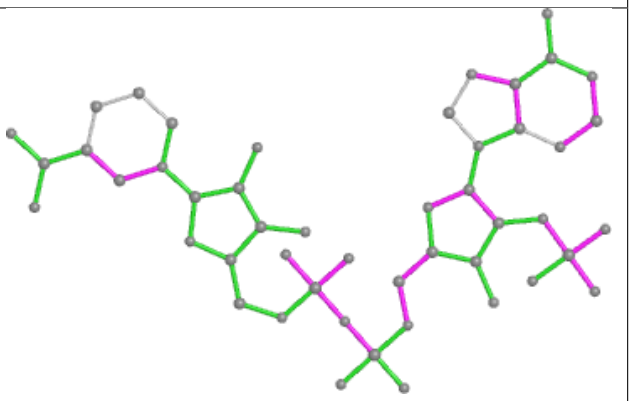


Rings

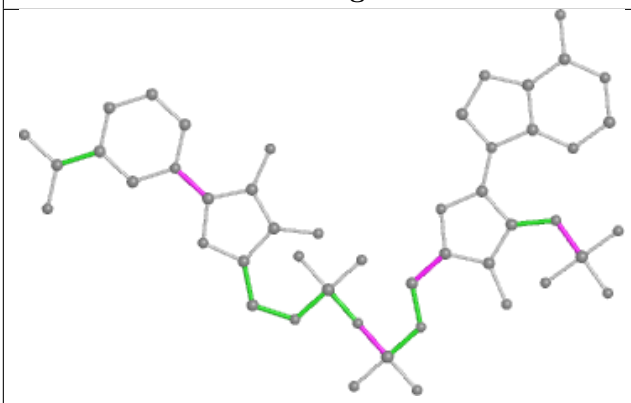
Ligand NDP C 301



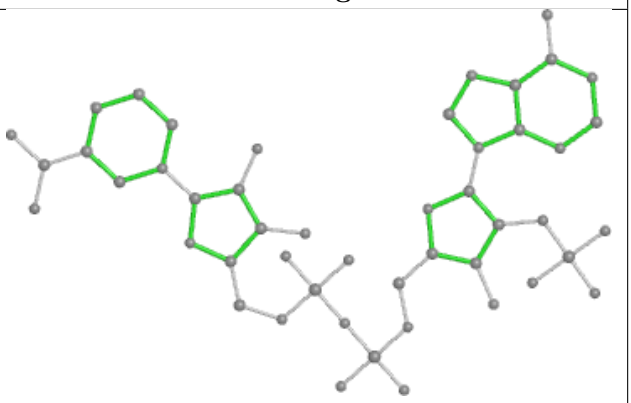
Bond lengths



Bond angles

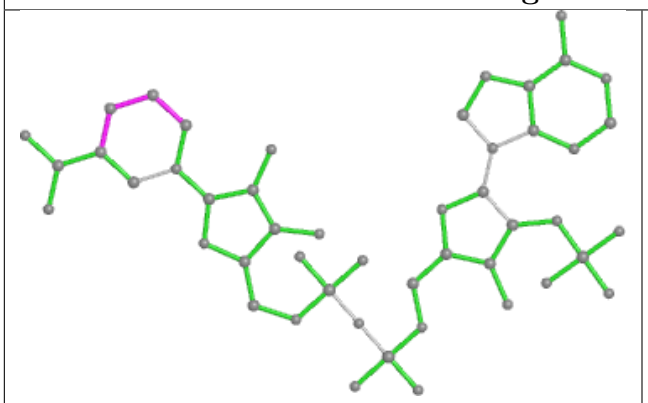


Torsions

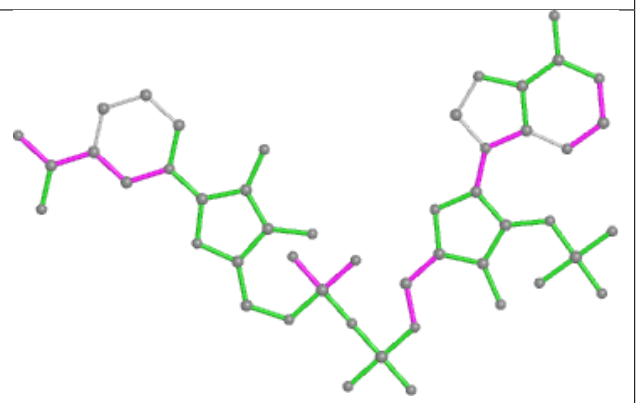


Rings

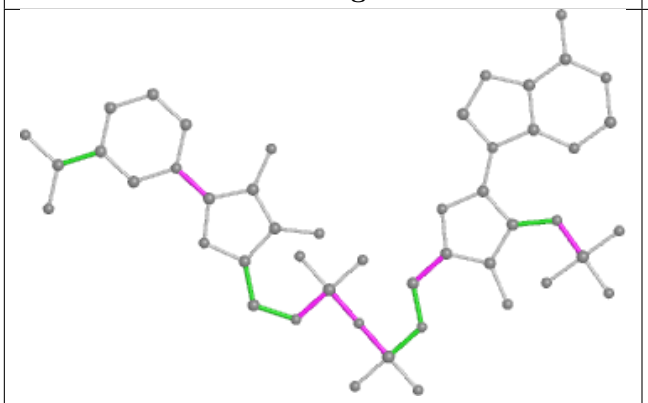
Ligand NDP D 301



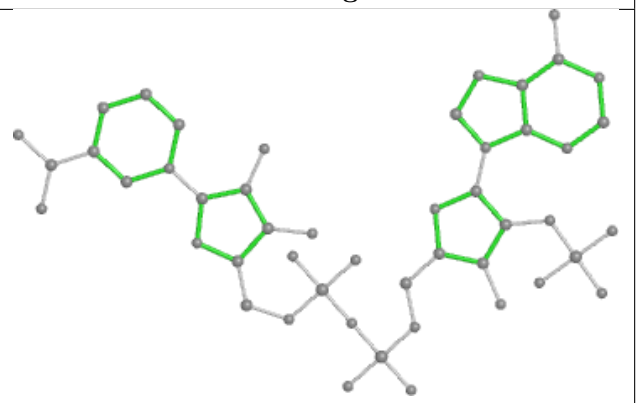
Bond lengths



Bond angles

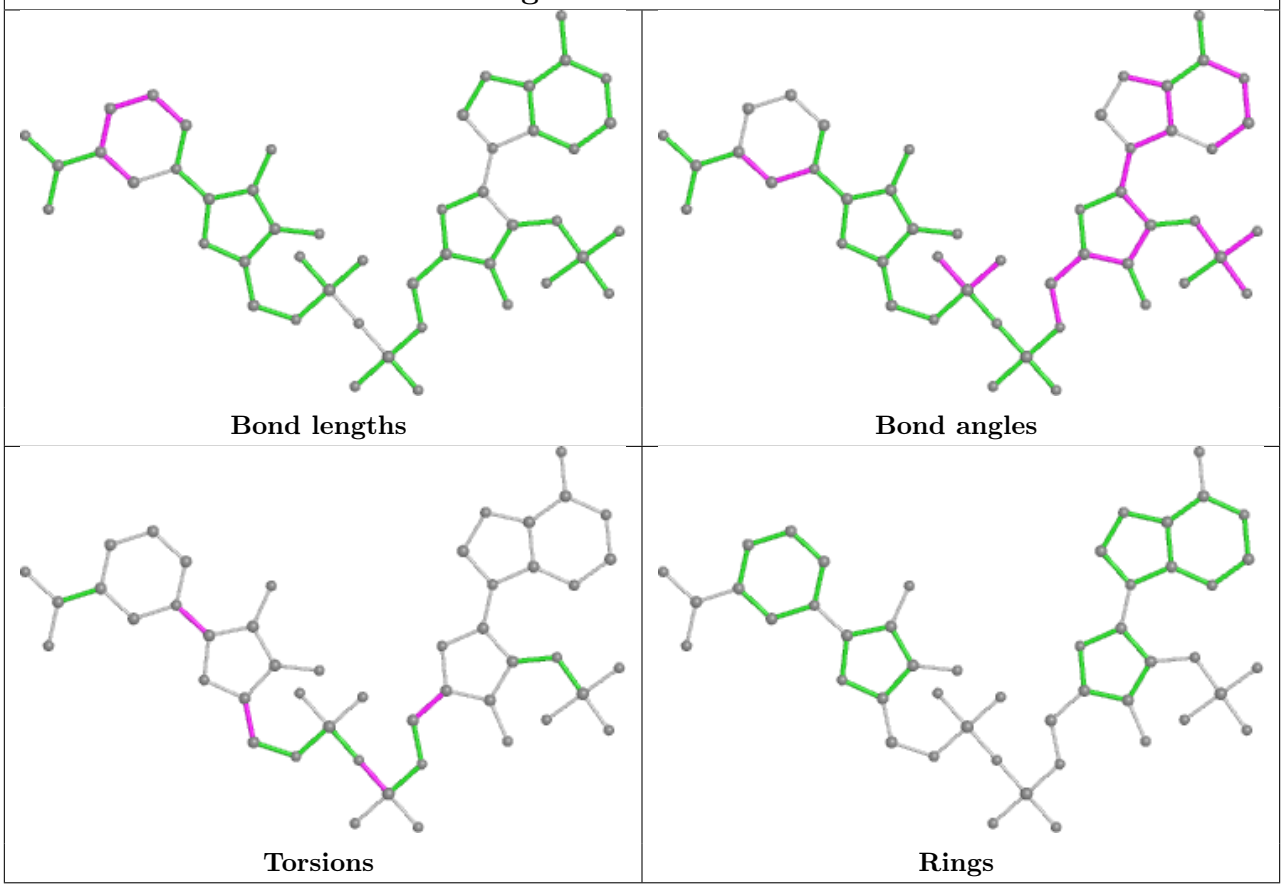


Torsions

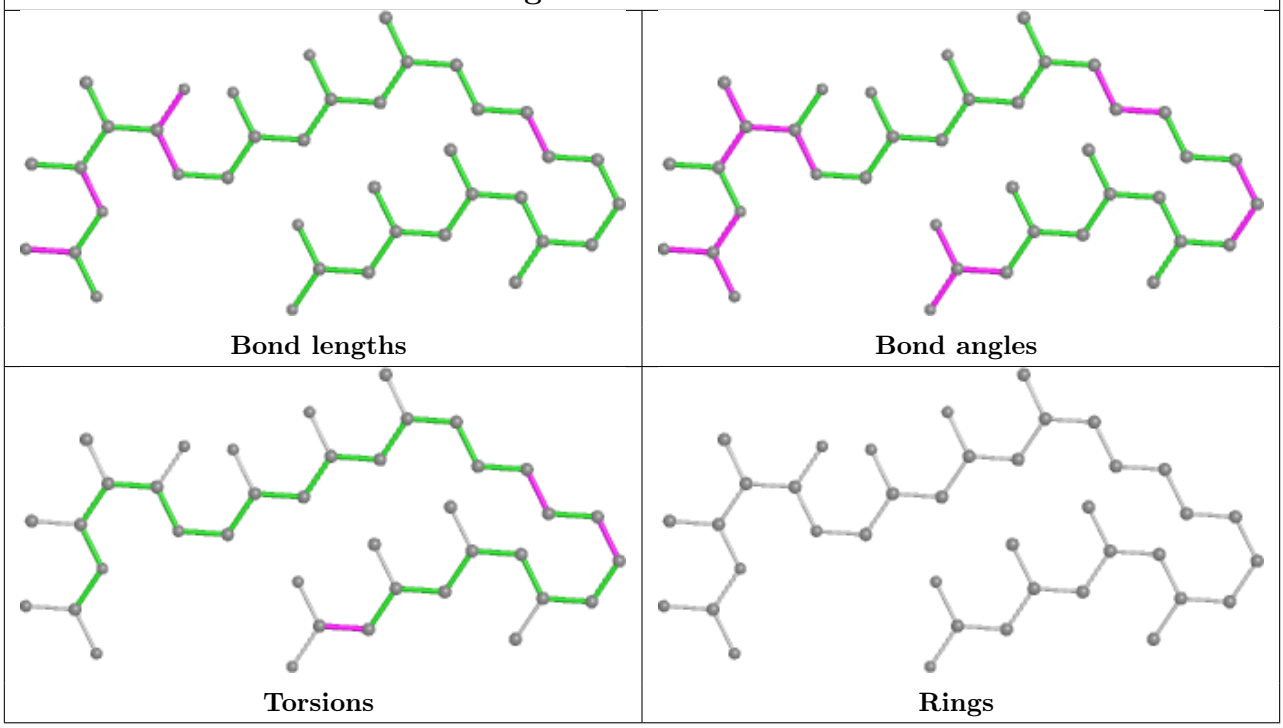


Rings

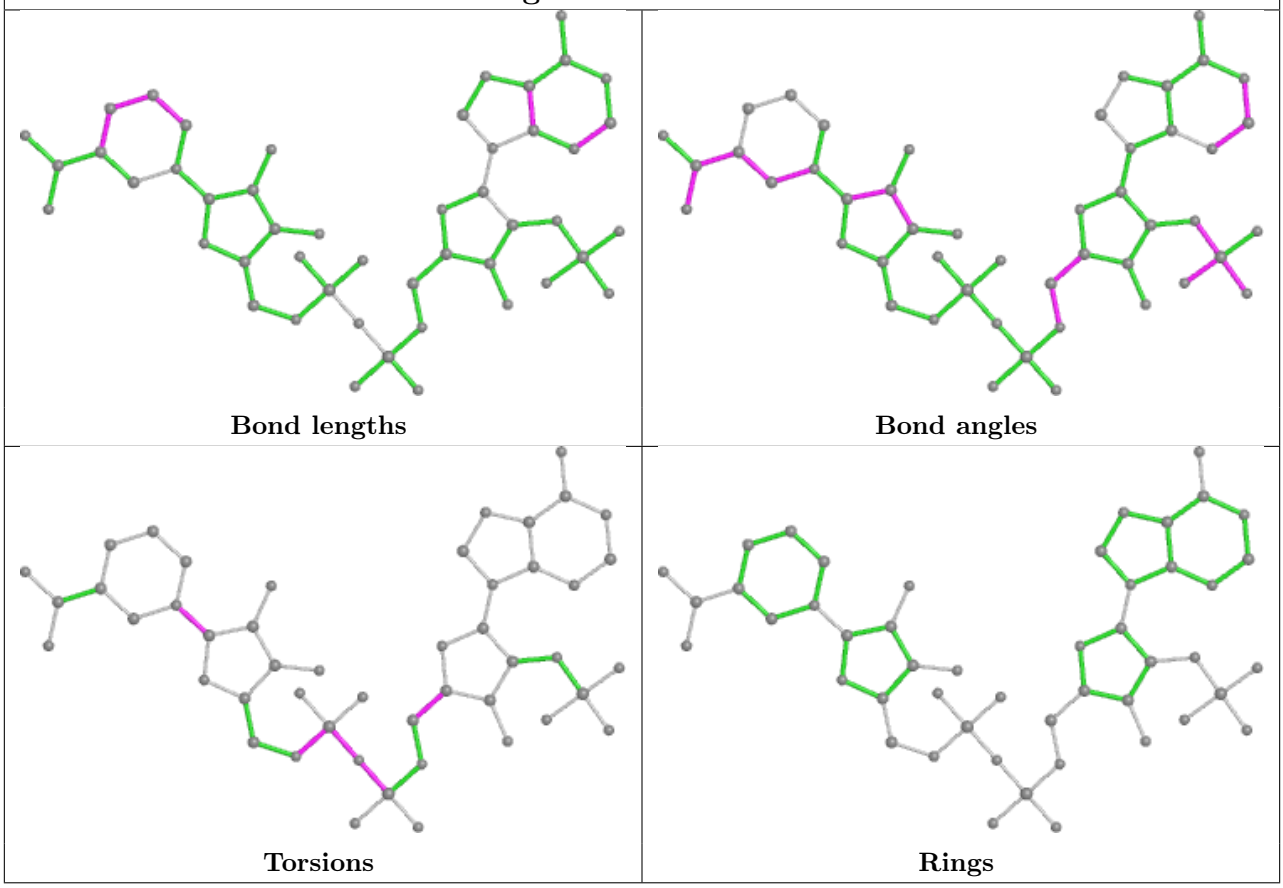
Ligand NDP G 301



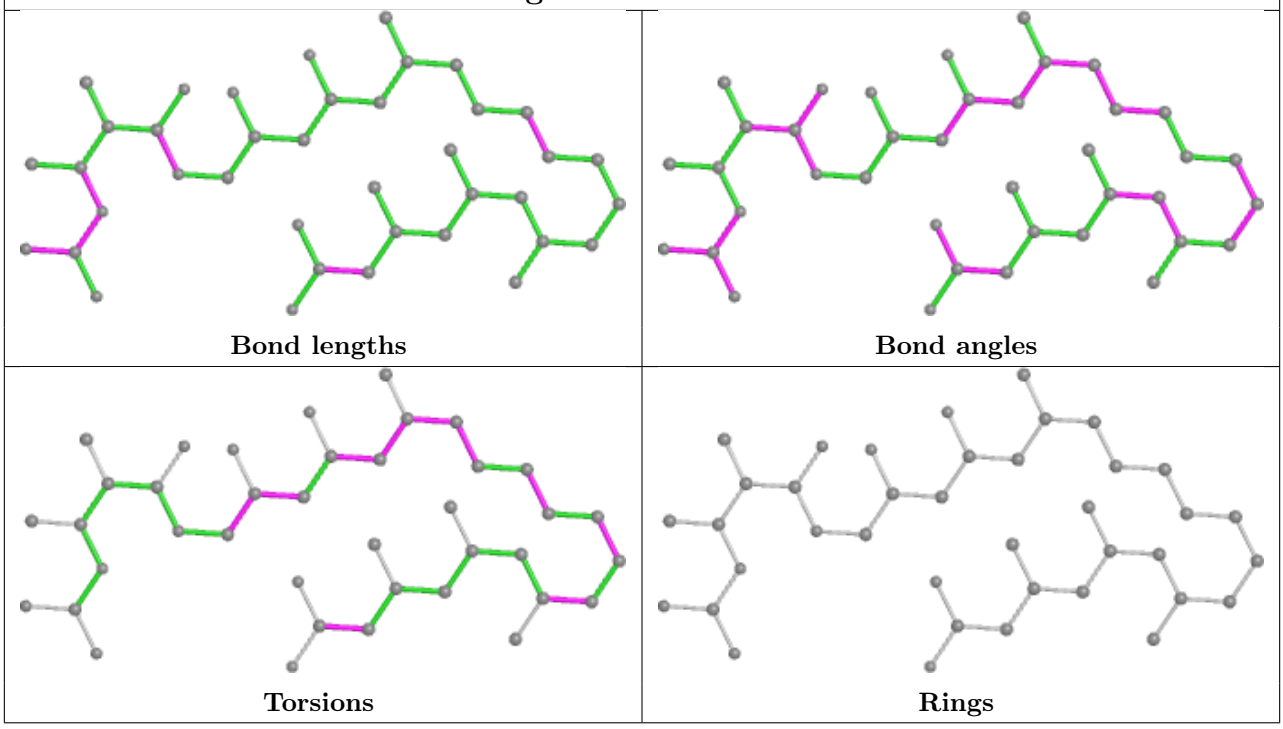
Ligand N5H H 302



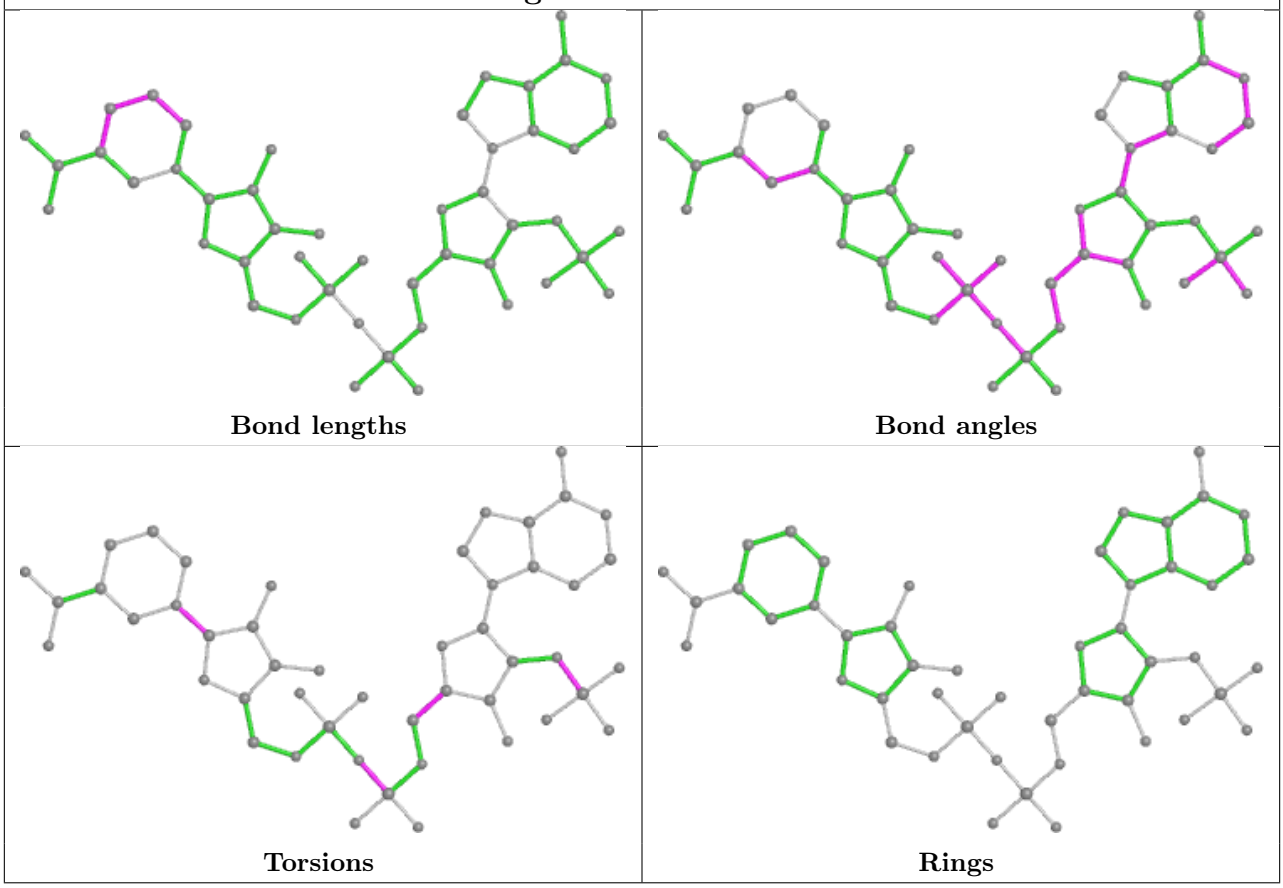
Ligand NDP B 301



Ligand N5H C 302



Ligand NDP F 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/261 (99%)	0.56	36 (13%)	2	3	69, 94, 146, 175	0
1	B	260/261 (99%)	0.58	29 (11%)	5	7	69, 95, 139, 154	0
1	C	259/261 (99%)	0.42	24 (9%)	8	10	64, 89, 133, 178	2 (0%)
1	D	258/261 (98%)	0.61	42 (16%)	1	1	68, 93, 145, 171	0
1	E	258/261 (98%)	0.52	34 (13%)	3	4	63, 91, 136, 160	0
1	F	258/261 (98%)	0.53	29 (11%)	5	7	63, 90, 137, 160	0
1	G	259/261 (99%)	0.97	53 (20%)	1	1	71, 103, 155, 191	0
1	H	258/261 (98%)	0.77	39 (15%)	2	2	67, 98, 141, 162	0
All	All	2070/2088 (99%)	0.62	286 (13%)	2	3	63, 95, 142, 191	2 (0%)

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	94	ILE	8.6
1	H	93	SER	7.8
1	H	92	HIS	7.3
1	H	12	MET	7.0
1	G	200	GLY	6.6
1	H	13	GLY	6.4
1	D	93	SER	6.3
1	H	201	VAL	6.3
1	G	12	MET	6.2
1	E	91	TYR	6.2
1	D	92	HIS	6.1
1	G	91	TYR	6.1
1	G	38	THR	6.0
1	G	46	LYS	5.9
1	F	93	SER	5.8
1	D	94	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	92	HIS	5.7
1	H	145	THR	5.7
1	D	199	LYS	5.7
1	C	-1	MET	5.6
1	B	13	GLY	5.5
1	B	12	MET	5.5
1	D	12	MET	5.5
1	D	13	GLY	5.3
1	G	93	SER	5.2
1	F	13	GLY	5.1
1	A	145	THR	5.1
1	D	90	VAL	5.0
1	H	200	GLY	4.9
1	G	138	GLU	4.8
1	G	143	VAL	4.8
1	H	91	TYR	4.8
1	G	13	GLY	4.8
1	A	93	SER	4.8
1	G	11	ILE	4.7
1	B	92	HIS	4.7
1	G	94	ILE	4.7
1	D	21	ALA	4.7
1	B	93	SER	4.6
1	B	94	ILE	4.6
1	G	90	VAL	4.5
1	E	12	MET	4.5
1	A	53	GLU	4.5
1	B	11	ILE	4.5
1	B	21	ALA	4.4
1	G	53	GLU	4.4
1	A	199	LYS	4.4
1	B	144	ALA	4.3
1	H	11	ILE	4.3
1	G	42	GLU	4.2
1	D	144	ALA	4.2
1	E	92	HIS	4.2
1	E	93	SER	4.1
1	G	10	VAL	4.1
1	A	92	HIS	4.0
1	A	200	GLY	4.0
1	A	12	MET	4.0
1	D	143	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	91	TYR	3.9
1	B	145	THR	3.9
1	G	145	THR	3.9
1	B	90	VAL	3.9
1	C	143	VAL	3.9
1	F	91	TYR	3.9
1	F	6	ASN	3.9
1	E	143	VAL	3.9
1	E	11	ILE	3.9
1	B	50	LYS	3.9
1	B	143	VAL	3.9
1	A	143	VAL	3.8
1	H	38	THR	3.8
1	D	60	ALA	3.8
1	G	144	ALA	3.8
1	B	46	LYS	3.8
1	A	91	TYR	3.8
1	H	143	VAL	3.8
1	H	144	ALA	3.8
1	A	50	LYS	3.8
1	C	12	MET	3.7
1	F	188	ILE	3.7
1	G	43	ARG	3.7
1	A	46	LYS	3.7
1	E	90	VAL	3.7
1	A	6	ASN	3.7
1	H	125	LEU	3.7
1	F	92	HIS	3.7
1	B	103	ARG	3.6
1	A	13	GLY	3.6
1	D	53	GLU	3.6
1	G	6	ASN	3.6
1	H	90	VAL	3.6
1	F	12	MET	3.6
1	G	203	GLY	3.6
1	A	52	LEU	3.6
1	E	144	ALA	3.6
1	D	188	ILE	3.5
1	E	13	GLY	3.5
1	D	202	GLY	3.4
1	G	21	ALA	3.4
1	C	11	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	93	SER	3.4
1	C	50	LYS	3.4
1	E	50	LYS	3.4
1	H	21	ALA	3.4
1	D	10	VAL	3.4
1	B	38	THR	3.3
1	D	46	LYS	3.3
1	G	142	ILE	3.3
1	D	24	VAL	3.3
1	D	145	THR	3.3
1	B	91	TYR	3.3
1	A	90	VAL	3.3
1	C	-2	HIS	3.2
1	A	187	ALA	3.2
1	B	10	VAL	3.2
1	D	49	GLU	3.2
1	G	60	ALA	3.2
1	F	94	ILE	3.2
1	D	142	ILE	3.2
1	H	59	GLU	3.2
1	F	43	ARG	3.2
1	C	91	TYR	3.1
1	A	49	GLU	3.1
1	F	11	ILE	3.1
1	E	49	GLU	3.1
1	D	11	ILE	3.1
1	B	142	ILE	3.1
1	F	143	VAL	3.1
1	D	58	PRO	3.1
1	D	50	LYS	3.1
1	E	21	ALA	3.1
1	C	89	GLY	3.0
1	E	60	ALA	3.0
1	E	10	VAL	3.0
1	G	137	PRO	3.0
1	D	200	GLY	3.0
1	A	128	VAL	3.0
1	D	45	ARG	3.0
1	B	51	LEU	3.0
1	H	116	LEU	3.0
1	E	200	GLY	3.0
1	H	100	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	201	VAL	2.9
1	G	205	ASN	2.9
1	G	188	ILE	2.9
1	E	187	ALA	2.9
1	B	-2	HIS	2.9
1	F	90	VAL	2.9
1	H	103	ARG	2.9
1	F	145	THR	2.9
1	G	202	GLY	2.9
1	G	204	PHE	2.9
1	A	188	ILE	2.8
1	G	49	GLU	2.8
1	A	94	ILE	2.8
1	E	89	GLY	2.8
1	E	94	ILE	2.8
1	F	204	PHE	2.8
1	G	51	LEU	2.8
1	C	141	SER	2.8
1	D	206	THR	2.7
1	A	144	ALA	2.7
1	G	85	GLY	2.7
1	C	21	ALA	2.7
1	F	138	GLU	2.7
1	E	2	LEU	2.7
1	H	50	LYS	2.7
1	D	43	ARG	2.7
1	E	142	ILE	2.7
1	G	58	PRO	2.6
1	E	54	GLN	2.6
1	B	99	MET	2.6
1	B	138	GLU	2.6
1	A	96	PHE	2.6
1	D	20	ILE	2.6
1	C	92	HIS	2.6
1	F	21	ALA	2.6
1	F	144	ALA	2.6
1	C	46	LYS	2.6
1	D	41	LYS	2.6
1	H	142	ILE	2.6
1	G	61	HIS	2.6
1	G	50	LYS	2.6
1	G	89	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	43	ARG	2.6
1	E	53	GLU	2.6
1	G	194	ARG	2.6
1	A	42	GLU	2.6
1	G	199	LYS	2.5
1	E	145	THR	2.5
1	G	206	THR	2.5
1	H	128	VAL	2.5
1	E	188	ILE	2.5
1	G	86	ASN	2.5
1	G	96	PHE	2.5
1	F	58	PRO	2.5
1	D	44	SER	2.5
1	E	46	LYS	2.5
1	A	203	GLY	2.5
1	C	49	GLU	2.5
1	A	209	LYS	2.5
1	G	198	ALA	2.5
1	G	128	VAL	2.4
1	F	104	GLY	2.4
1	G	54	GLN	2.4
1	C	90	VAL	2.4
1	E	43	ARG	2.4
1	C	10	VAL	2.4
1	F	10	VAL	2.4
1	H	10	VAL	2.4
1	C	60	ALA	2.4
1	H	46	LYS	2.4
1	E	9	TYR	2.4
1	B	-3	SER	2.4
1	C	43	ARG	2.4
1	G	84	VAL	2.4
1	H	53	GLU	2.4
1	A	45	ARG	2.4
1	D	42	GLU	2.4
1	G	81	GLY	2.4
1	G	82	LYS	2.4
1	E	201	VAL	2.3
1	H	138	GLU	2.3
1	C	82	LYS	2.3
1	G	156	ASN	2.3
1	H	112	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	218	LYS	2.3
1	C	13	GLY	2.3
1	F	53	GLU	2.3
1	A	202	GLY	2.3
1	H	71	GLU	2.3
1	H	14	ILE	2.3
1	E	103	ARG	2.3
1	A	82	LYS	2.3
1	F	14	ILE	2.3
1	G	214	ARG	2.3
1	A	205	ASN	2.3
1	D	124	SER	2.3
1	H	124	SER	2.3
1	A	125	LEU	2.3
1	B	167	LEU	2.3
1	B	43	ARG	2.2
1	H	96	PHE	2.2
1	B	213	GLU	2.2
1	A	54	GLN	2.2
1	H	167	LEU	2.2
1	E	83	ASP	2.2
1	F	128	VAL	2.2
1	E	45	ARG	2.2
1	B	146	THR	2.2
1	H	6	ASN	2.2
1	G	83	ASP	2.2
1	H	209	LYS	2.2
1	F	82	LYS	2.2
1	C	142	ILE	2.2
1	H	37	PHE	2.2
1	A	146	THR	2.1
1	G	65	ILE	2.1
1	F	59	GLU	2.1
1	B	82	LYS	2.1
1	F	54	GLN	2.1
1	D	194	ARG	2.1
1	F	194	ARG	2.1
1	D	59	GLU	2.1
1	D	52	LEU	2.1
1	D	89	GLY	2.1
1	C	94	ILE	2.1
1	A	194	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLU	2.1
1	F	202	GLY	2.1
1	D	209	LYS	2.1
1	E	141	SER	2.1
1	E	79	GLN	2.1
1	C	59	GLU	2.1
1	H	146	THR	2.1
1	B	125	LEU	2.1
1	D	37	PHE	2.1
1	H	78	GLU	2.1
1	D	85	GLY	2.0
1	A	11	ILE	2.0
1	H	199	LYS	2.0
1	D	203	GLY	2.0
1	G	45	ARG	2.0
1	D	128	VAL	2.0
1	F	45	ARG	2.0
1	C	53	GLU	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 monosaccharides 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	N5H	H	302	39/39	0.86	0.27	72,97,128,131	0
3	N5H	B	302	39/39	0.88	0.25	84,95,116,118	0
3	N5H	A	302	39/39	0.91	0.24	88,105,128,134	0
3	N5H	G	302	39/39	0.92	0.22	82,108,121,126	0
3	N5H	E	302	39/39	0.93	0.20	73,90,107,112	0

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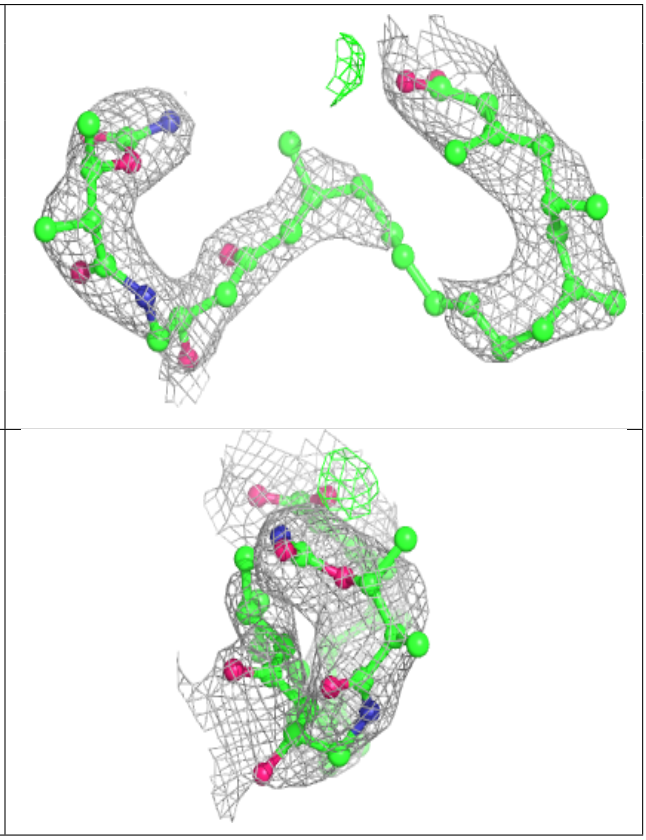
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDP	G	301	48/48	0.93	0.14	82,102,127,140	0
3	N5H	D	302	39/39	0.93	0.21	77,99,118,132	0
2	NDP	H	301	48/48	0.94	0.18	73,90,112,117	0
3	N5H	F	302	39/39	0.94	0.18	75,94,111,122	0
3	N5H	C	302	39/39	0.94	0.15	73,91,105,112	0
2	NDP	D	301	48/48	0.94	0.15	77,89,111,121	0
2	NDP	A	301	48/48	0.95	0.16	79,97,112,122	0
2	NDP	F	301	48/48	0.95	0.17	65,84,105,112	0
2	NDP	B	301	48/48	0.95	0.18	73,84,118,128	0
2	NDP	E	301	48/48	0.96	0.14	55,87,103,106	0
2	NDP	C	301	48/48	0.97	0.14	71,83,97,105	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.

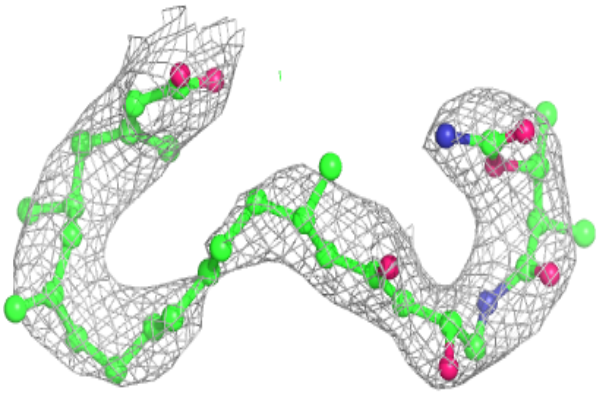
Electron density around N5H H 302:

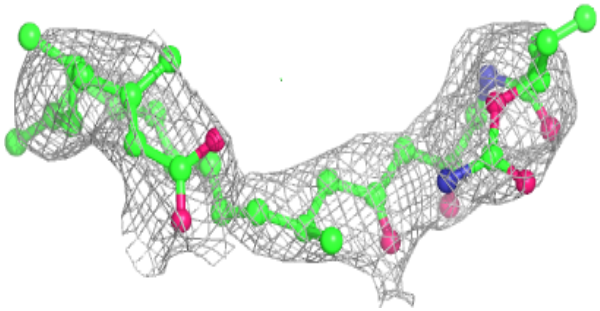
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N5H B 302:

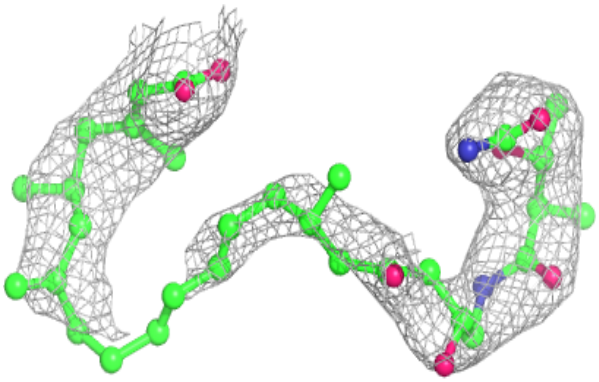
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

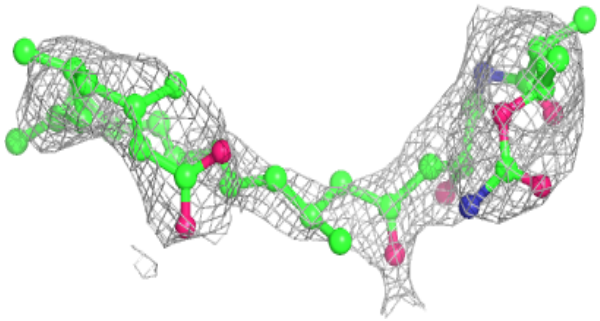


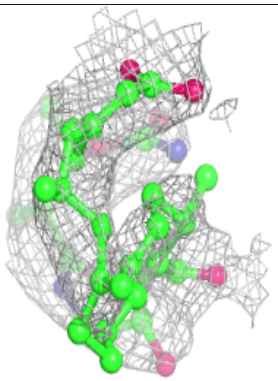


Electron density around N5H A 302:

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

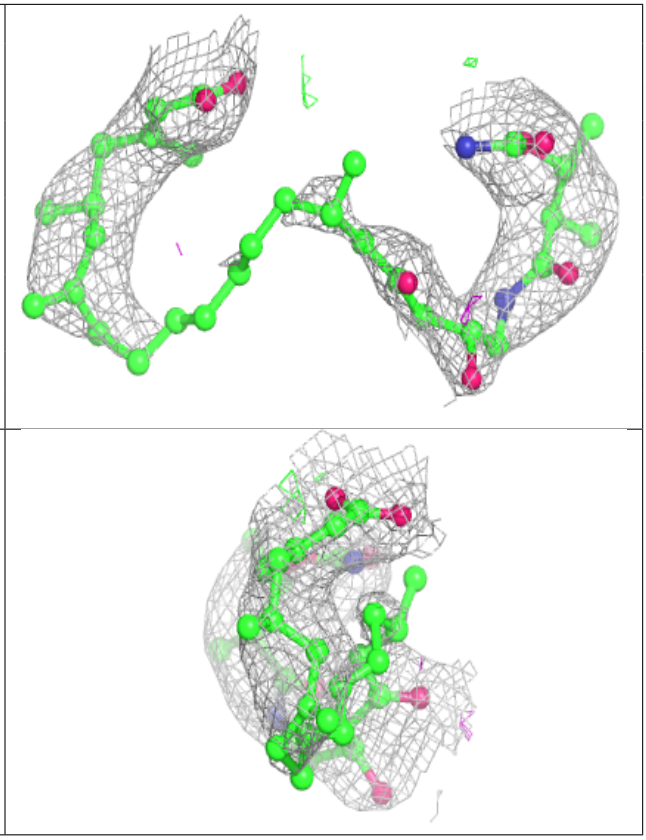






Electron density around N5H G 302:

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



Electron density around N5H E 302:

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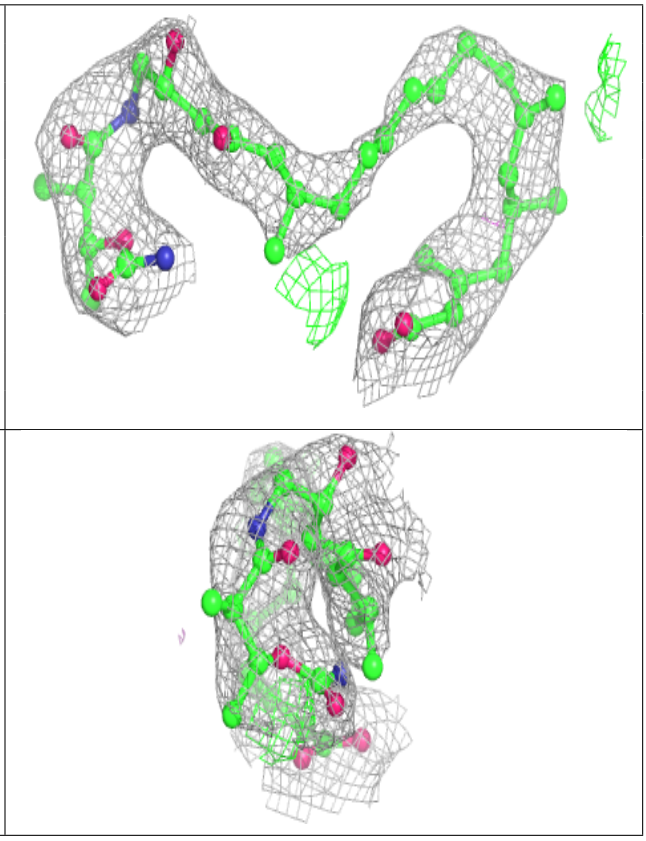
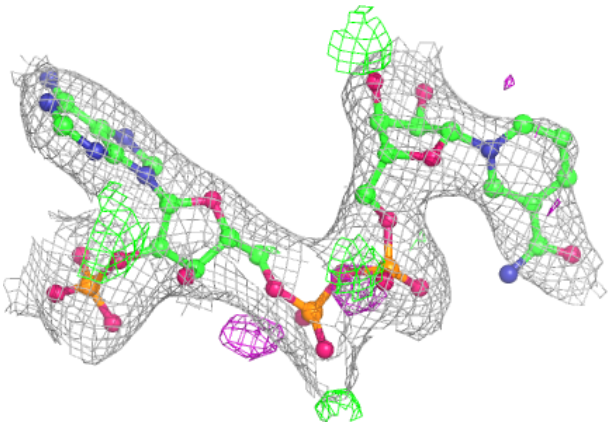
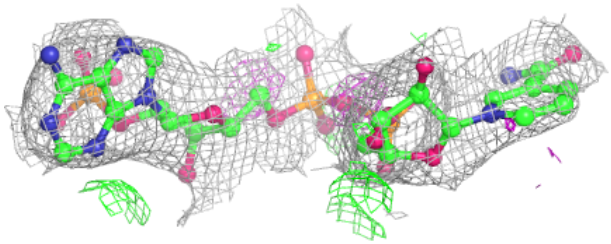
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

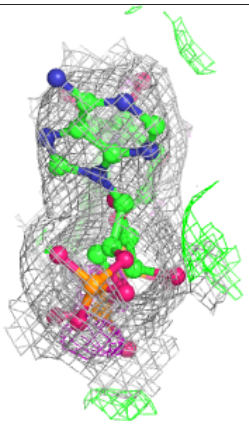


Electron density around NDP G 301:

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

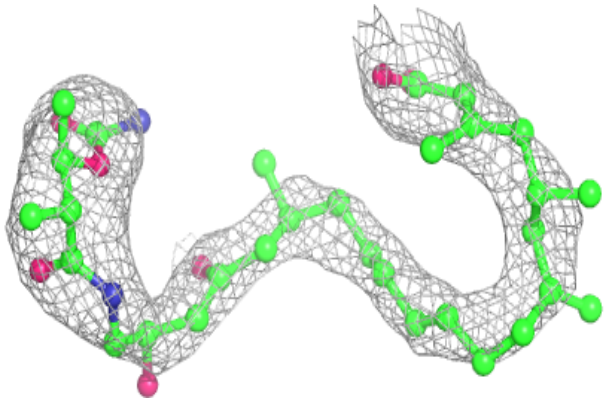


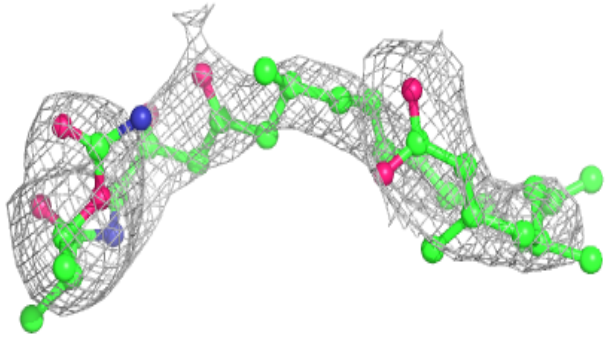


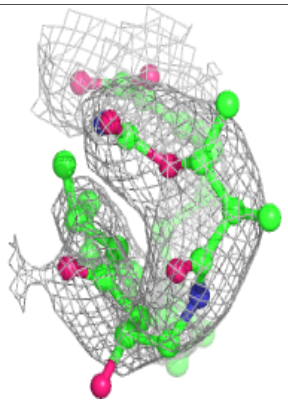


Electron density around N5H D 302:

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

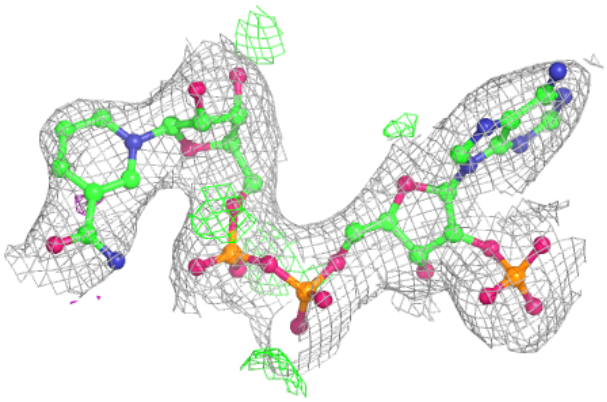


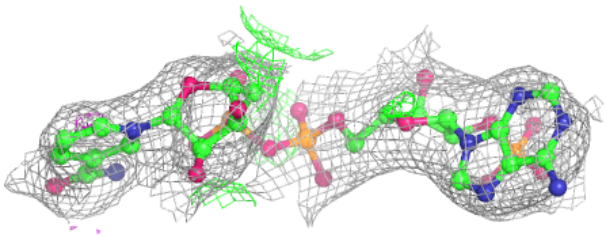


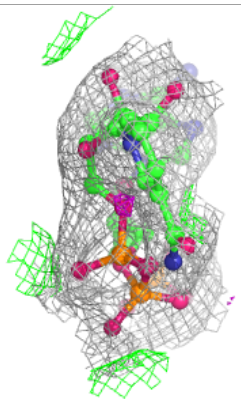


Electron density around NDP H 301:

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

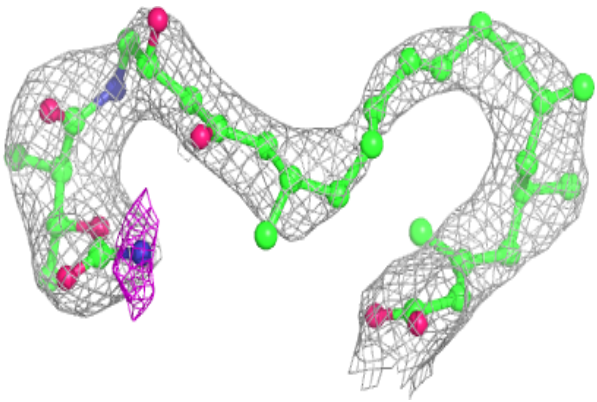


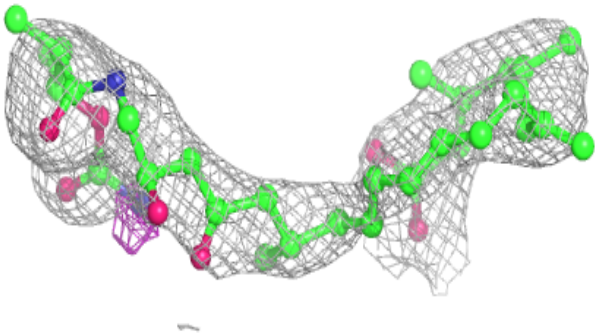


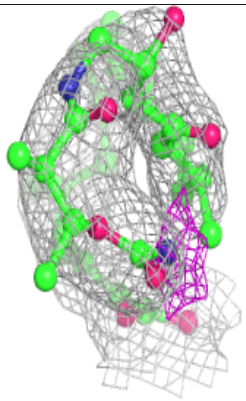


Electron density around N5H F 302:

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

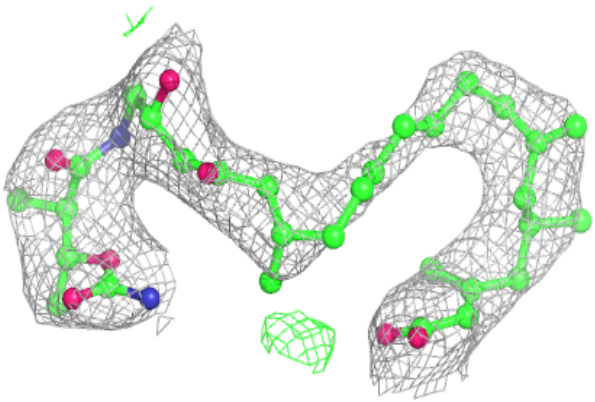


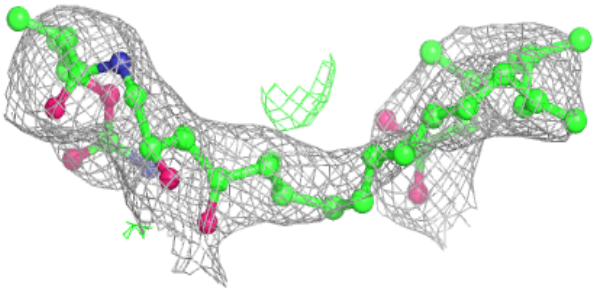


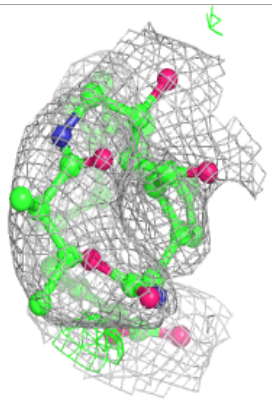


Electron density around N5H C 302:

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

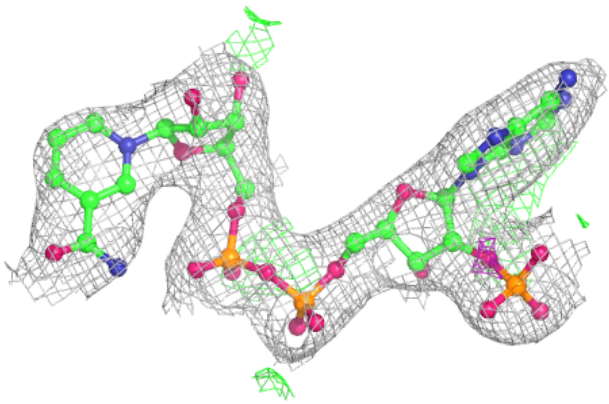


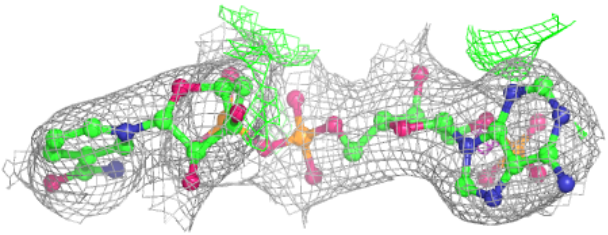


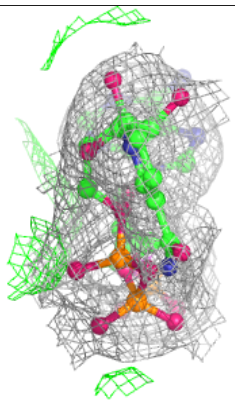


Electron density around NDP D 301:

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

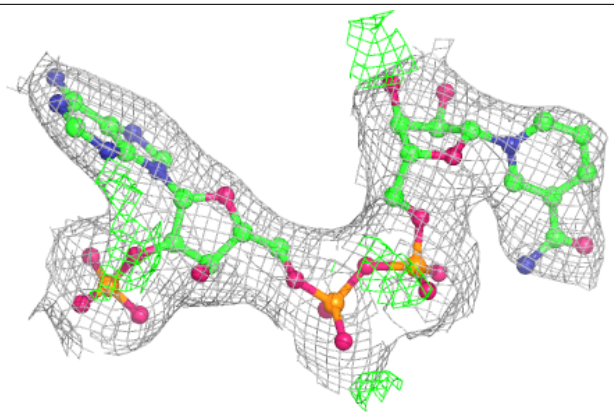


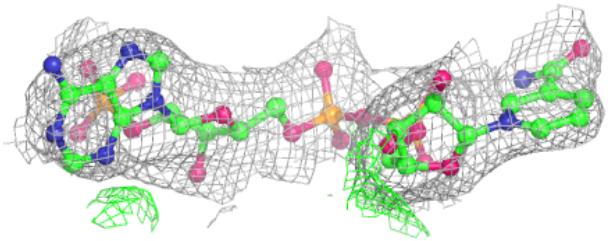


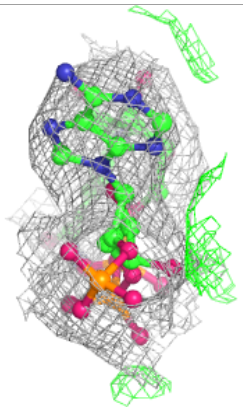


Electron density around NDP A 301:

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

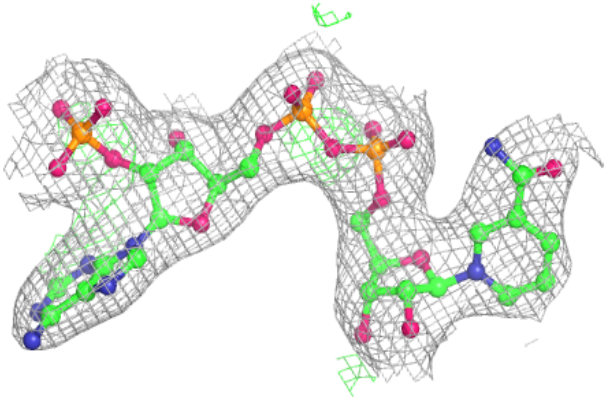


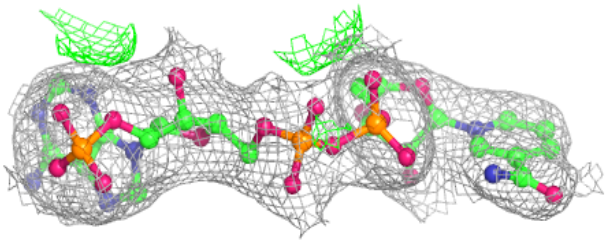


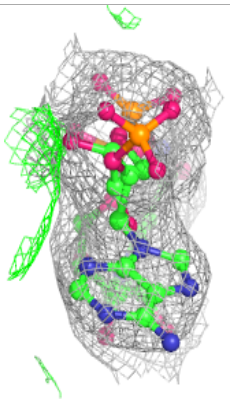


Electron density around NDP F 301:

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

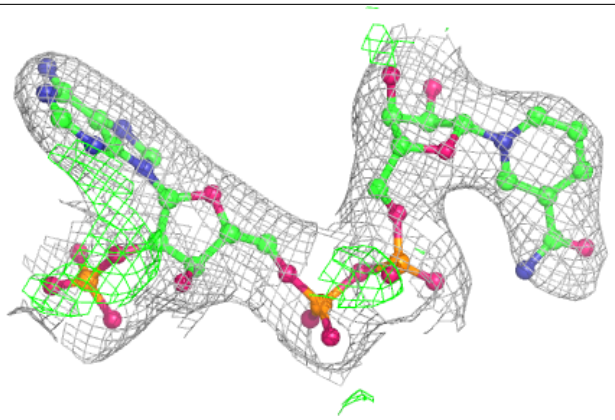


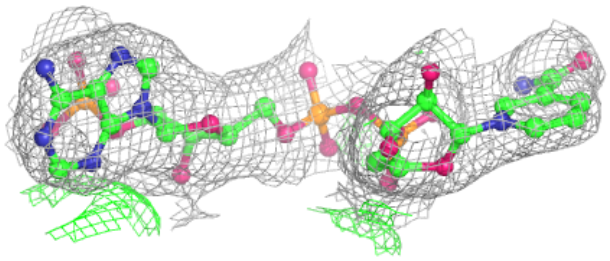


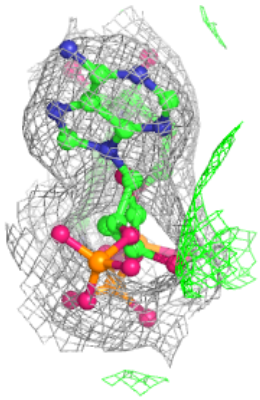


Electron density around NDP B 301:

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

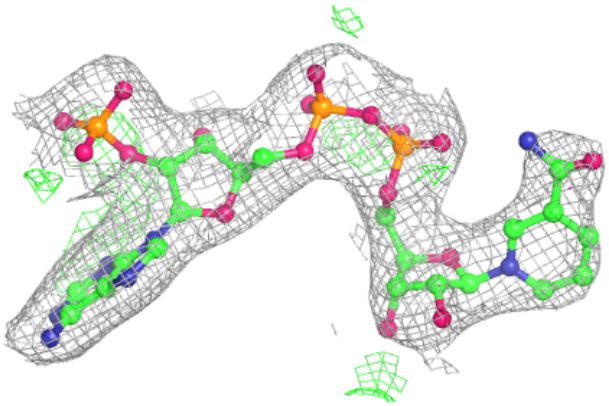


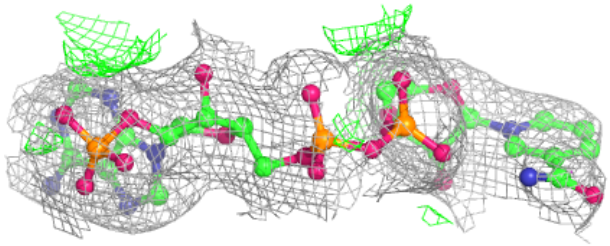


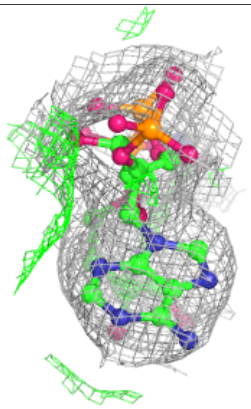


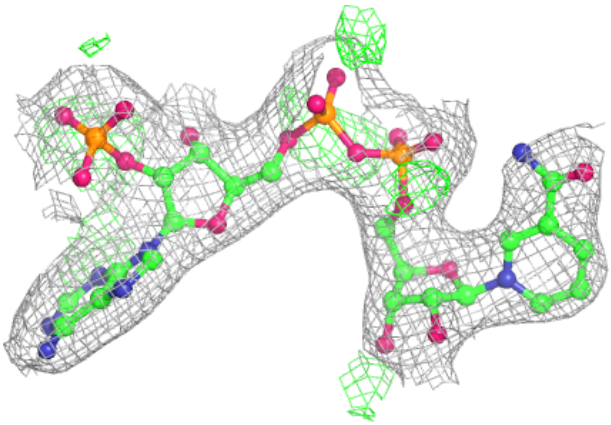
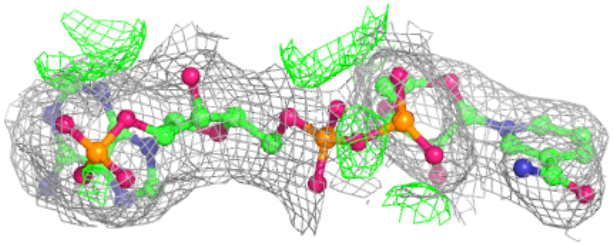
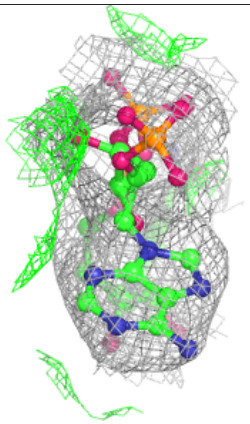
Electron density around NDP E 301:

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







Electron density around NDP C 301: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.