Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 12:38 AM EDT

PDB ID	:	4K1L
Title	:	4,4-Dioxo-5,6-dihydro-[1,4,3]oxathiazines, a novel class of 11 beta-HSD1 inhibitors for the treatment of diabetes
Authors	:	Loenze, P.; Schimanski-Breves, S.; Von der Heyden, C.; Engel, C.K.
Deposited on	:	2013-04-05
Resolution	:	1.96 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:

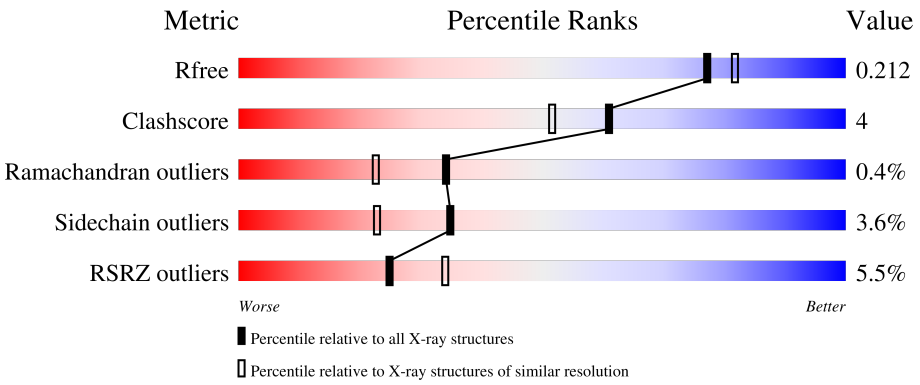
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	286	5% 82% 8% • 8%
1	B	286	5% 84% 7% • 7%
1	C	286	5% 83% 8% • 8%
1	D	286	5% 83% 9% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9120 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2038	1302	342	379	15	0	7	0
1	B	266	2086	1332	351	386	17	0	11	0
1	C	263	2062	1314	349	384	15	0	11	0
1	D	264	2053	1308	348	381	16	0	9	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	expression tag	UNP P28845
C	8	LYS	-	expression tag	UNP P28845
C	9	HIS	-	expression tag	UNP P28845
C	10	GLN	-	expression tag	UNP P28845
C	11	HIS	-	expression tag	UNP P28845
C	12	GLN	-	expression tag	UNP P28845
C	13	HIS	-	expression tag	UNP P28845
C	14	GLN	-	expression tag	UNP P28845
C	15	HIS	-	expression tag	UNP P28845
C	16	GLN	-	expression tag	UNP P28845
C	17	HIS	-	expression tag	UNP P28845
C	18	GLN	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	GLN	-	expression tag	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	expression tag	UNP P28845
D	8	LYS	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	GLN	-	expression tag	UNP P28845
D	11	HIS	-	expression tag	UNP P28845
D	12	GLN	-	expression tag	UNP P28845
D	13	HIS	-	expression tag	UNP P28845
D	14	GLN	-	expression tag	UNP P28845
D	15	HIS	-	expression tag	UNP P28845

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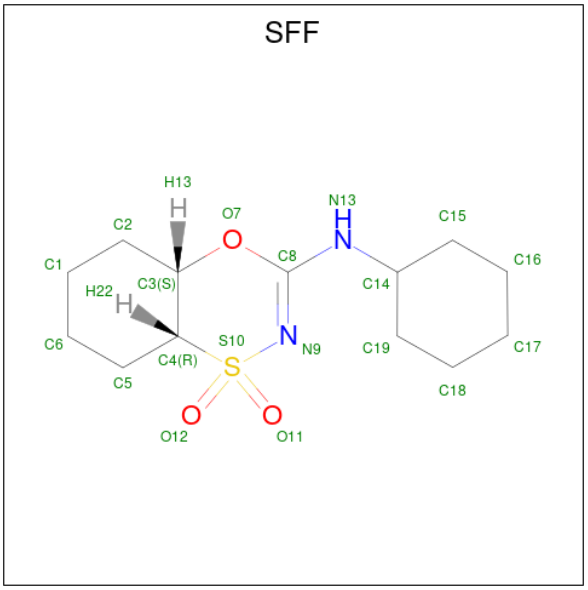
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

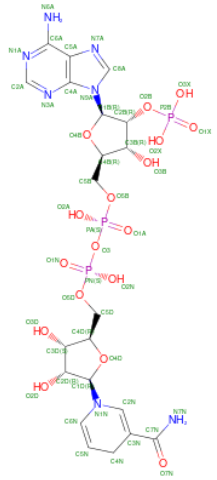
- Molecule 2 is (4aS,8aR)-N-cyclohexyl-4a,5,6,7,8,8a-hexahydro-4,1,2-benzoxathiazin-3-amine 1,1-dioxide (three-letter code: SFF) (formula: $C_{13}H_{22}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			19	13	2	3	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP



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

- Molecule 4 is water.

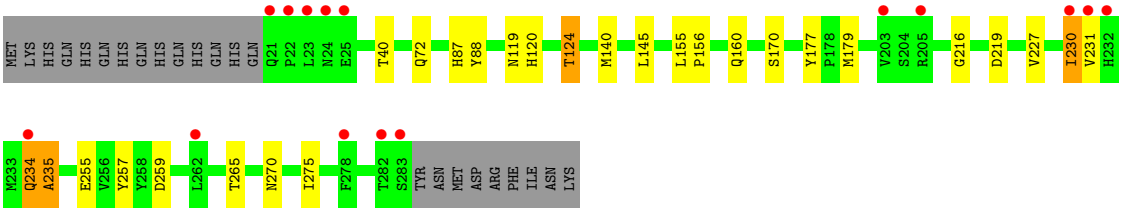
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	153	153	153	0	0
4	B	180	180	180	0	0
4	C	141	141	141	0	0
4	D	139	139	139	0	0

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.

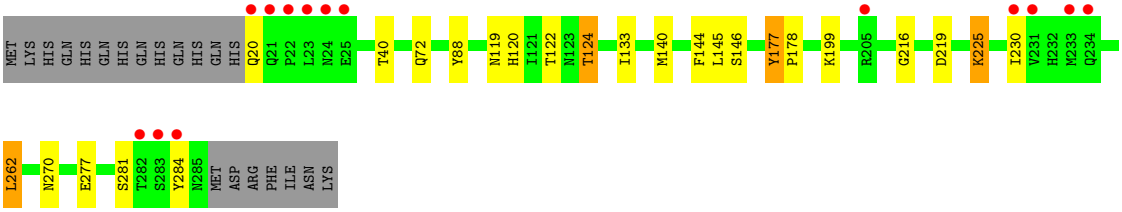
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain A:



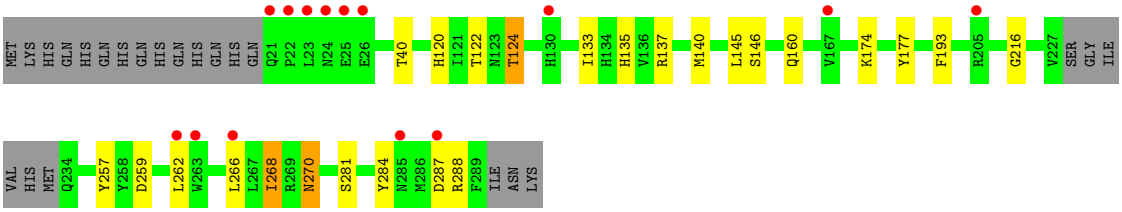
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain B:



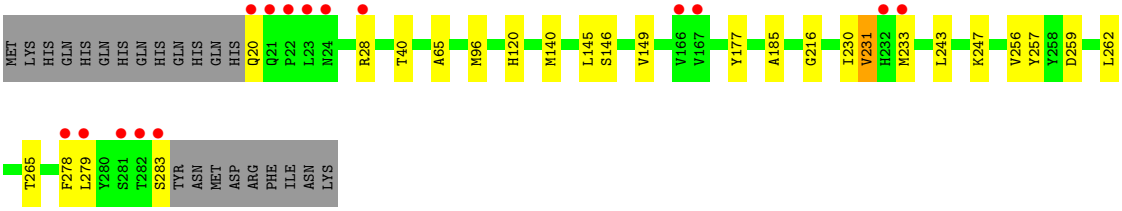
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain C:



• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain D:


MET
LYS
HIS
GLN
HIS
GLN
HIS
GLN
HIS
GLN
HIS
Q20
Q21
P22
L23
N24
R28
T40
A65
M96
H120
M140
L145
S146
V149
V166
V167
Y177
A185
G216
I230
V231
H232
M233
L243
K247
V256
Y257
Y258
D259
L262
T265
F278
L279
Y280
S281
T282
S283
TYR
ASN
MET
ASP
ARG
PHE
ILE
ASN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.36Å 150.94Å 74.17Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	28.62 – 1.96 28.62 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.62-1.96) 99.8 (28.62-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 1.96Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.167 , 0.202 0.173 , 0.212	Depositor DCC
R_{free} test set	4409 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9120	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, SFF

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	0.51	1/2102 (0.0%)	0.67	1/2841 (0.0%)
1	B	0.56	1/2170 (0.0%)	0.68	2/2931 (0.1%)
1	C	0.50	0/2145	0.63	0/2895
1	D	0.49	0/2127	0.63	0/2872
All	All	0.51	2/8544 (0.0%)	0.65	3/11539 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	PRO	N-CD	5.23	1.55	1.47
1	B	178	PRO	N-CD	5.22	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177[A]	TYR	C-N-CD	5.73	140.43	128.40
1	B	177[B]	TYR	C-N-CD	5.73	140.43	128.40
1	A	155	LEU	C-N-CD	5.53	140.01	128.40

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	2038	0	2085	29	0
1	B	2086	0	2126	22	0
1	C	2062	0	2098	17	0
1	D	2053	0	2095	17	0
2	A	19	0	22	1	0
2	B	19	0	22	1	0
2	C	19	0	22	1	0
2	D	19	0	22	1	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
3	C	48	0	26	2	0
3	D	48	0	26	2	0
4	A	153	0	0	4	0
4	B	180	0	0	1	0
4	C	141	0	0	1	0
4	D	139	0	0	0	0
All	All	9120	0	8596	77	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 4.

All (77) 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:A:179:MET:SD	1:A:230:ILE:HD11	2.11	0.91
1:B:140[B]:MET:CE	1:B:145[B]:LEU:HG	2.07	0.85
1:A:234:GLN:NE2	1:A:234:GLN:H	1.77	0.80
1:C:140:MET:HG3	1:D:140[B]:MET:HE3	1.67	0.76
1:A:234:GLN:H	1:A:234:GLN:HE21	1.32	0.75
1:A:234:GLN:CB	1:A:235:ALA:HB3	2.16	0.75
1:A:231:VAL:HG22	1:B:284:TYR:HB3	1.70	0.74
1:B:140[B]:MET:HE1	1:B:145[B]:LEU:HG	1.70	0.71
1:C:174:LYS:HG3	1:C:268:ILE:HD11	1.73	0.70
1:B:140[B]:MET:HE2	1:B:145[B]:LEU:HG	1.72	0.70
1:C:124[B]:THR:HG21	4:C:401:HOH:O	1.89	0.70
1:C:284:TYR:HB3	1:D:231:VAL:HG13	1.79	0.64
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.82	0.63
1:A:179:MET:CE	1:A:230:ILE:HD11	2.29	0.62
1:D:140[B]:MET:HE2	1:D:145:LEU:HB2	1.82	0.61
1:A:234:GLN:HA	1:A:235:ALA:CB	2.29	0.61
1:B:199:LYS:HE2	1:B:277:GLU:HB3	1.84	0.60
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72[A]:GLN:HG2	1:B:88:TYR:CE2	2.38	0.59
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.85	0.58
1:B:281:SER:HA	1:B:284:TYR:CZ	2.38	0.58
1:A:179:MET:HE1	1:A:230:ILE:HD11	1.86	0.57
1:B:140[B]:MET:CE	1:B:144:PHE:HD2	2.17	0.57
1:A:234:GLN:HB3	1:A:235:ALA:HB3	1.85	0.57
1:A:234:GLN:CA	1:A:235:ALA:HB3	2.34	0.57
1:C:40:THR:OG1	1:C:120:HIS:HD2	1.88	0.56
1:D:140[B]:MET:CE	1:D:145:LEU:HB2	2.35	0.56
1:A:234:GLN:CA	1:A:235:ALA:CB	2.85	0.55
2:B:301:SFF:C8	3:B:302:NDP:H41N	2.37	0.55
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.07	0.54
1:B:140[B]:MET:HE3	1:B:144:PHE:HD2	1.72	0.54
1:A:140:MET:HG3	1:B:140[B]:MET:CE	2.38	0.54
1:C:288:ARG:HD2	1:D:230:ILE:HD11	1.88	0.54
1:C:137[A]:ARG:HH22	1:D:96:MET:HG3	1.73	0.54
1:A:140:MET:HG3	1:B:140[B]:MET:HE3	1.91	0.53
1:D:216:GLY:HA3	1:D:259:ASP:OD1	2.10	0.51
1:A:216:GLY:O	3:A:302:NDP:H42N	2.11	0.51
1:A:255:GLU:OE2	1:A:257:TYR:OH	2.19	0.51
1:B:216:GLY:O	3:B:302:NDP:H42N	2.11	0.49
1:A:275:ILE:HD11	1:D:265:THR:OG1	2.13	0.49
1:A:124:THR:HG21	4:A:407:HOH:O	2.13	0.49
1:D:216:GLY:O	3:D:302:NDP:H42N	2.13	0.49
1:A:234:GLN:HA	1:A:235:ALA:HB3	1.94	0.49
1:D:120:HIS:HE1	1:D:146:SER:OG	1.95	0.49
1:D:257:TYR:CE1	1:D:265:THR:HG22	2.49	0.48
1:A:231:VAL:HG22	1:B:284:TYR:CB	2.43	0.48
2:C:301:SFF:C8	3:C:302:NDP:H41N	2.45	0.47
1:C:124[B]:THR:HG22	1:C:135:HIS:HE1	1.78	0.47
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.96	0.47
1:C:216:GLY:O	3:C:302:NDP:H42N	2.14	0.47
1:A:119:ASN:ND2	3:A:302:NDP:H4D	2.30	0.47
1:C:133:ILE:HD13	1:D:149:VAL:HG22	1.97	0.47
1:B:120:HIS:HE1	1:B:146:SER:OG	1.98	0.47
1:D:262:LEU:O	1:D:265:THR:HG23	2.15	0.47
1:C:122:THR:O	1:C:124[A]:THR:HG22	2.14	0.46
1:C:120:HIS:HE1	1:C:146:SER:OG	1.98	0.46
1:A:72:GLN:HG3	1:A:88:TYR:CE2	2.51	0.46
1:A:140:MET:HG2	4:A:430:HOH:O	2.15	0.46
1:A:87:HIS:HE1	4:A:522:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:SER:HA	1:C:284:TYR:CZ	2.51	0.45
1:C:216:GLY:HA3	1:C:259:ASP:OD1	2.17	0.44
1:D:231:VAL:HG12	1:D:233:MET:HG2	1.99	0.44
2:A:301:SFF:C8	3:A:302:NDP:H41N	2.47	0.44
1:A:145[A]:LEU:HG	1:B:133:ILE:HD11	2.00	0.43
1:B:199:LYS:CE	1:B:277:GLU:HB3	2.48	0.43
1:B:140[B]:MET:HE3	1:B:144:PHE:CD2	2.52	0.43
1:A:227:VAL:HB	1:A:231:VAL:HB	2.02	0.42
1:C:257:TYR:CE1	1:C:268:ILE:HD12	2.55	0.42
2:D:301:SFF:C8	3:D:302:NDP:H41N	2.50	0.42
1:B:122:THR:O	1:B:124:THR:HG22	2.21	0.41
1:B:225:LYS:HD3	4:B:488:HOH:O	2.20	0.41
1:C:270:ASN:C	1:C:270:ASN:HD22	2.24	0.41
1:D:243:LEU:HG	1:D:247:LYS:HE3	2.02	0.41
1:B:119:ASN:ND2	3:B:302:NDP:H4D	2.36	0.41
1:A:87:HIS:HD2	4:A:434:HOH:O	2.03	0.41
1:A:234:GLN:HA	1:A:235:ALA:HB2	2.02	0.40
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.97	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	268/286 (94%)	257 (96%)	9 (3%)	2 (1%)	22 11
1	B	275/286 (96%)	261 (95%)	13 (5%)	1 (0%)	34 22
1	C	270/286 (94%)	261 (97%)	9 (3%)	0	100 100
1	D	271/286 (95%)	261 (96%)	9 (3%)	1 (0%)	34 22
All	All	1084/1144 (95%)	1040 (96%)	40 (4%)	4 (0%)	34 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ALA
1	D	65	ALA
1	A	219	ASP
1	B	219	ASP

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	227/243 (93%)	218 (96%)	9 (4%)	31	19
1	B	234/243 (96%)	226 (97%)	8 (3%)	37	25
1	C	232/243 (96%)	221 (95%)	11 (5%)	26	13
1	D	230/243 (95%)	222 (96%)	8 (4%)	36	24
All	All	923/972 (95%)	887 (96%)	36 (4%)	35	19

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	160	GLN
1	A	170	SER
1	A	177[A]	TYR
1	A	177[B]	TYR
1	A	230	ILE
1	A	234	GLN
1	A	265	THR
1	A	270	ASN
1	B	20	GLN
1	B	124	THR
1	B	177[A]	TYR
1	B	177[B]	TYR
1	B	225	LYS
1	B	230	ILE
1	B	262	LEU
1	B	270	ASN
1	C	124[A]	THR

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Mol	Chain	Res	Type
1	C	124[B]	THR
1	C	145[A]	LEU
1	C	145[B]	LEU
1	C	160	GLN
1	C	177	TYR
1	C	262	LEU
1	C	266	LEU
1	C	268	ILE
1	C	270	ASN
1	C	287	ASP
1	D	20	GLN
1	D	28	ARG
1	D	177	TYR
1	D	231	VAL
1	D	256	VAL
1	D	278	PHE
1	D	279	LEU
1	D	283	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	234	GLN
1	A	270	ASN
1	B	87	HIS
1	B	105	GLN
1	B	119	ASN
1	B	120	HIS
1	B	127	ASN
1	B	270	ASN
1	C	87	HIS
1	C	105	GLN
1	C	119	ASN
1	C	120	HIS
1	C	135	HIS
1	C	253	GLN
1	C	270	ASN
1	C	285	ASN
1	D	87	HIS

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Mol	Chain	Res	Type
1	D	119	ASN
1	D	120	HIS
1	D	127	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SFF	B	301	-	19,21,21	2.52	6 (31%)	19,30,30	1.71	4 (21%)
2	SFF	C	301	-	19,21,21	2.39	6 (31%)	19,30,30	1.93	4 (21%)
3	NDP	A	302	-	45,52,52	0.59	0	53,80,80	0.93	3 (5%)
3	NDP	D	302	-	45,52,52	0.67	0	53,80,80	0.99	3 (5%)
2	SFF	A	301	-	19,21,21	2.69	7 (36%)	19,30,30	1.58	4 (21%)
2	SFF	D	301	-	19,21,21	2.30	5 (26%)	19,30,30	1.50	2 (10%)
3	NDP	C	302	-	45,52,52	0.68	0	53,80,80	0.88	3 (5%)
3	NDP	B	302	-	45,52,52	0.66	0	53,80,80	0.99	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SFF	B	301	-	-	0/2/38/38	0/2/3/3
2	SFF	C	301	-	-	0/2/38/38	0/2/3/3
3	NDP	A	302	-	-	2/30/77/77	0/5/5/5
3	NDP	D	302	-	-	5/30/77/77	0/5/5/5
2	SFF	A	301	-	-	0/2/38/38	0/2/3/3
2	SFF	D	301	-	-	0/2/38/38	0/2/3/3
3	NDP	C	302	-	-	5/30/77/77	0/5/5/5
3	NDP	B	302	-	-	4/30/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SFF	C8-N9	5.84	1.40	1.29
2	B	301	SFF	O7-C3	-5.75	1.38	1.46
2	C	301	SFF	C8-N9	5.61	1.39	1.29
2	B	301	SFF	C8-N9	5.57	1.39	1.29
2	D	301	SFF	O7-C3	-5.24	1.39	1.46
2	A	301	SFF	O7-C3	-5.23	1.39	1.46
2	C	301	SFF	O7-C3	-5.05	1.39	1.46
2	D	301	SFF	C8-N9	5.02	1.38	1.29
2	A	301	SFF	O12-S10	4.83	1.50	1.44
2	A	301	SFF	O11-S10	4.68	1.50	1.44
2	C	301	SFF	O12-S10	4.54	1.49	1.44
2	D	301	SFF	O12-S10	4.23	1.49	1.44
2	B	301	SFF	O12-S10	3.74	1.48	1.44
2	B	301	SFF	O11-S10	3.55	1.48	1.44
2	D	301	SFF	O11-S10	3.20	1.48	1.44
2	A	301	SFF	C5-C4	3.03	1.57	1.53
2	C	301	SFF	C5-C4	2.99	1.57	1.53
2	B	301	SFF	O7-C8	2.67	1.39	1.34
2	C	301	SFF	O7-C8	2.64	1.39	1.34
2	C	301	SFF	O11-S10	2.60	1.47	1.44
2	B	301	SFF	C5-C4	2.59	1.56	1.53
2	D	301	SFF	O7-C8	2.37	1.38	1.34
2	A	301	SFF	O7-C8	2.20	1.38	1.34
2	A	301	SFF	C15-C14	2.07	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SFF	O12-S10-O11	-6.14	113.13	118.44
2	B	301	SFF	O12-S10-O11	-5.61	113.59	118.44
2	D	301	SFF	O12-S10-O11	-4.47	114.57	118.44
2	A	301	SFF	O12-S10-O11	-4.10	114.89	118.44
2	A	301	SFF	O11-S10-C4	-3.25	104.23	108.91
2	B	301	SFF	O12-S10-N9	2.78	112.92	108.92
3	C	302	NDP	O2N-PN-O1N	2.76	125.90	112.24
2	D	301	SFF	O12-S10-C4	-2.66	105.09	108.91
3	D	302	NDP	O2A-PA-O1A	2.66	125.37	112.24
3	D	302	NDP	O2N-PN-O1N	2.59	125.07	112.24
2	C	301	SFF	O11-S10-N9	2.51	112.53	108.92
2	C	301	SFF	O7-C3-C4	2.39	114.71	111.09
3	B	302	NDP	O2A-PA-O1A	2.37	123.95	112.24
3	C	302	NDP	O7N-C7N-C3N	-2.31	116.55	120.90
3	B	302	NDP	C5A-C6A-N6A	2.26	123.78	120.35
2	A	301	SFF	O12-S10-N9	2.25	112.16	108.92
3	D	302	NDP	C5A-C6A-N6A	2.23	123.75	120.35
3	C	302	NDP	C5A-C6A-N6A	2.22	123.72	120.35
3	A	302	NDP	C5A-C6A-N6A	2.20	123.69	120.35
2	C	301	SFF	O11-S10-C4	-2.19	105.76	108.91
3	A	302	NDP	O2A-PA-O1A	2.17	122.99	112.24
2	A	301	SFF	O11-S10-N9	2.09	111.92	108.92
2	B	301	SFF	O11-S10-C4	-2.08	105.92	108.91
3	A	302	NDP	O7N-C7N-C3N	-2.06	117.01	120.90
3	B	302	NDP	O7N-C7N-C3N	-2.03	117.07	120.90
2	B	301	SFF	O12-S10-C4	-2.00	106.03	108.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	NDP	O4D-C1D-N1N-C6N
3	D	302	NDP	O4D-C1D-N1N-C6N
3	A	302	NDP	O4D-C1D-N1N-C6N
3	C	302	NDP	O4D-C1D-N1N-C6N
3	D	302	NDP	C3B-C2B-O2B-P2B
3	D	302	NDP	C1B-C2B-O2B-P2B
3	A	302	NDP	O4B-C4B-C5B-O5B
3	B	302	NDP	C3B-C2B-O2B-P2B
3	C	302	NDP	C3B-C2B-O2B-P2B
3	B	302	NDP	C5D-O5D-PN-O3
3	C	302	NDP	C2B-O2B-P2B-O2X
3	D	302	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	D	302	NDP	C2N-C3N-C7N-N7N
3	B	302	NDP	O4B-C4B-C5B-O5B
3	C	302	NDP	O4B-C4B-C5B-O5B
3	C	302	NDP	C1B-C2B-O2B-P2B

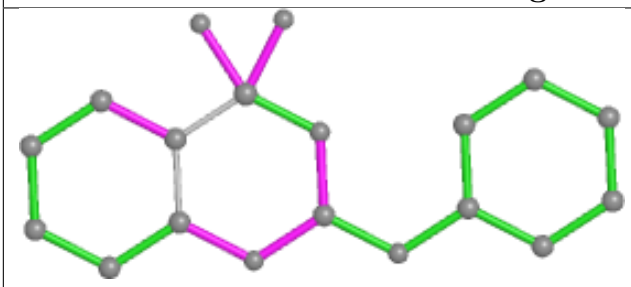
There are no ring outliers.

8 monomers are involved in 10 short contacts:

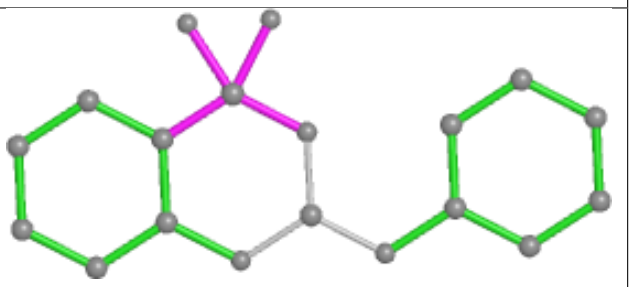
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SFF	1	0
2	C	301	SFF	1	0
3	A	302	NDP	3	0
3	D	302	NDP	2	0
2	A	301	SFF	1	0
2	D	301	SFF	1	0
3	C	302	NDP	2	0
3	B	302	NDP	3	0

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 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.

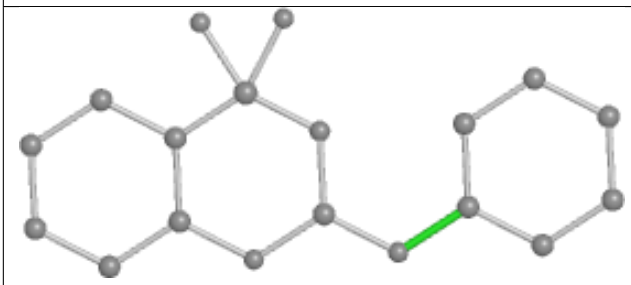
Ligand SFF B 301



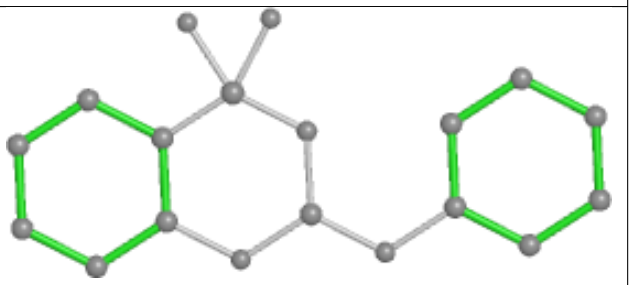
Bond lengths



Bond angles

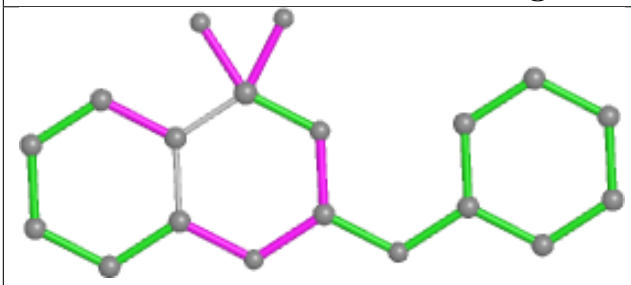


Torsions



Rings

Ligand SFF C 301



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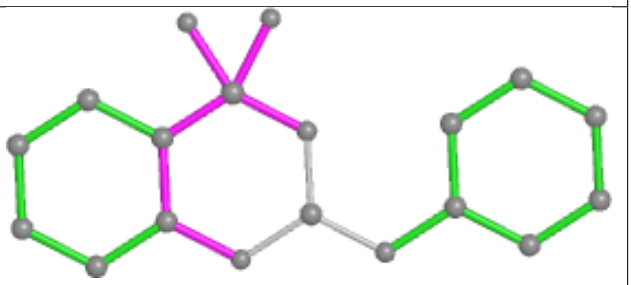

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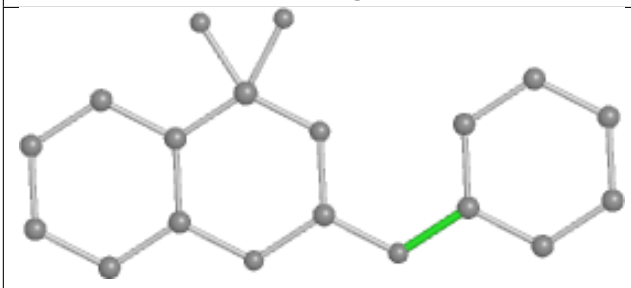

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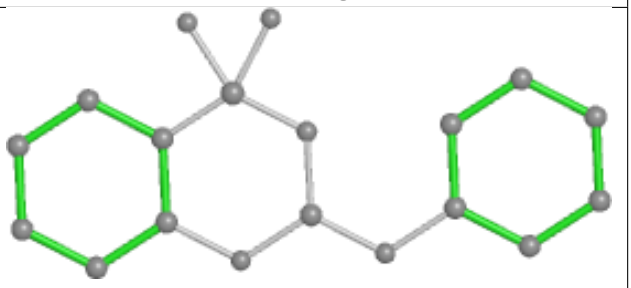
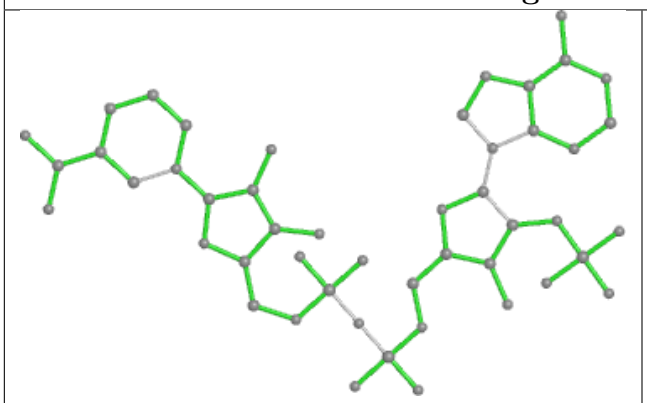


Rings

Ligand NDP A 302



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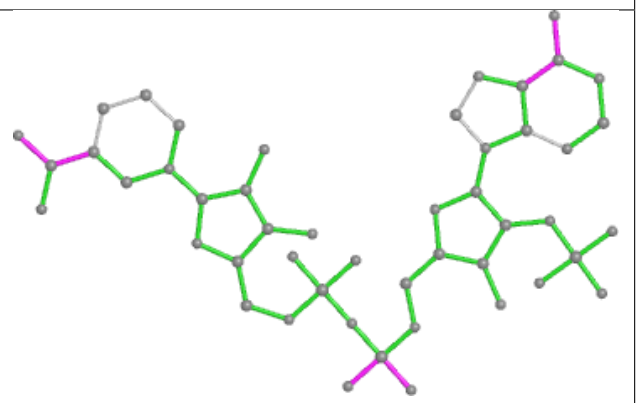

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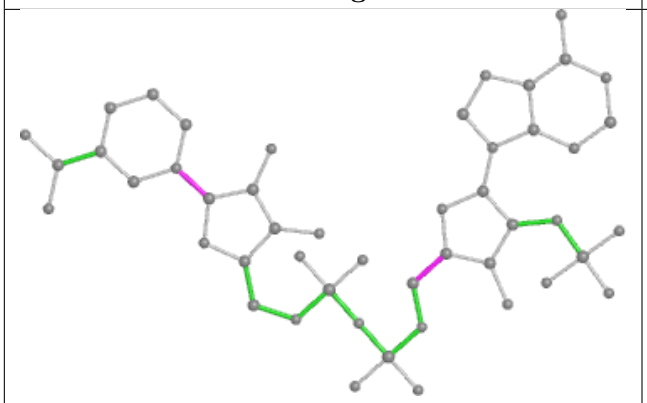

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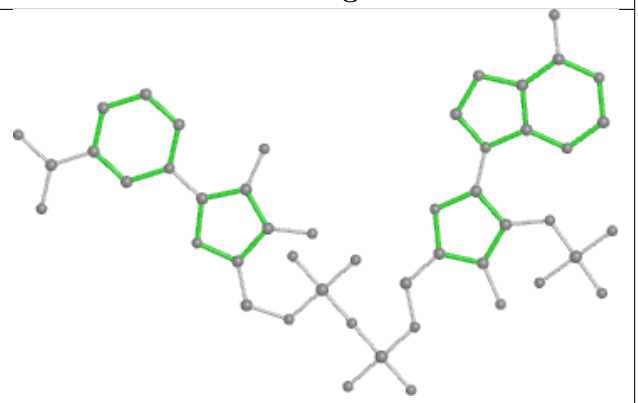

Rings

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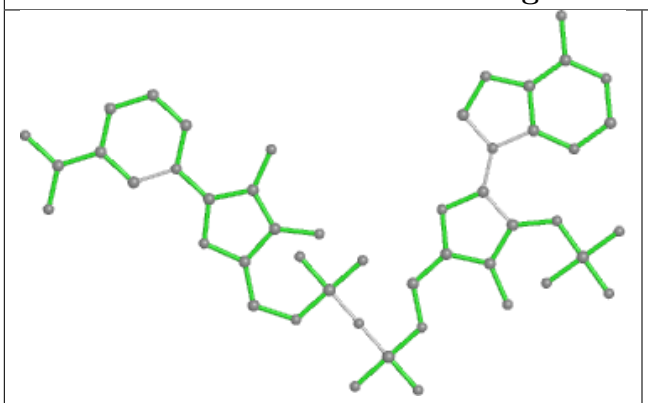
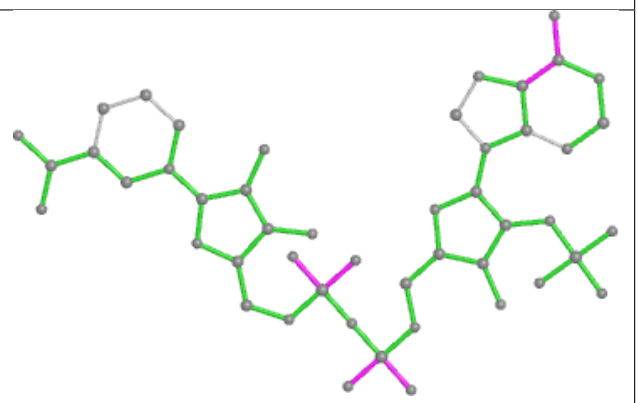
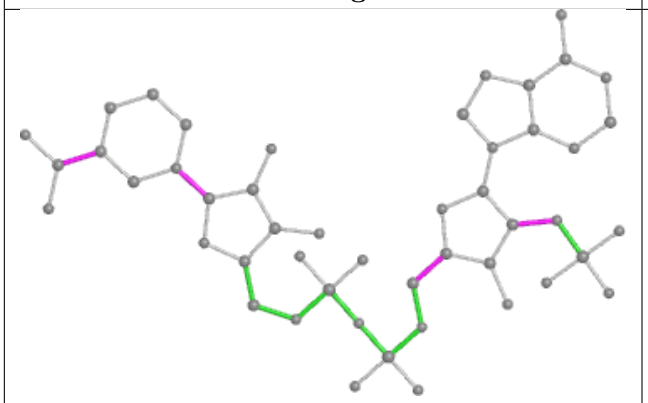


Bond lengths



Bond angles



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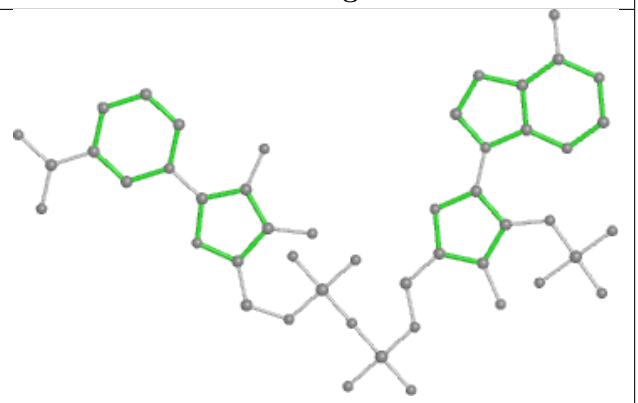
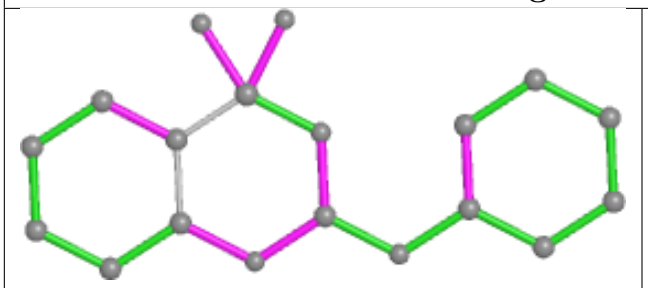


Rings

Ligand SFF A 301



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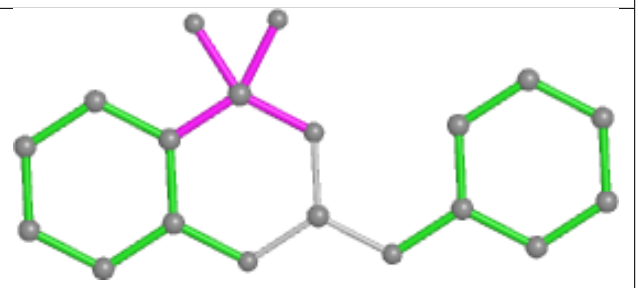
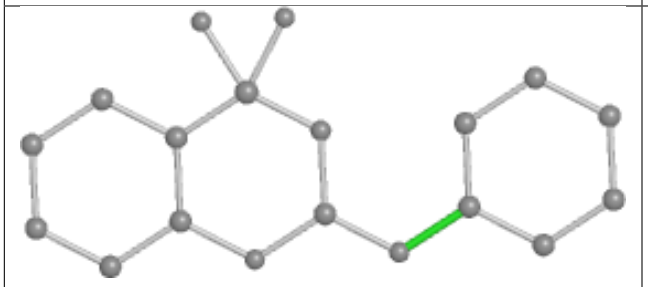
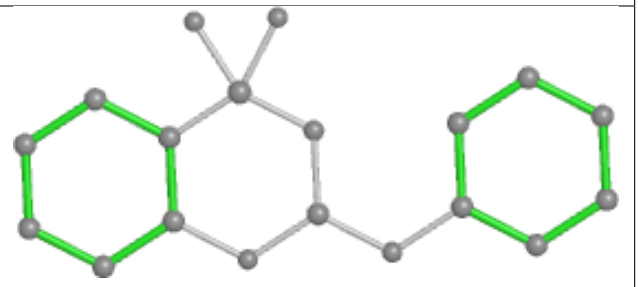


Bond angles

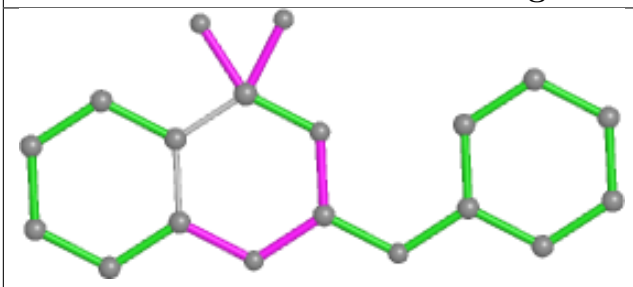


Torsions

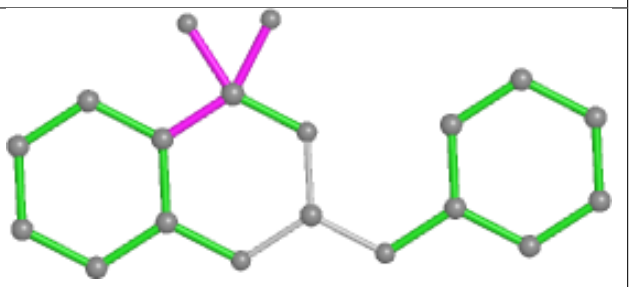


Rings

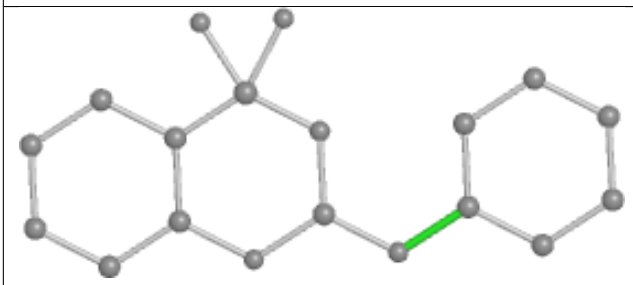
Ligand SFF D 301



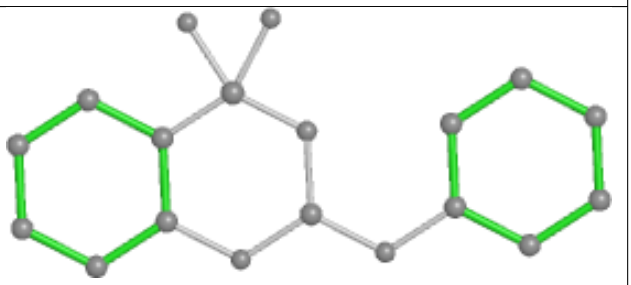
Bond lengths



Bond angles

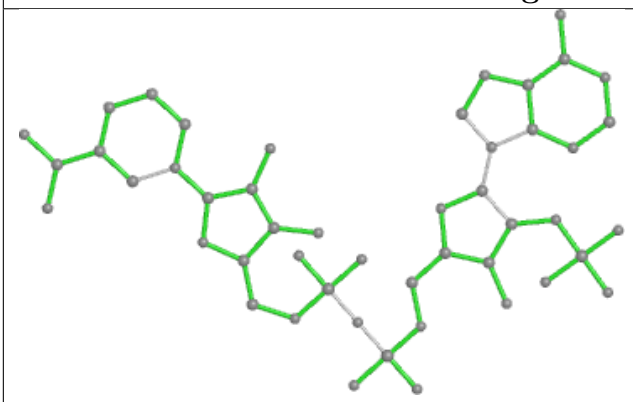


Torsions

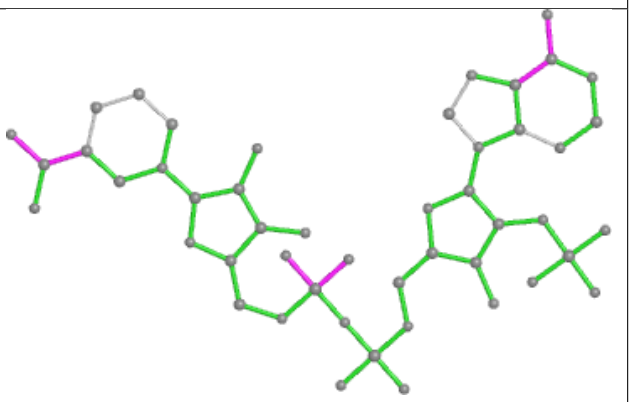


Rings

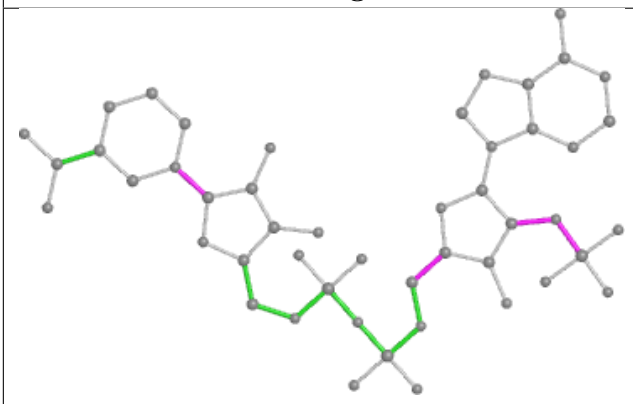
Ligand NDP C 302



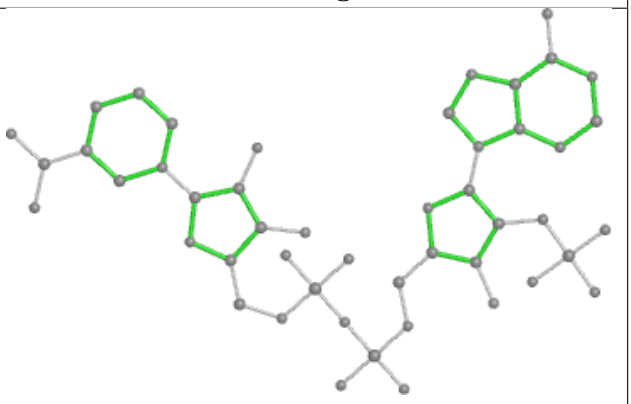
Bond lengths



Bond angles

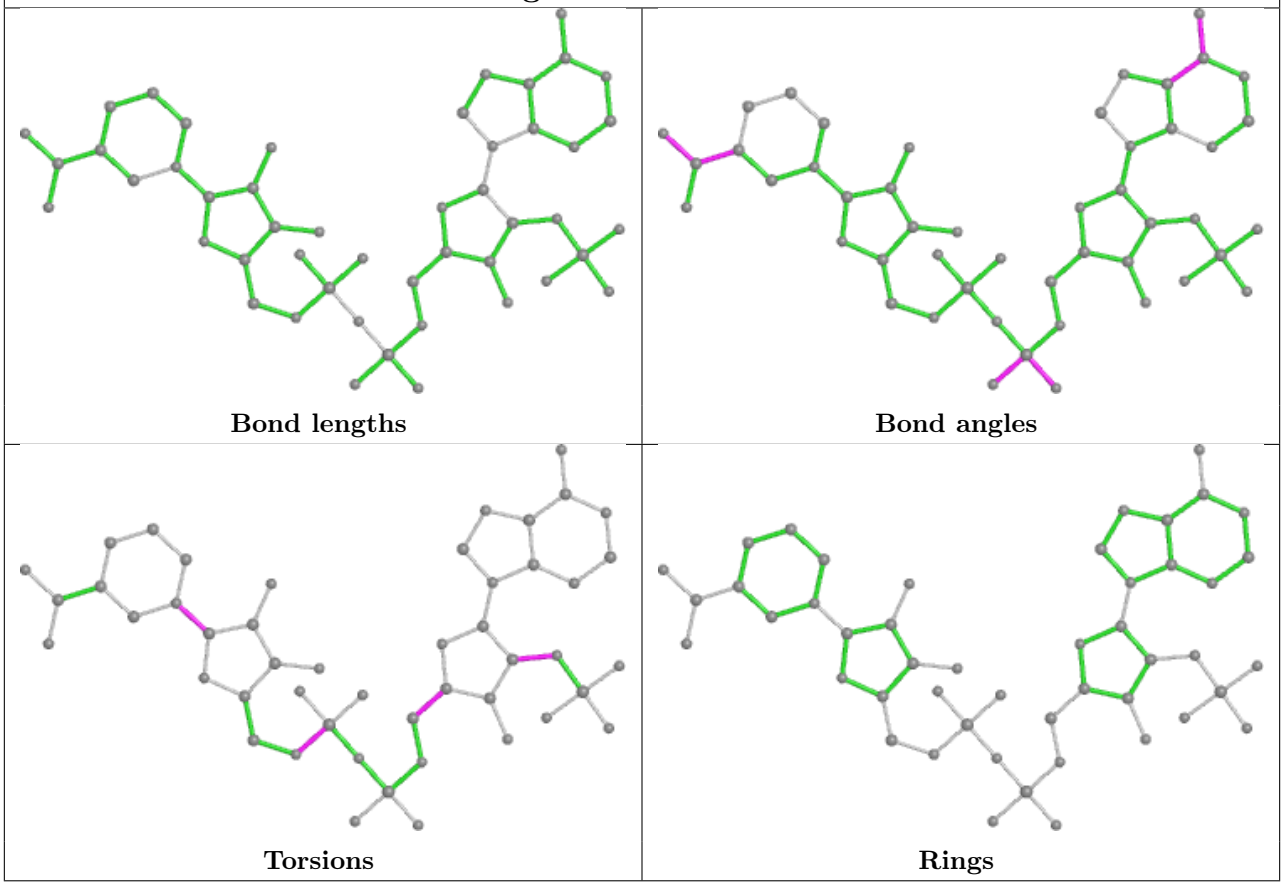


Torsions



Rings

Ligand NDP B 302



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	263/286 (91%)	0.22	15 (5%)	23	32	10, 22, 52, 83	0
1	B	266/286 (93%)	0.01	14 (5%)	26	35	9, 17, 39, 77	0
1	C	263/286 (91%)	0.04	14 (5%)	26	35	10, 21, 46, 78	0
1	D	264/286 (92%)	0.07	15 (5%)	23	32	10, 22, 52, 79	0
All	All	1056/1144 (92%)	0.08	58 (5%)	25	34	9, 21, 49, 83	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	7.2
1	D	232	HIS	6.1
1	A	24	ASN	6.1
1	A	262	LEU	6.1
1	C	263	TRP	5.8
1	C	24	ASN	5.6
1	D	24	ASN	5.1
1	A	232	HIS	5.0
1	A	231	VAL	4.9
1	B	21	GLN	4.8
1	A	21	GLN	4.5
1	A	23	LEU	4.5
1	D	21	GLN	4.4
1	C	21	GLN	4.3
1	D	23	LEU	4.3
1	D	282	THR	4.1
1	C	262	LEU	4.1
1	C	205	ARG	4.0
1	B	23	LEU	3.9
1	D	278	PHE	3.9
1	C	23	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	22	PRO	3.6
1	A	205	ARG	3.4
1	A	22	PRO	3.3
1	C	25	GLU	3.2
1	B	205	ARG	3.2
1	D	22	PRO	3.0
1	A	234	GLN	3.0
1	A	282	THR	2.9
1	B	230	ILE	2.9
1	B	234	GLN	2.8
1	A	230	ILE	2.8
1	B	231	VAL	2.8
1	D	283	SER	2.8
1	B	20	GLN	2.7
1	B	233	MET	2.7
1	D	281	SER	2.7
1	B	284	TYR	2.7
1	D	20	GLN	2.5
1	C	287	ASP	2.4
1	D	279	LEU	2.3
1	C	130[A]	HIS	2.3
1	A	203	VAL	2.3
1	C	285	ASN	2.3
1	A	283	SER	2.2
1	D	233	MET	2.2
1	B	282	THR	2.2
1	C	26	GLU	2.2
1	C	22	PRO	2.2
1	C	266	LEU	2.1
1	A	278	PHE	2.1
1	A	25	GLU	2.1
1	C	167	VAL	2.1
1	D	167	VAL	2.1
1	B	283	SER	2.1
1	D	28	ARG	2.1
1	D	166	VAL	2.0
1	B	25	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)

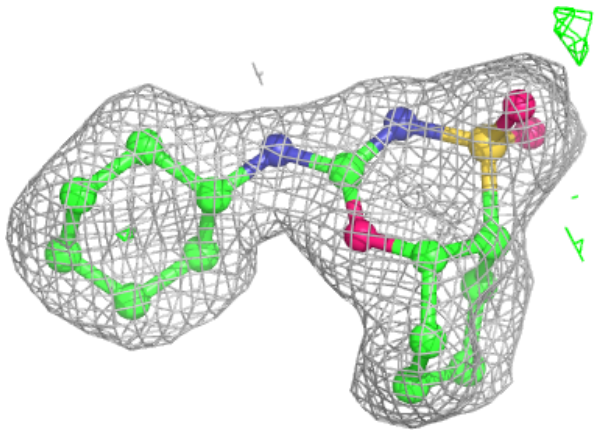
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

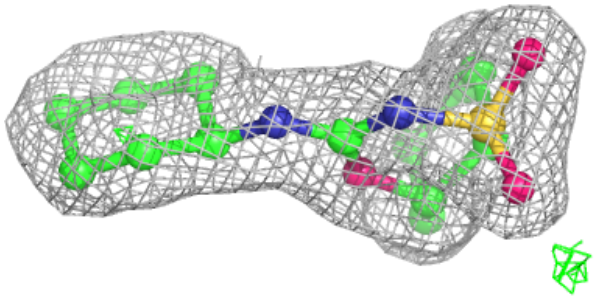
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SFF	D	301	19/19	0.97	0.09	13,18,20,20	0
3	NDP	A	302	48/48	0.97	0.08	10,17,25,27	0
3	NDP	D	302	48/48	0.97	0.07	12,16,19,24	0
2	SFF	C	301	19/19	0.98	0.08	14,19,22,24	0
3	NDP	C	302	48/48	0.98	0.07	9,15,21,24	0
2	SFF	A	301	19/19	0.98	0.08	14,16,19,19	0
2	SFF	B	301	19/19	0.99	0.07	11,14,17,17	0
3	NDP	B	302	48/48	0.99	0.07	8,13,17,19	0

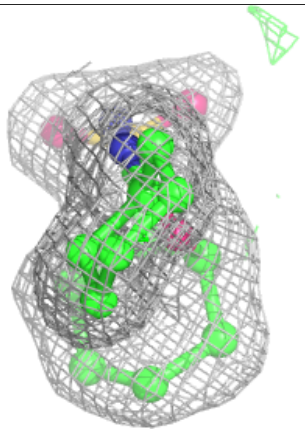
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SFF 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)

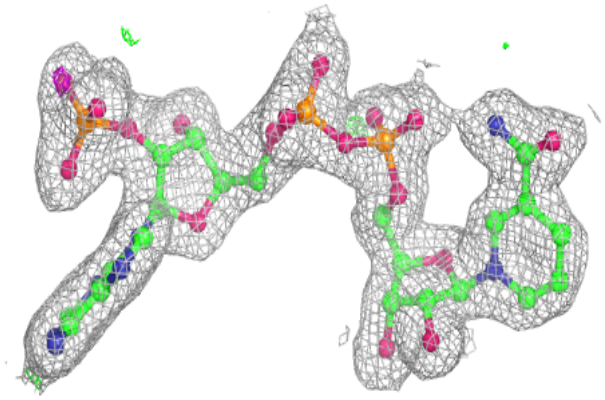


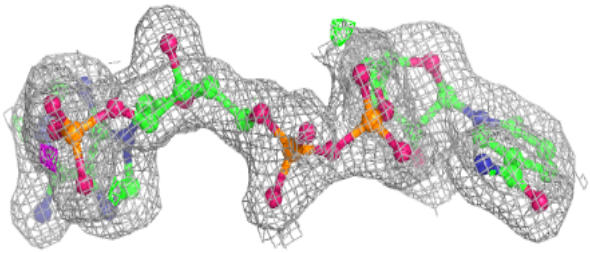


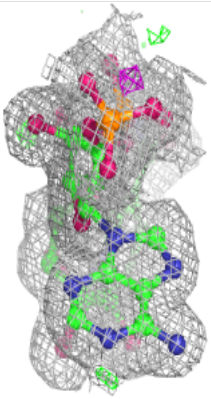


Electron density around NDP A 302:

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

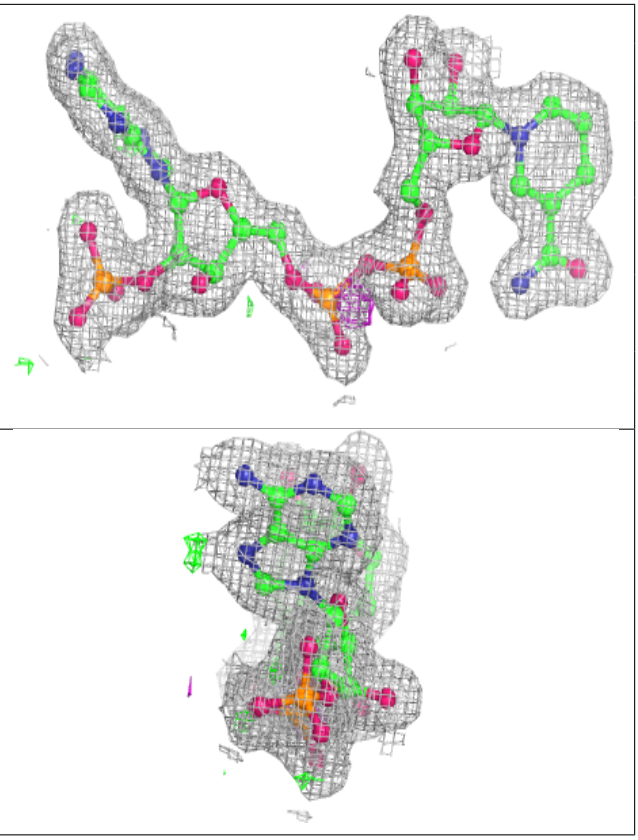






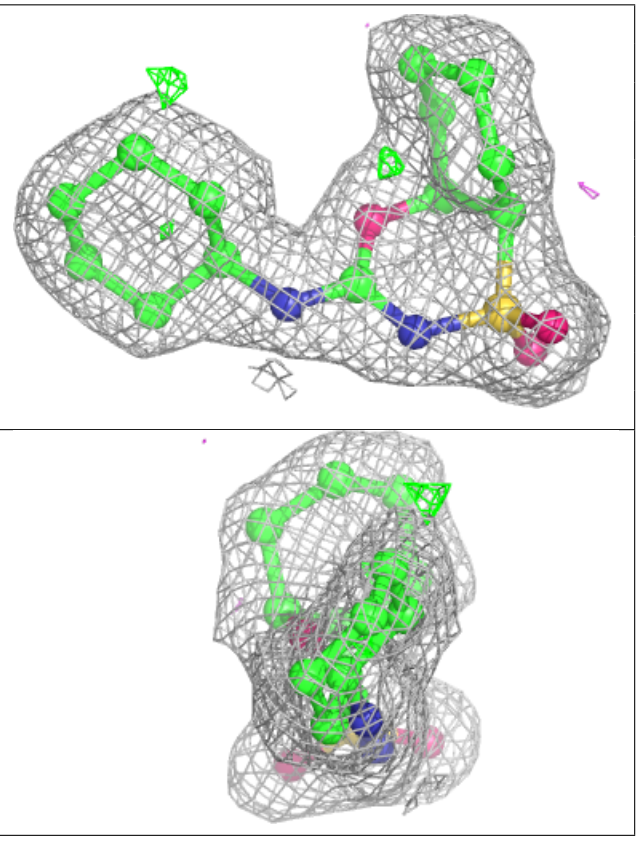
Electron density around NDP D 302:

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



Electron density around SFF 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)



Electron density around NDP C 302:

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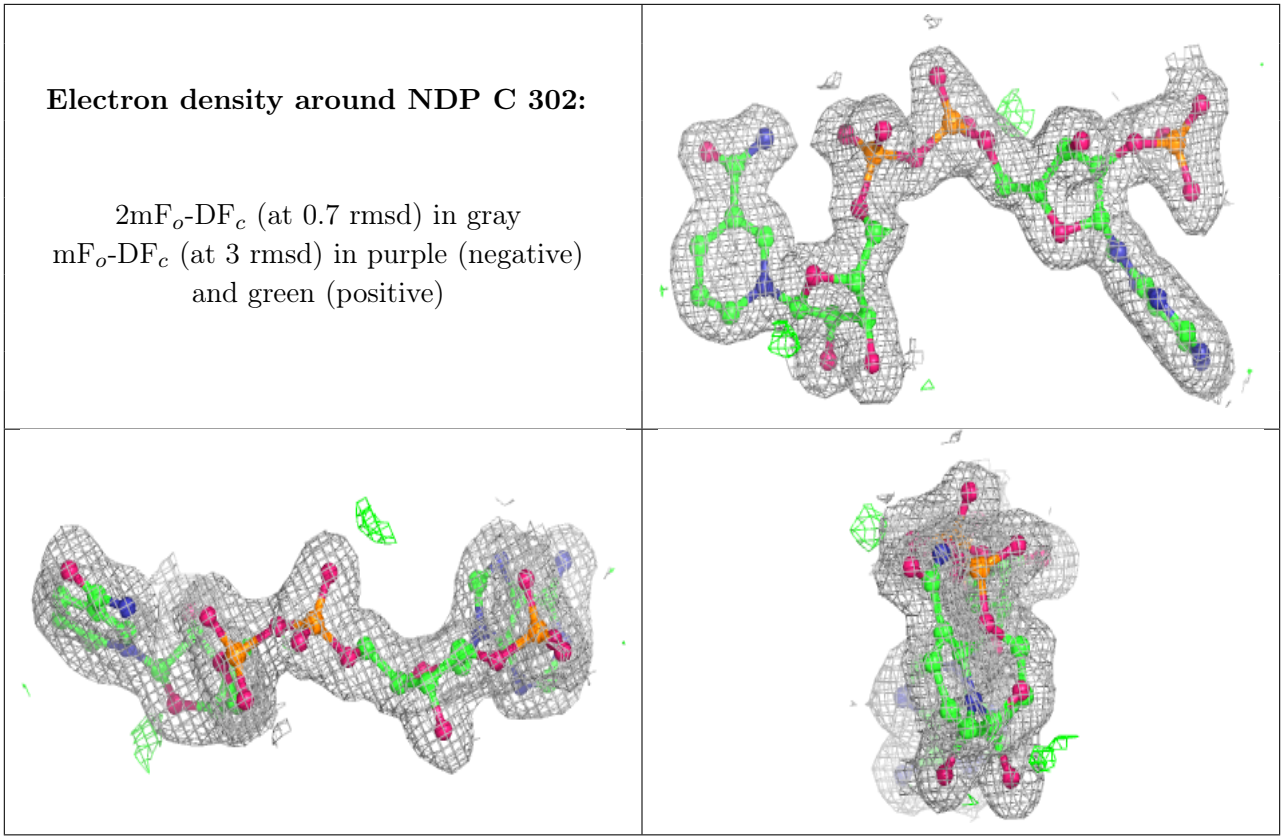
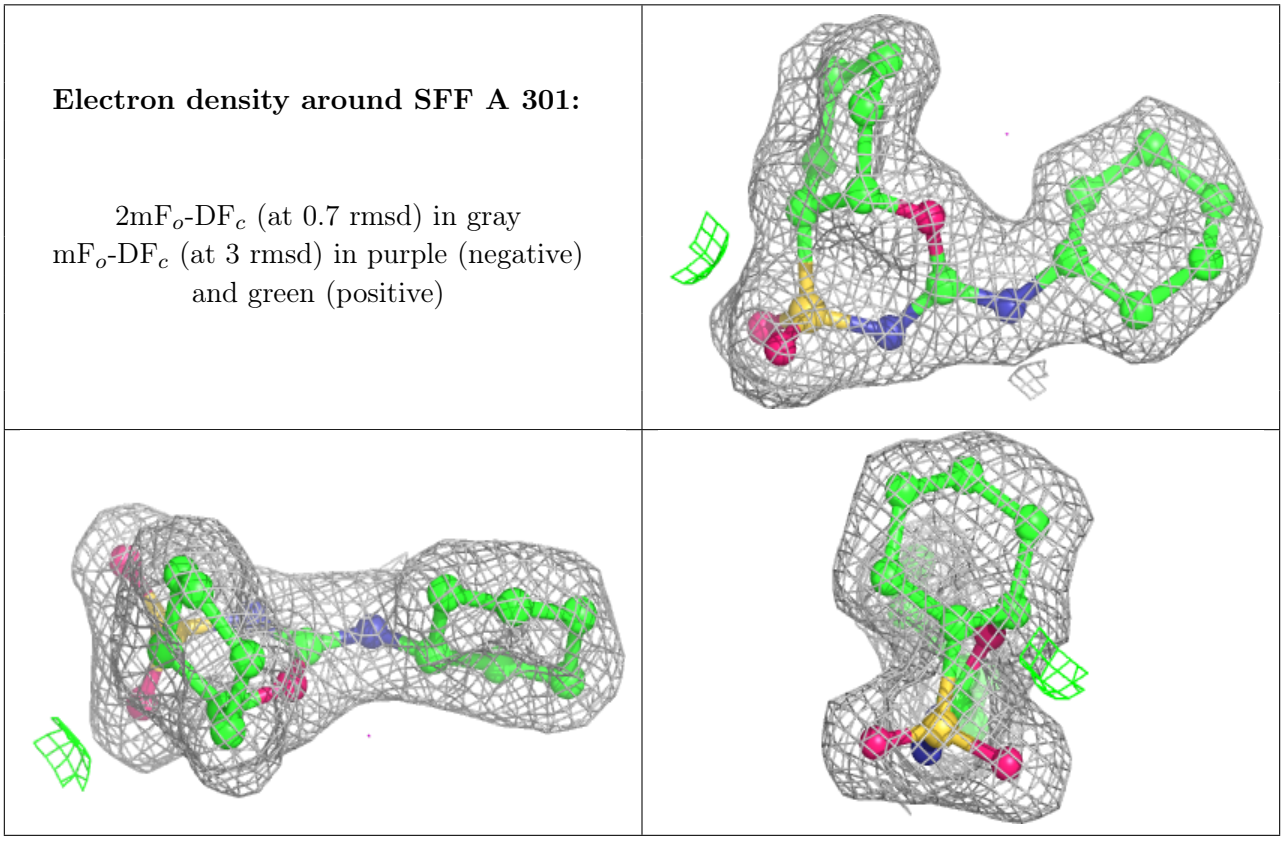
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SFF 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 SFF B 301:

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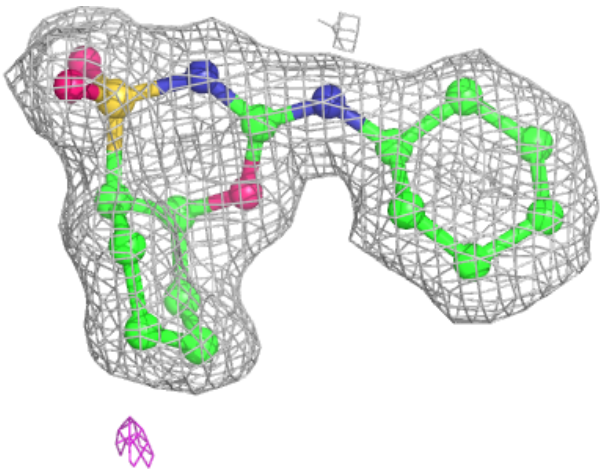
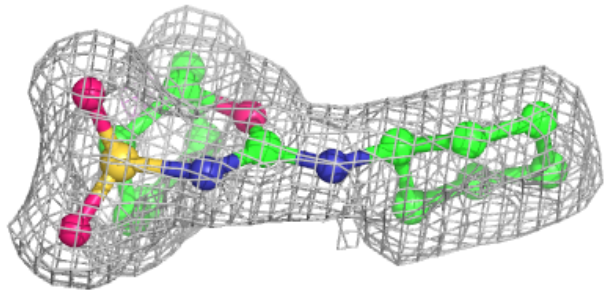
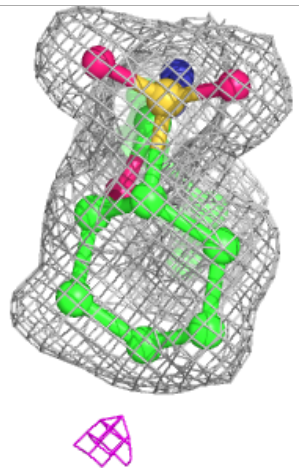
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

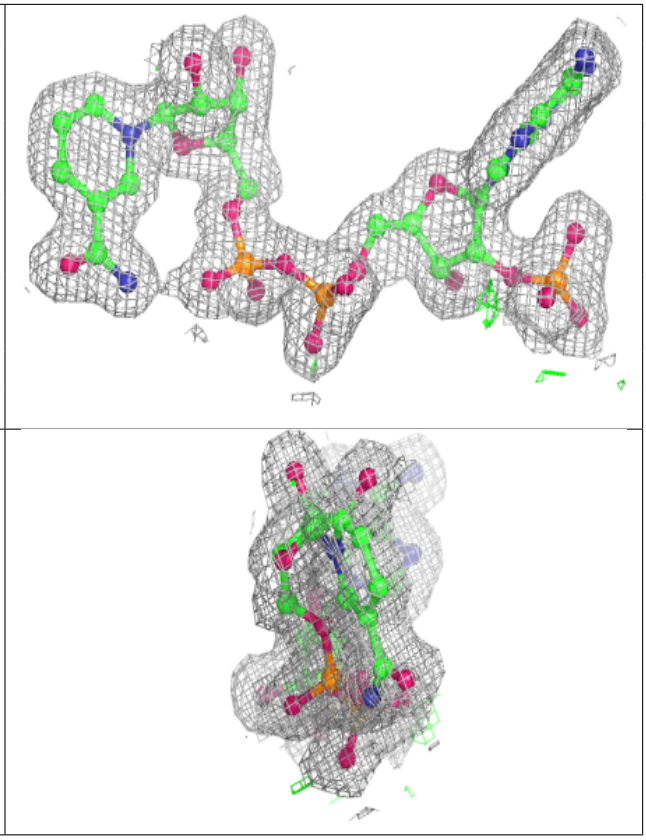






Electron density around NDP B 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.