Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 02:42 PM JST

PDB ID	:	7CS7
Title	:	IiPLR1 with NADP+ and (+)secoisolariciresinol
Authors	:	Shao, K.; Zhang, P.
Deposited on	:	2020-08-14
Resolution	:	2.30 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:

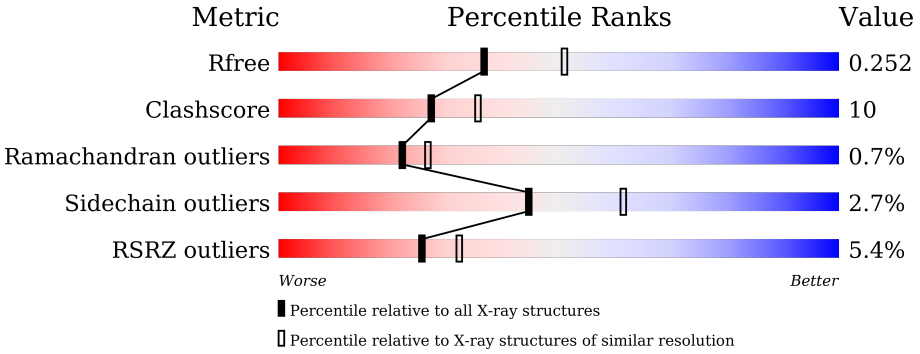
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	317	4% 76% 12% •• 10%
1	B	317	11% 71% 17% • 9%
1	C	317	5% 75% 14% • 10%
1	D	317	3% 72% 17% • 11%
1	E	317	3% 78% 11% • 10%
1	F	317	2% 78% 14% • 8%

2 Entry composition (i)

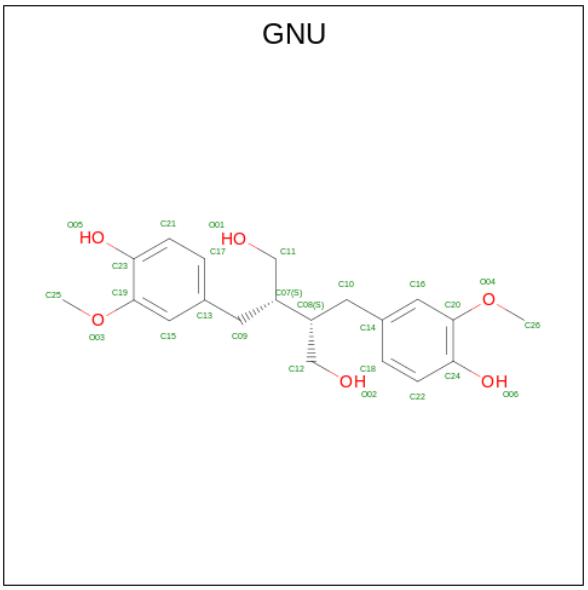
There are 4 unique types of molecules in this entry. The entry contains 15020 atoms, of which 312 are hydrogens and 0 are deuteriums.

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 Pinoresinol-lariciresinol reductase.

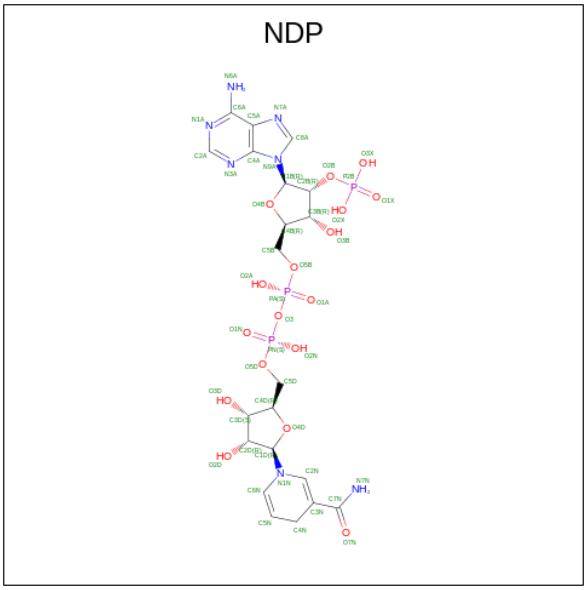
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2243	1426	379	429	9	0	0	0
1	B	287	2263	1441	383	430	9	0	0	0
1	C	284	2233	1420	376	428	9	0	0	0
1	D	283	2229	1418	375	427	9	0	0	0
1	E	286	2247	1428	380	430	9	0	0	0
1	F	293	2308	1469	392	438	9	0	0	0

- Molecule 2 is (2S,3S)-2,3-bis[(3-methoxy-4-oxidanyl-phenyl)methyl]butane-1,4-diol (three-letter code: GNU) (formula: $C_{20}H_{26}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	52	20	26	6	0	0
2	B	1	52	20	26	6	0	0
2	C	1	52	20	26	6	0	0
2	D	1	52	20	26	6	0	0
2	E	1	52	20	26	6	0	0
2	F	1	52	20	26	6	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	74	21	26	7	17	3	0	0
3	B	1	74	21	26	7	17	3	0	0
3	C	1	74	21	26	7	17	3	0	0
3	D	1	74	21	26	7	17	3	0	0
3	E	1	74	21	26	7	17	3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	F	1	74	21	26	7	17	3	0	0

- Molecule 4 is water.

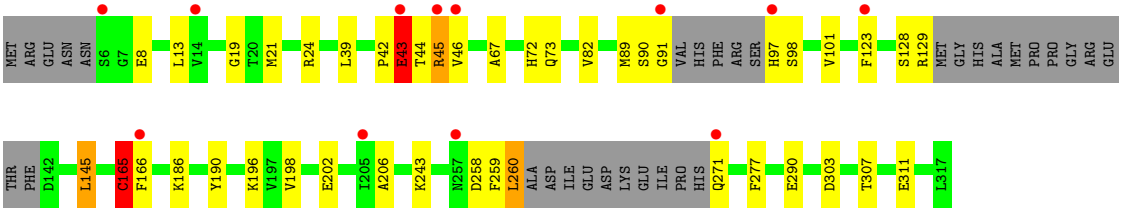
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	141	141	141	0	0
4	B	124	124	124	0	0
4	C	103	103	103	0	0
4	D	102	102	102	0	0
4	E	133	133	133	0	0
4	F	138	138	138	0	0

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.

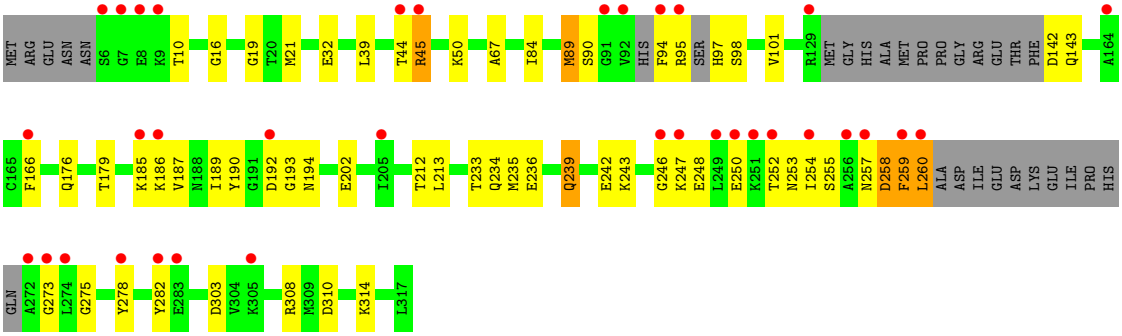
• Molecule 1: Pinoresinol-lariciresinol reductase

Chain A:



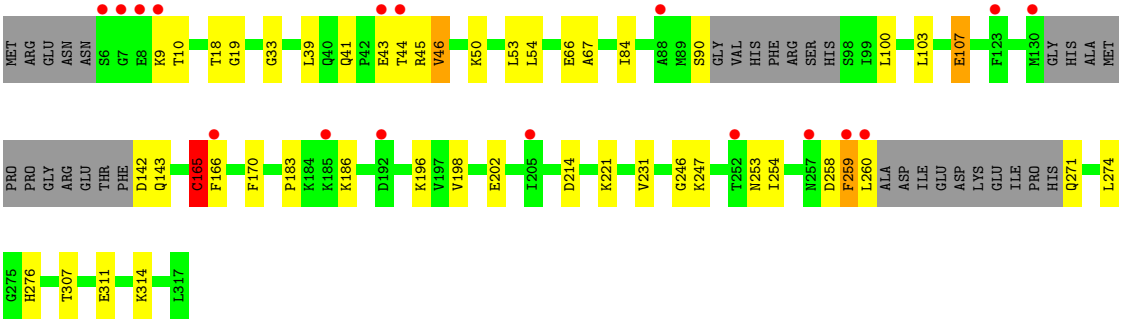
• Molecule 1: Pinoresinol-lariciresinol reductase

Chain B:



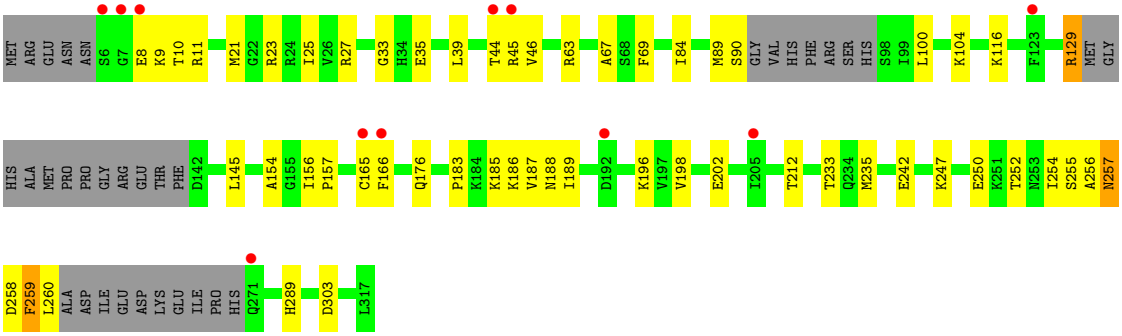
• Molecule 1: Pinoresinol-lariciresinol reductase

Chain C:



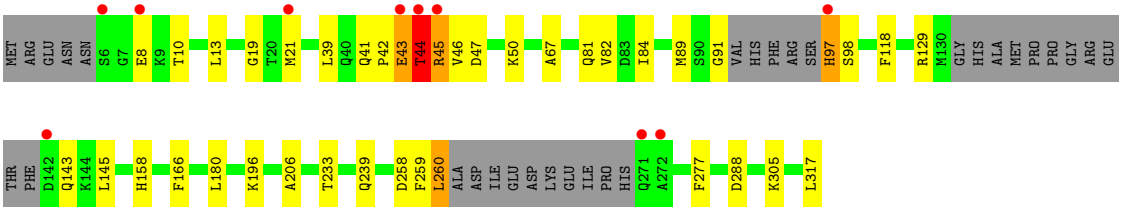
- Molecule 1: Pinoresinol-lariciresinol reductase

Chain D:



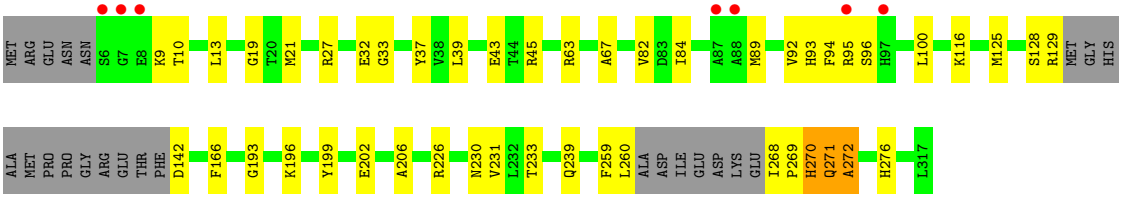
- Molecule 1: Pinoresinol-lariciresinol reductase

Chain E:



- Molecule 1: Pinoresinol-lariciresinol reductase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	243.61Å 243.61Å 76.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.25 – 2.30 32.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.25-2.30) 91.9 (32.25-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.197 , 0.252 0.197 , 0.252	Depositor DCC
R_{free} test set	1994 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15020	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1300e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, GNU

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	0.45	1/2280 (0.0%)	0.59	0/3079
1	B	0.39	0/2300	0.57	0/3104
1	C	0.42	1/2269 (0.0%)	0.56	0/3064
1	D	0.39	0/2265	0.55	0/3059
1	E	0.41	0/2284	0.57	0/3084
1	F	0.41	0/2349	0.58	0/3175
All	All	0.41	2/13747 (0.0%)	0.57	0/18565

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	A	0	1
1	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	CYS	CB-SG	-7.39	1.69	1.82
1	C	165	CYS	CB-SG	-5.21	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	HIS	Peptide
1	E	44	THR	Peptide

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	2243	0	2248	36	0
1	B	2263	0	2270	64	0
1	C	2233	0	2239	43	0
1	D	2229	0	2238	48	0
1	E	2247	0	2249	39	0
1	F	2308	0	2312	39	0
2	A	26	26	0	0	0
2	B	26	26	0	0	0
2	C	26	26	0	1	0
2	D	26	26	0	2	0
2	E	26	26	0	1	0
2	F	26	26	0	2	0
3	A	48	26	25	9	0
3	B	48	26	26	6	0
3	C	48	26	25	7	0
3	D	48	26	24	12	0
3	E	48	26	25	6	0
3	F	48	26	23	2	0
4	A	141	0	0	7	0
4	B	124	0	0	11	0
4	C	103	0	0	11	0
4	D	102	0	0	5	0
4	E	133	0	0	7	0
4	F	138	0	0	9	0
All	All	14708	312	13704	279	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 10.

All (279) 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)
3:D:402:NDP:O4D	3:D:402:NDP:C1D	1.64	1.27
3:E:402:NDP:O4D	3:E:402:NDP:C1D	1.63	1.13
1:C:19:GLY:HA3	3:C:402:NDP:H52A	1.44	0.97
1:B:142:ASP:N	4:B:501:HOH:O	1.97	0.97
1:F:268:ILE:HG22	1:F:269:PRO:HD3	1.48	0.93
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.50	0.92
1:A:42:PRO:HB2	1:A:45:ARG:HH22	1.34	0.91
1:F:239:GLN:NE2	4:F:502:HOH:O	2.05	0.89
1:E:260:LEU:HD13	1:E:260:LEU:H	1.39	0.85
1:A:91:GLY:O	4:A:501:HOH:O	1.94	0.83
1:F:270:HIS:HA	1:F:271:GLN:HB3	1.60	0.83
1:F:27:ARG:NH1	4:F:503:HOH:O	2.12	0.82
1:B:19:GLY:HA3	3:B:402:NDP:H52A	1.62	0.81
1:F:21:MET:CE	1:F:206:ALA:HB2	2.10	0.81
1:A:45:ARG:H	1:A:45:ARG:HD3	1.46	0.81
1:E:45:ARG:H	1:E:45:ARG:HD2	1.45	0.81
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.62	0.81
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.63	0.80
1:C:100:LEU:HD21	1:C:143:GLN:HG2	1.62	0.80
1:F:21:MET:HE1	1:F:206:ALA:HB2	1.63	0.80
1:B:233:THR:HG22	1:B:236:GLU:OE1	1.82	0.79
1:D:10:THR:HG21	1:D:84:ILE:HD12	1.65	0.78
1:B:258:ASP:OD1	4:B:502:HOH:O	2.02	0.77
1:E:91:GLY:O	4:E:501:HOH:O	2.02	0.77
1:B:257:ASN:N	4:B:502:HOH:O	2.17	0.75
1:B:185:LYS:NZ	1:B:250:GLU:OE2	2.19	0.75
1:A:73:GLN:OE1	4:A:502:HOH:O	2.05	0.75
1:C:44:THR:HG21	1:C:54:LEU:CD1	2.17	0.75
1:B:247:LYS:NZ	1:B:248:GLU:O	2.18	0.75
1:B:233:THR:HG23	1:B:236:GLU:H	1.51	0.74
1:F:202:GLU:OE2	4:F:501:HOH:O	2.04	0.74
1:B:95:ARG:HA	1:B:143:GLN:CD	2.07	0.74
1:C:44:THR:HG21	1:C:54:LEU:HD12	1.68	0.73
1:C:247:LYS:NZ	4:C:505:HOH:O	2.22	0.72
1:A:260:LEU:HD22	1:A:260:LEU:H	1.53	0.71
1:F:93:HIS:ND1	1:F:271:GLN:O	2.24	0.71
1:C:45:ARG:NH2	4:C:501:HOH:O	1.95	0.70
1:B:89:MET:HE2	1:B:89:MET:H	1.55	0.70
1:A:202:GLU:OE2	4:A:503:HOH:O	2.09	0.69
1:C:260:LEU:H	1:C:260:LEU:HD22	1.58	0.69
1:C:18:THR:OG1	3:C:402:NDP:O1X	2.08	0.69
1:A:42:PRO:O	1:A:44:THR:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:HG23	1:B:45:ARG:HD3	1.74	0.69
1:C:271:GLN:HB2	1:C:274:LEU:HD12	1.75	0.69
1:D:8:GLU:OE2	1:D:8:GLU:HA	1.92	0.69
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.73	0.68
1:D:183:PRO:O	4:D:501:HOH:O	2.11	0.68
1:E:42:PRO:HD2	1:E:43:GLU:HG2	1.76	0.68
1:D:44:THR:HG22	1:D:45:ARG:HG3	1.75	0.68
1:E:39:LEU:HD11	1:E:67:ALA:HB3	1.73	0.68
1:B:44:THR:O	1:B:45:ARG:HG3	1.94	0.68
1:B:193:GLY:O	1:B:233:THR:OG1	2.11	0.68
1:E:305:LYS:NZ	4:E:505:HOH:O	2.25	0.68
1:D:185:LYS:NZ	1:D:250:GLU:OE1	2.27	0.67
1:F:271:GLN:HA	4:F:512:HOH:O	1.94	0.67
1:E:19:GLY:HA3	3:E:402:NDP:H52A	1.76	0.67
1:D:166:PHE:HB3	1:D:202:GLU:OE1	1.95	0.66
1:D:258:ASP:O	1:D:260:LEU:HD22	1.96	0.66
1:D:166:PHE:H	3:D:402:NDP:H72N	1.41	0.66
1:D:257:ASN:OD1	4:D:502:HOH:O	2.14	0.66
1:A:39:LEU:HD11	1:A:67:ALA:HB3	1.79	0.65
1:F:270:HIS:HA	1:F:271:GLN:CB	2.22	0.65
1:D:202:GLU:OE2	4:D:503:HOH:O	2.15	0.65
1:C:9:LYS:HD3	1:C:33:GLY:O	1.97	0.64
1:B:94:PHE:N	4:B:508:HOH:O	2.29	0.64
1:F:94:PHE:HZ	1:F:125:MET:HE1	1.61	0.64
1:C:214:ASP:OD2	4:C:502:HOH:O	2.14	0.64
1:E:21:MET:CE	1:E:206:ALA:HB2	2.27	0.64
1:A:43:GLU:O	1:A:43:GLU:HG2	1.99	0.62
1:B:98:SER:O	1:B:101:VAL:HG12	1.98	0.62
1:C:165:CYS:HB2	1:C:198:VAL:O	1.99	0.62
1:A:43:GLU:O	1:A:43:GLU:CG	2.48	0.61
1:F:10:THR:HG21	1:F:84:ILE:HD12	1.81	0.61
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.81	0.61
1:B:275:GLY:N	4:B:505:HOH:O	2.24	0.61
1:E:44:THR:HG21	4:E:553:HOH:O	2.01	0.61
1:B:19:GLY:CA	3:B:402:NDP:H52A	2.31	0.60
1:D:9:LYS:HD2	1:D:33:GLY:O	2.01	0.60
1:C:196:LYS:HD2	1:C:231:VAL:HG12	1.82	0.60
1:E:97:HIS:N	1:E:143:GLN:HE22	2.00	0.60
1:B:89:MET:HE2	1:B:89:MET:N	2.17	0.60
1:C:45:ARG:NH2	1:C:66:GLU:OE1	2.34	0.60
1:D:257:ASN:N	4:D:502:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ASP:O	1:E:260:LEU:N	2.35	0.60
1:B:254:ILE:HG23	1:B:258:ASP:HB2	1.84	0.59
1:D:186:LYS:HE2	1:D:252:THR:HB	1.84	0.59
1:A:123:PHE:O	3:A:402:NDP:H2N	2.01	0.59
1:C:100:LEU:HD21	1:C:143:GLN:CG	2.32	0.59
1:B:186:LYS:HG2	1:B:250:GLU:HB3	1.84	0.59
1:A:165:CYS:HB2	1:A:198:VAL:O	2.03	0.59
1:E:41:GLN:OE1	4:E:502:HOH:O	2.16	0.58
1:B:90:SER:OG	3:B:402:NDP:H8A	2.03	0.58
1:C:170:PHE:HE2	3:C:402:NDP:N7N	2.01	0.58
1:B:190:TYR:HD2	1:B:234:GLN:OE1	1.86	0.58
1:C:90:SER:OG	1:C:90:SER:O	2.21	0.58
1:D:189:ILE:HD12	1:D:235:MET:HE2	1.85	0.58
1:F:94:PHE:HB3	1:F:142:ASP:HB3	1.86	0.58
1:F:94:PHE:CZ	1:F:125:MET:HE1	2.40	0.57
1:B:278:TYR:CD1	1:B:282:TYR:HB2	2.39	0.57
1:E:10:THR:HG21	1:E:84:ILE:HD12	1.87	0.57
1:B:242:GLU:HG2	1:B:247:LYS:O	2.05	0.57
1:F:43:GLU:HG2	4:F:623:HOH:O	2.05	0.57
3:A:402:NDP:O1X	3:A:402:NDP:O3B	2.23	0.57
1:D:35:GLU:OE2	1:D:63:ARG:NH1	2.38	0.57
1:B:16:GLY:N	4:B:514:HOH:O	2.39	0.56
1:C:10:THR:HG21	1:C:84:ILE:HD12	1.87	0.56
1:D:186:LYS:HE2	1:D:252:THR:CB	2.34	0.56
1:F:92:VAL:O	2:F:401:GNU:O01	2.24	0.56
1:B:202:GLU:CD	1:B:202:GLU:H	2.08	0.56
1:A:307:THR:HG23	1:A:311:GLU:HG2	1.88	0.56
1:C:271:GLN:NE2	4:C:511:HOH:O	2.39	0.56
1:B:314:LYS:NZ	4:B:512:HOH:O	2.36	0.55
1:F:271:GLN:O	1:F:272:ALA:HB3	2.06	0.55
1:A:166:PHE:H	3:A:402:NDP:H72N	1.54	0.55
1:E:45:ARG:H	1:E:45:ARG:CD	2.19	0.55
1:E:44:THR:OG1	1:E:46:VAL:HG22	2.07	0.55
1:D:129:ARG:HH12	1:D:289:HIS:CD2	2.23	0.55
1:D:196:LYS:HD3	1:D:233:THR:HG23	1.89	0.55
1:E:97:HIS:N	4:E:510:HOH:O	2.40	0.55
1:D:255:SER:HB3	1:D:258:ASP:OD2	2.07	0.54
1:F:125:MET:HE2	1:F:276:HIS:CD2	2.42	0.54
1:F:196:LYS:HE2	1:F:233:THR:HG23	1.88	0.54
1:B:254:ILE:CG2	1:B:258:ASP:HB2	2.37	0.54
1:F:268:ILE:CG2	1:F:269:PRO:HD3	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:HG2	4:C:501:HOH:O	2.06	0.54
1:C:246:GLY:C	1:C:247:LYS:HD2	2.28	0.54
1:C:166:PHE:CD1	3:C:402:NDP:H41N	2.42	0.54
1:E:41:GLN:HB3	1:E:43:GLU:HG2	1.89	0.54
1:A:13:LEU:HB2	1:A:82:VAL:HG11	1.90	0.53
1:B:95:ARG:O	1:B:143:GLN:NE2	2.42	0.53
1:F:269:PRO:O	1:F:270:HIS:CB	2.56	0.53
1:B:278:TYR:HD1	1:B:282:TYR:HB2	1.73	0.53
1:B:258:ASP:O	1:B:260:LEU:HD13	2.08	0.53
1:D:89:MET:O	3:D:402:NDP:H52N	2.07	0.53
1:B:189:ILE:O	1:B:253:ASN:HA	2.09	0.53
1:D:166:PHE:HB2	3:D:402:NDP:N7N	2.24	0.53
1:B:21:MET:HE3	1:B:166:PHE:CZ	2.43	0.53
1:B:176:GLN:NE2	1:B:187:VAL:HG23	2.24	0.53
1:D:90:SER:HA	3:D:402:NDP:PA	2.48	0.53
1:B:44:THR:HG22	4:B:510:HOH:O	2.08	0.52
1:C:166:PHE:HB3	1:C:202:GLU:OE2	2.09	0.52
1:D:186:LYS:HE2	1:D:252:THR:OG1	2.09	0.52
1:E:129:ARG:NH2	1:E:288:ASP:OD2	2.42	0.52
1:A:42:PRO:HB2	1:A:45:ARG:NH2	2.16	0.51
1:A:72:HIS:ND1	4:A:510:HOH:O	2.35	0.51
1:F:226:ARG:NH1	4:F:504:HOH:O	2.27	0.51
1:E:89:MET:O	3:E:402:NDP:H52N	2.11	0.51
1:A:190:TYR:CE2	1:A:277:PHE:HE2	2.29	0.51
1:E:196:LYS:HE3	1:E:233:THR:HG23	1.93	0.51
1:E:260:LEU:H	1:E:260:LEU:CD1	2.18	0.51
1:F:32:GLU:HG3	4:F:515:HOH:O	2.11	0.51
1:C:183:PRO:O	4:C:503:HOH:O	2.19	0.50
1:B:190:TYR:CD2	1:B:234:GLN:OE1	2.64	0.50
1:C:142:ASP:N	4:C:516:HOH:O	2.44	0.50
1:E:21:MET:HE3	1:E:206:ALA:HB2	1.92	0.50
1:D:23:ARG:O	1:D:27:ARG:HG3	2.12	0.50
1:F:116:LYS:NZ	4:F:516:HOH:O	2.45	0.50
1:B:166:PHE:H	3:B:402:NDP:H72N	1.60	0.49
1:D:69:PHE:O	1:D:104:LYS:HD3	2.12	0.49
1:E:47:ASP:OD2	1:E:50:LYS:HD2	2.11	0.49
1:E:239:GLN:OE1	4:E:503:HOH:O	2.20	0.49
1:D:166:PHE:N	3:D:402:NDP:H72N	2.09	0.49
2:C:401:GNU:C09	3:C:402:NDP:H42N	2.43	0.49
1:C:253:ASN:C	1:C:254:ILE:HD12	2.33	0.49
1:A:89:MET:O	3:A:402:NDP:H52N	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HD12	1:D:254:ILE:N	2.27	0.49
1:A:166:PHE:CD1	3:A:402:NDP:C7N	2.96	0.49
1:B:255:SER:HB2	1:B:258:ASP:OD1	2.12	0.49
1:F:270:HIS:N	4:F:512:HOH:O	2.39	0.49
1:B:273:GLY:HA2	4:B:554:HOH:O	2.12	0.48
1:B:239:GLN:NE2	4:B:516:HOH:O	2.43	0.48
1:D:189:ILE:HD12	1:D:235:MET:CE	2.43	0.48
1:C:45:ARG:NH1	4:C:501:HOH:O	2.43	0.48
1:D:166:PHE:CD2	3:D:402:NDP:C7N	2.96	0.48
1:D:165:CYS:HB2	1:D:198:VAL:O	2.13	0.48
1:B:192:ASP:OD1	1:B:192:ASP:O	2.31	0.48
1:F:271:GLN:O	1:F:272:ALA:CB	2.62	0.48
1:F:13:LEU:HB2	1:F:82:VAL:HG11	1.96	0.48
1:C:221:LYS:NZ	4:C:504:HOH:O	2.19	0.47
1:D:11:ARG:HG2	1:D:35:GLU:HB3	1.95	0.47
1:C:271:GLN:N	4:C:511:HOH:O	2.47	0.47
1:E:45:ARG:CD	1:E:45:ARG:N	2.77	0.47
1:A:44:THR:O	1:A:46:VAL:N	2.48	0.47
1:F:93:HIS:HB2	1:F:95:ARG:O	2.15	0.47
1:C:103:LEU:O	1:C:107:GLU:HG2	2.15	0.47
1:C:170:PHE:HE2	3:C:402:NDP:H71N	1.62	0.47
1:C:254:ILE:HD12	1:C:254:ILE:N	2.30	0.47
1:A:98:SER:O	1:A:101:VAL:HB	2.15	0.47
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.97	0.47
1:A:258:ASP:O	1:A:260:LEU:HD13	2.15	0.46
1:B:166:PHE:CD2	3:B:402:NDP:H41N	2.50	0.46
1:C:41:GLN:O	1:C:44:THR:HB	2.14	0.46
1:C:46:VAL:O	1:C:46:VAL:HG13	2.14	0.46
1:D:89:MET:O	3:D:402:NDP:H3D	2.16	0.46
1:B:235:MET:SD	1:B:239:GLN:OE1	2.74	0.46
1:D:154:ALA:HB3	1:D:156:ILE:HD12	1.97	0.46
1:A:290:GLU:HG3	4:A:504:HOH:O	2.15	0.46
1:C:258:ASP:O	1:C:260:LEU:N	2.48	0.46
1:D:188:ASN:OD1	1:D:254:ILE:HD11	2.16	0.46
1:A:128:SER:HA	1:A:145:LEU:HD11	1.97	0.46
1:B:303:ASP:OD1	1:B:303:ASP:N	2.47	0.46
1:C:254:ILE:HG23	1:C:258:ASP:HB2	1.97	0.46
1:E:97:HIS:CG	1:E:98:SER:H	2.34	0.46
1:B:44:THR:C	1:B:45:ARG:HG3	2.35	0.46
1:A:303:ASP:OD1	1:A:303:ASP:N	2.43	0.46
1:A:90:SER:HA	3:A:402:NDP:O3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:THR:HG21	1:B:84:ILE:HD12	1.99	0.45
1:B:97:HIS:HA	1:B:143:GLN:HE22	1.81	0.45
1:F:128:SER:O	1:F:129:ARG:HB3	2.16	0.45
1:C:166:PHE:CD2	3:C:402:NDP:O7N	2.70	0.45
1:E:81:GLN:NE2	4:E:504:HOH:O	2.21	0.45
1:E:97:HIS:N	1:E:97:HIS:HD1	2.14	0.45
1:B:258:ASP:OD1	1:B:258:ASP:N	2.49	0.45
1:B:194:ASN:HA	1:B:233:THR:OG1	2.17	0.45
1:D:90:SER:OG	3:D:402:NDP:H8A	2.17	0.45
1:E:42:PRO:O	1:E:43:GLU:C	2.56	0.45
1:E:44:THR:OG1	1:E:46:VAL:CG2	2.64	0.45
1:C:45:ARG:HG3	1:C:45:ARG:HH11	1.82	0.44
1:D:303:ASP:OD2	1:D:303:ASP:N	2.50	0.44
1:A:166:PHE:CD2	3:A:402:NDP:H41N	2.52	0.44
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.75	0.44
3:D:402:NDP:O5D	3:D:402:NDP:H6N	2.17	0.44
1:D:116:LYS:O	1:D:157:PRO:HG2	2.18	0.44
1:B:243:LYS:HA	1:B:243:LYS:HD2	1.76	0.44
1:D:90:SER:HA	3:D:402:NDP:O3	2.18	0.44
1:E:145:LEU:HD12	1:E:145:LEU:HA	1.82	0.44
1:A:21:MET:CE	1:A:206:ALA:HB2	2.47	0.44
1:B:190:TYR:HD1	1:B:259:PHE:CE1	2.36	0.44
1:B:194:ASN:O	1:B:194:ASN:OD1	2.36	0.44
1:C:307:THR:HG23	1:C:311:GLU:HG2	1.99	0.44
1:A:24:ARG:NH1	4:A:522:HOH:O	2.51	0.43
1:A:45:ARG:O	1:A:46:VAL:C	2.56	0.43
1:D:9:LYS:NZ	4:D:507:HOH:O	2.31	0.43
2:F:401:GNU:O02	2:F:401:GNU:C11	2.67	0.43
1:F:37:TYR:CE2	1:F:63:ARG:HD2	2.54	0.43
1:B:84:ILE:HD13	1:B:213:LEU:O	2.18	0.43
1:D:196:LYS:HD3	1:D:233:THR:CG2	2.49	0.43
1:C:314:LYS:NZ	4:C:513:HOH:O	2.42	0.43
1:D:21:MET:HE2	1:D:25:ILE:HD11	2.01	0.43
1:F:268:ILE:N	1:F:269:PRO:CD	2.81	0.43
1:B:260:LEU:HD13	1:B:260:LEU:N	2.34	0.42
1:A:43:GLU:HA	1:A:45:ARG:NE	2.35	0.42
1:A:186:LYS:HE2	1:A:186:LYS:HB2	1.79	0.42
1:D:176:GLN:CD	1:D:187:VAL:HG23	2.39	0.42
1:F:199:TYR:O	1:F:230:ASN:HB3	2.20	0.42
1:B:308:ARG:HB2	1:B:310:ASP:OD1	2.20	0.42
2:D:401:GNU:O01	2:D:401:GNU:C13	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:402:NDP:O3B	3:D:402:NDP:P2B	2.78	0.42
1:B:260:LEU:HD22	1:B:260:LEU:H	1.84	0.42
1:A:259:PHE:O	1:A:260:LEU:C	2.58	0.42
1:E:97:HIS:N	1:E:143:GLN:NE2	2.67	0.42
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.92	0.42
1:D:255:SER:OG	1:D:256:ALA:N	2.53	0.42
1:E:13:LEU:HB2	1:E:82:VAL:HG11	2.02	0.42
1:B:166:PHE:CD1	3:B:402:NDP:C7N	3.03	0.41
1:B:252:THR:O	1:B:252:THR:HG22	2.20	0.41
1:C:246:GLY:O	1:C:247:LYS:HD2	2.19	0.41
1:F:193:GLY:O	1:F:233:THR:HB	2.20	0.41
1:B:254:ILE:HG23	1:B:258:ASP:CB	2.49	0.41
1:B:255:SER:HB2	4:B:502:HOH:O	2.19	0.41
1:B:242:GLU:O	1:B:246:GLY:N	2.49	0.41
1:E:166:PHE:CD2	3:E:402:NDP:H41N	2.55	0.41
1:F:196:LYS:HD2	1:F:231:VAL:HG12	2.03	0.41
1:B:190:TYR:O	1:B:193:GLY:N	2.53	0.41
1:B:95:ARG:HA	1:B:143:GLN:OE1	2.19	0.41
1:F:9:LYS:HG2	1:F:33:GLY:O	2.20	0.41
1:F:166:PHE:CD2	3:F:402:NDP:H41N	2.55	0.41
1:D:46:VAL:HG13	1:E:180:LEU:HD21	2.02	0.41
1:E:43:GLU:H	1:E:43:GLU:CD	2.22	0.41
3:A:402:NDP:HO3A	3:A:402:NDP:P2B	2.43	0.41
2:E:401:GNU:C09	3:E:402:NDP:H42N	2.51	0.41
1:D:242:GLU:HG2	1:D:247:LYS:O	2.21	0.40
1:E:118:PHE:O	1:E:158:HIS:HA	2.21	0.40
1:E:317:LEU:HA	1:E:317:LEU:HD23	1.86	0.40
1:C:44:THR:HG21	1:C:54:LEU:HD11	1.99	0.40
2:D:401:GNU:O01	2:D:401:GNU:C15	2.69	0.40
1:A:243:LYS:HE3	4:A:629:HOH:O	2.21	0.40
1:D:89:MET:O	1:D:90:SER:C	2.60	0.40
1:E:166:PHE:CD1	3:E:402:NDP:C7N	3.04	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	277/317 (87%)	267 (96%)	8 (3%)	2 (1%)	22	26
1	B	277/317 (87%)	267 (96%)	9 (3%)	1 (0%)	34	42
1	C	276/317 (87%)	268 (97%)	7 (2%)	1 (0%)	34	42
1	D	275/317 (87%)	265 (96%)	9 (3%)	1 (0%)	34	42
1	E	278/317 (88%)	269 (97%)	6 (2%)	3 (1%)	14	15
1	F	287/317 (90%)	274 (96%)	9 (3%)	4 (1%)	11	11
All	All	1670/1902 (88%)	1610 (96%)	48 (3%)	12 (1%)	22	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	45	ARG
1	F	270	HIS
1	C	259	PHE
1	E	43	GLU
1	E	259	PHE
1	E	44	THR
1	F	271	GLN
1	F	272	ALA
1	D	259	PHE
1	B	259	PHE
1	F	45	ARG

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	243/271 (90%)	235 (97%)	8 (3%)	38	53
1	B	245/271 (90%)	236 (96%)	9 (4%)	34	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	242/271 (89%)	233 (96%)	9 (4%)	34	48
1	D	242/271 (89%)	237 (98%)	5 (2%)	53	70
1	E	243/271 (90%)	238 (98%)	5 (2%)	53	70
1	F	250/271 (92%)	246 (98%)	4 (2%)	62	78
All	All	1465/1626 (90%)	1425 (97%)	40 (3%)	44	61

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	43	GLU
1	A	129	ARG
1	A	145	LEU
1	A	165	CYS
1	A	196	LYS
1	A	260	LEU
1	A	271	GLN
1	B	32	GLU
1	B	45	ARG
1	B	50	LYS
1	B	89	MET
1	B	179	THR
1	B	212	THR
1	B	239	GLN
1	B	258	ASP
1	B	260	LEU
1	C	43	GLU
1	C	46	VAL
1	C	50	LYS
1	C	53	LEU
1	C	107	GLU
1	C	165	CYS
1	C	186	LYS
1	C	259	PHE
1	C	276	HIS
1	D	100	LEU
1	D	129	ARG
1	D	212	THR
1	D	257	ASN
1	D	259	PHE
1	E	8	GLU

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Mol	Chain	Res	Type
1	E	45	ARG
1	E	97	HIS
1	E	260	LEU
1	E	277	PHE
1	F	89	MET
1	F	96	SER
1	F	259	PHE
1	F	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	ASN
1	E	41	GLN
1	E	239	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	NDP	B	402	-	45,52,52	3.95	19 (42%)	53,80,80	1.99	6 (11%)
3	NDP	F	402	-	45,52,52	3.94	18 (40%)	53,80,80	1.98	6 (11%)
2	GNU	D	401	-	27,27,27	1.25	2 (7%)	30,36,36	1.30	3 (10%)
3	NDP	A	402	-	45,52,52	4.09	20 (44%)	53,80,80	2.09	5 (9%)
2	GNU	F	401	-	27,27,27	1.14	3 (11%)	30,36,36	1.09	2 (6%)
2	GNU	B	401	-	27,27,27	1.05	3 (11%)	30,36,36	1.01	2 (6%)
2	GNU	A	401	-	27,27,27	1.00	2 (7%)	30,36,36	1.33	4 (13%)
3	NDP	C	402	-	45,52,52	4.18	23 (51%)	53,80,80	2.08	5 (9%)
2	GNU	E	401	-	27,27,27	1.18	3 (11%)	30,36,36	1.10	2 (6%)
3	NDP	D	402	-	45,52,52	4.17	19 (42%)	53,80,80	2.09	7 (13%)
2	GNU	C	401	-	27,27,27	1.06	2 (7%)	30,36,36	0.92	2 (6%)
3	NDP	E	402	-	45,52,52	4.17	19 (42%)	53,80,80	1.92	5 (9%)

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	NDP	B	402	-	-	5/30/77/77	0/5/5/5
3	NDP	F	402	-	-	8/30/77/77	0/5/5/5
2	GNU	D	401	-	-	4/20/20/20	0/2/2/2
3	NDP	A	402	-	-	6/30/77/77	0/5/5/5
2	GNU	F	401	-	-	3/20/20/20	0/2/2/2
2	GNU	B	401	-	-	4/20/20/20	0/2/2/2
2	GNU	A	401	-	-	0/20/20/20	0/2/2/2
3	NDP	C	402	-	-	8/30/77/77	0/5/5/5
2	GNU	E	401	-	-	6/20/20/20	0/2/2/2
3	NDP	D	402	-	-	10/30/77/77	0/5/5/5
2	GNU	C	401	-	-	4/20/20/20	0/2/2/2
3	NDP	E	402	-	-	4/30/77/77	0/5/5/5

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NDP	O4B-C1B	15.54	1.62	1.41
3	D	402	NDP	O4B-C1B	15.51	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	NDP	O4B-C1B	15.46	1.62	1.41
3	A	402	NDP	O4B-C1B	14.73	1.61	1.41
3	F	402	NDP	O4B-C1B	14.35	1.61	1.41
3	B	402	NDP	O4B-C1B	13.93	1.60	1.41
3	E	402	NDP	C6N-C5N	12.65	1.55	1.33
3	C	402	NDP	C6N-C5N	12.55	1.55	1.33
3	D	402	NDP	C6N-C5N	12.32	1.55	1.33
3	A	402	NDP	C6N-C5N	12.30	1.55	1.33
3	B	402	NDP	C6N-C5N	12.25	1.55	1.33
3	F	402	NDP	C6N-C5N	11.62	1.54	1.33
3	D	402	NDP	O4D-C1D	9.27	1.64	1.42
3	E	402	NDP	O4D-C1D	9.14	1.63	1.42
3	A	402	NDP	O4D-C1D	8.96	1.63	1.42
3	C	402	NDP	O4D-C1D	8.93	1.63	1.42
3	F	402	NDP	O4D-C1D	8.33	1.61	1.42
3	B	402	NDP	O4D-C1D	8.27	1.61	1.42
3	F	402	NDP	C2D-C1D	-6.91	1.31	1.53
3	E	402	NDP	C2D-C1D	-6.85	1.31	1.53
3	A	402	NDP	C2D-C1D	-6.69	1.32	1.53
3	C	402	NDP	C2D-C1D	-6.68	1.32	1.53
3	B	402	NDP	C2D-C1D	-6.65	1.32	1.53
3	D	402	NDP	C2D-C1D	-6.64	1.32	1.53
3	F	402	NDP	O4B-C4B	-6.53	1.30	1.45
3	B	402	NDP	O4B-C4B	-6.44	1.30	1.45
3	A	402	NDP	O4B-C4B	-6.32	1.30	1.45
3	E	402	NDP	O4B-C4B	-6.18	1.31	1.45
3	E	402	NDP	O4D-C4D	-6.15	1.31	1.45
3	C	402	NDP	O4D-C4D	-6.14	1.31	1.45
3	B	402	NDP	O4D-C4D	-6.13	1.31	1.45
3	F	402	NDP	O4D-C4D	-6.12	1.31	1.45
3	D	402	NDP	O4D-C4D	-6.11	1.31	1.45
3	A	402	NDP	O4D-C4D	-6.09	1.31	1.45
3	C	402	NDP	O4B-C4B	-6.08	1.31	1.45
3	C	402	NDP	C2N-C3N	6.06	1.51	1.34
3	D	402	NDP	C2N-C3N	6.05	1.51	1.34
3	A	402	NDP	C2N-C3N	5.86	1.51	1.34
3	D	402	NDP	O4B-C4B	-5.73	1.32	1.45
3	E	402	NDP	C2N-C3N	5.67	1.50	1.34
3	B	402	NDP	C2N-C3N	5.63	1.50	1.34
3	F	402	NDP	C2N-C3N	5.55	1.50	1.34
3	E	402	NDP	C7N-N7N	4.55	1.45	1.33
3	D	402	NDP	C7N-N7N	4.51	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	C7N-N7N	4.44	1.45	1.33
3	B	402	NDP	C7N-N7N	4.37	1.45	1.33
3	C	402	NDP	C7N-N7N	4.37	1.45	1.33
3	F	402	NDP	C7N-N7N	4.17	1.44	1.33
3	D	402	NDP	C6A-N6A	3.94	1.48	1.34
3	C	402	NDP	C6A-N6A	3.85	1.48	1.34
3	E	402	NDP	C6A-N6A	3.67	1.47	1.34
3	B	402	NDP	C6A-N6A	3.64	1.47	1.34
3	F	402	NDP	C6A-N6A	3.57	1.47	1.34
3	A	402	NDP	C6A-N6A	3.50	1.46	1.34
3	E	402	NDP	O2D-C2D	3.44	1.51	1.43
3	D	402	NDP	O2D-C2D	3.38	1.50	1.43
3	C	402	NDP	C4N-C5N	3.33	1.57	1.48
3	A	402	NDP	O2D-C2D	3.30	1.50	1.43
3	B	402	NDP	O2D-C2D	3.29	1.50	1.43
3	D	402	NDP	C2A-N3A	3.28	1.37	1.32
3	D	402	NDP	C4N-C5N	3.28	1.57	1.48
3	D	402	NDP	C6N-N1N	3.28	1.45	1.37
3	F	402	NDP	O2D-C2D	3.24	1.50	1.43
3	C	402	NDP	O2D-C2D	3.22	1.50	1.43
3	C	402	NDP	C6N-N1N	3.20	1.45	1.37
3	A	402	NDP	P2B-O2B	3.20	1.65	1.59
3	E	402	NDP	C2A-N3A	3.20	1.37	1.32
2	D	401	GNU	O03-C19	3.16	1.42	1.37
3	E	402	NDP	C4N-C5N	3.14	1.57	1.48
3	A	402	NDP	C2A-N3A	3.13	1.37	1.32
3	A	402	NDP	C4N-C5N	3.11	1.57	1.48
3	E	402	NDP	C6N-N1N	3.06	1.44	1.37
3	C	402	NDP	C2A-N3A	3.05	1.37	1.32
3	C	402	NDP	C4N-C3N	3.03	1.55	1.49
2	C	401	GNU	O04-C20	3.03	1.42	1.37
3	A	402	NDP	C6N-N1N	3.03	1.44	1.37
3	B	402	NDP	C4N-C5N	2.98	1.56	1.48
3	F	402	NDP	O3B-C3B	-2.94	1.36	1.43
3	A	402	NDP	C7N-C3N	2.93	1.55	1.48
3	C	402	NDP	C7N-C3N	2.93	1.55	1.48
3	D	402	NDP	P2B-O2B	2.92	1.64	1.59
3	F	402	NDP	C2A-N3A	2.90	1.36	1.32
2	E	401	GNU	O03-C19	2.82	1.41	1.37
3	A	402	NDP	C4N-C3N	2.81	1.55	1.49
3	C	402	NDP	O3D-C3D	-2.81	1.36	1.43
3	D	402	NDP	O3B-C3B	-2.80	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	NDP	O3D-C3D	-2.78	1.36	1.43
2	D	401	GNU	O04-C20	2.78	1.41	1.37
3	A	402	NDP	O3D-C3D	-2.76	1.36	1.43
3	E	402	NDP	C7N-C3N	2.73	1.54	1.48
3	B	402	NDP	C6N-N1N	2.71	1.44	1.37
3	B	402	NDP	C2A-N3A	2.68	1.36	1.32
2	F	401	GNU	O03-C19	2.67	1.41	1.37
3	E	402	NDP	O3B-C3B	-2.66	1.36	1.43
3	D	402	NDP	O3D-C3D	-2.63	1.36	1.43
3	B	402	NDP	C4N-C3N	2.61	1.55	1.49
2	B	401	GNU	O04-C20	2.59	1.41	1.37
3	F	402	NDP	C4N-C5N	2.56	1.55	1.48
2	A	401	GNU	O04-C20	2.51	1.41	1.37
3	B	402	NDP	O3D-C3D	-2.50	1.37	1.43
3	F	402	NDP	C6N-N1N	2.50	1.43	1.37
2	A	401	GNU	O03-C19	2.49	1.41	1.37
3	B	402	NDP	C5A-C4A	-2.49	1.34	1.40
3	E	402	NDP	O3D-C3D	-2.49	1.37	1.43
3	D	402	NDP	C7N-C3N	2.49	1.54	1.48
3	D	402	NDP	C4N-C3N	2.48	1.54	1.49
3	E	402	NDP	C4N-C3N	2.48	1.54	1.49
3	F	402	NDP	C4N-C3N	2.45	1.54	1.49
3	F	402	NDP	C5A-C4A	-2.43	1.34	1.40
3	C	402	NDP	O3B-C3B	-2.42	1.37	1.43
3	F	402	NDP	P2B-O2B	2.40	1.63	1.59
2	E	401	GNU	O05-C23	2.38	1.41	1.36
3	A	402	NDP	O3B-C3B	-2.36	1.37	1.43
2	B	401	GNU	O05-C23	2.36	1.41	1.36
3	E	402	NDP	P2B-O2B	2.35	1.63	1.59
3	D	402	NDP	O7N-C7N	-2.34	1.18	1.24
3	C	402	NDP	PN-O5D	2.34	1.68	1.59
2	E	401	GNU	O04-C20	2.30	1.40	1.37
3	B	402	NDP	C7N-C3N	2.29	1.53	1.48
3	B	402	NDP	O3B-C3B	-2.27	1.37	1.43
2	F	401	GNU	O05-C23	2.25	1.41	1.36
3	A	402	NDP	O7N-C7N	-2.23	1.19	1.24
2	B	401	GNU	O06-C24	2.23	1.40	1.36
3	C	402	NDP	PA-O5B	2.21	1.68	1.59
3	C	402	NDP	C5A-C4A	-2.19	1.35	1.40
3	A	402	NDP	C5A-C4A	-2.17	1.35	1.40
3	C	402	NDP	O7N-C7N	-2.15	1.19	1.24
3	C	402	NDP	C5D-C4D	2.07	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	GNU	O04-C20	2.06	1.40	1.37
2	C	401	GNU	O06-C24	2.05	1.40	1.36
3	C	402	NDP	P2B-O2B	2.05	1.63	1.59
3	B	402	NDP	PA-O5B	2.03	1.67	1.59
3	E	402	NDP	O7N-C7N	-2.02	1.19	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	NDP	C5A-C6A-N6A	9.36	134.58	120.35
3	A	402	NDP	C5A-C6A-N6A	9.23	134.37	120.35
3	C	402	NDP	C5A-C6A-N6A	8.26	132.91	120.35
3	C	402	NDP	C1B-N9A-C4A	-8.18	112.27	126.64
3	B	402	NDP	C5A-C6A-N6A	8.14	132.72	120.35
3	E	402	NDP	C5A-C6A-N6A	8.09	132.64	120.35
3	F	402	NDP	C5A-C6A-N6A	7.72	132.08	120.35
3	F	402	NDP	C1B-N9A-C4A	-7.34	113.75	126.64
3	A	402	NDP	C1B-N9A-C4A	-6.99	114.36	126.64
3	A	402	NDP	N6A-C6A-N1A	-6.75	104.56	118.57
3	B	402	NDP	C1B-N9A-C4A	-6.49	115.23	126.64
3	D	402	NDP	N6A-C6A-N1A	-6.36	105.38	118.57
3	D	402	NDP	C1B-N9A-C4A	-6.09	115.94	126.64
3	E	402	NDP	C1B-N9A-C4A	-6.08	115.96	126.64
3	C	402	NDP	N6A-C6A-N1A	-5.79	106.55	118.57
3	B	402	NDP	N6A-C6A-N1A	-5.63	106.89	118.57
3	E	402	NDP	N6A-C6A-N1A	-5.43	107.31	118.57
3	F	402	NDP	N6A-C6A-N1A	-5.30	107.56	118.57
3	F	402	NDP	N3A-C2A-N1A	-5.08	120.74	128.68
3	B	402	NDP	N3A-C2A-N1A	-5.05	120.78	128.68
3	C	402	NDP	N3A-C2A-N1A	-4.95	120.95	128.68
3	A	402	NDP	N3A-C2A-N1A	-4.89	121.03	128.68
3	D	402	NDP	N3A-C2A-N1A	-4.87	121.06	128.68
3	E	402	NDP	N3A-C2A-N1A	-4.86	121.08	128.68
2	A	401	GNU	C26-O04-C20	3.92	123.45	117.53
2	D	401	GNU	C26-O04-C20	3.61	122.97	117.53
2	E	401	GNU	C14-C10-C08	-3.45	107.98	113.65
2	F	401	GNU	C26-O04-C20	3.23	122.41	117.53
2	D	401	GNU	C25-O03-C19	3.15	122.29	117.53
3	F	402	NDP	C3N-C2N-N1N	-3.02	118.78	123.10
3	E	402	NDP	PN-O3-PA	-3.00	122.53	132.83
2	F	401	GNU	C14-C10-C08	-2.98	108.75	113.65
2	B	401	GNU	C13-C09-C07	2.90	118.41	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GNU	C25-O03-C19	2.82	121.79	117.53
3	D	402	NDP	PN-O3-PA	-2.72	123.48	132.83
2	E	401	GNU	O04-C20-C24	2.69	118.46	114.57
2	A	401	GNU	O03-C19-C23	2.64	118.39	114.57
2	C	401	GNU	O04-C20-C24	2.63	118.38	114.57
3	B	402	NDP	PN-O3-PA	-2.58	123.96	132.83
2	B	401	GNU	O04-C20-C24	2.55	118.27	114.57
2	A	401	GNU	O04-C20-C24	2.46	118.14	114.57
3	A	402	NDP	PN-O3-PA	-2.44	124.47	132.83
3	C	402	NDP	O2B-C2B-C1B	-2.36	101.59	110.10
3	B	402	NDP	O5B-C5B-C4B	2.33	117.01	108.99
2	C	401	GNU	O03-C19-C23	2.31	117.91	114.57
3	F	402	NDP	PN-O3-PA	-2.14	125.47	132.83
3	D	402	NDP	C3N-C2N-N1N	-2.12	120.07	123.10
3	D	402	NDP	C5B-C4B-C3B	-2.08	107.37	115.18
2	D	401	GNU	C09-C13-C15	2.02	123.89	120.44

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	GNU	C11-C07-C08-C12
3	C	402	NDP	C5D-O5D-PN-O1N
3	C	402	NDP	C2N-C3N-C7N-O7N
3	C	402	NDP	C2N-C3N-C7N-N7N
3	D	402	NDP	C5B-O5B-PA-O1A
3	D	402	NDP	C5B-O5B-PA-O3
3	F	402	NDP	C2N-C3N-C7N-O7N
2	E	401	GNU	C24-C20-O04-C26
2	C	401	GNU	C24-C20-O04-C26
2	D	401	GNU	C23-C19-O03-C25
2	C	401	GNU	C16-C20-O04-C26
2	E	401	GNU	C16-C20-O04-C26
3	D	402	NDP	C3B-C2B-O2B-P2B
2	C	401	GNU	C23-C19-O03-C25
2	D	401	GNU	C15-C19-O03-C25
2	C	401	GNU	C15-C19-O03-C25
3	A	402	NDP	C1B-C2B-O2B-P2B
3	F	402	NDP	C1B-C2B-O2B-P2B
3	A	402	NDP	C3B-C2B-O2B-P2B
3	B	402	NDP	C3B-C2B-O2B-P2B
3	F	402	NDP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
3	B	402	NDP	C1B-C2B-O2B-P2B
2	E	401	GNU	C23-C19-O03-C25
3	D	402	NDP	C3B-C4B-C5B-O5B
3	D	402	NDP	O4D-C4D-C5D-O5D
2	E	401	GNU	C15-C19-O03-C25
3	A	402	NDP	C2D-C1D-N1N-C2N
3	D	402	NDP	O4B-C4B-C5B-O5B
3	C	402	NDP	C2B-O2B-P2B-O1X
2	B	401	GNU	C24-C20-O04-C26
3	C	402	NDP	C2B-O2B-P2B-O2X
3	C	402	NDP	C5D-O5D-PN-O3
3	A	402	NDP	O4D-C1D-N1N-C2N
3	C	402	NDP	C5D-O5D-PN-O2N
3	F	402	NDP	C2N-C3N-C7N-N7N
2	E	401	GNU	C09-C07-C08-C10
2	F	401	GNU	C09-C07-C08-C10
2	E	401	GNU	C11-C07-C08-C12
2	F	401	GNU	C09-C07-C08-C12
3	A	402	NDP	C2D-C1D-N1N-C6N
2	D	401	GNU	C07-C09-C13-C15
3	A	402	NDP	O4D-C1D-N1N-C6N
3	C	402	NDP	O4D-C1D-N1N-C2N
3	E	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	O4D-C1D-N1N-C2N
3	F	402	NDP	O4D-C1D-N1N-C2N
2	B	401	GNU	C16-C20-O04-C26
3	B	402	NDP	O4D-C1D-N1N-C2N
3	B	402	NDP	C2D-C1D-N1N-C2N
3	D	402	NDP	C3D-C4D-C5D-O5D
3	E	402	NDP	C2B-O2B-P2B-O1X
3	F	402	NDP	C2B-O2B-P2B-O1X
2	D	401	GNU	C07-C09-C13-C17
3	B	402	NDP	C2B-O2B-P2B-O2X
3	E	402	NDP	C2B-O2B-P2B-O3X
3	F	402	NDP	C2B-O2B-P2B-O2X
3	D	402	NDP	PN-O3-PA-O1A
3	D	402	NDP	PN-O3-PA-O2A
2	B	401	GNU	C11-C07-C09-C13
3	E	402	NDP	C2N-C3N-C7N-N7N
2	B	401	GNU	C08-C07-C09-C13
3	F	402	NDP	C2D-C1D-N1N-C2N

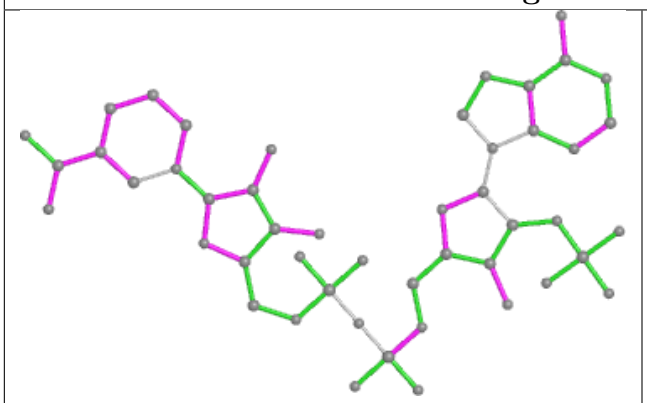
There are no ring outliers.

10 monomers are involved in 46 short contacts:

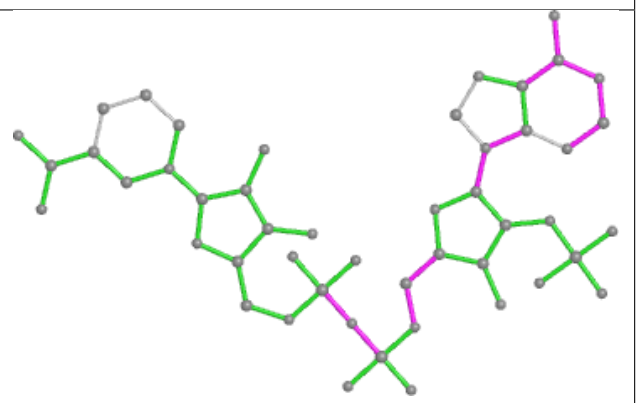
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NDP	6	0
3	F	402	NDP	2	0
2	D	401	GNU	2	0
3	A	402	NDP	9	0
2	F	401	GNU	2	0
3	C	402	NDP	7	0
2	E	401	GNU	1	0
3	D	402	NDP	12	0
2	C	401	GNU	1	0
3	E	402	NDP	6	0

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.

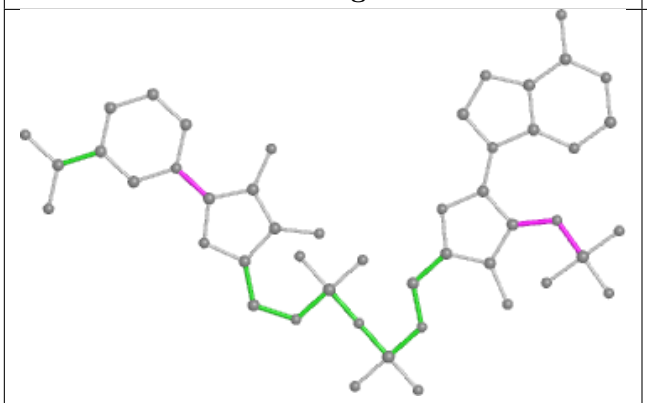
Ligand NDP B 402



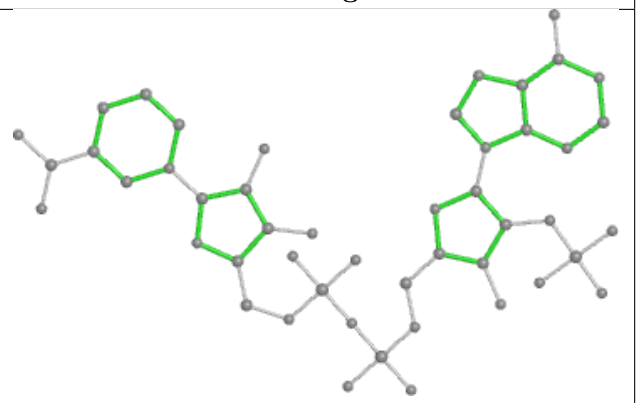
Bond lengths



Bond angles

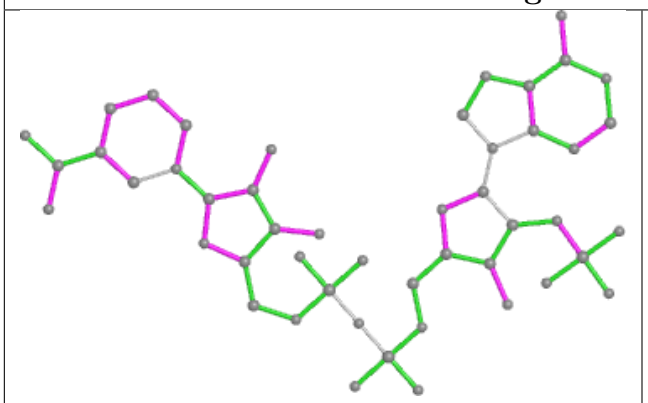


Torsions

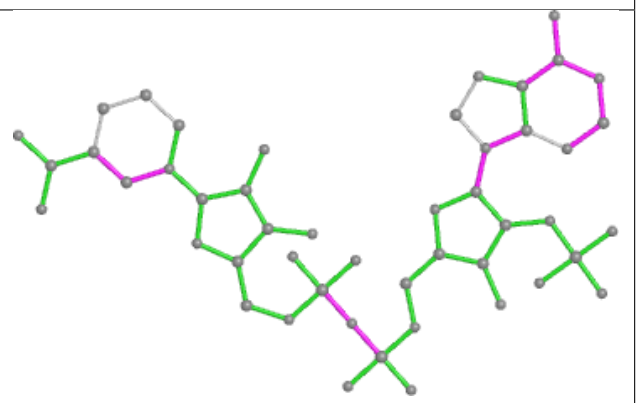


Rings

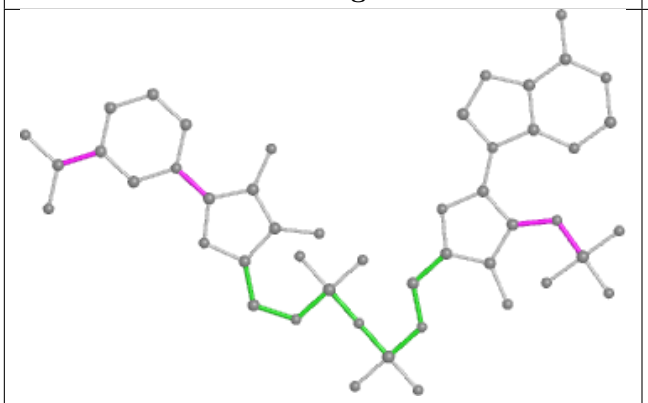
Ligand NDP F 402



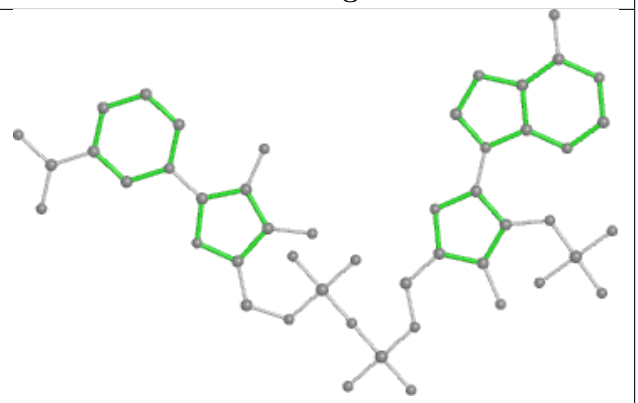
Bond lengths



Bond angles

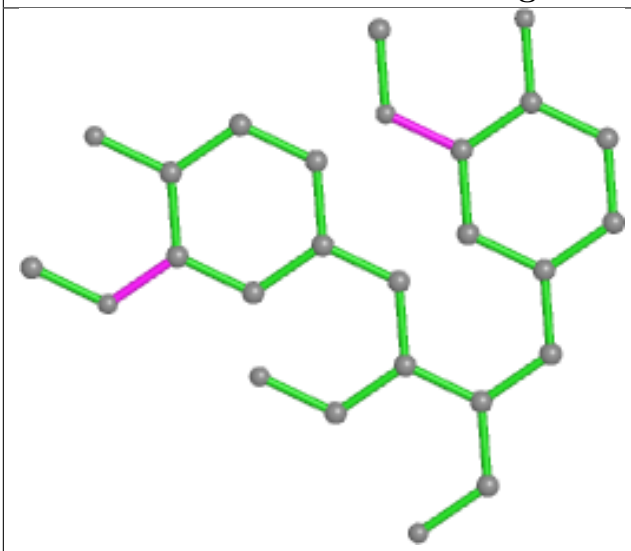


Torsions

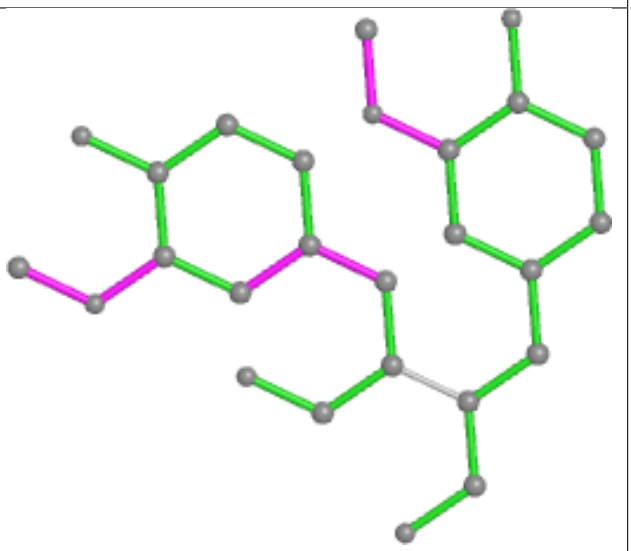


Rings

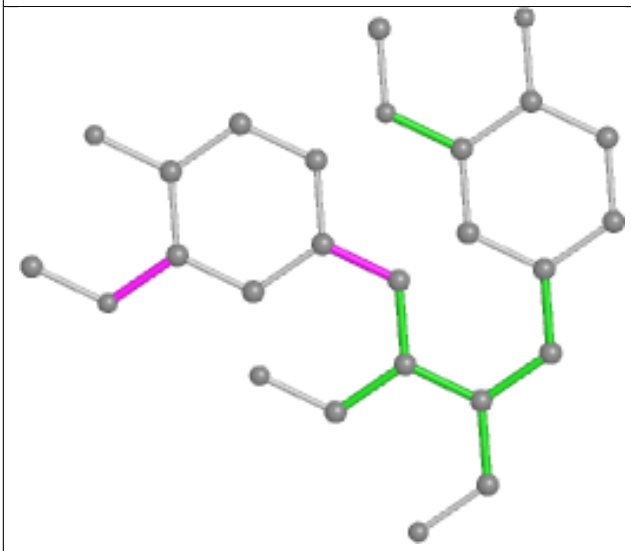
Ligand GNU D 401



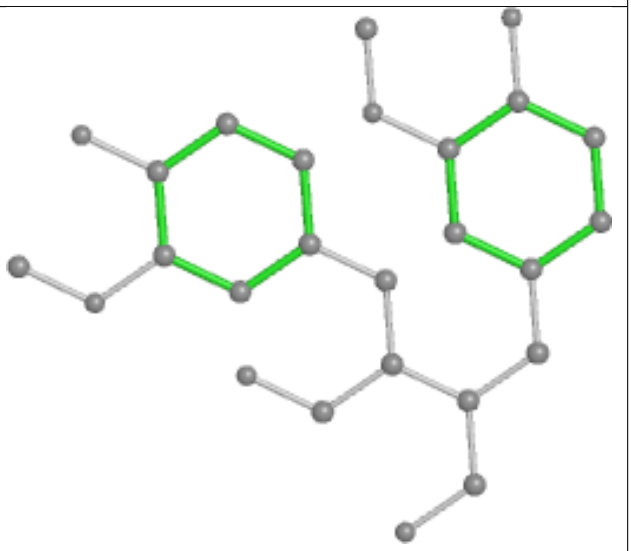
Bond lengths



Bond angles

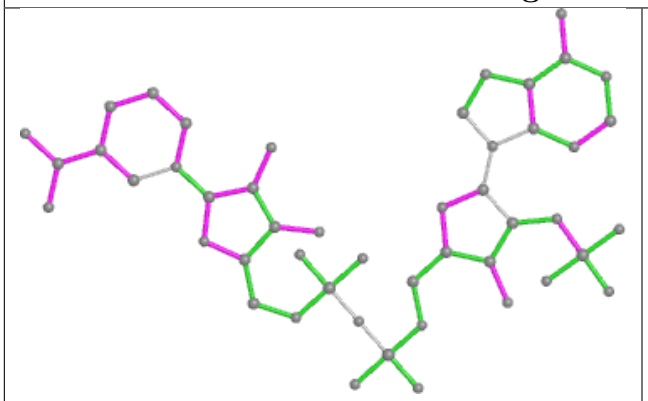


Torsions

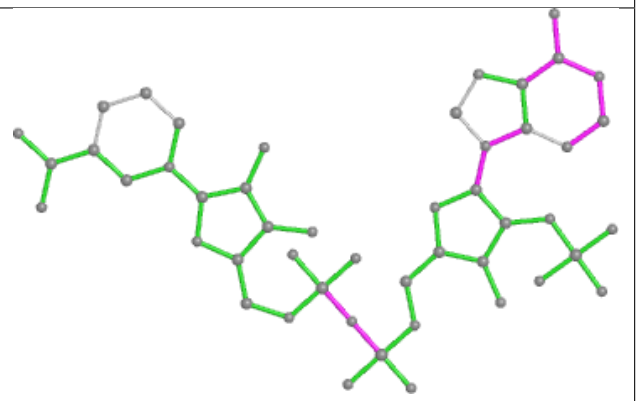


Rings

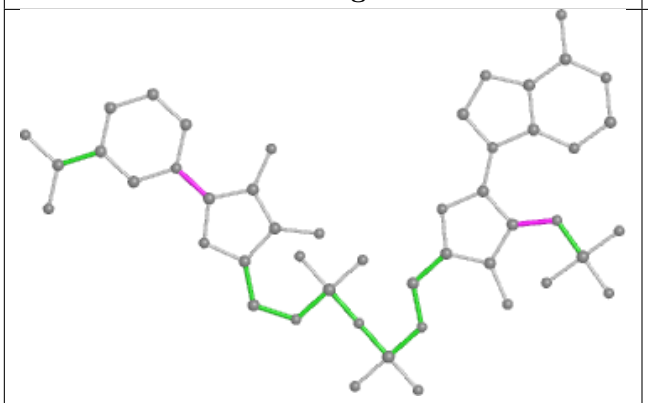
Ligand NDP A 402



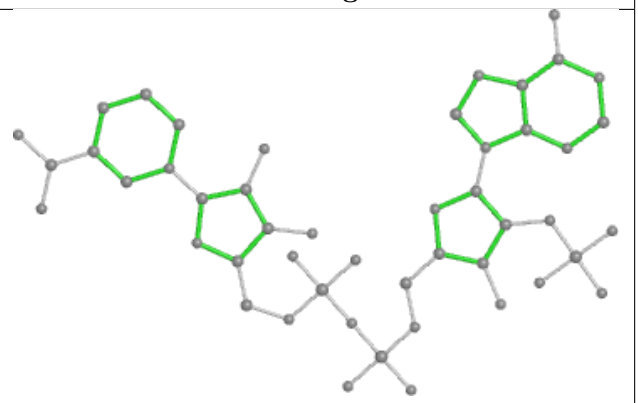
Bond lengths



Bond angles

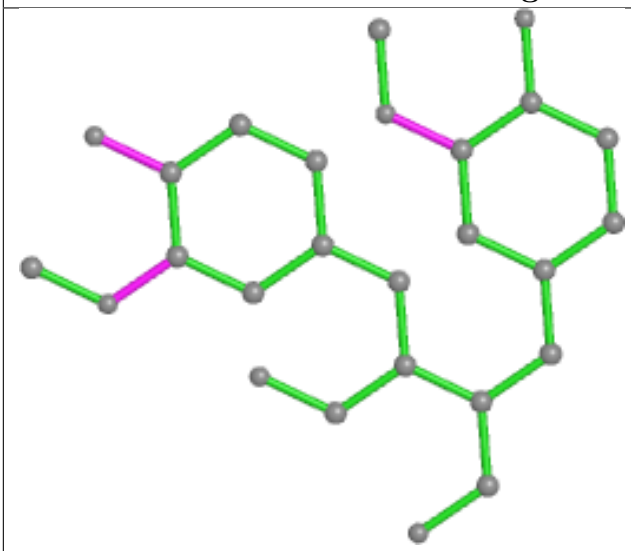


Torsions

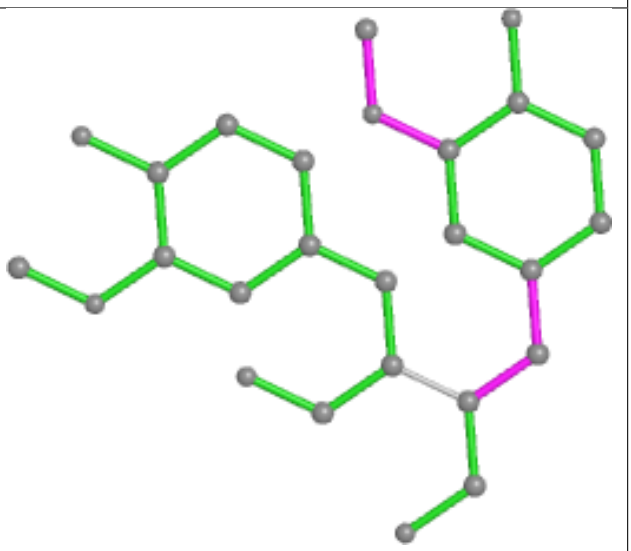


Rings

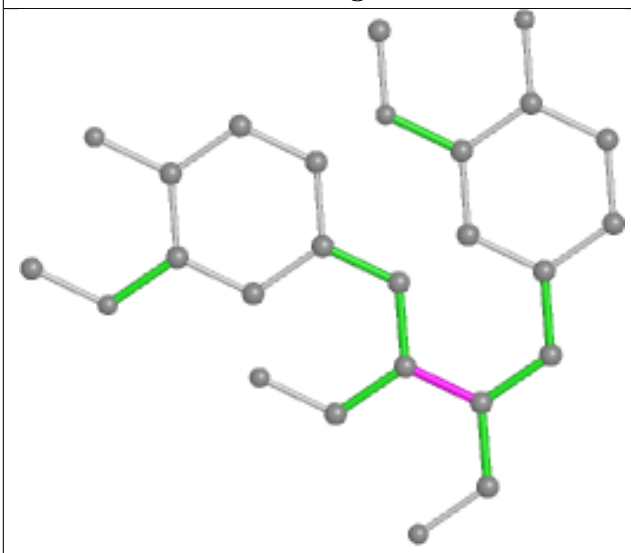
Ligand GNU F 401



Bond lengths



Bond angles



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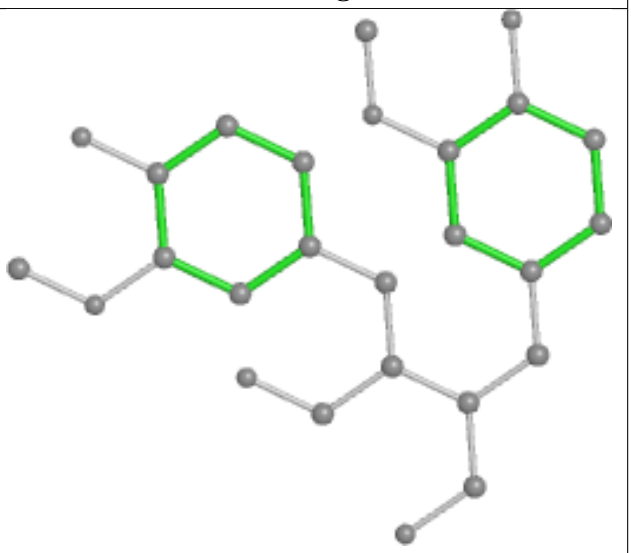
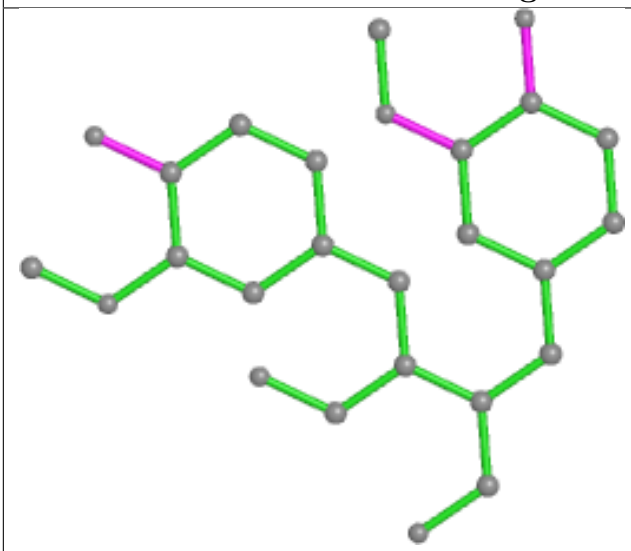


Rings

Ligand GNU B 401



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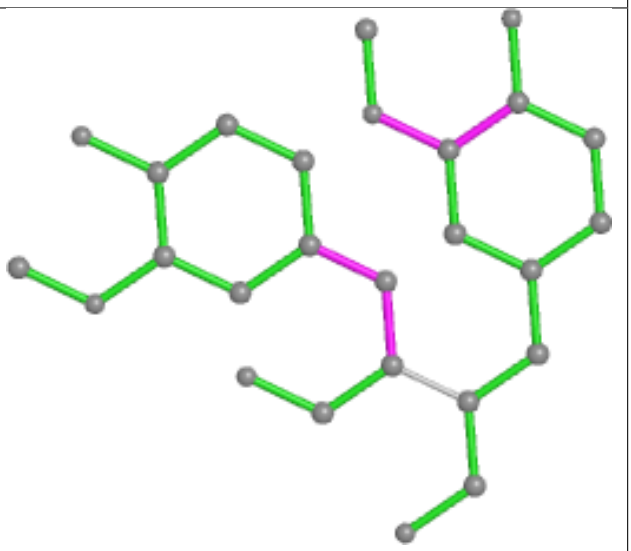

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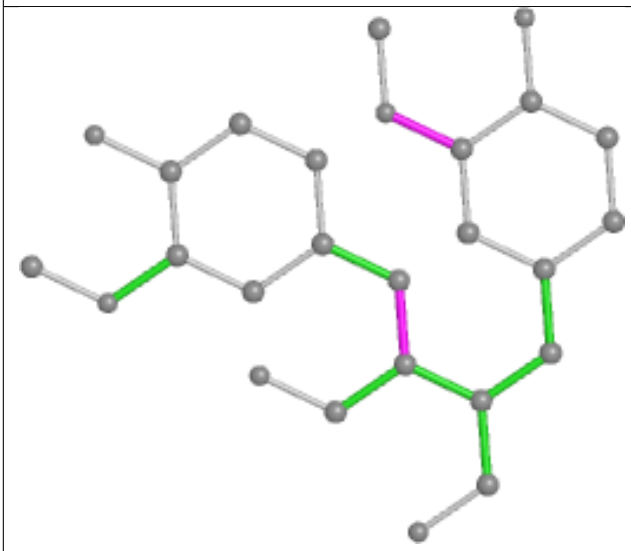
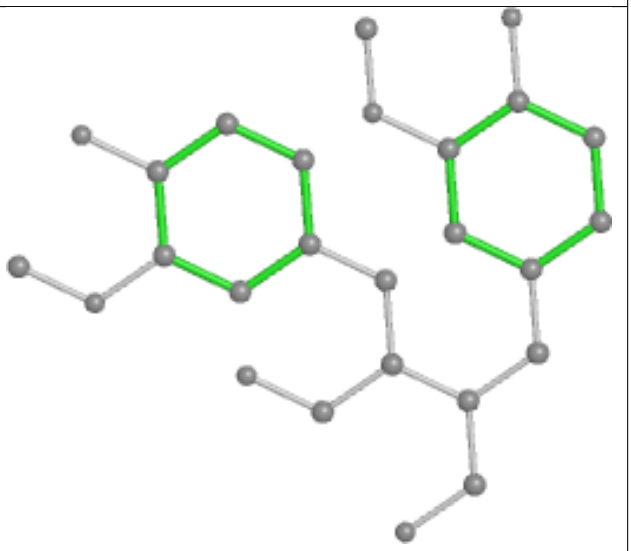
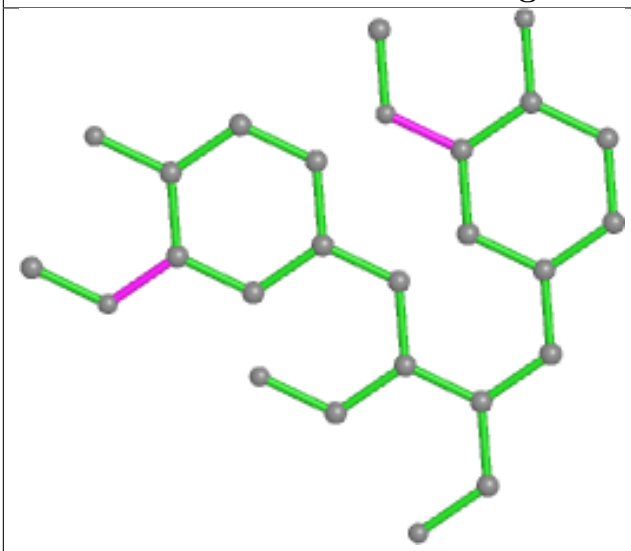


Torsions



Rings

Ligand GNU A 401



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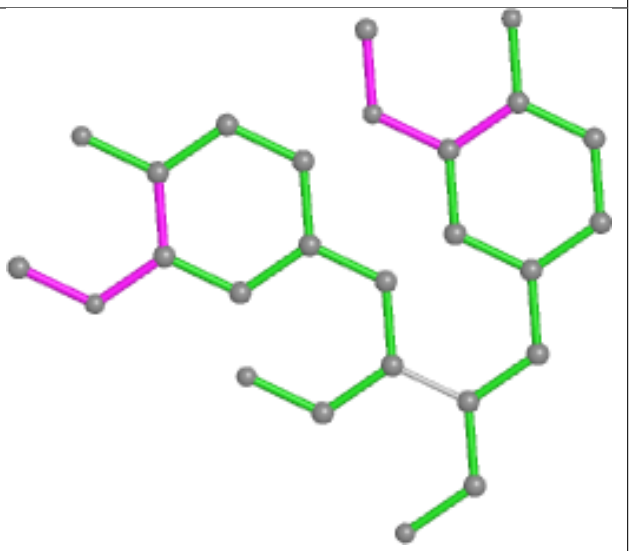

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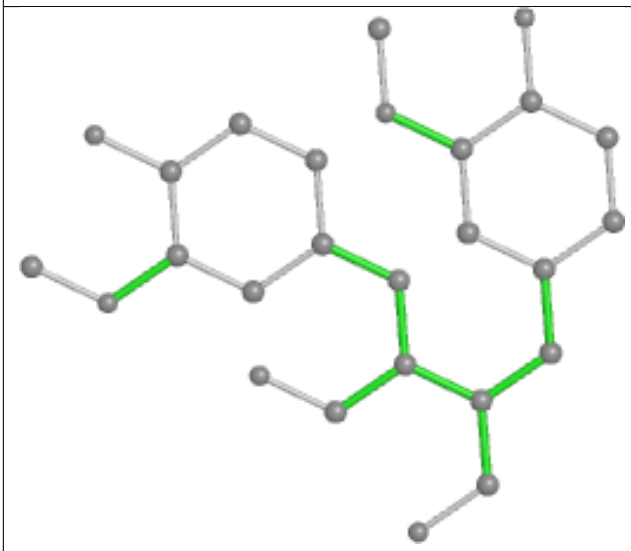

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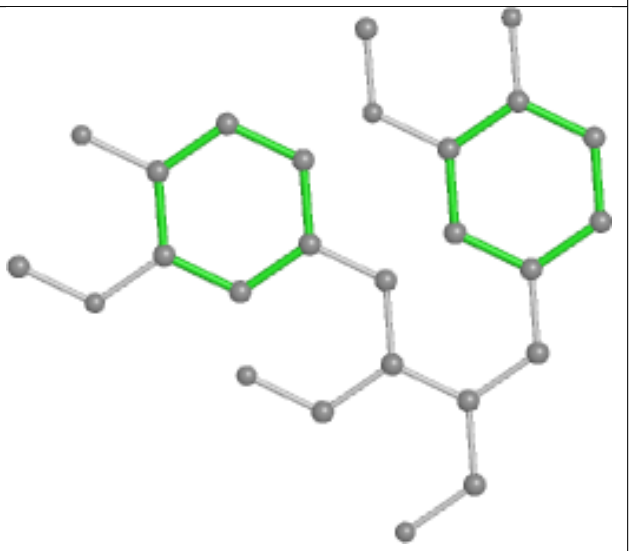
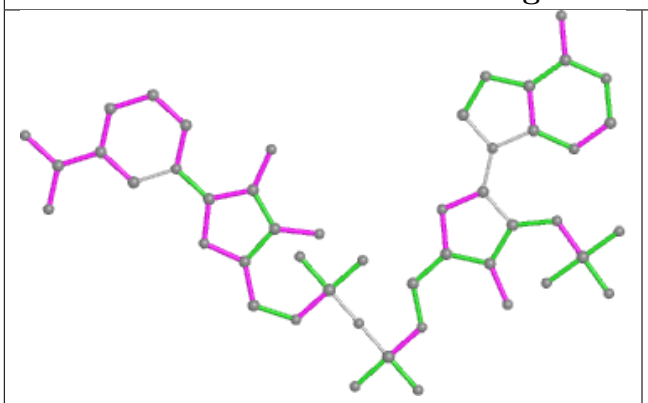


Rings

Ligand NDP C 402



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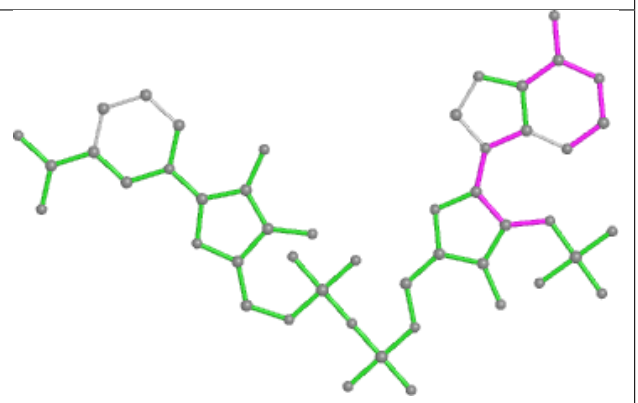
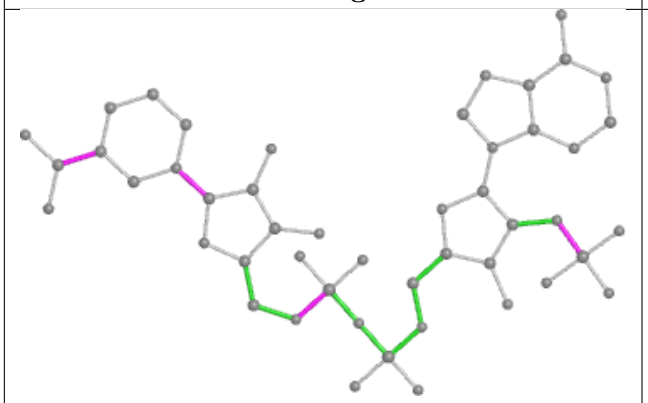
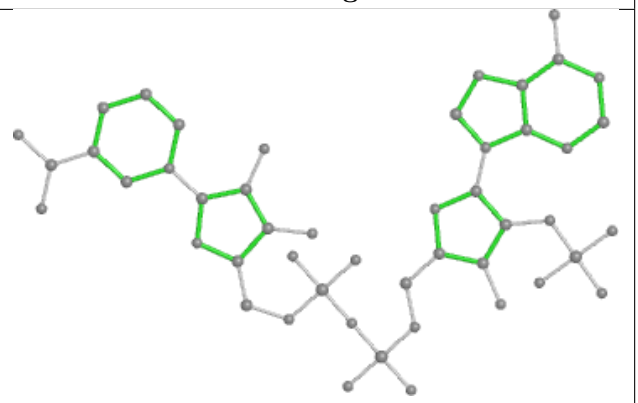


Bond angles

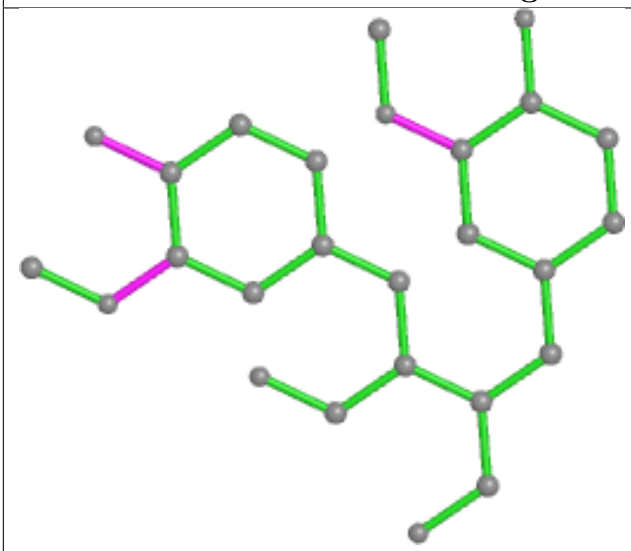


Torsions



Rings

Ligand GNU E 401



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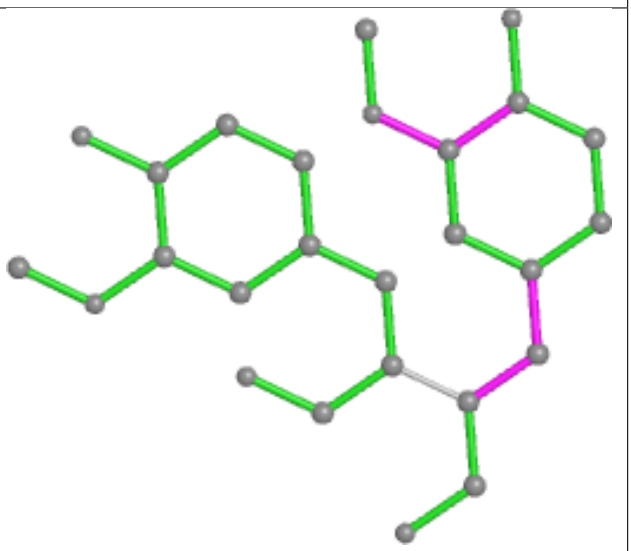
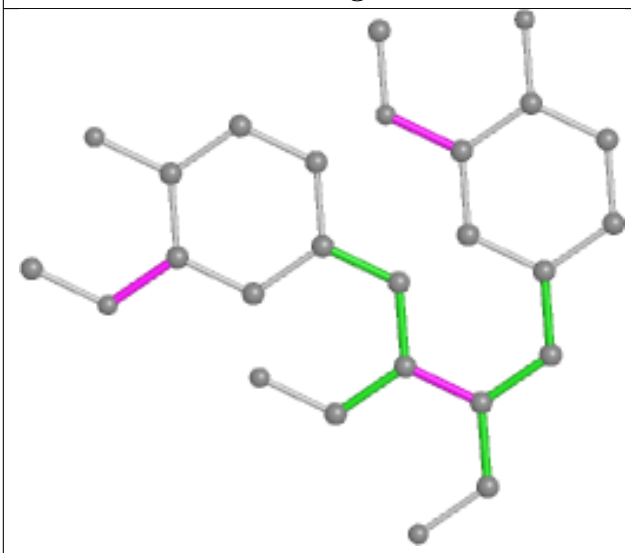
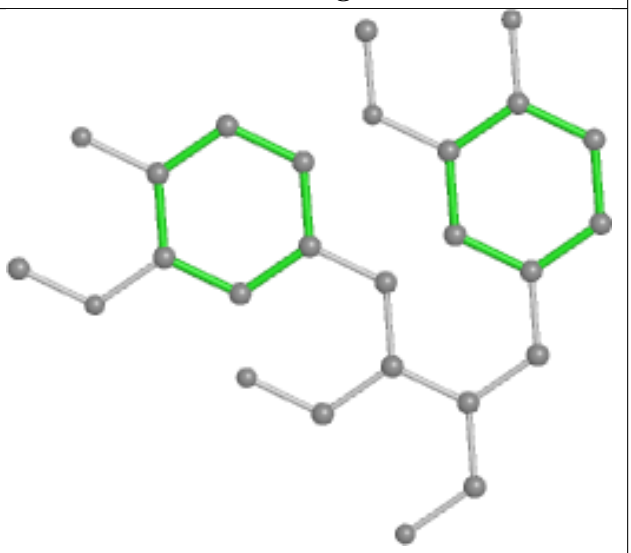


Bond angles

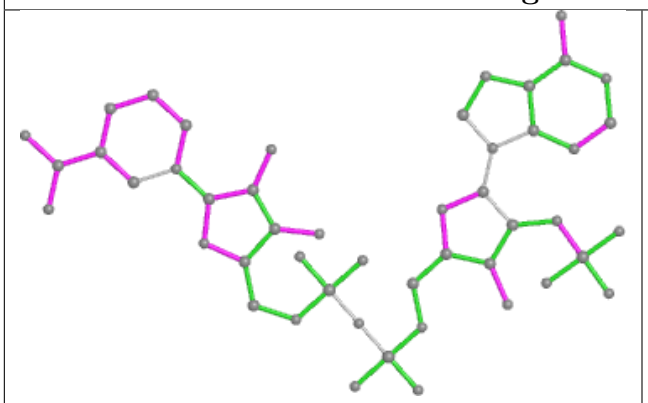


Torsions



Rings

Ligand NDP D 402



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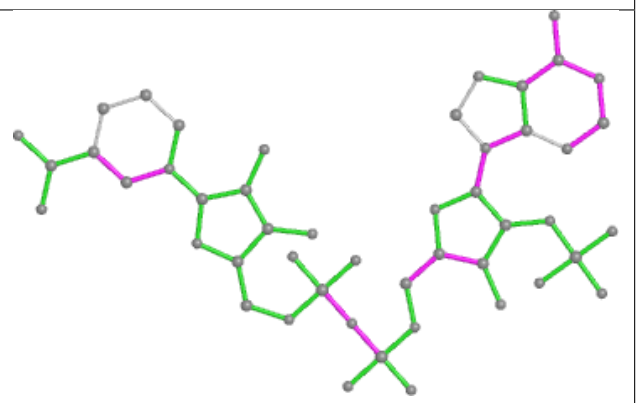
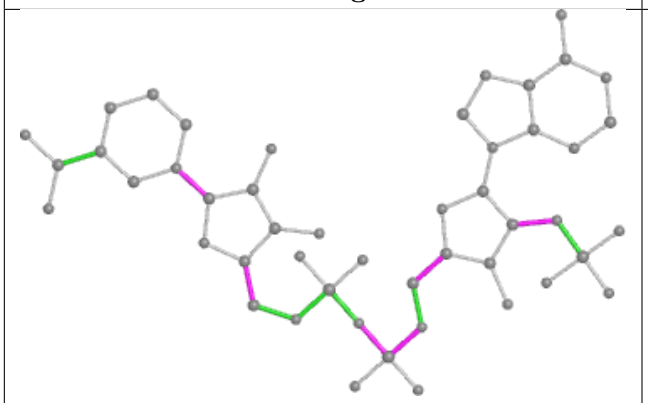
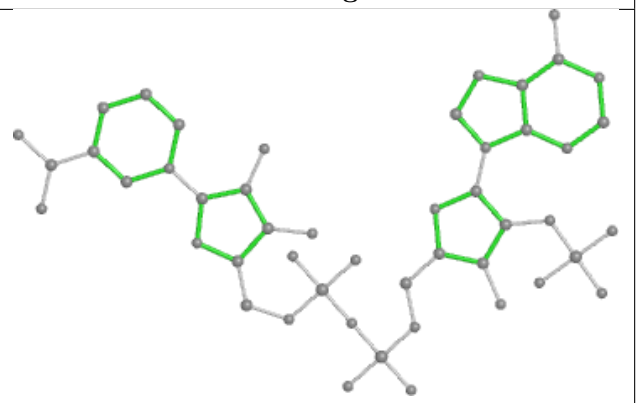


Bond angles

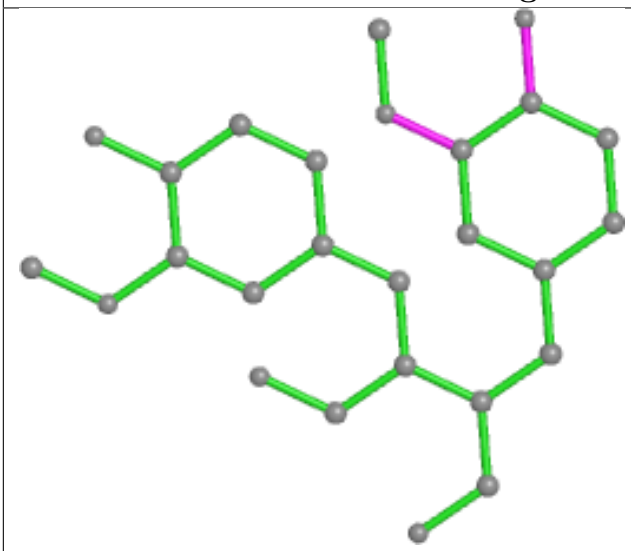


Torsions



Rings

Ligand GNU C 401



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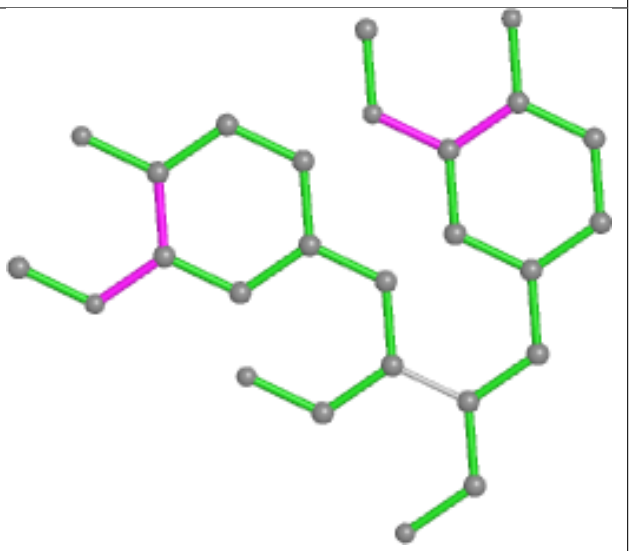
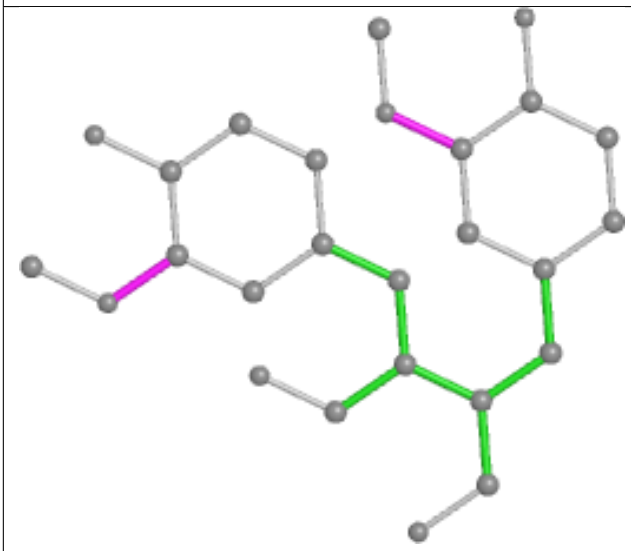
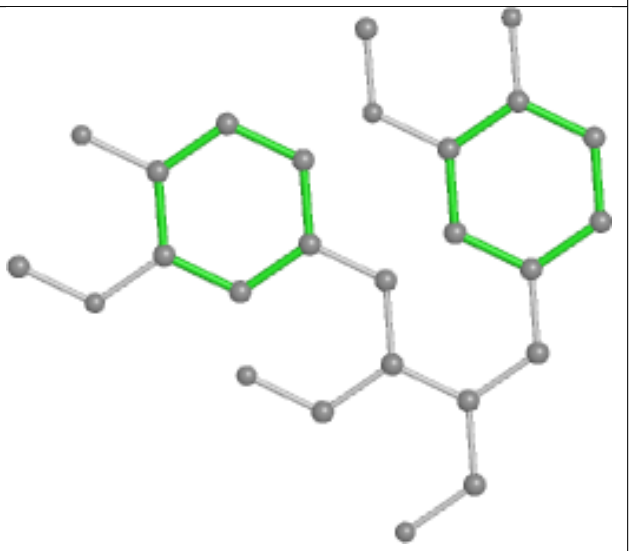


Bond angles

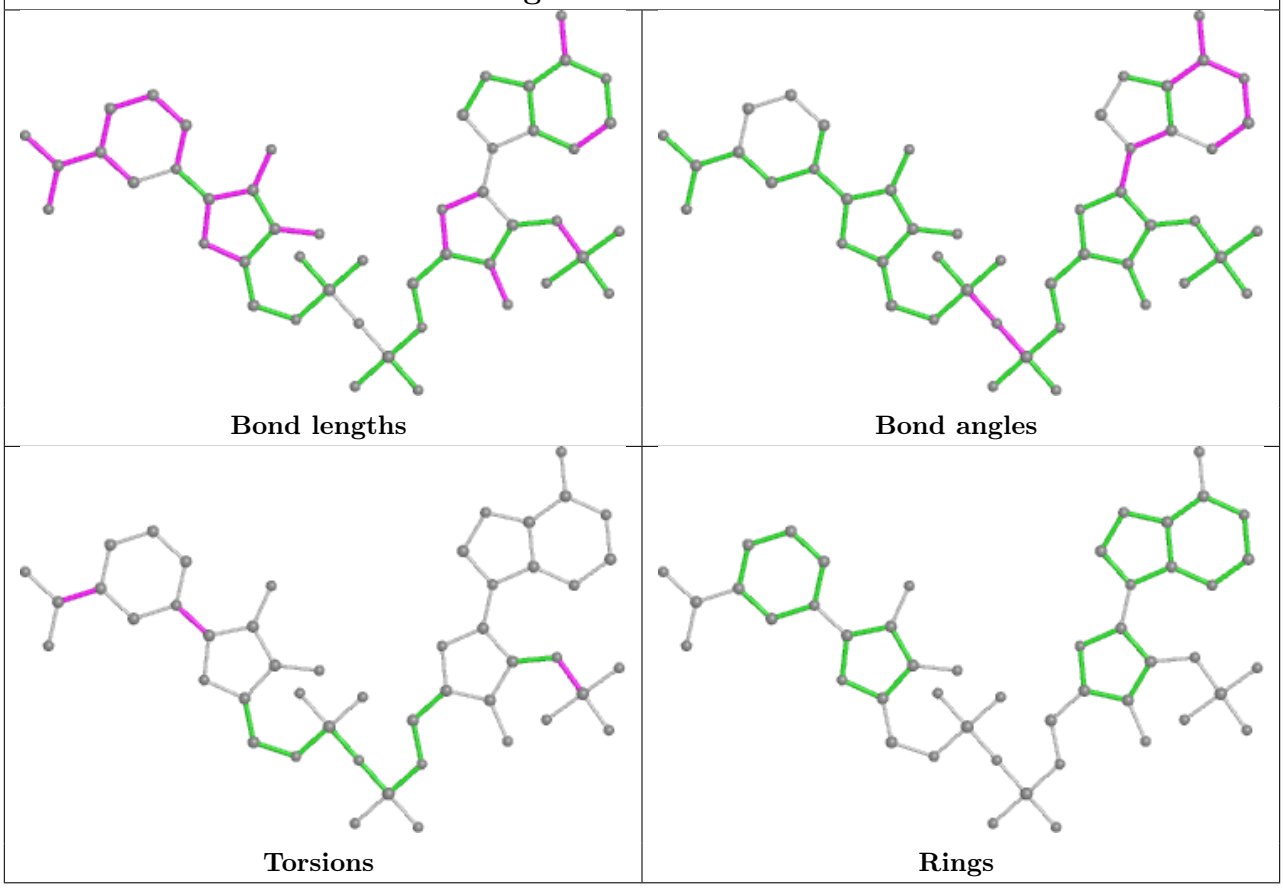


Torsions



Rings

Ligand NDP E 402



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	285/317 (89%)	0.03	12 (4%)	36	43	20, 29, 49, 68	0
1	B	287/317 (90%)	0.37	35 (12%)	4	6	20, 32, 66, 88	0
1	C	284/317 (89%)	0.24	17 (5%)	21	28	20, 33, 59, 84	0
1	D	283/317 (89%)	0.18	11 (3%)	39	46	21, 33, 57, 84	0
1	E	286/317 (90%)	-0.01	10 (3%)	44	51	19, 28, 52, 72	0
1	F	293/317 (92%)	-0.02	7 (2%)	59	66	20, 28, 49, 72	0
All	All	1718/1902 (90%)	0.13	92 (5%)	25	32	19, 30, 58, 88	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	SER	20.0
1	D	6	SER	17.6
1	B	6	SER	13.8
1	D	7	GLY	11.2
1	C	7	GLY	10.4
1	E	6	SER	8.2
1	A	6	SER	8.1
1	E	44	THR	7.0
1	B	7	GLY	6.9
1	F	6	SER	6.2
1	A	45	ARG	5.3
1	B	249	LEU	5.0
1	B	94	PHE	5.0
1	F	95	ARG	4.9
1	A	97	HIS	4.8
1	B	257	ASN	4.5
1	D	44	THR	4.3
1	E	271	GLN	4.2
1	B	272	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	274	LEU	3.8
1	B	95	ARG	3.8
1	D	271	GLN	3.7
1	C	192	ASP	3.6
1	A	46	VAL	3.5
1	E	43	GLU	3.5
1	B	260	LEU	3.4
1	D	45	ARG	3.4
1	B	254	ILE	3.4
1	E	272	ALA	3.3
1	B	278	TYR	3.3
1	B	259	PHE	3.2
1	B	250	GLU	3.2
1	B	185	LYS	3.2
1	C	8	GLU	3.1
1	B	247	LYS	3.1
1	F	87	ALA	3.1
1	D	165	CYS	3.1
1	B	166	PHE	3.0
1	B	44	THR	3.0
1	C	260	LEU	3.0
1	E	142	ASP	2.9
1	B	256	ALA	2.8
1	E	45	ARG	2.8
1	C	123	PHE	2.8
1	D	192	ASP	2.7
1	B	246	GLY	2.7
1	D	166	PHE	2.7
1	C	259	PHE	2.6
1	B	8	GLU	2.6
1	C	252	THR	2.6
1	A	271	GLN	2.6
1	F	7	GLY	2.6
1	B	282	TYR	2.5
1	C	257	ASN	2.5
1	B	205	ILE	2.5
1	F	97	HIS	2.5
1	A	205	ILE	2.5
1	B	45	ARG	2.5
1	A	257	ASN	2.5
1	B	9	LYS	2.5
1	D	8	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	92	VAL	2.5
1	B	252	THR	2.5
1	A	91	GLY	2.5
1	A	123	PHE	2.4
1	E	21	MET	2.4
1	B	273	GLY	2.4
1	A	166	PHE	2.4
1	F	88	ALA	2.3
1	F	8	GLU	2.3
1	B	305	LYS	2.3
1	D	205	ILE	2.3
1	E	8	GLU	2.3
1	C	44	THR	2.3
1	C	43	GLU	2.3
1	A	43	GLU	2.2
1	B	192	ASP	2.2
1	C	88	ALA	2.2
1	C	205	ILE	2.2
1	B	91	GLY	2.2
1	A	14	VAL	2.2
1	D	123	PHE	2.2
1	C	185	LYS	2.1
1	B	129	ARG	2.1
1	B	283	GLU	2.1
1	B	164	ALA	2.1
1	C	166	PHE	2.1
1	B	186	LYS	2.1
1	B	251	LYS	2.0
1	C	9	LYS	2.0
1	C	130	MET	2.0
1	E	97	HIS	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)

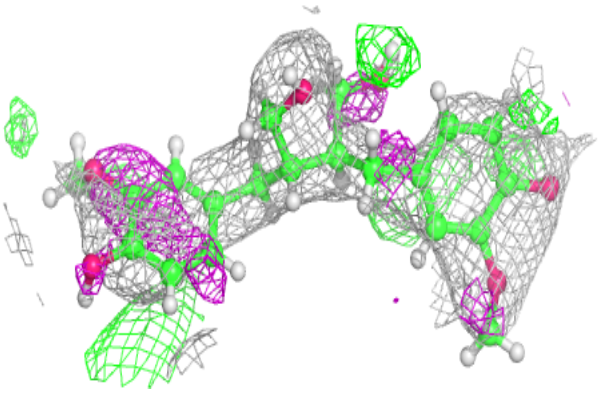
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

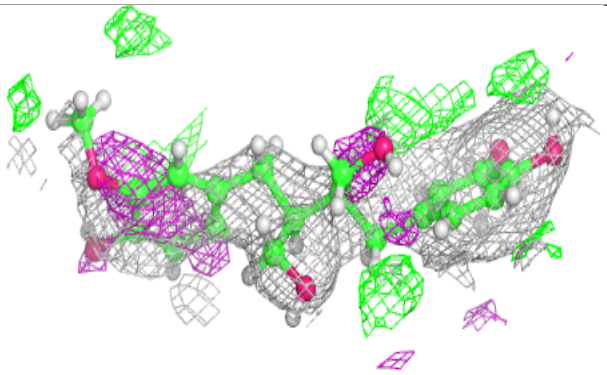
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GNU	C	401	26/26	0.66	0.29	49,61,73,81	0
2	GNU	D	401	26/26	0.70	0.30	48,59,71,75	0
2	GNU	A	401	26/26	0.72	0.31	38,56,68,79	0
2	GNU	B	401	26/26	0.73	0.21	42,55,68,74	0
2	GNU	E	401	26/26	0.86	0.22	38,49,64,76	0
3	NDP	C	402	48/48	0.90	0.18	37,53,64,80	0
3	NDP	B	402	48/48	0.92	0.15	30,38,49,50	0
3	NDP	A	402	48/48	0.92	0.19	35,50,61,63	0
3	NDP	D	402	48/48	0.92	0.16	40,50,59,64	0
3	NDP	E	402	48/48	0.92	0.15	30,43,52,56	0
2	GNU	F	401	26/26	0.93	0.14	26,33,40,53	0
3	NDP	F	402	48/48	0.97	0.10	23,31,42,47	0

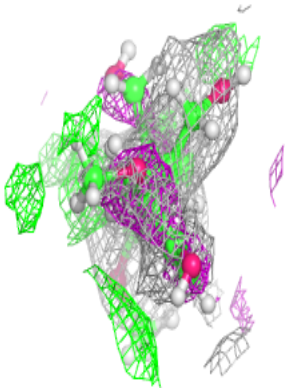
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNU C 401:

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

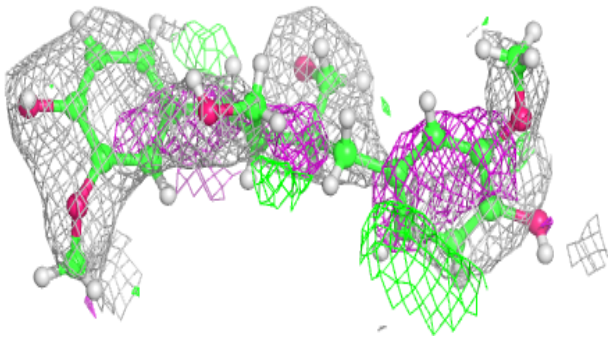


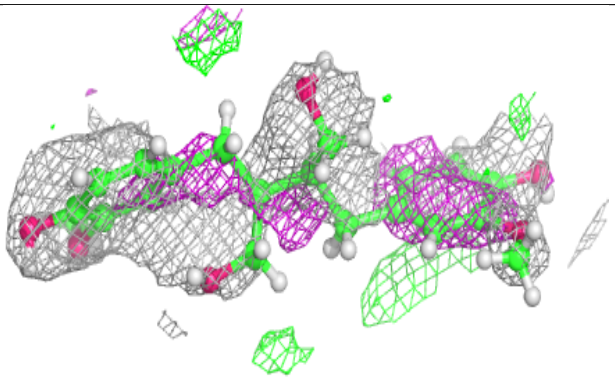


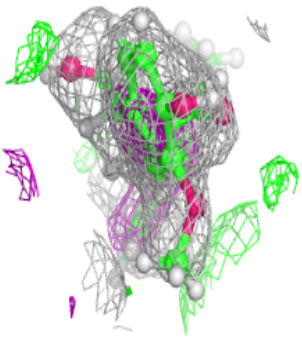


Electron density around GNU D 401:

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

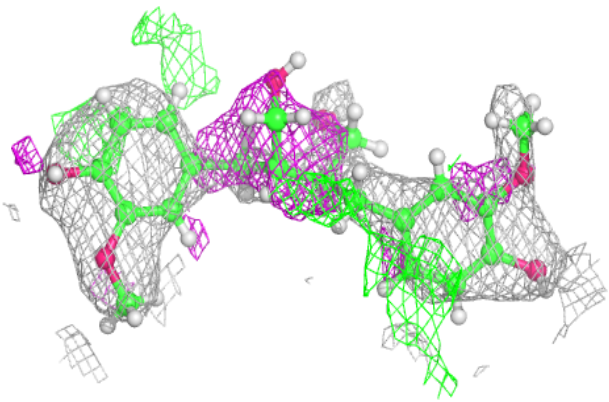


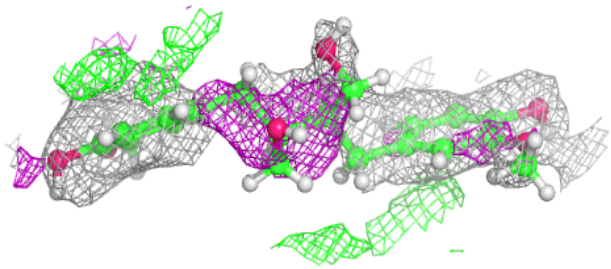


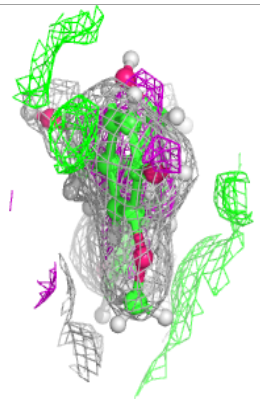


Electron density around GNU A 401:

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







Electron density around GNU B 401:

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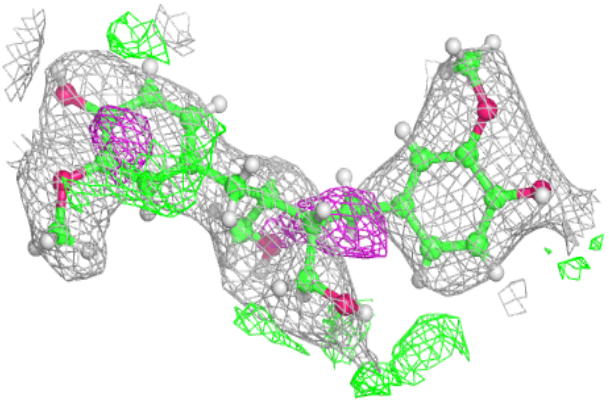
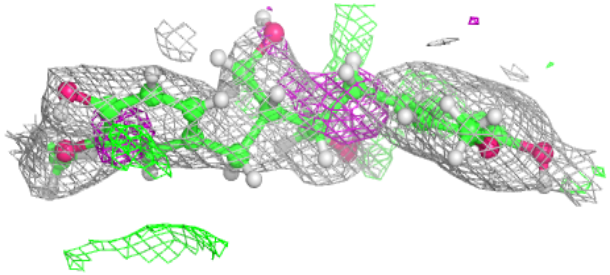
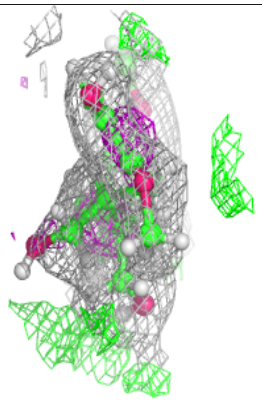
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

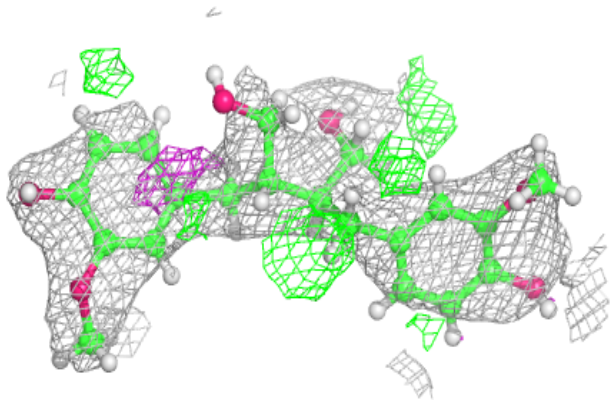


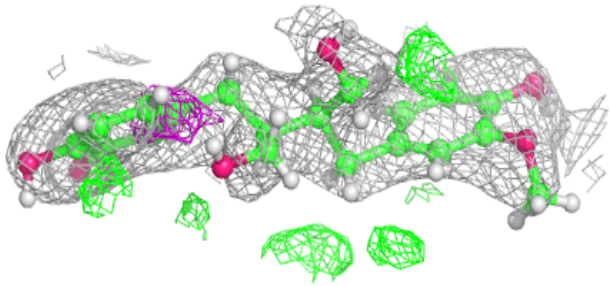


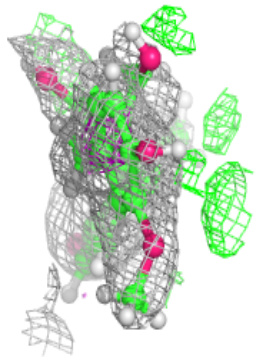


Electron density around GNU E 401:

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

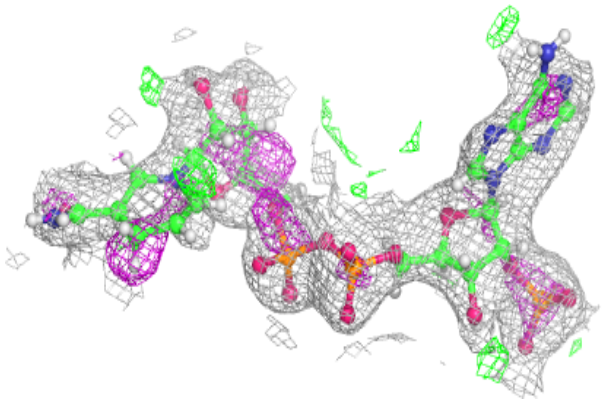


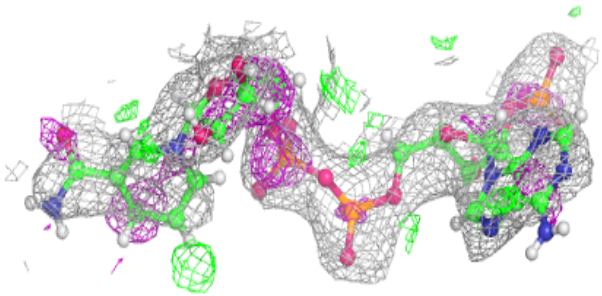


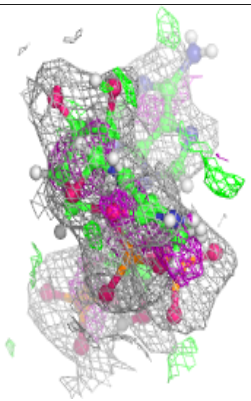


Electron density around NDP C 402:

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

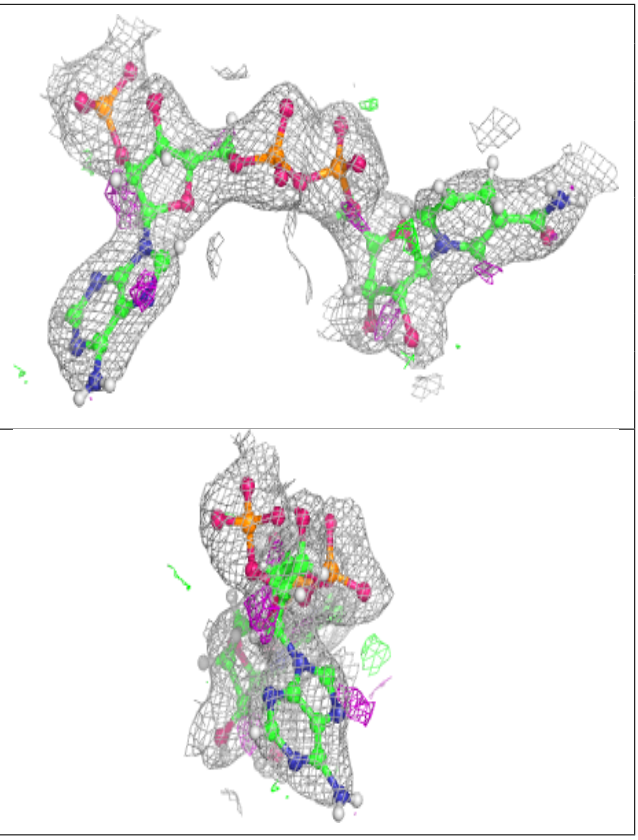






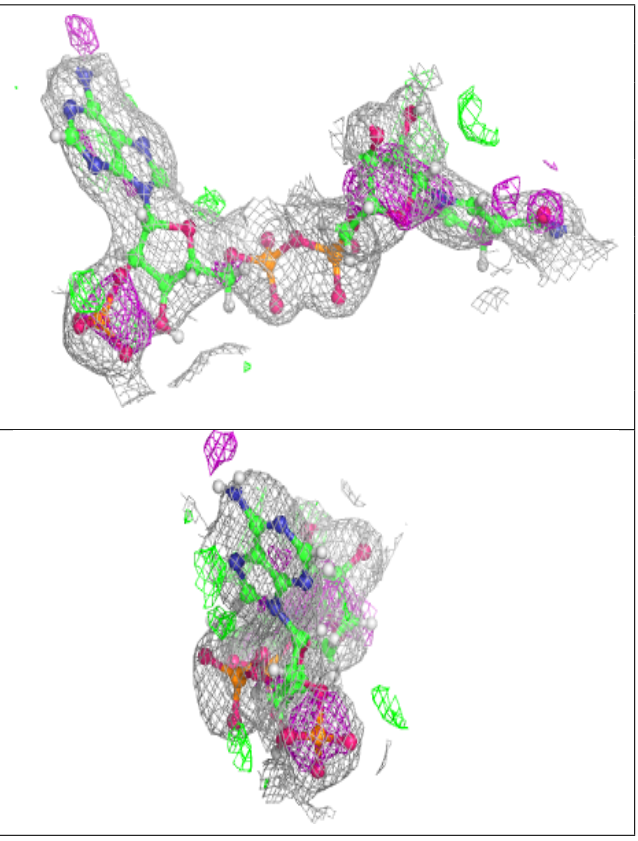
Electron density around NDP B 402:

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



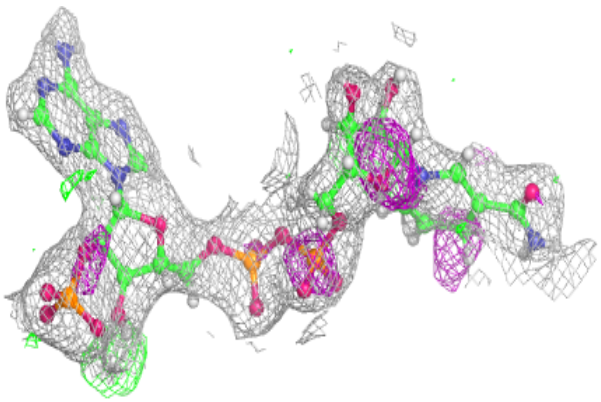
Electron density around NDP A 402:

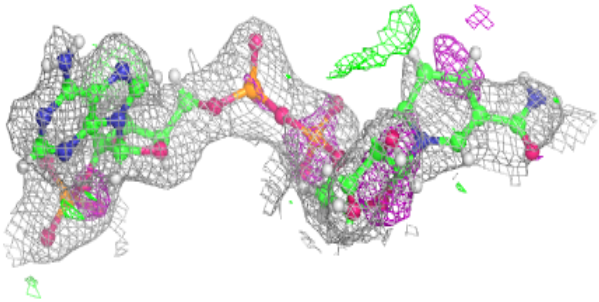
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

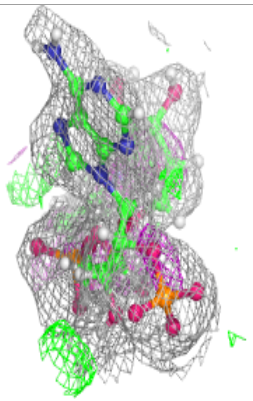


Electron density around NDP D 402:

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

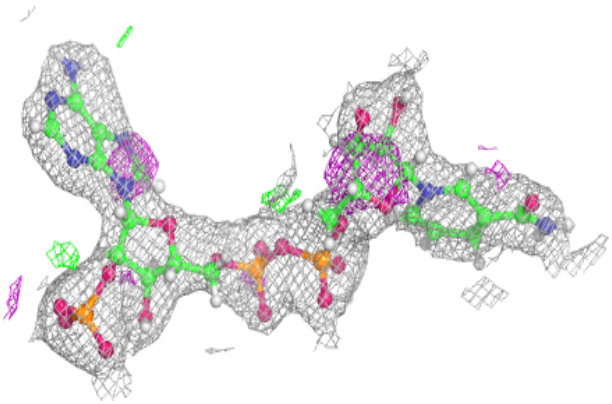


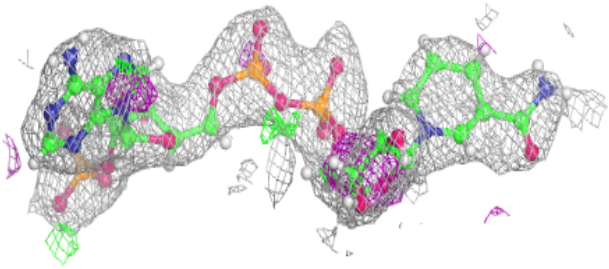


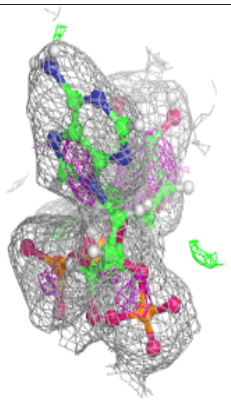


Electron density around NDP E 402:

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

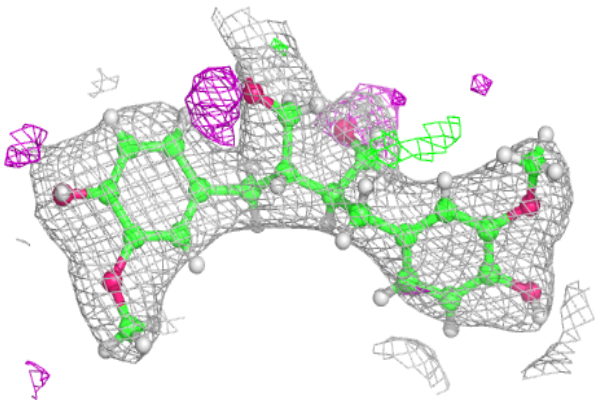


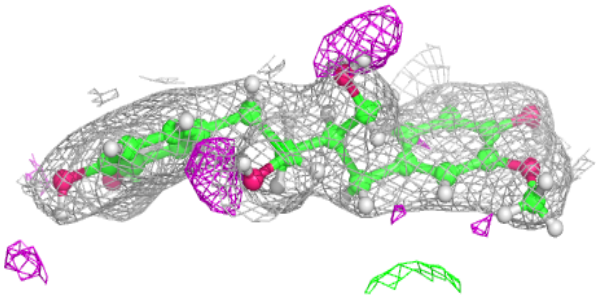


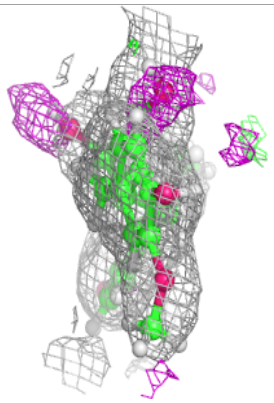


Electron density around GNU F 401:

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

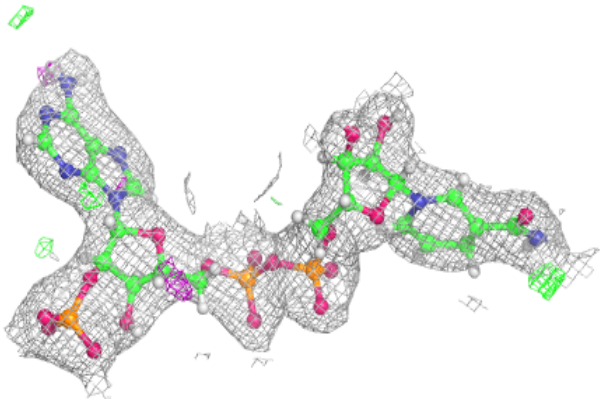


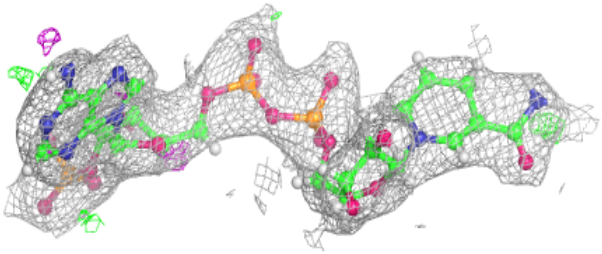


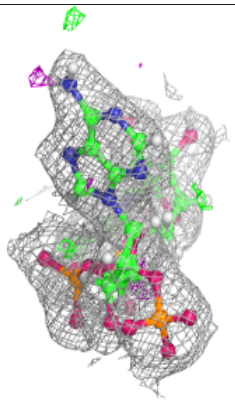


Electron density around NDP F 402:

$2mF_o$-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.