



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2021 – 04:14 PM JST

PDB ID : 7CS3  
Title : liPLR1 with NADP+  
Authors : Shao, K.; Zhang, P.  
Deposited on : 2020-08-14  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.19  
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) : 2.19

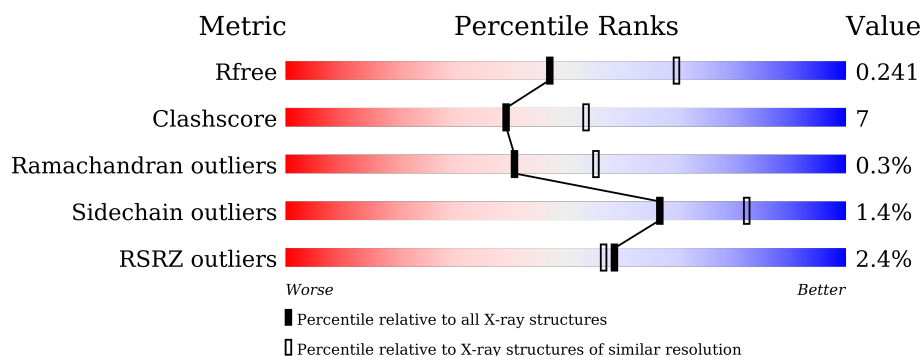
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	317	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	317	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	317	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	317	<div> <div>0%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	317	<div> <div>0%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition ⓘ

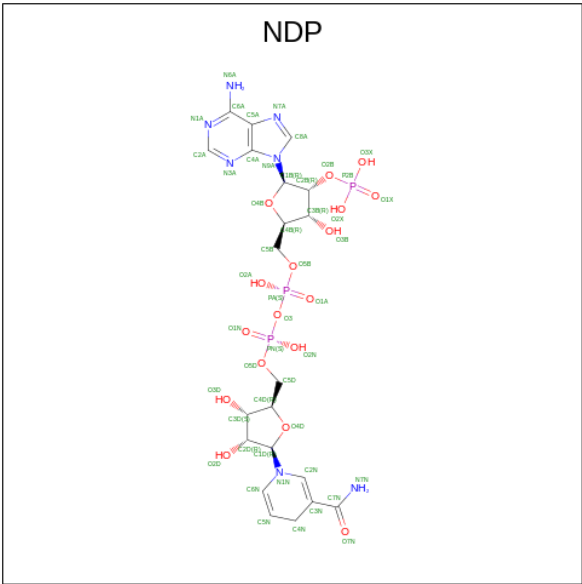
There are 3 unique types of molecules in this entry. The entry contains 14569 atoms, of which 156 are hydrogens and 0 are deuteriums.

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 Pinorexinol-lariciresinol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2307	1470	389	438	10			
1	B	295	Total	C	N	O	S	0	0	0
			2330	1481	397	442	10			
1	C	292	Total	C	N	O	S	0	0	0
			2303	1466	389	438	10			
1	D	290	Total	C	N	O	S	0	0	0
			2286	1455	385	436	10			
1	E	289	Total	C	N	O	S	0	0	0
			2282	1453	384	435	10			
1	F	282	Total	C	N	O	S	0	0	0
			2221	1415	375	422	9			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

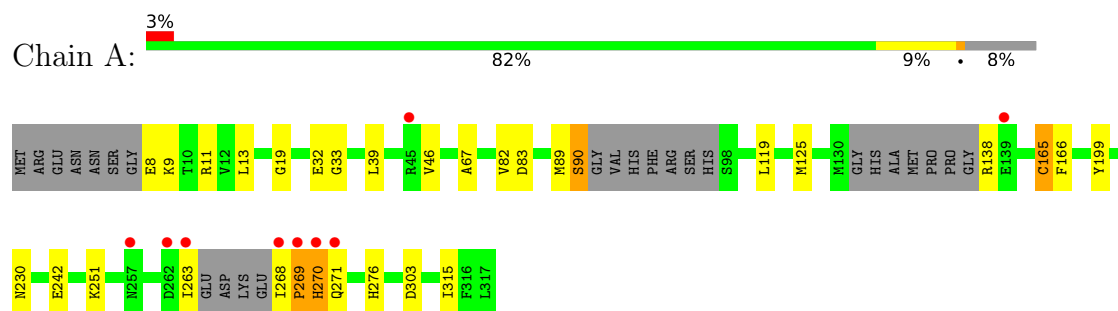
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O		
			66	66	0	0
3	B	76	Total	O		
			76	76	0	0
3	C	58	Total	O		
			58	58	0	0
3	D	57	Total	O		
			57	57	0	0
3	E	80	Total	O		
			80	80	0	0
3	F	59	Total	O		
			59	59	0	0

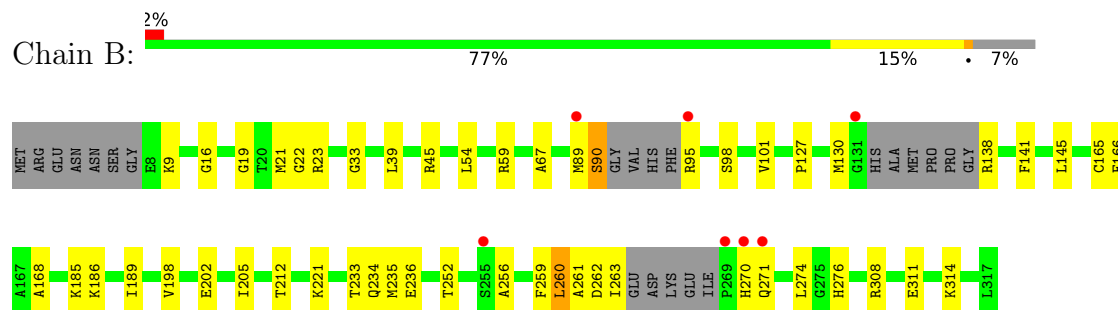
### 3 Residue-property plots

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.

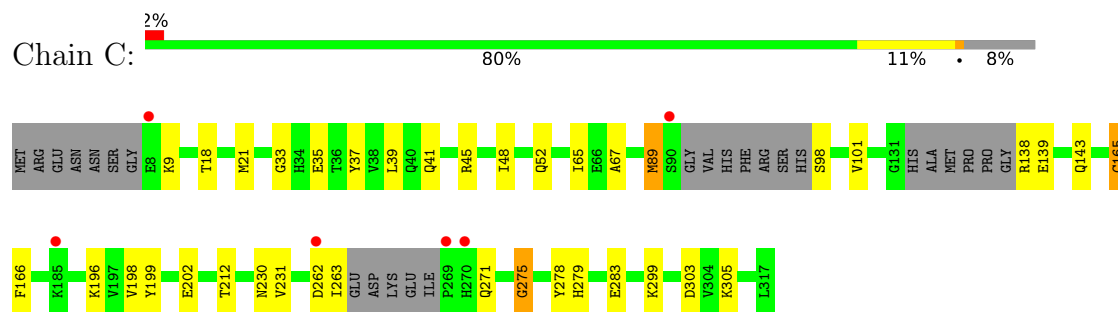
#### • Molecule 1: Pinoresinol-lariciresinol reductase



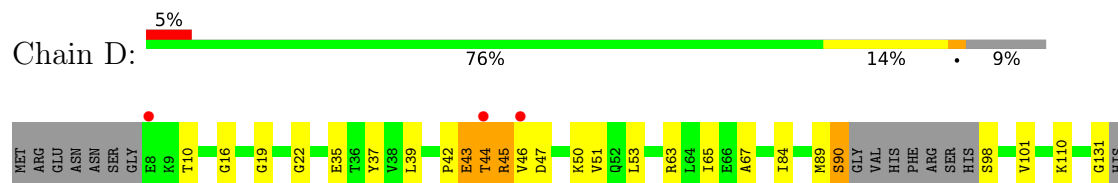
#### • Molecule 1: Pinoresinol-lariciresinol reductase



#### • Molecule 1: Pinoresinol-lariciresinol reductase

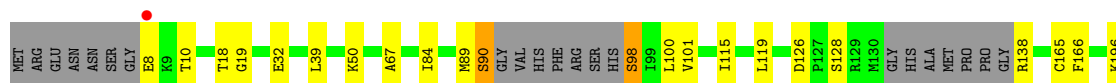
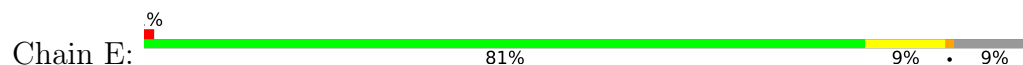


#### • Molecule 1: Pinoresinol-lariciresinol reductase

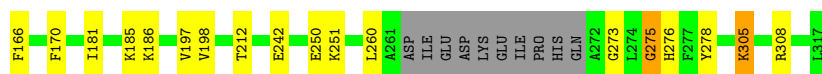
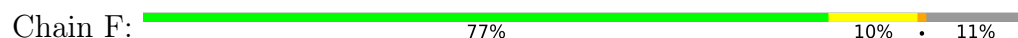




- Molecule 1: Pinoresinol-lariciresinol reductase



- Molecule 1: Pinoresinol-lariciresinol reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.90Å 243.90Å 76.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.94 – 2.40 39.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.94-2.40) 92.1 (39.45-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10_2155, PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.196 , 0.241 0.198 , 0.241	Depositor DCC
$R_{free}$ test set	2005 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 30.82 % 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 1.2258e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

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	0.50	1/2346 (0.0%)	0.59	0/3170
1	B	0.45	0/2370	0.57	0/3200
1	C	0.48	1/2342 (0.0%)	0.59	0/3163
1	D	0.46	1/2323 (0.0%)	0.60	0/3137
1	E	0.48	1/2319 (0.0%)	0.58	0/3132
1	F	0.49	0/2258	0.59	0/3051
All	All	0.48	4/13958 (0.0%)	0.59	0/18853

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	C	0	2
1	D	0	3
1	F	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	CYS	CB-SG	-5.55	1.72	1.81
1	D	165	CYS	CB-SG	-5.19	1.73	1.81
1	A	165	CYS	CB-SG	-5.12	1.73	1.81
1	E	165	CYS	CB-SG	-5.07	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.



All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	HIS	Peptide
1	C	275	GLY	Peptide
1	C	89	MET	Peptide
1	D	42	PRO	Peptide
1	D	44	THR	Peptide
1	D	45	ARG	Peptide
1	F	275	GLY	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	2307	0	2315	28	0
1	B	2330	0	2333	39	0
1	C	2303	0	2308	39	0
1	D	2286	0	2293	36	0
1	E	2282	0	2290	26	0
1	F	2221	0	2230	35	0
2	A	48	26	24	8	0
2	B	48	26	24	3	0
2	C	48	26	24	9	0
2	D	48	26	24	8	0
2	E	48	26	25	7	0
2	F	48	26	25	9	0
3	A	66	0	0	4	0
3	B	76	0	0	7	0
3	C	58	0	0	5	0
3	D	57	0	0	4	0
3	E	80	0	0	4	0
3	F	59	0	0	4	0
All	All	14413	156	13915	206	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 7.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:NDP:C1D	2:F:401:NDP:O4D	1.63	1.21
2:C:401:NDP:O4D	2:C:401:NDP:C1D	1.64	1.17
1:D:45:ARG:HG2	1:D:47:ASP:H	1.23	1.01
1:F:97:HIS:N	3:F:501:HOH:O	2.03	0.90
1:F:98:SER:OG	2:F:401:NDP:N6A	2.06	0.89
1:F:185:LYS:NZ	1:F:250:GLU:OE2	2.07	0.86
1:E:8:GLU:N	3:E:501:HOH:O	2.11	0.84
1:C:263:ILE:O	1:C:271:GLN:NE2	2.10	0.84
1:F:89:MET:O	1:F:90:SER:HB2	1.76	0.83
1:C:98:SER:N	3:C:501:HOH:O	2.10	0.83
1:A:19:GLY:HA3	2:A:401:NDP:H52A	1.61	0.83
1:A:8:GLU:N	3:A:501:HOH:O	2.11	0.82
1:D:192:ASP:OD1	1:D:194:ASN:HB3	1.81	0.81
1:F:100:LEU:HD11	1:F:143:GLN:HB3	1.63	0.78
1:D:262:ASP:O	1:D:263:ILE:HG22	1.83	0.76
1:C:262:ASP:O	1:C:263:ILE:HG12	1.85	0.76
1:D:235:MET:O	1:D:239:GLN:HG3	1.86	0.76
1:B:202:GLU:OE2	3:B:501:HOH:O	2.04	0.75
1:F:185:LYS:HG3	1:F:186:LYS:HG3	1.68	0.75
1:C:18:THR:OG1	2:C:401:NDP:O1X	2.02	0.74
1:A:138:ARG:N	1:A:276:HIS:HE2	1.85	0.73
1:C:166:PHE:H	2:C:401:NDP:H71N	1.35	0.73
1:A:39:LEU:HD11	1:A:67:ALA:HB3	1.70	0.73
1:B:98:SER:O	1:B:101:VAL:HG22	1.90	0.71
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.70	0.71
1:B:23:ARG:NH2	1:F:49:GLU:OE2	2.22	0.70
1:B:19:GLY:HA3	2:B:401:NDP:H52A	1.74	0.70
1:B:95:ARG:HG3	1:B:270:HIS:NE2	2.06	0.70
1:D:202:GLU:OE2	3:D:501:HOH:O	2.08	0.70
1:C:305:LYS:O	1:C:305:LYS:HD3	1.91	0.69
1:F:89:MET:O	2:F:401:NDP:H3D	1.93	0.69
1:F:8:GLU:N	3:F:502:HOH:O	2.25	0.69
1:F:8:GLU:OE2	3:F:502:HOH:O	2.11	0.68
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.75	0.67
1:D:45:ARG:HD3	1:D:51:VAL:HG21	1.77	0.67
1:D:90:SER:HB3	2:D:401:NDP:H3D	1.77	0.65
1:D:45:ARG:HG2	1:D:47:ASP:N	2.05	0.65
1:F:19:GLY:HA3	2:F:401:NDP:H52A	1.80	0.64
1:C:305:LYS:NZ	3:C:504:HOH:O	2.26	0.64
1:E:19:GLY:HA3	2:E:401:NDP:H52A	1.79	0.64
1:C:202:GLU:OE2	3:C:503:HOH:O	2.15	0.64
1:A:268:ILE:O	1:A:270:HIS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:OE2	3:B:502:HOH:O	2.15	0.63
1:C:21:MET:CE	1:C:166:PHE:CZ	2.82	0.63
1:B:233:THR:OG1	1:B:236:GLU:HG3	1.98	0.63
1:B:252:THR:HG23	3:B:511:HOH:O	1.98	0.63
1:B:21:MET:HE3	1:B:166:PHE:CZ	2.34	0.63
1:E:98:SER:O	1:E:101:VAL:HG22	1.99	0.62
1:E:202:GLU:OE1	3:E:502:HOH:O	2.16	0.62
1:D:98:SER:N	3:D:506:HOH:O	2.32	0.61
1:C:21:MET:HE3	1:C:166:PHE:CZ	2.37	0.60
1:B:202:GLU:H	1:B:202:GLU:CD	2.05	0.60
1:E:263:ILE:O	3:E:503:HOH:O	2.16	0.59
1:F:8:GLU:N	1:F:8:GLU:OE2	2.35	0.59
1:D:19:GLY:HA3	2:D:401:NDP:H52A	1.83	0.59
1:D:217:ARG:NH2	1:D:300:LEU:HD23	2.17	0.59
1:F:44:THR:HG21	1:F:54:LEU:HD12	1.85	0.59
1:A:165:CYS:HA	2:A:401:NDP:H72N	1.68	0.59
1:D:39:LEU:HD11	1:D:67:ALA:HB3	1.86	0.58
1:B:263:ILE:O	3:B:503:HOH:O	2.17	0.57
1:A:166:PHE:N	2:A:401:NDP:N7N	2.50	0.57
1:C:305:LYS:HD3	1:C:305:LYS:C	2.24	0.57
1:E:39:LEU:HD11	1:E:67:ALA:HB3	1.87	0.56
1:B:39:LEU:CD1	1:B:67:ALA:HB3	2.36	0.56
1:D:139:GLU:O	1:D:143:GLN:HG3	2.05	0.56
1:B:9:LYS:HD2	1:B:33:GLY:O	2.06	0.56
1:C:138:ARG:O	1:C:138:ARG:HD2	2.06	0.56
1:D:138:ARG:N	1:D:276:HIS:HE2	2.03	0.55
1:F:21:MET:HE3	1:F:166:PHE:CZ	2.41	0.55
1:A:32:GLU:OE2	3:A:502:HOH:O	2.18	0.55
1:C:166:PHE:HB3	1:C:202:GLU:OE1	2.06	0.55
1:C:45:ARG:NH2	3:C:512:HOH:O	2.39	0.55
1:F:89:MET:O	1:F:90:SER:CB	2.51	0.55
1:D:45:ARG:HD3	1:D:51:VAL:CG2	2.36	0.55
1:B:314:LYS:NZ	3:B:509:HOH:O	2.38	0.55
1:A:269:PRO:HA	1:A:271:GLN:HG2	1.88	0.55
1:D:19:GLY:CA	2:D:401:NDP:H52A	2.38	0.55
1:F:166:PHE:H	2:F:401:NDP:H72N	1.56	0.54
1:F:275:GLY:HA2	1:F:278:TYR:HB3	1.88	0.54
1:B:130:MET:HG3	1:B:141:PHE:CD2	2.43	0.54
2:D:401:NDP:O5D	2:D:401:NDP:H6N	2.07	0.54
1:C:299:LYS:NZ	3:C:511:HOH:O	2.38	0.54
1:F:16:GLY:HA2	2:F:401:NDP:H4B	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:CD1	1:E:67:ALA:HB3	2.39	0.53
1:F:242:GLU:OE1	1:F:251:LYS:NZ	2.41	0.53
1:A:19:GLY:CA	2:A:401:NDP:H52A	2.36	0.53
1:C:275:GLY:HA2	1:C:278:TYR:HB3	1.91	0.53
1:C:165:CYS:HB2	1:C:198:VAL:O	2.08	0.53
1:A:46:VAL:O	1:A:46:VAL:HG22	2.07	0.53
1:D:166:PHE:H	2:D:401:NDP:H72N	1.57	0.53
1:D:16:GLY:O	1:D:22:GLY:HA3	2.08	0.53
1:B:259:PHE:O	1:B:261:ALA:N	2.43	0.52
1:B:259:PHE:C	1:B:261:ALA:H	2.12	0.52
1:E:138:ARG:N	1:E:276:HIS:HE2	2.07	0.52
1:F:97:HIS:CD2	1:F:143:GLN:HE22	2.29	0.51
1:C:48:ILE:O	1:C:52:GLN:HG3	2.09	0.51
1:B:168:ALA:N	1:B:202:GLU:OE1	2.40	0.50
1:C:279:HIS:ND1	1:C:283:GLU:OE1	2.41	0.50
1:A:90:SER:HB2	2:A:401:NDP:H3D	1.94	0.50
1:B:19:GLY:CA	2:B:401:NDP:H52A	2.41	0.50
1:D:192:ASP:OD2	1:D:192:ASP:N	2.45	0.50
1:A:242:GLU:OE1	1:A:251:LYS:NZ	2.45	0.50
1:B:166:PHE:H	2:B:401:NDP:H72N	1.58	0.49
1:C:89:MET:O	2:C:401:NDP:O5B	2.30	0.49
1:F:305:LYS:CE	1:F:305:LYS:HA	2.37	0.49
1:A:13:LEU:HB2	1:A:82:VAL:HG11	1.93	0.49
1:D:131:GLY:O	3:D:503:HOH:O	2.20	0.49
1:E:262:ASP:O	1:E:263:ILE:HG13	2.13	0.49
1:D:169:TYR:OH	3:D:502:HOH:O	2.16	0.48
1:F:99:ILE:HG22	1:F:100:LEU:HD12	1.95	0.48
1:D:37:TYR:CD2	1:D:65:ILE:HD11	2.48	0.48
1:B:89:MET:O	1:B:90:SER:C	2.50	0.48
1:C:98:SER:O	1:C:101:VAL:HG22	2.13	0.48
1:D:259:PHE:CZ	1:D:274:LEU:HD12	2.49	0.48
1:A:90:SER:OG	3:A:503:HOH:O	2.20	0.48
1:F:275:GLY:HA2	1:F:278:TYR:CB	2.43	0.48
1:B:189:ILE:HD12	1:B:235:MET:HE2	1.96	0.48
1:E:89:MET:O	1:E:90:SER:C	2.52	0.48
1:B:234:GLN:O	1:B:234:GLN:HG2	2.13	0.47
1:E:199:TYR:O	1:E:230:ASN:HB3	2.14	0.47
1:F:197:VAL:CG1	1:F:198:VAL:N	2.77	0.47
1:D:50:LYS:HE3	2:D:401:NDP:O3X	2.14	0.47
1:D:45:ARG:HG2	1:D:46:VAL:N	2.30	0.47
1:E:90:SER:HB2	2:E:401:NDP:H3D	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LEU:CD1	1:F:143:GLN:HB3	2.39	0.47
1:D:89:MET:O	1:D:90:SER:C	2.52	0.46
1:F:170:PHE:CE2	2:F:401:NDP:N7N	2.83	0.46
1:E:138:ARG:HG3	1:E:272:ALA:CB	2.46	0.46
1:D:19:GLY:HA3	2:D:401:NDP:C5B	2.45	0.46
1:E:50:LYS:HE3	2:E:401:NDP:O3X	2.16	0.46
1:E:89:MET:O	2:E:401:NDP:O4B	2.32	0.46
1:C:21:MET:HE2	1:C:166:PHE:CZ	2.50	0.46
2:F:401:NDP:O1X	2:F:401:NDP:O3B	2.30	0.46
1:B:59:ARG:NH2	3:B:505:HOH:O	2.31	0.45
1:B:127:PRO:HB2	1:B:145:LEU:HD13	1.98	0.45
1:D:273:GLY:O	1:D:276:HIS:HB2	2.17	0.45
1:B:45:ARG:HE	1:F:181:ILE:HD11	1.80	0.45
1:C:303:ASP:OD1	1:C:303:ASP:N	2.49	0.45
1:E:32:GLU:OE2	3:E:504:HOH:O	2.21	0.45
1:A:119:LEU:HD12	1:A:119:LEU:N	2.32	0.45
1:D:110:LYS:HD2	1:D:154:ALA:HB1	1.99	0.44
1:C:35:GLU:HG2	1:C:37:TYR:CE1	2.53	0.44
1:C:39:LEU:CD1	1:C:67:ALA:HB3	2.45	0.44
1:C:196:LYS:HD2	1:C:231:VAL:HG12	2.00	0.44
1:C:202:GLU:CD	1:C:202:GLU:H	2.21	0.44
1:A:89:MET:O	1:A:90:SER:C	2.56	0.44
1:A:263:ILE:HB	1:A:268:ILE:HG12	2.00	0.44
1:D:35:GLU:OE2	1:D:63:ARG:NH1	2.49	0.44
1:E:119:LEU:HD12	1:E:119:LEU:N	2.33	0.44
1:A:89:MET:O	2:A:401:NDP:O4B	2.34	0.44
1:B:138:ARG:N	1:B:276:HIS:HE2	2.16	0.44
1:C:165:CYS:HA	2:C:401:NDP:H72N	1.83	0.44
1:E:19:GLY:CA	2:E:401:NDP:H52A	2.45	0.43
1:D:10:THR:HG21	1:D:84:ILE:HD12	2.01	0.43
1:F:44:THR:HG21	1:F:54:LEU:CD1	2.48	0.43
1:D:262:ASP:O	1:D:263:ILE:CG2	2.60	0.43
1:B:185:LYS:HB3	1:B:185:LYS:HE3	1.75	0.43
1:B:259:PHE:C	1:B:261:ALA:N	2.71	0.43
1:D:202:GLU:H	1:D:202:GLU:CD	2.21	0.43
1:E:262:ASP:C	1:E:263:ILE:HG13	2.38	0.43
1:F:41:GLN:NE2	3:F:503:HOH:O	2.28	0.43
1:E:18:THR:OG1	2:E:401:NDP:O1X	2.29	0.43
1:E:196:LYS:HD2	1:E:231:VAL:HG12	2.01	0.43
1:B:165:CYS:HB2	1:B:198:VAL:O	2.19	0.43
1:F:10:THR:HG21	1:F:84:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:O	1:A:230:ASN:HB3	2.19	0.43
1:C:9:LYS:HD2	1:C:33:GLY:O	2.19	0.43
1:C:21:MET:N	2:C:401:NDP:O1N	2.43	0.42
1:F:260:LEU:HA	1:F:260:LEU:HD23	1.78	0.42
1:E:115:ILE:HD13	1:E:115:ILE:HA	1.90	0.42
1:E:166:PHE:CD2	2:E:401:NDP:H41N	2.53	0.42
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.87	0.42
1:C:139:GLU:O	1:C:143:GLN:HG3	2.18	0.42
1:B:256:ALA:O	1:B:260:LEU:HG	2.20	0.42
1:A:9:LYS:HE3	1:A:33:GLY:O	2.20	0.42
1:B:130:MET:HG3	1:B:141:PHE:CE2	2.54	0.42
1:C:21:MET:HB2	2:C:401:NDP:O1N	2.19	0.42
1:D:43:GLU:HA	1:D:45:ARG:NH1	2.35	0.42
1:E:32:GLU:O	1:E:32:GLU:HG3	2.20	0.42
1:A:166:PHE:CD1	2:A:401:NDP:H41N	2.55	0.42
1:E:126:ASP:OD1	1:E:128:SER:OG	2.31	0.42
1:A:125:MET:HE3	3:A:517:HOH:O	2.21	0.41
1:A:268:ILE:N	1:A:269:PRO:HD3	2.35	0.41
1:B:202:GLU:HA	1:B:205:ILE:HD12	2.03	0.41
1:F:39:LEU:HD11	1:F:67:ALA:HB3	2.02	0.41
1:B:186:LYS:HB3	3:B:511:HOH:O	2.21	0.41
1:D:98:SER:O	1:D:101:VAL:HG22	2.20	0.41
1:A:303:ASP:OD2	1:A:303:ASP:N	2.51	0.41
1:B:262:ASP:N	1:B:262:ASP:OD1	2.52	0.41
1:C:199:TYR:O	1:C:230:ASN:HB3	2.21	0.41
1:A:11:ARG:NH2	1:A:83:ASP:OD2	2.43	0.41
1:A:166:PHE:H	2:A:401:NDP:H72N	1.60	0.41
1:C:37:TYR:CD2	1:C:65:ILE:HD11	2.56	0.41
1:C:262:ASP:N	1:C:262:ASP:OD1	2.52	0.41
1:C:275:GLY:O	1:C:279:HIS:CD2	2.74	0.41
1:F:305:LYS:HA	1:F:305:LYS:HE3	2.03	0.41
1:C:166:PHE:H	2:C:401:NDP:H72N	1.56	0.40
1:E:10:THR:HG21	1:E:84:ILE:HD12	2.02	0.40
1:F:273:GLY:O	1:F:276:HIS:HB2	2.22	0.40
1:A:315:ILE:HD12	1:A:315:ILE:HA	1.71	0.40
1:B:16:GLY:O	1:B:22:GLY:HA3	2.22	0.40
1:B:221:LYS:HE3	1:B:221:LYS:HB3	1.95	0.40
1:C:41:GLN:OE1	2:C:401:NDP:H2A	2.22	0.40
1:D:166:PHE:HB2	2:D:401:NDP:H71N	1.87	0.40
1:F:100:LEU:CD1	1:F:100:LEU:N	2.85	0.40
2:F:401:NDP:O3B	2:F:401:NDP:P2B	2.79	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	284/317 (90%)	276 (97%)	7 (2%)	1 (0%)	34	48
1	B	287/317 (90%)	279 (97%)	7 (2%)	1 (0%)	41	55
1	C	284/317 (90%)	276 (97%)	8 (3%)	0	100	100
1	D	282/317 (89%)	270 (96%)	9 (3%)	3 (1%)	14	20
1	E	281/317 (89%)	276 (98%)	5 (2%)	0	100	100
1	F	274/317 (86%)	265 (97%)	9 (3%)	0	100	100
All	All	1692/1902 (89%)	1642 (97%)	45 (3%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	261	ALA
1	A	269	PRO
1	B	260	LEU
1	D	262	ASP
1	D	43	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/271 (92%)	249 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	252/271 (93%)	247 (98%)	5 (2%)	55	74
1	C	249/271 (92%)	248 (100%)	1 (0%)	91	96
1	D	247/271 (91%)	243 (98%)	4 (2%)	62	79
1	E	247/271 (91%)	242 (98%)	5 (2%)	55	74
1	F	240/271 (89%)	235 (98%)	5 (2%)	53	72
All	All	1485/1626 (91%)	1464 (99%)	21 (1%)	67	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	B	90	SER
1	B	212	THR
1	B	271	GLN
1	B	274	LEU
1	B	308	ARG
1	C	212	THR
1	D	44	THR
1	D	53	LEU
1	D	90	SER
1	D	271	GLN
1	E	90	SER
1	E	98	SER
1	E	100	LEU
1	E	212	THR
1	E	248	GLU
1	F	90	SER
1	F	100	LEU
1	F	212	THR
1	F	305	LYS
1	F	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	97	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	NDP	E	401	-	45,52,52	3.99	20 (44%)	53,80,80	1.96	8 (15%)
2	NDP	A	401	-	45,52,52	3.98	19 (42%)	53,80,80	2.38	11 (20%)
2	NDP	D	401	-	45,52,52	3.99	19 (42%)	53,80,80	2.09	9 (16%)
2	NDP	C	401	-	45,52,52	4.20	20 (44%)	53,80,80	2.06	10 (18%)
2	NDP	F	401	-	45,52,52	4.19	24 (53%)	53,80,80	2.55	15 (28%)
2	NDP	B	401	-	45,52,52	3.90	20 (44%)	53,80,80	2.34	11 (20%)

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	NDP	E	401	-	-	2/30/77/77	0/5/5/5
2	NDP	A	401	-	-	12/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	D	401	-	-	10/30/77/77	0/5/5/5
2	NDP	C	401	-	-	9/30/77/77	0/5/5/5
2	NDP	F	401	-	-	7/30/77/77	0/5/5/5
2	NDP	B	401	-	-	4/30/77/77	0/5/5/5

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NDP	O4B-C1B	14.95	1.61	1.41
2	A	401	NDP	O4B-C1B	13.79	1.60	1.41
2	D	401	NDP	O4B-C1B	13.72	1.60	1.41
2	E	401	NDP	O4B-C1B	13.63	1.60	1.41
2	F	401	NDP	O4B-C1B	13.43	1.59	1.41
2	B	401	NDP	O4B-C1B	13.28	1.59	1.41
2	F	401	NDP	C6N-C5N	12.97	1.56	1.33
2	C	401	NDP	C6N-C5N	12.34	1.55	1.33
2	A	401	NDP	C6N-C5N	12.12	1.55	1.33
2	E	401	NDP	C6N-C5N	11.62	1.54	1.33
2	D	401	NDP	C6N-C5N	11.48	1.53	1.33
2	B	401	NDP	C6N-C5N	11.42	1.53	1.33
2	C	401	NDP	O4D-C1D	9.43	1.64	1.42
2	F	401	NDP	O4D-C1D	9.22	1.63	1.42
2	E	401	NDP	O4D-C1D	8.89	1.63	1.42
2	D	401	NDP	O4D-C1D	8.88	1.63	1.42
2	B	401	NDP	O4D-C1D	7.97	1.60	1.42
2	A	401	NDP	O4D-C1D	7.94	1.60	1.42
2	E	401	NDP	C2D-C1D	-7.55	1.29	1.53
2	F	401	NDP	C2D-C1D	-7.42	1.29	1.53
2	D	401	NDP	C2D-C1D	-7.40	1.29	1.53
2	B	401	NDP	C2D-C1D	-7.39	1.29	1.53
2	A	401	NDP	C2D-C1D	-7.26	1.30	1.53
2	C	401	NDP	O4D-C4D	-7.18	1.28	1.45
2	C	401	NDP	C2D-C1D	-7.16	1.30	1.53
2	B	401	NDP	O4D-C4D	-6.95	1.29	1.45
2	E	401	NDP	O4D-C4D	-6.89	1.29	1.45
2	A	401	NDP	O4D-C4D	-6.80	1.29	1.45
2	B	401	NDP	O4B-C4B	-6.74	1.29	1.45
2	A	401	NDP	O4B-C4B	-6.69	1.30	1.45
2	D	401	NDP	O4D-C4D	-6.64	1.30	1.45
2	C	401	NDP	O4B-C4B	-6.46	1.30	1.45
2	D	401	NDP	O4B-C4B	-6.45	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	NDP	O4B-C4B	-6.38	1.30	1.45
2	F	401	NDP	O4D-C4D	-5.97	1.31	1.45
2	F	401	NDP	C2N-C3N	5.90	1.51	1.34
2	D	401	NDP	C2N-C3N	5.85	1.51	1.34
2	C	401	NDP	C2N-C3N	5.81	1.51	1.34
2	F	401	NDP	O4B-C4B	-5.64	1.32	1.45
2	F	401	NDP	P2B-O2B	5.57	1.69	1.59
2	E	401	NDP	C2N-C3N	5.55	1.50	1.34
2	A	401	NDP	C2N-C3N	5.53	1.50	1.34
2	B	401	NDP	C2N-C3N	5.06	1.49	1.34
2	C	401	NDP	P2B-O2B	4.63	1.68	1.59
2	F	401	NDP	C6A-N6A	4.49	1.50	1.34
2	D	401	NDP	C6A-N6A	4.30	1.49	1.34
2	B	401	NDP	P2B-O2B	4.10	1.67	1.59
2	A	401	NDP	C6A-N6A	4.10	1.49	1.34
2	E	401	NDP	C6A-N6A	4.10	1.49	1.34
2	B	401	NDP	C6A-N6A	4.01	1.48	1.34
2	E	401	NDP	P2B-O2B	3.92	1.66	1.59
2	C	401	NDP	C6A-N6A	3.91	1.48	1.34
2	A	401	NDP	C4N-C3N	3.79	1.57	1.49
2	F	401	NDP	C4N-C5N	3.79	1.58	1.48
2	F	401	NDP	C2A-N3A	3.75	1.38	1.32
2	C	401	NDP	O2D-C2D	3.70	1.51	1.43
2	D	401	NDP	C2A-N3A	3.65	1.38	1.32
2	F	401	NDP	C4N-C3N	3.63	1.57	1.49
2	F	401	NDP	O2D-C2D	3.58	1.51	1.43
2	A	401	NDP	C2A-N3A	3.51	1.37	1.32
2	C	401	NDP	C2A-N3A	3.50	1.37	1.32
2	A	401	NDP	C6N-N1N	3.49	1.46	1.37
2	D	401	NDP	O2D-C2D	3.49	1.51	1.43
2	E	401	NDP	C7N-N7N	3.43	1.42	1.33
2	F	401	NDP	C6N-N1N	3.40	1.45	1.37
2	A	401	NDP	P2B-O2B	3.38	1.65	1.59
2	C	401	NDP	C4N-C5N	3.27	1.57	1.48
2	B	401	NDP	O2D-C2D	3.25	1.50	1.43
2	D	401	NDP	C7N-N7N	3.23	1.42	1.33
2	E	401	NDP	C2A-N3A	3.18	1.37	1.32
2	D	401	NDP	P2B-O2B	3.14	1.65	1.59
2	A	401	NDP	C4N-C5N	3.09	1.57	1.48
2	B	401	NDP	O3B-C3B	-3.07	1.35	1.43
2	D	401	NDP	O3B-C3B	-3.05	1.35	1.43
2	D	401	NDP	O7N-C7N	-3.04	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NDP	C7N-N7N	2.98	1.41	1.33
2	C	401	NDP	C6N-N1N	2.97	1.44	1.37
2	B	401	NDP	C2A-N3A	2.96	1.36	1.32
2	E	401	NDP	O2D-C2D	2.95	1.49	1.43
2	B	401	NDP	C4N-C5N	2.90	1.56	1.48
2	B	401	NDP	C7N-N7N	2.84	1.40	1.33
2	A	401	NDP	O2D-C2D	2.81	1.49	1.43
2	E	401	NDP	C4N-C3N	2.81	1.55	1.49
2	C	401	NDP	C7N-N7N	2.78	1.40	1.33
2	C	401	NDP	O3D-C3D	-2.69	1.36	1.43
2	B	401	NDP	O7N-C7N	-2.66	1.18	1.24
2	C	401	NDP	PN-O5D	2.66	1.70	1.59
2	A	401	NDP	O3B-C3B	-2.65	1.36	1.43
2	E	401	NDP	O3D-C3D	-2.63	1.36	1.43
2	D	401	NDP	C4N-C5N	2.61	1.55	1.48
2	F	401	NDP	C2A-N1A	2.58	1.38	1.33
2	F	401	NDP	O3B-C3B	-2.52	1.37	1.43
2	F	401	NDP	C7N-C3N	2.51	1.54	1.48
2	E	401	NDP	O3B-C3B	-2.46	1.37	1.43
2	B	401	NDP	O3D-C3D	-2.44	1.37	1.43
2	F	401	NDP	PN-O5D	2.43	1.69	1.59
2	A	401	NDP	O3D-C3D	-2.38	1.37	1.43
2	E	401	NDP	O7N-C7N	-2.36	1.18	1.24
2	A	401	NDP	PN-O5D	2.35	1.68	1.59
2	B	401	NDP	C6N-N1N	2.35	1.43	1.37
2	F	401	NDP	PA-O5B	2.34	1.68	1.59
2	E	401	NDP	C6N-N1N	2.32	1.43	1.37
2	D	401	NDP	C6N-N1N	2.30	1.43	1.37
2	C	401	NDP	PA-O5B	2.28	1.68	1.59
2	D	401	NDP	O3D-C3D	-2.26	1.37	1.43
2	C	401	NDP	C4N-C3N	2.23	1.54	1.49
2	D	401	NDP	C7N-C3N	2.23	1.53	1.48
2	F	401	NDP	C4A-N3A	2.21	1.38	1.35
2	E	401	NDP	C4N-C5N	2.20	1.54	1.48
2	C	401	NDP	O3B-C3B	-2.15	1.37	1.43
2	A	401	NDP	C7N-N7N	2.13	1.39	1.33
2	F	401	NDP	O7N-C7N	-2.12	1.19	1.24
2	C	401	NDP	C2A-N1A	2.11	1.37	1.33
2	B	401	NDP	C5A-C4A	-2.11	1.35	1.40
2	B	401	NDP	C7N-C3N	2.11	1.53	1.48
2	B	401	NDP	C5B-C4B	2.10	1.58	1.51
2	A	401	NDP	C7N-C3N	2.10	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NDP	C5D-C4D	2.07	1.58	1.51
2	E	401	NDP	C5D-C4D	2.06	1.58	1.51
2	F	401	NDP	C8A-N7A	2.03	1.38	1.34
2	E	401	NDP	PN-O5D	2.02	1.67	1.59
2	D	401	NDP	C4N-C3N	2.01	1.53	1.49

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NDP	C5A-C6A-N6A	10.35	136.07	120.35
2	A	401	NDP	C5A-C6A-N6A	9.45	134.71	120.35
2	B	401	NDP	C5A-C6A-N6A	9.09	134.17	120.35
2	C	401	NDP	C5A-C6A-N6A	8.00	132.50	120.35
2	E	401	NDP	C5A-C6A-N6A	7.73	132.10	120.35
2	D	401	NDP	C5A-C6A-N6A	7.28	131.41	120.35
2	F	401	NDP	N3A-C2A-N1A	-7.26	117.33	128.68
2	F	401	NDP	N6A-C6A-N1A	-6.74	104.58	118.57
2	B	401	NDP	N3A-C2A-N1A	-6.29	118.85	128.68
2	A	401	NDP	N6A-C6A-N1A	-6.21	105.68	118.57
2	B	401	NDP	C1B-N9A-C4A	-6.01	116.09	126.64
2	D	401	NDP	C1B-N9A-C4A	-5.85	116.37	126.64
2	E	401	NDP	N3A-C2A-N1A	-5.80	119.62	128.68
2	C	401	NDP	N3A-C2A-N1A	-5.68	119.79	128.68
2	A	401	NDP	O4B-C4B-C3B	-5.66	93.91	105.11
2	B	401	NDP	N6A-C6A-N1A	-5.62	106.90	118.57
2	C	401	NDP	N6A-C6A-N1A	-5.57	107.00	118.57
2	A	401	NDP	C1B-N9A-C4A	-5.46	117.05	126.64
2	A	401	NDP	N3A-C2A-N1A	-5.37	120.29	128.68
2	C	401	NDP	C1B-N9A-C4A	-5.36	117.23	126.64
2	D	401	NDP	N3A-C2A-N1A	-5.23	120.50	128.68
2	E	401	NDP	C1B-N9A-C4A	-5.05	117.77	126.64
2	F	401	NDP	C1B-N9A-C4A	-4.87	118.09	126.64
2	E	401	NDP	N6A-C6A-N1A	-4.52	109.20	118.57
2	A	401	NDP	C3N-C7N-N7N	-4.41	109.83	117.67
2	D	401	NDP	PN-O3-PA	-4.30	118.08	132.83
2	D	401	NDP	N6A-C6A-N1A	-4.27	109.71	118.57
2	D	401	NDP	C3N-C2N-N1N	-4.22	117.07	123.10
2	D	401	NDP	O4B-C4B-C3B	-4.04	97.12	105.11
2	E	401	NDP	O4B-C4B-C3B	-3.88	97.44	105.11
2	F	401	NDP	O4B-C4B-C3B	-3.77	97.65	105.11
2	E	401	NDP	C3N-C2N-N1N	-3.60	117.96	123.10
2	B	401	NDP	O3B-C3B-C4B	-3.11	102.05	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NDP	O4B-C4B-C3B	-3.11	98.96	105.11
2	C	401	NDP	C3N-C2N-N1N	-3.01	118.80	123.10
2	B	401	NDP	O7N-C7N-N7N	-2.97	115.94	122.88
2	F	401	NDP	C3N-C2N-N1N	-2.91	118.95	123.10
2	F	401	NDP	O4D-C1D-C2D	-2.79	100.55	106.64
2	F	401	NDP	O7N-C7N-C3N	2.76	126.10	120.90
2	F	401	NDP	C4A-C5A-N7A	-2.73	106.56	109.40
2	B	401	NDP	C3N-C2N-N1N	-2.66	119.30	123.10
2	F	401	NDP	C4D-O4D-C1D	-2.57	103.80	109.47
2	F	401	NDP	O4D-C1D-N1N	2.52	112.98	108.06
2	B	401	NDP	O3B-C3B-C2B	2.50	118.28	111.17
2	F	401	NDP	O3X-P2B-O2B	2.50	117.20	105.99
2	C	401	NDP	O2B-C2B-C3B	-2.46	102.75	111.68
2	B	401	NDP	C3N-C7N-N7N	2.43	121.99	117.67
2	A	401	NDP	O5B-PA-O1A	-2.43	99.58	109.07
2	A	401	NDP	O3B-C3B-C2B	2.42	118.03	111.17
2	F	401	NDP	C2A-N1A-C6A	2.34	122.76	118.75
2	A	401	NDP	O4D-C1D-C2D	-2.31	101.61	106.64
2	A	401	NDP	O7N-C7N-N7N	2.28	128.21	122.88
2	F	401	NDP	O3X-P2B-O2X	-2.28	98.93	107.64
2	F	401	NDP	O4D-C4D-C3D	-2.26	100.64	105.11
2	C	401	NDP	C5B-C4B-C3B	-2.21	106.91	115.18
2	C	401	NDP	O2A-PA-O5B	2.21	117.99	107.75
2	D	401	NDP	O7N-C7N-N7N	-2.20	117.74	122.88
2	D	401	NDP	C1D-N1N-C6N	-2.18	116.14	120.83
2	B	401	NDP	O2B-C2B-C1B	-2.16	102.31	110.10
2	C	401	NDP	C2D-C3D-C4D	2.15	106.81	102.64
2	E	401	NDP	C2B-C3B-C4B	-2.12	97.39	101.99
2	C	401	NDP	C4D-O4D-C1D	-2.11	104.83	109.47
2	A	401	NDP	C3N-C2N-N1N	-2.09	120.12	123.10
2	E	401	NDP	C2D-C3D-C4D	2.04	106.61	102.64

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NDP	C5D-O5D-PN-O1N
2	A	401	NDP	C5D-O5D-PN-O2N
2	A	401	NDP	C2N-C3N-C7N-N7N
2	C	401	NDP	C5B-O5B-PA-O3
2	C	401	NDP	O4D-C1D-N1N-C2N
2	C	401	NDP	C2N-C3N-C7N-O7N

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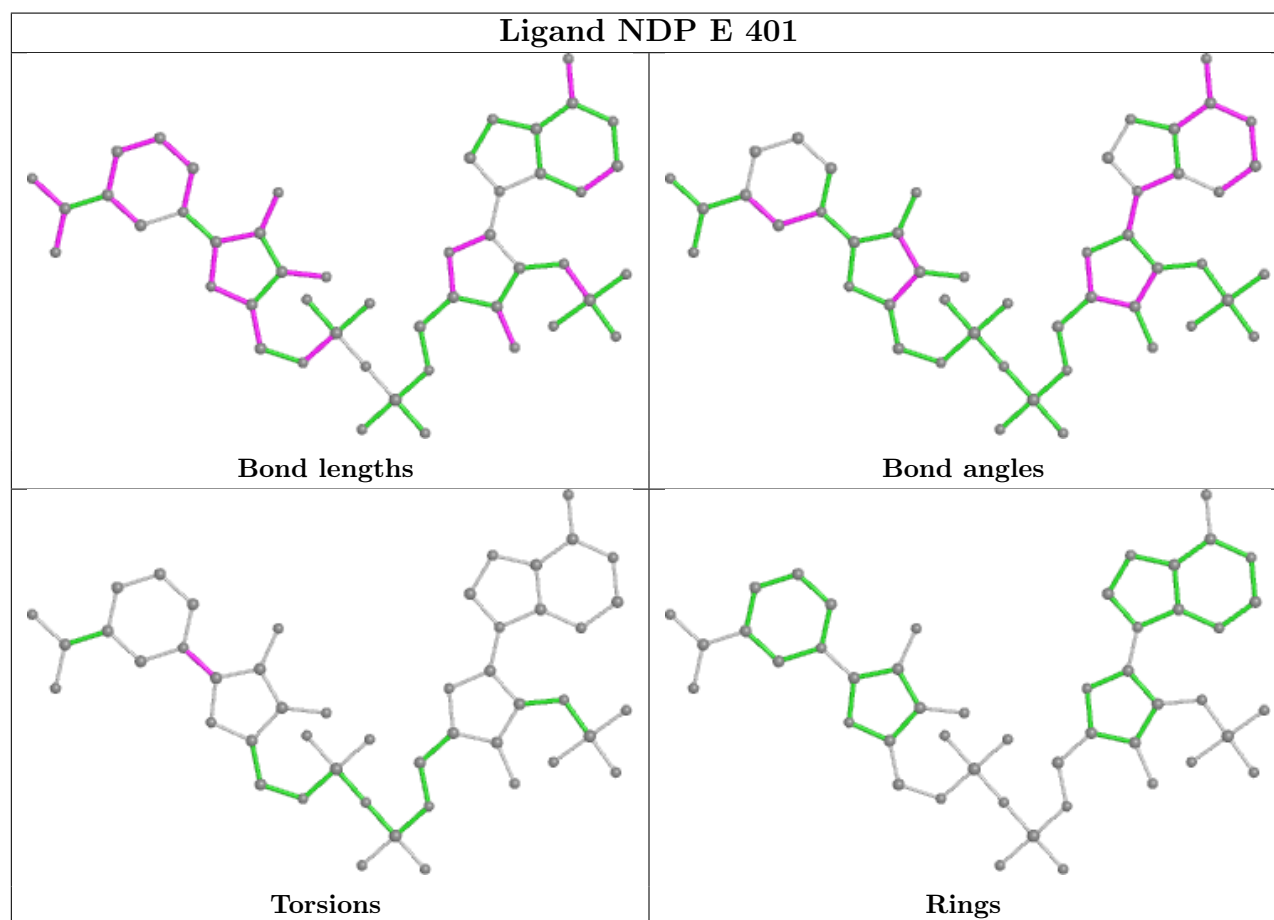
Mol	Chain	Res	Type	Atoms
2	C	401	NDP	C2N-C3N-C7N-N7N
2	F	401	NDP	C3B-C2B-O2B-P2B
2	F	401	NDP	C5D-O5D-PN-O1N
2	D	401	NDP	O4B-C4B-C5B-O5B
2	B	401	NDP	C1B-C2B-O2B-P2B
2	A	401	NDP	C3B-C2B-O2B-P2B
2	B	401	NDP	C3B-C2B-O2B-P2B
2	A	401	NDP	C1B-C2B-O2B-P2B
2	D	401	NDP	C1B-C2B-O2B-P2B
2	D	401	NDP	C3B-C2B-O2B-P2B
2	D	401	NDP	O4D-C4D-C5D-O5D
2	B	401	NDP	O4D-C1D-N1N-C2N
2	D	401	NDP	O4D-C1D-N1N-C2N
2	C	401	NDP	C2B-O2B-P2B-O1X
2	A	401	NDP	C5B-O5B-PA-O3
2	A	401	NDP	C5D-O5D-PN-O3
2	F	401	NDP	C2B-O2B-P2B-O3X
2	F	401	NDP	C5D-O5D-PN-O3
2	C	401	NDP	C5B-O5B-PA-O1A
2	C	401	NDP	C5D-O5D-PN-O2N
2	F	401	NDP	C5D-O5D-PN-O2N
2	F	401	NDP	O4D-C1D-N1N-C2N
2	A	401	NDP	C2N-C3N-C7N-O7N
2	A	401	NDP	C2D-C1D-N1N-C2N
2	A	401	NDP	O4D-C1D-N1N-C2N
2	E	401	NDP	O4D-C1D-N1N-C2N
2	A	401	NDP	C2D-C1D-N1N-C6N
2	F	401	NDP	C2D-C1D-N1N-C2N
2	D	401	NDP	C2B-O2B-P2B-O1X
2	E	401	NDP	C2D-C1D-N1N-C2N
2	B	401	NDP	C2B-O2B-P2B-O2X
2	C	401	NDP	C5D-O5D-PN-O3
2	D	401	NDP	C2B-O2B-P2B-O2X
2	D	401	NDP	C2B-O2B-P2B-O3X
2	C	401	NDP	PN-O3-PA-O2A
2	A	401	NDP	C5B-O5B-PA-O2A
2	D	401	NDP	C5B-O5B-PA-O1A
2	D	401	NDP	C5D-O5D-PN-O1N

There are no ring outliers.

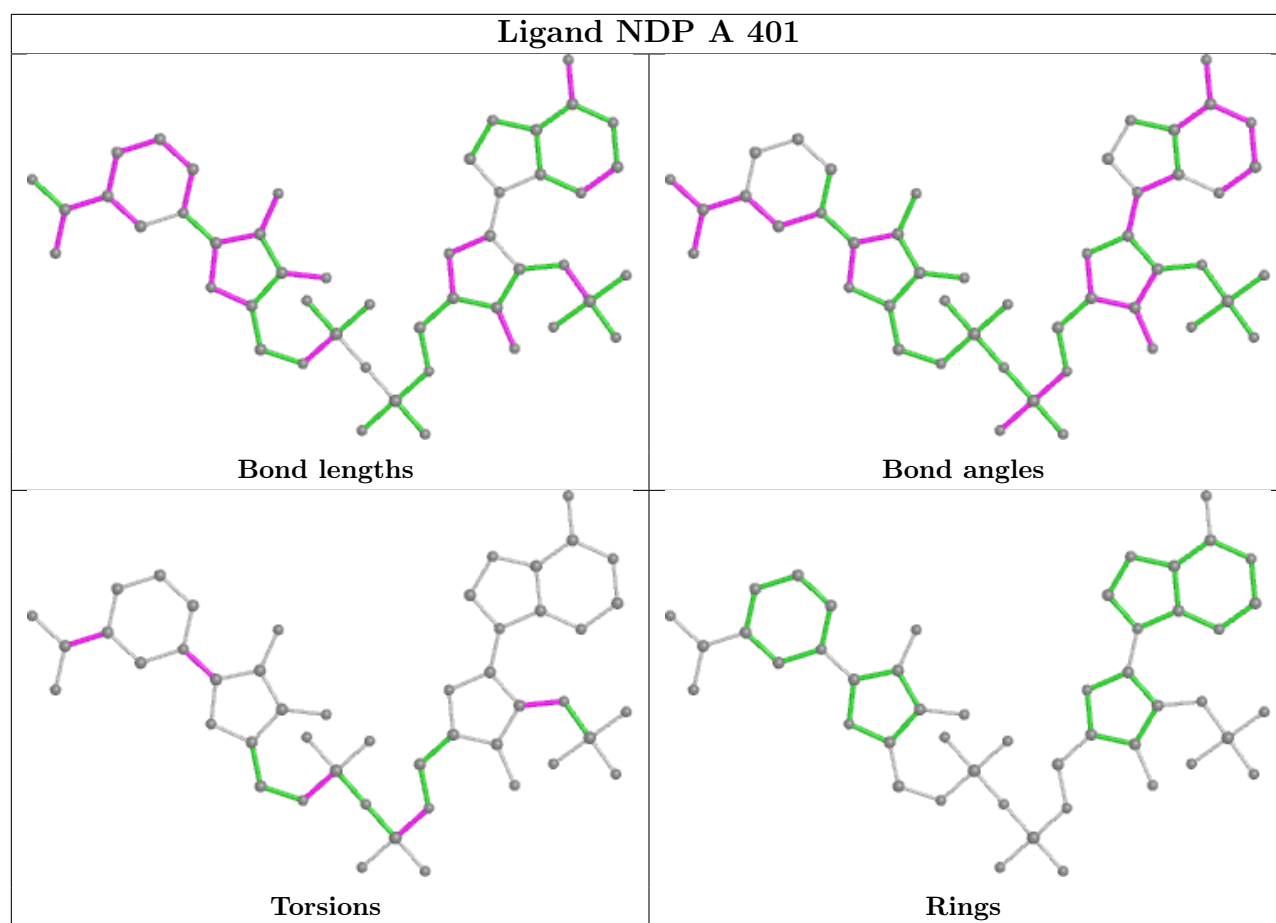
6 monomers are involved in 44 short contacts:

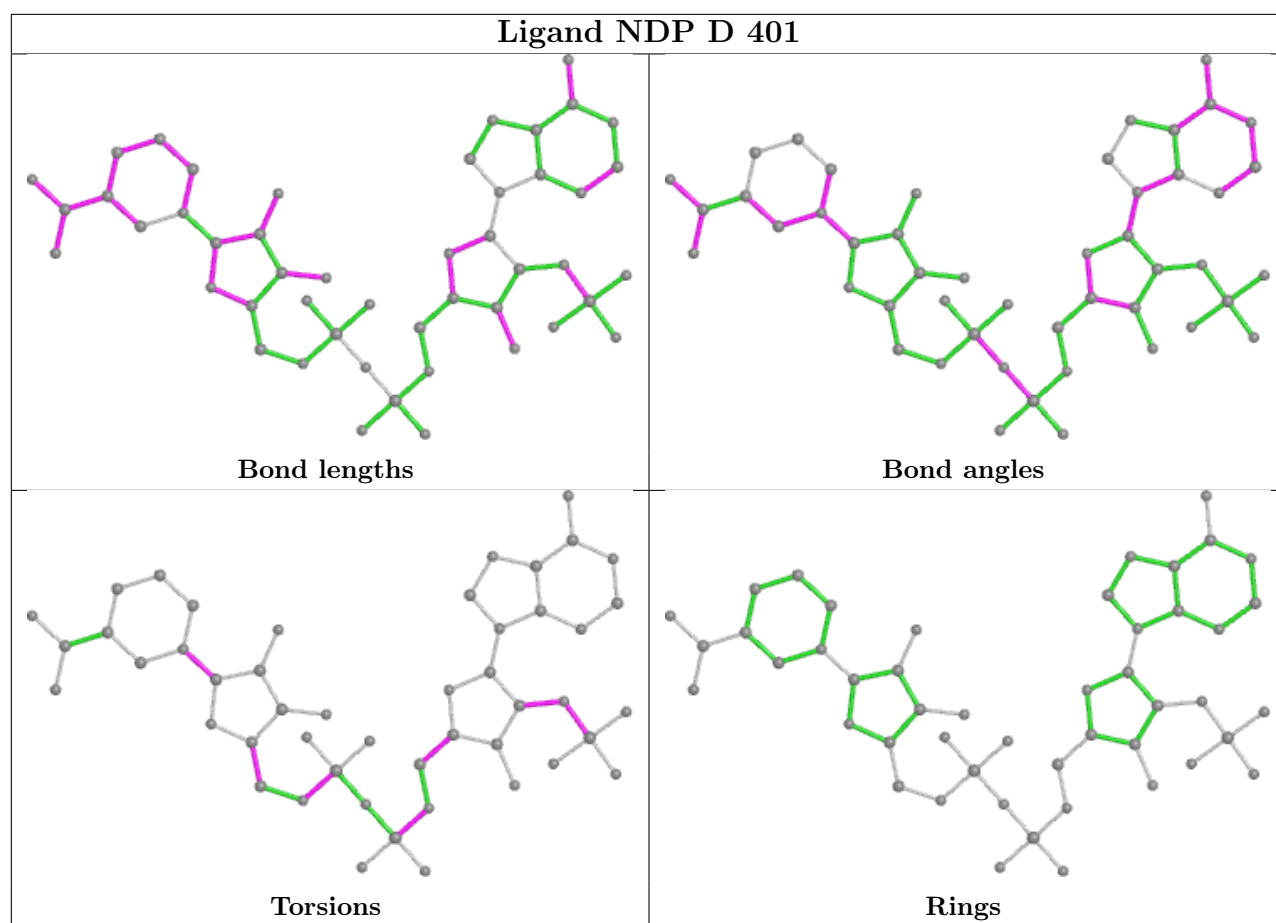
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	NDP	7	0
2	A	401	NDP	8	0
2	D	401	NDP	8	0
2	C	401	NDP	9	0
2	F	401	NDP	9	0
2	B	401	NDP	3	0

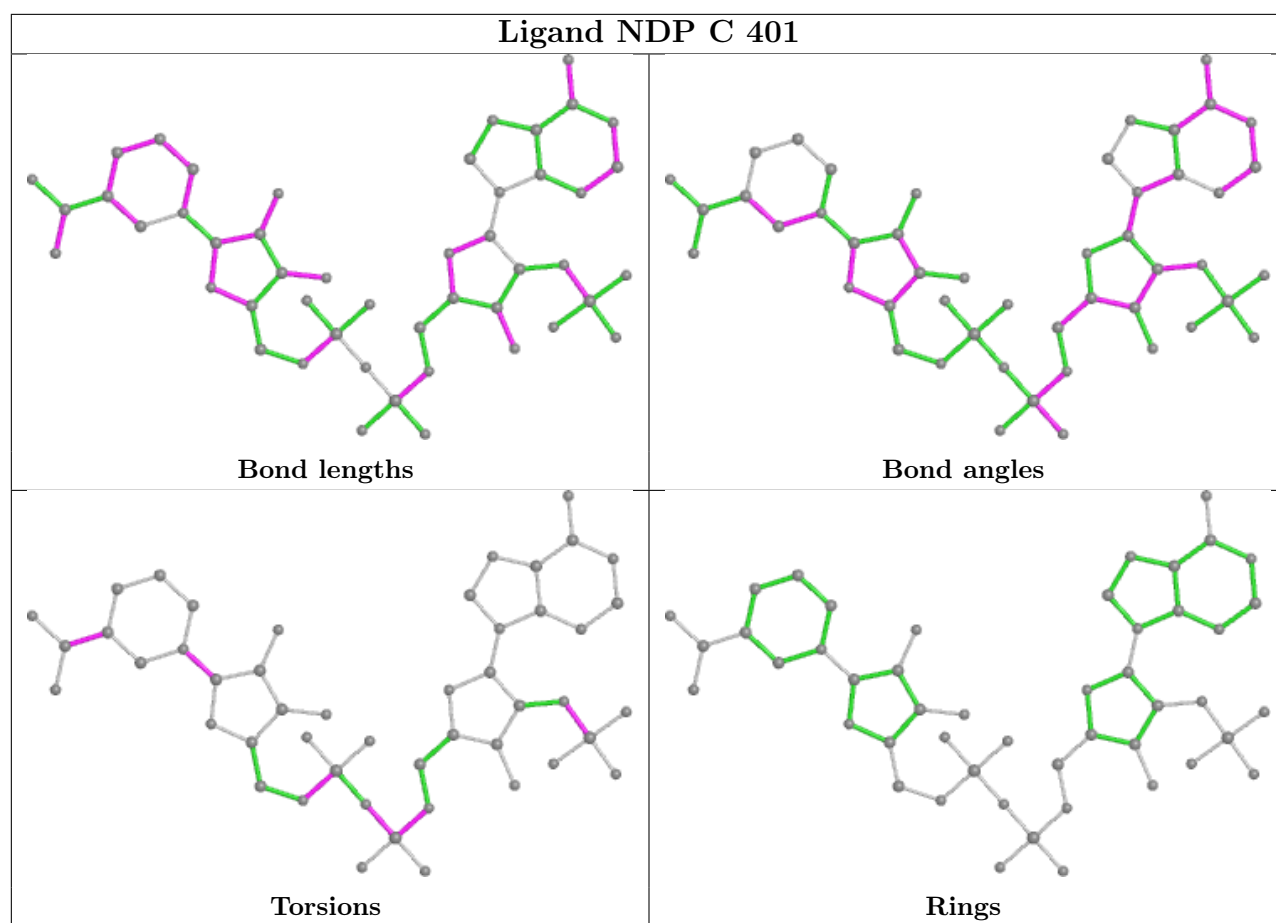
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

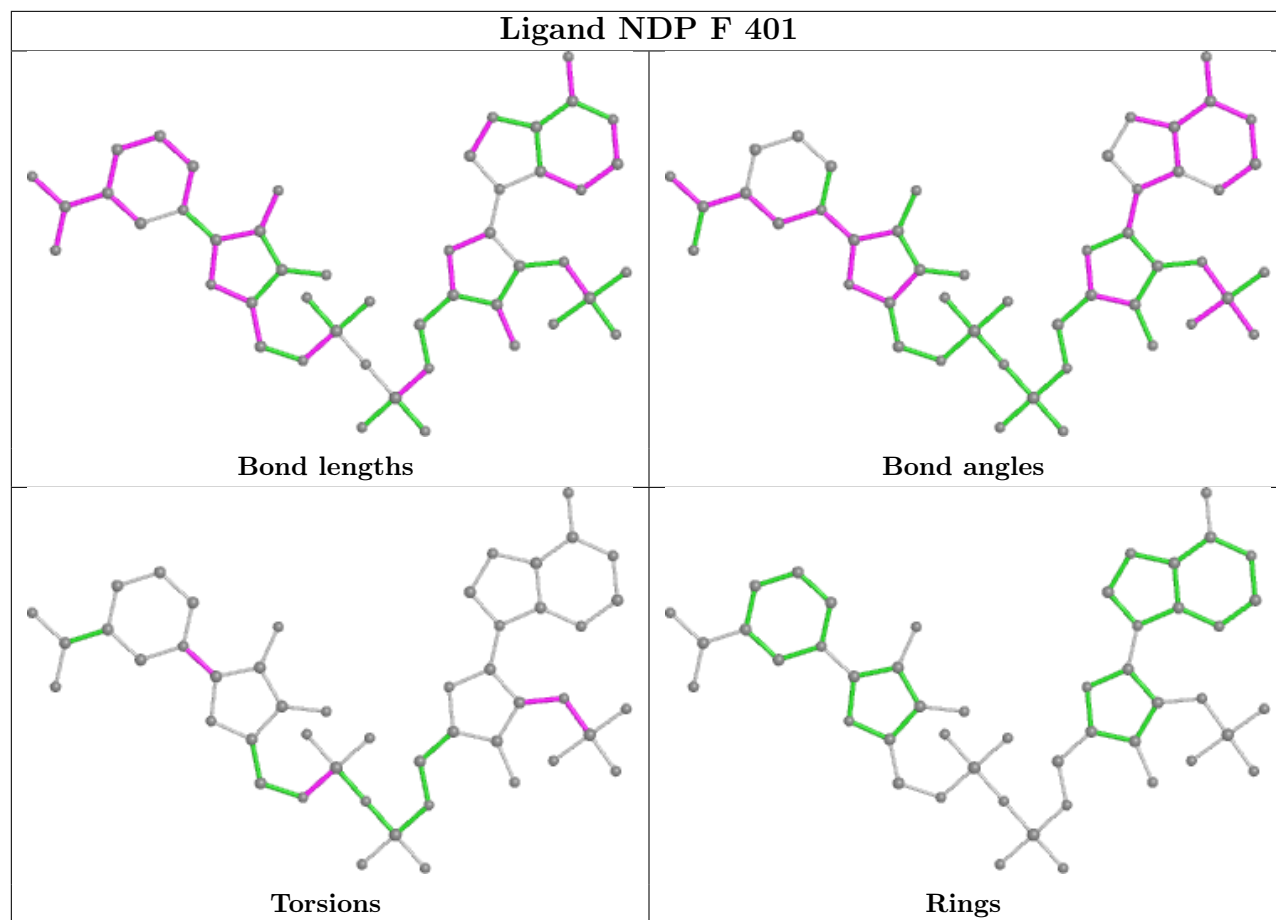


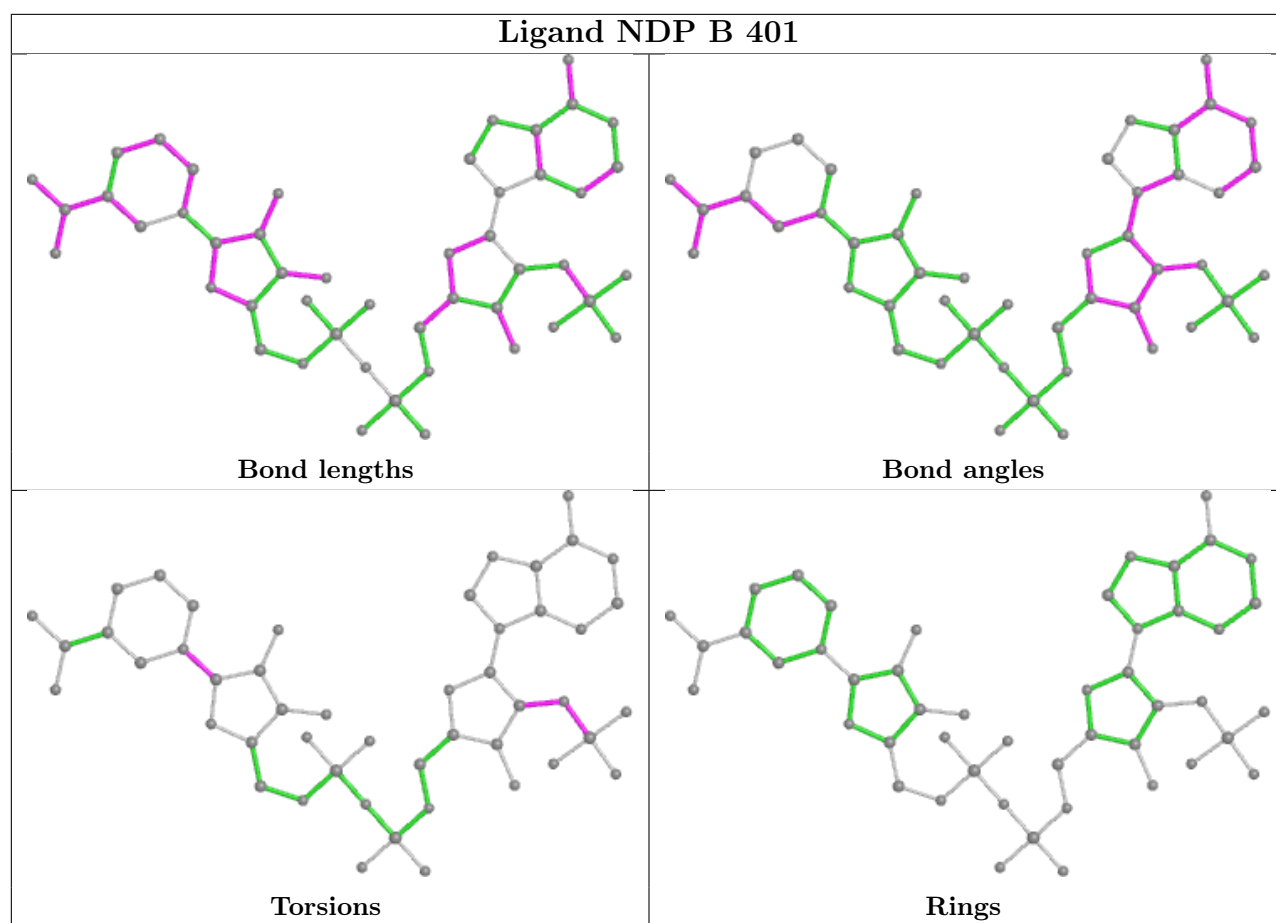












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	292/317 (92%)	-0.28	9 (3%)	49	47	25, 30, 51, 76	0
1	B	295/317 (93%)	-0.23	7 (2%)	59	57	25, 31, 49, 74	0
1	C	292/317 (92%)	-0.33	6 (2%)	63	61	26, 32, 51, 74	0
1	D	290/317 (91%)	-0.05	15 (5%)	27	26	26, 33, 56, 86	0
1	E	289/317 (91%)	-0.39	3 (1%)	82	80	24, 28, 45, 61	0
1	F	282/317 (88%)	-0.32	1 (0%)	92	91	25, 31, 49, 69	0
All	All	1740/1902 (91%)	-0.27	41 (2%)	59	57	24, 31, 51, 86	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	PHE	6.0
1	D	263	ILE	5.5
1	B	270	HIS	5.0
1	A	270	HIS	4.7
1	A	269	PRO	4.4
1	B	269	PRO	4.3
1	C	262	ASP	3.2
1	B	131	GLY	3.1
1	A	263	ILE	3.1
1	D	260	LEU	3.0
1	D	8	GLU	3.0
1	D	44	THR	3.0
1	A	268	ILE	2.9
1	D	262	ASP	2.8
1	A	271	GLN	2.8
1	B	255	SER	2.6
1	A	139	GLU	2.6
1	C	8	GLU	2.6
1	A	45	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	272	ALA	2.5
1	B	95	ARG	2.5
1	C	185	LYS	2.5
1	D	255	SER	2.4
1	E	262	ASP	2.3
1	D	192	ASP	2.3
1	C	270	HIS	2.3
1	D	46	VAL	2.3
1	D	254	ILE	2.2
1	B	271	GLN	2.2
1	C	269	PRO	2.1
1	C	90	SER	2.1
1	E	263	ILE	2.1
1	A	257	ASN	2.1
1	D	141	PHE	2.1
1	D	274	LEU	2.1
1	E	8	GLU	2.1
1	A	262	ASP	2.1
1	F	97	HIS	2.1
1	B	89	MET	2.1
1	D	257	ASN	2.0
1	D	138	ARG	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, 95<sup>th</sup> 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.

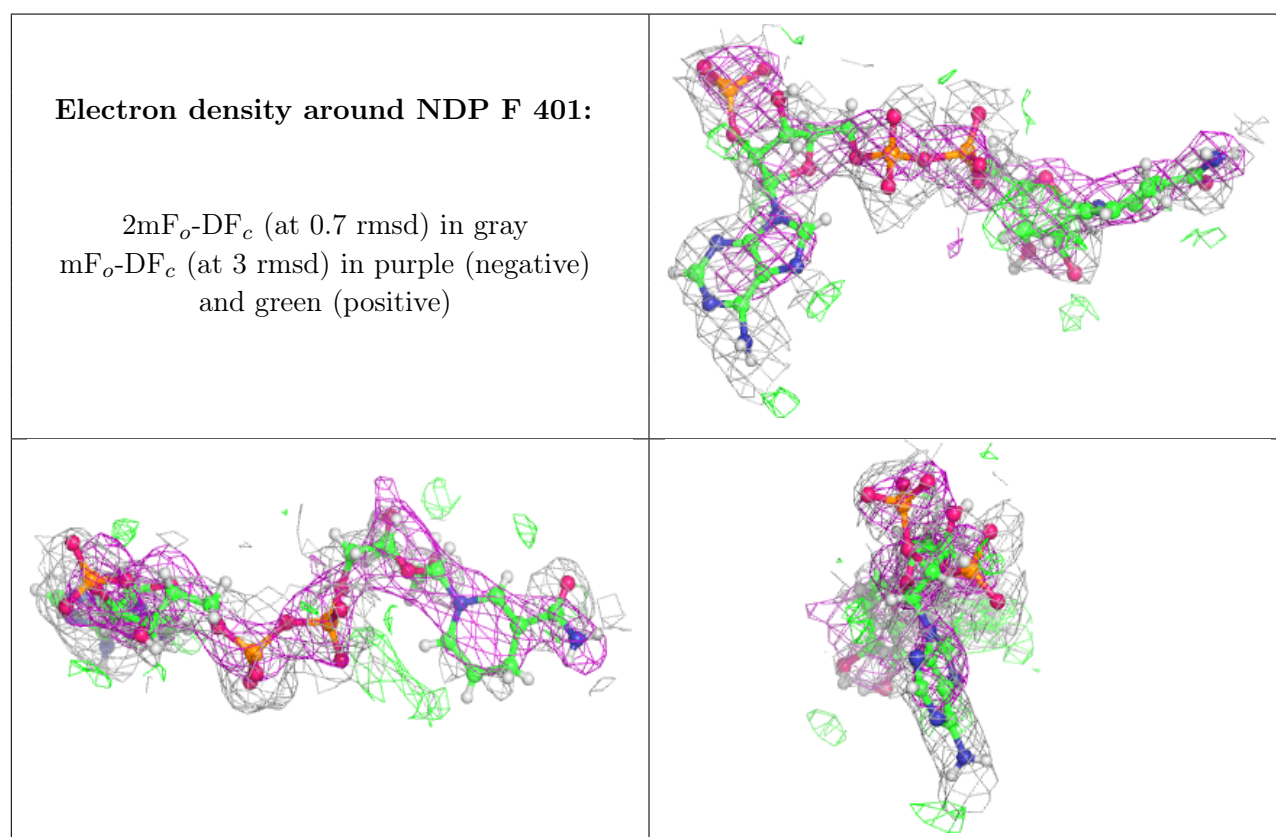
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NDP	F	401	48/48	0.78	0.34	40,50,60,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	A	401	48/48	0.90	0.17	36,45,53,56	0
2	NDP	C	401	48/48	0.91	0.20	38,44,53,72	0
2	NDP	E	401	48/48	0.94	0.14	29,37,45,56	0
2	NDP	D	401	48/48	0.94	0.14	34,40,48,57	0
2	NDP	B	401	48/48	0.96	0.11	27,36,44,46	0

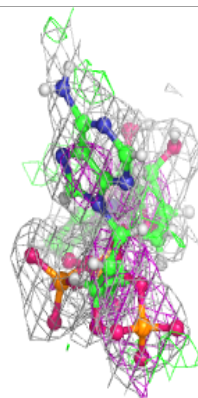
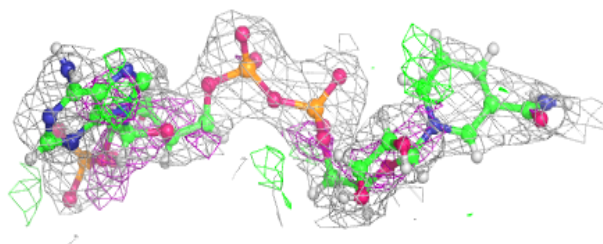
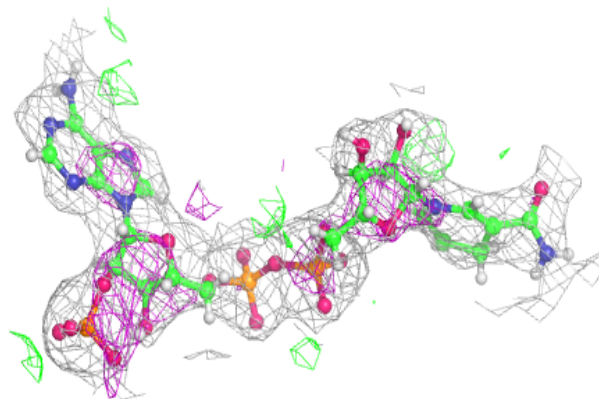
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



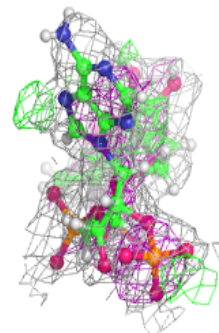
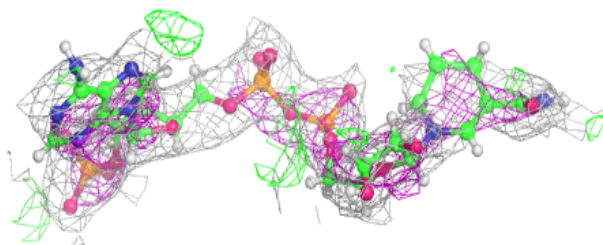
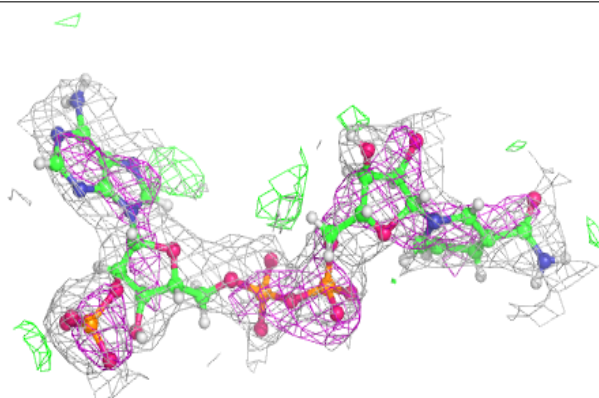


**Electron density around NDP A 401:**

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

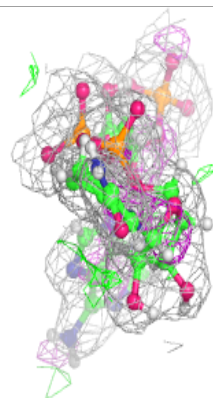
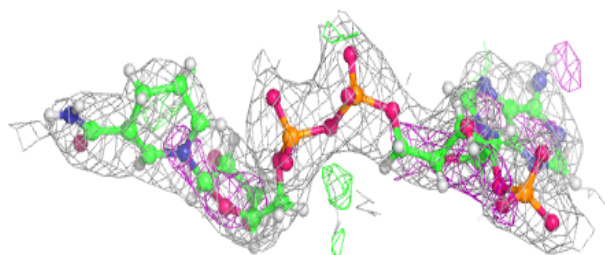
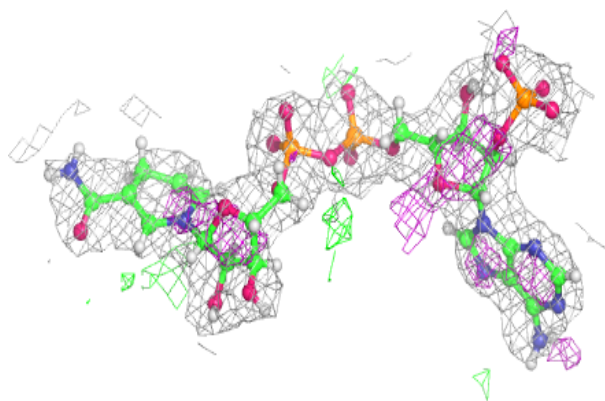
**Electron density around NDP C 401:**

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

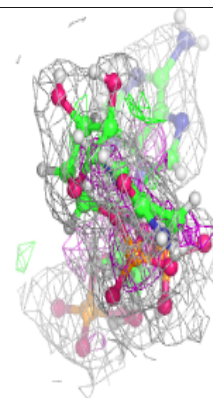
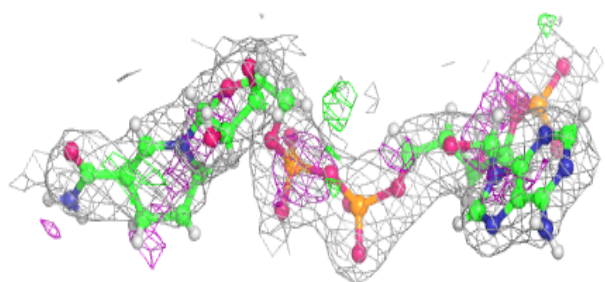
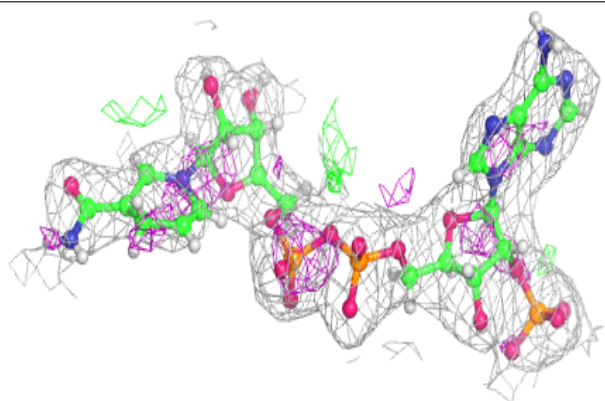


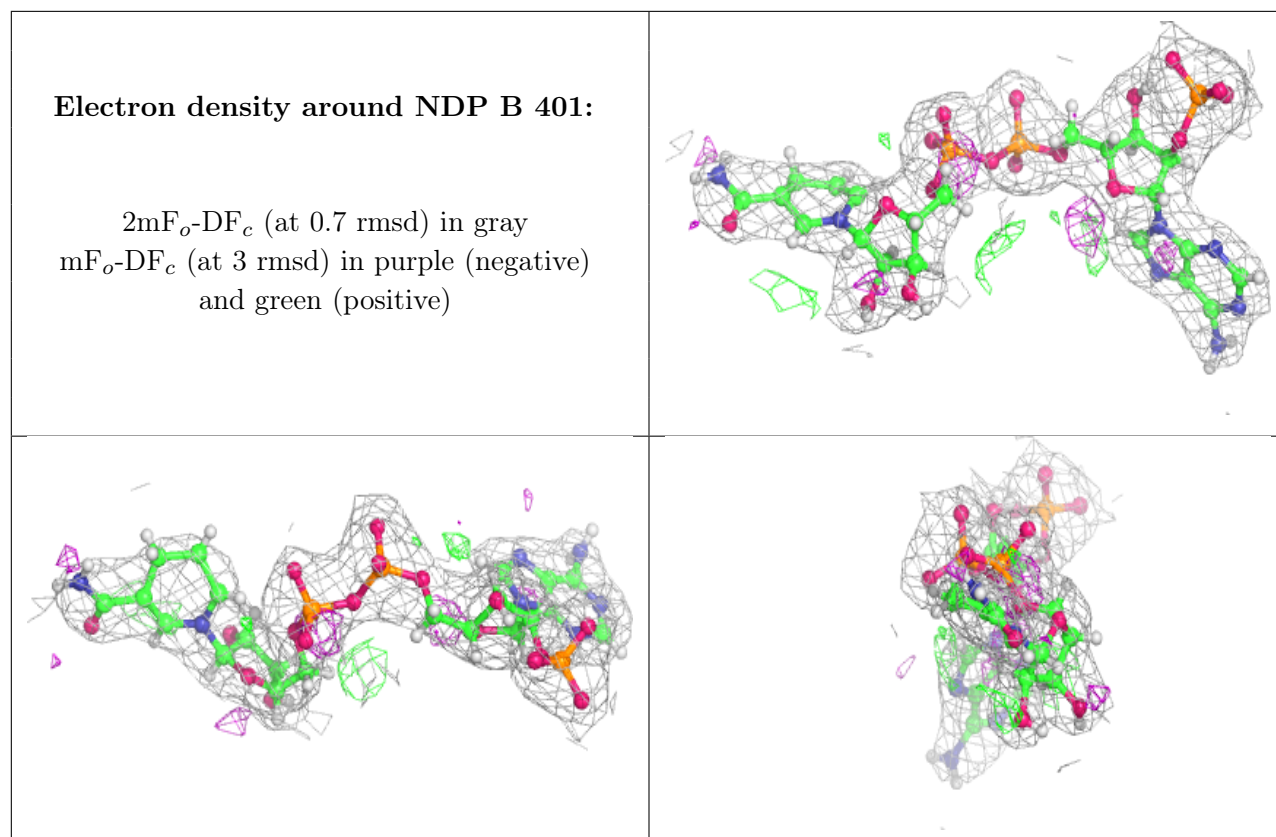
**Electron density around NDP E 401:**

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

**Electron density around NDP 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.