



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2026 – 10:15 AM JST

PDB ID : 24XI / pdb_000024xi
Title : Crystal structure of the diaminopimelate dehydrogenase from *Pyrococcus* sp. in its holo form
Authors : Matyuta, I.O.; Bezsudnova, E.Y.; Popov, V.O.; Boyko, K.M.
Deposited on : 2026-03-23
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

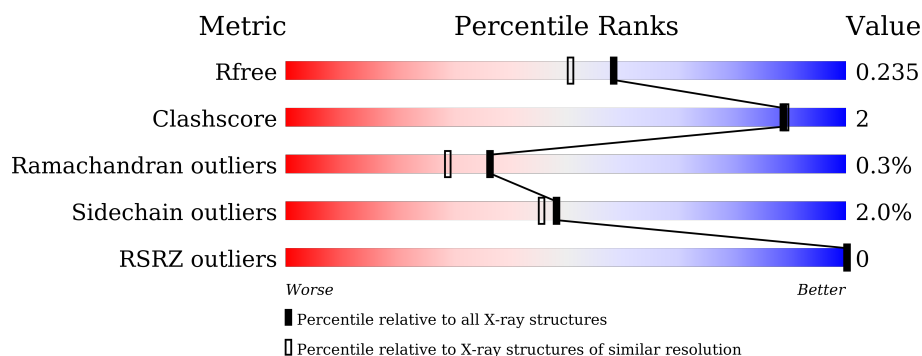
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	311	<div> <div>91%</div> <div>7% ..</div> </div>
1	B	311	<div> <div>94%</div> <div>5%</div> </div>
1	C	311	<div> <div>96%</div> <div>..</div> </div>
1	D	311	<div> <div>95%</div> <div>..</div> </div>
1	E	311	<div> <div>95%</div> <div>..</div> </div>
1	F	311	<div> <div>88%</div> <div>9% ..</div> </div>

2 Entry composition [i](#)

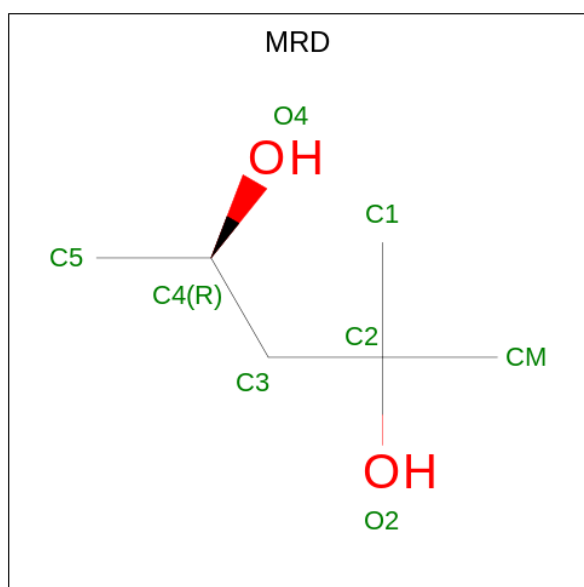
There are 6 unique types of molecules in this entry. The entry contains 15711 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Diaminopimelate dehydrogenase.

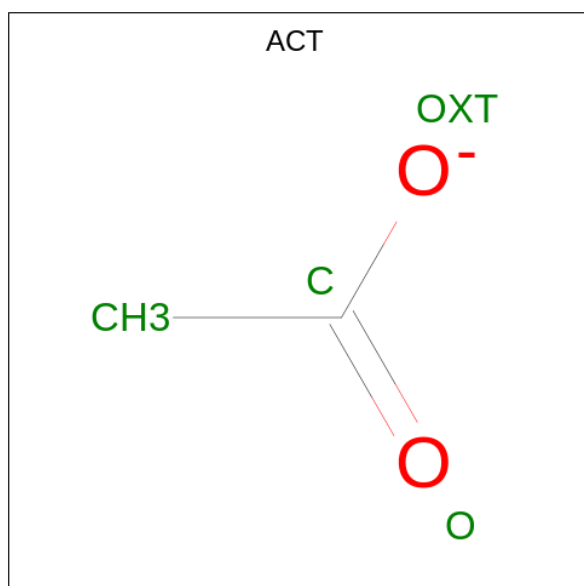
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	7	0
			2458	1578	402	466	12			
1	B	310	Total	C	N	O	S	0	3	0
			2431	1562	399	458	12			
1	C	309	Total	C	N	O	S	0	0	0
			2396	1539	396	449	12			
1	D	309	Total	C	N	O	S	0	2	0
			2387	1539	389	447	12			
1	E	308	Total	C	N	O	S	0	1	0
			2373	1527	387	447	12			
1	F	310	Total	C	N	O	S	0	2	0
			2375	1528	391	444	12			

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



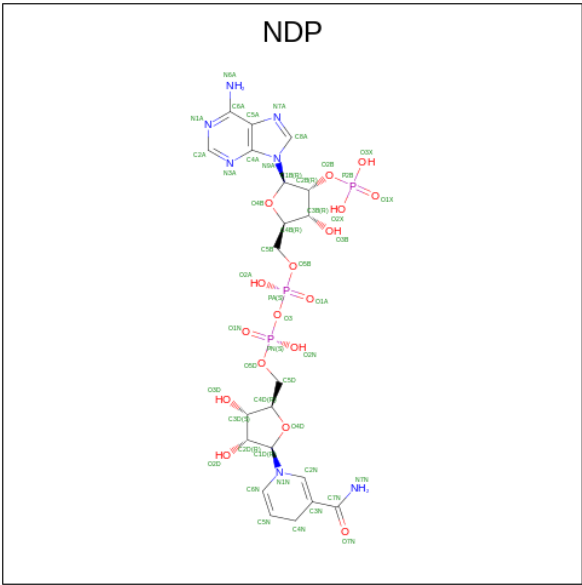
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



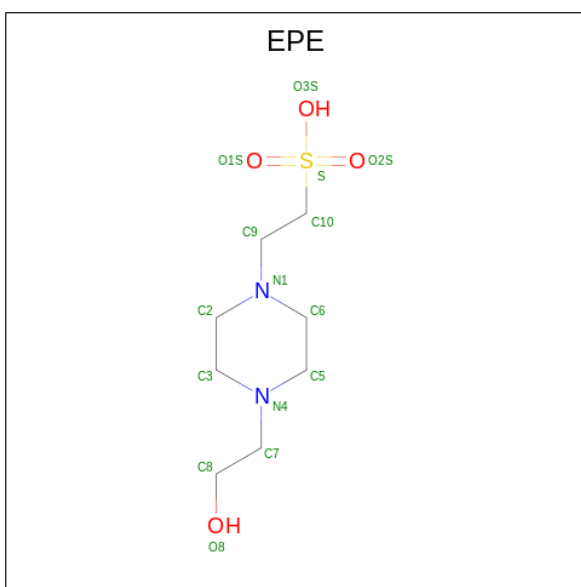
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	181	Total	O	0	1
			181	181		
6	B	164	Total	O	0	1
			164	164		
6	C	161	Total	O	0	1
			161	161		
6	D	155	Total	O	0	1
			155	155		
6	E	129	Total	O	0	0
			129	129		
6	F	139	Total	O	0	0
			139	139		

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: Diaminopimelate dehydrogenase

Chain A:  91% 7% ..



- Molecule 1: Diaminopimelate dehydrogenase

Chain B:  94% 5% ..



- Molecule 1: Diaminopimelate dehydrogenase

Chain C:  96% ..



- Molecule 1: Diaminopimelate dehydrogenase

Chain D:  95% ..




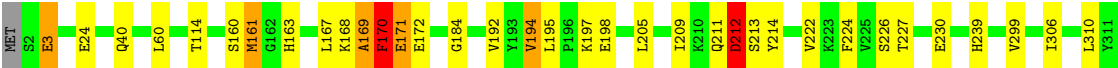
- Molecule 1: Diaminopimelate dehydrogenase

Chain E:  95% ..



- Molecule 1: Diaminopimelate dehydrogenase

Chain F:  88% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.89Å 165.90Å 82.87Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	22.08 – 1.90 22.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (22.08-1.90) 98.7 (22.08-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.229 0.205 , 0.235	Depositor DCC
R_{free} test set	8222 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15711	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, MRD, ACT, 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	1.18	5/2528 (0.2%)	1.32	3/3420 (0.1%)
1	B	1.11	1/2489 (0.0%)	1.31	5/3372 (0.1%)
1	C	1.10	0/2445	1.31	2/3314 (0.1%)
1	D	1.11	2/2442 (0.1%)	1.30	2/3313 (0.1%)
1	E	1.12	1/2425 (0.0%)	1.27	2/3292 (0.1%)
1	F	1.16	2/2429 (0.1%)	1.34	7/3297 (0.2%)
All	All	1.13	11/14758 (0.1%)	1.31	21/20008 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	239	HIS	CE1-NE2	7.00	1.39	1.32
1	A	244[A]	GLU	C-O	6.57	1.31	1.23
1	A	244[B]	GLU	C-O	6.57	1.31	1.23
1	A	103	HIS	CE1-NE2	6.36	1.39	1.32
1	A	172	GLU	CD-OE2	-5.44	1.15	1.25
1	D	244	GLU	C-O	5.41	1.29	1.23
1	F	239	HIS	C-O	5.37	1.30	1.23
1	B	239	HIS	CE1-NE2	5.36	1.38	1.32
1	E	244	GLU	C-O	5.23	1.29	1.23
1	D	103	HIS	CE1-NE2	5.20	1.37	1.32
1	A	58	TYR	C-O	5.09	1.30	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	212	ASP	CB-CA-C	-7.12	96.25	110.42
1	A	84	GLU	CB-CG-CD	7.00	124.50	112.60
1	F	184	GLY	CA-C-O	-6.73	117.58	122.23
1	F	3	GLU	CA-C-O	-6.07	114.44	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	230	GLU	N-CA-CB	5.44	118.71	110.28
1	F	170	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	135	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	172	GLU	CB-CG-CD	5.37	121.73	112.60
1	B	24	GLU	CA-C-N	5.34	127.43	120.28
1	B	24	GLU	C-N-CA	5.34	127.43	120.28
1	D	161	MET	CA-C-N	5.17	125.68	119.94
1	D	161	MET	C-N-CA	5.17	125.68	119.94
1	F	114	THR	CA-CB-OG1	-5.17	101.85	109.60
1	E	24	GLU	CA-C-N	5.16	127.19	120.28
1	E	24	GLU	C-N-CA	5.16	127.19	120.28
1	C	24	GLU	CA-C-N	5.13	127.15	120.28
1	C	24	GLU	C-N-CA	5.13	127.15	120.28
1	F	24	GLU	CA-C-N	5.08	127.09	120.28
1	F	24	GLU	C-N-CA	5.08	127.09	120.28
1	B	184	GLY	CA-C-O	-5.04	117.95	121.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2458	0	2508	11	0
1	B	2431	0	2456	9	0
1	C	2396	0	2411	3	0
1	D	2387	0	2391	5	0
1	E	2373	0	2362	4	0
1	F	2375	0	2369	21	0
2	A	24	0	42	2	0
2	C	16	0	28	2	0
2	D	8	0	14	1	0
2	E	8	0	14	2	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
4	A	48	0	26	0	0
4	B	48	0	26	0	0
4	C	48	0	26	1	0
4	D	48	0	26	0	0
4	E	48	0	26	0	0
4	F	31	0	11	1	0
5	F	15	0	18	0	0
6	A	181	0	0	3	0
6	B	164	0	0	1	0
6	C	161	0	0	2	0
6	D	155	0	0	1	0
6	E	129	0	0	0	0
6	F	139	0	0	0	0
All	All	15711	0	14769	56	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 2.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:OG1	1:A:230:GLU:HG2	1.83	0.78
1:F:161:MET:HE2	1:F:161:MET:HA	1.66	0.78
1:F:227:THR:HG23	1:F:230:GLU:H	1.55	0.72
1:D:114:THR:HG23	1:D:287:ALA:H	1.55	0.72
1:A:114[A]:THR:HG23	1:A:287:ALA:H	1.57	0.70
1:E:114:THR:HG23	1:E:287:ALA:H	1.58	0.69
2:E:401:MRD:H5C2	2:E:401:MRD:O2	1.96	0.66
1:A:282[B]:LYS:HE3	1:A:297:THR:HB	1.79	0.63
1:A:27:LYS:NZ	1:E:198:GLU:OE2	2.33	0.59
1:F:160:SER:OG	1:F:163:HIS:HD2	1.85	0.59
1:F:194:VAL:HG23	1:F:224:PHE:CD1	2.37	0.59
1:B:32:ARG:HD3	6:B:506:HOH:O	2.01	0.59
1:C:172:GLU:HG3	1:C:205:LEU:HD13	1.87	0.56
1:F:205:LEU:O	1:F:209:ILE:HG12	2.05	0.56
1:F:211:GLN:O	1:F:213:SER:N	2.37	0.56
1:F:170:PHE:O	1:F:172:GLU:N	2.33	0.56
6:A:536:HOH:O	1:B:271:GLN:CD	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:MRD:HMC1	2:E:401:MRD:O4	2.08	0.53
1:F:167:LEU:HD22	1:F:209:ILE:HD12	1.92	0.50
1:F:299:VAL:HG23	1:F:306[B]:ILE:HD11	1.94	0.49
1:A:271:GLN:OE1	6:A:501:HOH:O	2.20	0.49
2:C:401:MRD:HMC3	6:C:639:HOH:O	2.13	0.49
1:F:192:VAL:HG13	1:F:222:VAL:HA	1.95	0.48
1:F:212:ASP:O	1:F:214:TYR:N	2.43	0.48
1:F:161:MET:HA	1:F:161:MET:CE	2.43	0.47
1:F:167:LEU:HD13	1:F:192:VAL:HG21	1.96	0.47
2:A:405:MRD:C5	6:A:603:HOH:O	2.63	0.47
1:A:289:THR:HB	1:B:311:TYR:CZ	2.51	0.46
1:D:32:ARG:HD3	6:D:552:HOH:O	2.14	0.46
2:A:401:MRD:H1C2	2:A:401:MRD:O4	2.17	0.45
1:B:185:ASN:CG	1:D:181:ILE:CG2	2.90	0.45
1:F:168:LYS:O	1:F:169:ALA:HB3	2.17	0.45
1:B:108:GLU:O	1:B:111[A]:GLU:HG2	2.17	0.44
2:C:401:MRD:C5	2:C:401:MRD:HMC1	2.47	0.44
1:F:160:SER:OG	1:F:163:HIS:CD2	2.69	0.44
1:B:310:LEU:HD12	1:B:310:LEU:C	2.43	0.43
1:A:310:LEU:C	1:A:310:LEU:HD12	2.43	0.43
1:D:153:THR:HG21	2:D:401:MRD:HMC2	1.99	0.43
1:E:110:LYS:O	1:E:114:THR:OG1	2.32	0.42
1:C:310:LEU:C	1:C:310:LEU:HD12	2.44	0.42
1:A:311:TYR:CZ	1:B:289:THR:HB	2.53	0.42
1:D:310:LEU:C	1:D:310:LEU:HD12	2.44	0.42
1:F:169:ALA:O	1:F:171:GLU:N	2.53	0.42
1:A:225:VAL:HB	1:A:230:GLU:HG3	2.02	0.42
1:A:110:LYS:O	1:A:114[A]:THR:OG1	2.32	0.42
1:A:241:VAL:O	1:A:260:ASP:HA	2.20	0.42
1:F:211:GLN:C	1:F:213:SER:H	2.24	0.42
4:C:404:NDP:H8A	6:C:586:HOH:O	2.19	0.41
1:F:167:LEU:HD13	1:F:192:VAL:CG2	2.50	0.41
1:F:194:VAL:CG2	1:F:224:PHE:CD1	3.03	0.41
1:E:310:LEU:HD12	1:E:310:LEU:C	2.45	0.41
1:F:60:LEU:HD11	4:F:402:NDP:H2A	2.03	0.41
1:B:75:LEU:HD12	1:B:75:LEU:N	2.37	0.40
1:C:241:VAL:O	1:C:260:ASP:HA	2.21	0.40
1:F:310:LEU:C	1:F:310:LEU:HD12	2.46	0.40
1:B:241:VAL:O	1:B:260:ASP:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	314/311 (101%)	306 (98%)	8 (2%)	0	100	100
1	B	311/311 (100%)	305 (98%)	6 (2%)	0	100	100
1	C	307/311 (99%)	299 (97%)	8 (3%)	0	100	100
1	D	309/311 (99%)	303 (98%)	6 (2%)	0	100	100
1	E	307/311 (99%)	301 (98%)	6 (2%)	0	100	100
1	F	310/311 (100%)	297 (96%)	7 (2%)	6 (2%)	6	1
All	All	1858/1866 (100%)	1811 (98%)	41 (2%)	6 (0%)	36	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	170	PHE
1	F	171	GLU
1	F	197	LYS
1	F	198	GLU
1	F	212	ASP
1	F	169	ALA

5.3.2 Protein sidechains

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	275/274 (100%)	265 (96%)	10 (4%)	31	23
1	B	266/274 (97%)	263 (99%)	3 (1%)	65	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	260/274 (95%)	257 (99%)	3 (1%)	63	63
1	D	256/274 (93%)	252 (98%)	4 (2%)	55	54
1	E	254/274 (93%)	249 (98%)	5 (2%)	48	46
1	F	253/274 (92%)	246 (97%)	7 (3%)	38	32
All	All	1564/1644 (95%)	1532 (98%)	32 (2%)	48	46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	44	GLU
1	A	84	GLU
1	A	171	GLU
1	A	195	LEU
1	A	230	GLU
1	A	231	LEU
1	A	239	HIS
1	A	282[A]	LYS
1	A	282[B]	LYS
1	B	191	LEU
1	B	231	LEU
1	B	239	HIS
1	C	44	GLU
1	C	195	LEU
1	C	239	HIS
1	D	44	GLU
1	D	104	ASP
1	D	191	LEU
1	D	239	HIS
1	E	44	GLU
1	E	191	LEU
1	E	195	LEU
1	E	239	HIS
1	E	257	LEU
1	F	3	GLU
1	F	40	GLN
1	F	161	MET
1	F	170	PHE
1	F	194	VAL
1	F	195	LEU
1	F	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	B	271	GLN
1	C	40	GLN
1	D	271	GLN
1	F	148	ASN
1	F	163	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	MRD	A	405	-	7,7,7	0.34	0	9,10,10	0.82	0
4	NDP	A	404	-	49,52,52	0.97	2 (4%)	66,80,80	0.86	3 (4%)
2	MRD	C	401	-	7,7,7	0.52	0	9,10,10	0.98	0
3	ACT	E	402	-	3,3,3	0.91	0	3,3,3	1.10	0
4	NDP	E	403	-	49,52,52	0.71	2 (4%)	66,80,80	0.93	4 (6%)
2	MRD	A	401	-	7,7,7	0.49	0	9,10,10	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MRD	E	401	-	7,7,7	0.20	0	9,10,10	0.55	0
3	ACT	B	401	-	3,3,3	1.50	1 (33%)	3,3,3	0.82	0
2	MRD	A	402	-	7,7,7	0.38	0	9,10,10	1.07	0
3	ACT	A	403	-	3,3,3	1.00	0	3,3,3	1.04	0
2	MRD	C	403	-	7,7,7	0.26	0	9,10,10	0.71	0
4	NDP	F	402	-	31,33,52	0.89	2 (6%)	48,52,80	0.97	2 (4%)
4	NDP	C	404	-	49,52,52	0.74	1 (2%)	66,80,80	1.02	5 (7%)
5	EPE	F	401	-	15,15,15	0.55	0	18,20,20	1.91	3 (16%)
2	MRD	D	401	-	7,7,7	0.46	0	9,10,10	1.11	1 (11%)
3	ACT	D	402	-	3,3,3	1.30	1 (33%)	3,3,3	0.55	0
4	NDP	B	402	-	49,52,52	0.83	3 (6%)	66,80,80	1.04	3 (4%)
4	NDP	D	403	-	49,52,52	0.56	0	66,80,80	1.03	5 (7%)
3	ACT	C	402	-	3,3,3	1.06	0	3,3,3	0.84	0

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	MRD	A	405	-	-	1/5/5/5	-
2	MRD	E	401	-	-	1/5/5/5	-
5	EPE	F	401	-	-	0/9/19/19	0/1/1/1
2	MRD	D	401	-	-	2/5/5/5	-
2	MRD	C	403	-	-	0/5/5/5	-
4	NDP	A	404	-	-	3/34/77/77	0/5/5/5
2	MRD	C	401	-	-	2/5/5/5	-
4	NDP	F	402	-	-	3/21/37/77	0/3/3/5
4	NDP	E	403	-	-	5/34/77/77	0/5/5/5
4	NDP	D	403	-	-	5/34/77/77	0/5/5/5
2	MRD	A	401	-	-	1/5/5/5	-
4	NDP	B	402	-	-	5/34/77/77	0/5/5/5
4	NDP	C	404	-	-	4/34/77/77	0/5/5/5
2	MRD	A	402	-	-	2/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	NDP	P2B-O2B	4.58	1.68	1.59
4	F	402	NDP	P2B-O2B	2.99	1.64	1.59
4	E	403	NDP	P2B-O2B	2.80	1.64	1.59
4	B	402	NDP	P2B-O2B	2.63	1.64	1.59
4	C	404	NDP	P2B-O3X	-2.52	1.45	1.54
4	F	402	NDP	P2B-O2X	-2.27	1.46	1.54
4	B	402	NDP	P2B-O2X	-2.22	1.46	1.54
3	B	401	ACT	O-C	2.22	1.32	1.22
4	E	403	NDP	C2N-C3N	2.18	1.41	1.34
4	B	402	NDP	P2B-O3X	-2.11	1.46	1.54
4	A	404	NDP	P2B-O2X	-2.10	1.46	1.54
3	D	402	ACT	OXT-C	-2.04	1.21	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	EPE	O3S-S-C10	6.56	116.37	105.77
4	B	402	NDP	PN-O3-PA	-4.08	118.84	132.83
4	D	403	NDP	C3N-C7N-N7N	3.24	123.42	117.67
4	C	404	NDP	PN-O3-PA	-3.10	122.19	132.83
5	F	401	EPE	O3S-S-O2S	-3.05	103.83	111.27
4	D	403	NDP	O2X-P2B-O2B	-3.02	92.47	105.99
4	B	402	NDP	O7N-C7N-C3N	-2.76	115.69	120.90
4	C	404	NDP	O2B-P2B-O1X	-2.57	99.47	109.39
4	D	403	NDP	O7N-C7N-C3N	-2.50	116.18	120.90
4	F	402	NDP	O2B-P2B-O1X	-2.45	99.93	109.39
4	E	403	NDP	PN-O3-PA	-2.39	124.61	132.83
4	B	402	NDP	C3D-C2D-C1D	2.34	105.86	101.43
5	F	401	EPE	O2S-S-C10	-2.32	104.12	106.92
4	F	402	NDP	O2A-PA-O1A	2.29	123.57	112.24
4	A	404	NDP	O2B-C2B-C3B	-2.26	103.47	111.68
4	D	403	NDP	O4B-C1B-N9A	2.25	112.50	108.06
2	D	401	MRD	O2-C2-C3	-2.24	101.39	109.80
4	E	403	NDP	O3X-P2B-O2B	2.22	115.95	105.99
4	C	404	NDP	O2A-PA-O1A	2.09	122.59	112.24
4	C	404	NDP	C3N-C7N-N7N	2.08	121.37	117.67
4	A	404	NDP	O2X-P2B-O1X	2.07	118.79	110.68
4	E	403	NDP	O3X-P2B-O2X	2.05	115.47	107.64
4	E	403	NDP	O2B-C2B-C1B	2.05	117.48	110.10
4	A	404	NDP	O2B-P2B-O1X	-2.03	101.55	109.39
4	C	404	NDP	C3D-C2D-C1D	2.03	105.28	101.43
4	D	403	NDP	C3D-C2D-C1D	2.00	105.23	101.43

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	NDP	C2B-O2B-P2B-O1X
4	B	402	NDP	C2B-O2B-P2B-O1X
4	B	402	NDP	O4D-C1D-N1N-C2N
4	C	404	NDP	C2B-O2B-P2B-O1X
4	E	403	NDP	C2B-O2B-P2B-O1X
4	F	402	NDP	C2B-O2B-P2B-O1X
4	A	404	NDP	O4D-C1D-N1N-C2N
4	D	403	NDP	O4D-C1D-N1N-C2N
4	E	403	NDP	O4D-C1D-N1N-C2N
4	C	404	NDP	O4D-C1D-N1N-C2N
4	F	402	NDP	PN-O3-PA-O1A
4	F	402	NDP	PN-O3-PA-O2A
2	A	402	MRD	C2-C3-C4-C5
2	D	401	MRD	C2-C3-C4-C5
2	E	401	MRD	C2-C3-C4-C5
4	D	403	NDP	PN-O3-PA-O1A
4	E	403	NDP	PN-O3-PA-O1A
4	A	404	NDP	O4B-C4B-C5B-O5B
4	C	404	NDP	O4B-C4B-C5B-O5B
2	A	401	MRD	O2-C2-C3-C4
2	C	401	MRD	O2-C2-C3-C4
4	B	402	NDP	C2B-O2B-P2B-O3X
4	C	404	NDP	C2B-O2B-P2B-O3X
4	D	403	NDP	C2B-O2B-P2B-O2X
4	B	402	NDP	O4B-C4B-C5B-O5B
4	D	403	NDP	O4B-C4B-C5B-O5B
4	B	402	NDP	PN-O3-PA-O2A
4	E	403	NDP	PN-O3-PA-O2A
2	A	405	MRD	C2-C3-C4-C5
2	C	401	MRD	C2-C3-C4-C5
4	D	403	NDP	C2N-C3N-C7N-N7N
4	E	403	NDP	O4B-C4B-C5B-O5B
2	A	402	MRD	C2-C3-C4-O4
2	D	401	MRD	C2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 9 short contacts:

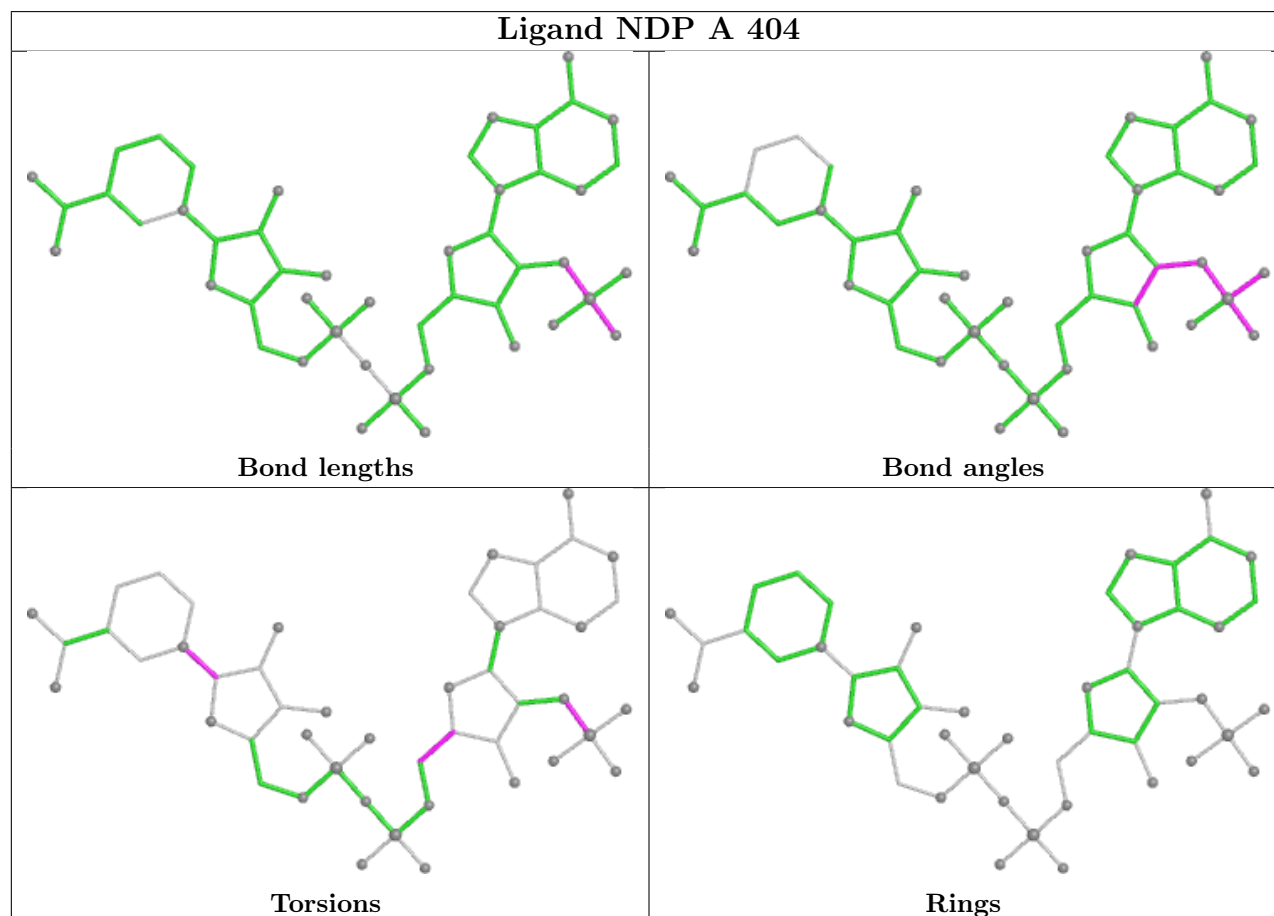
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	MRD	1	0

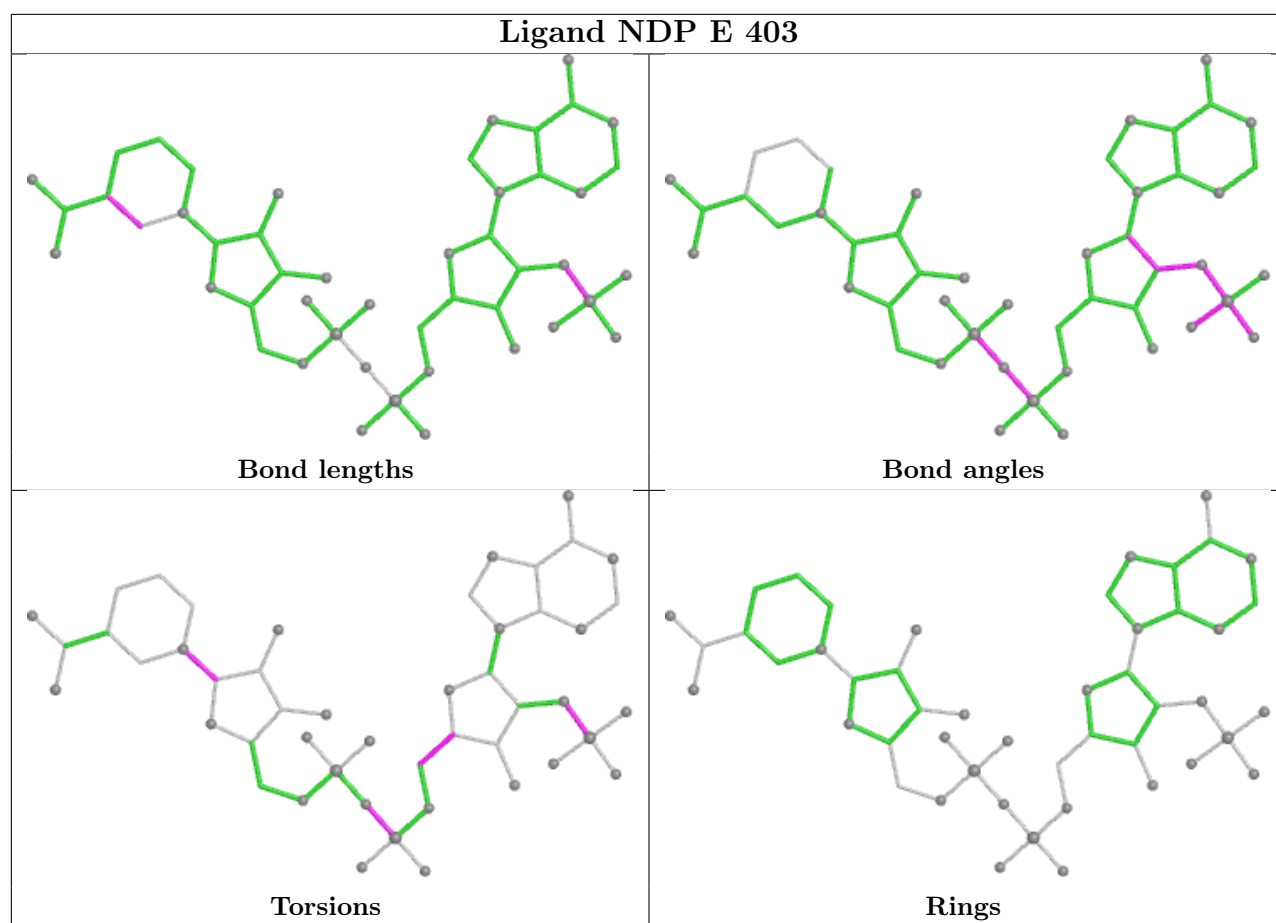
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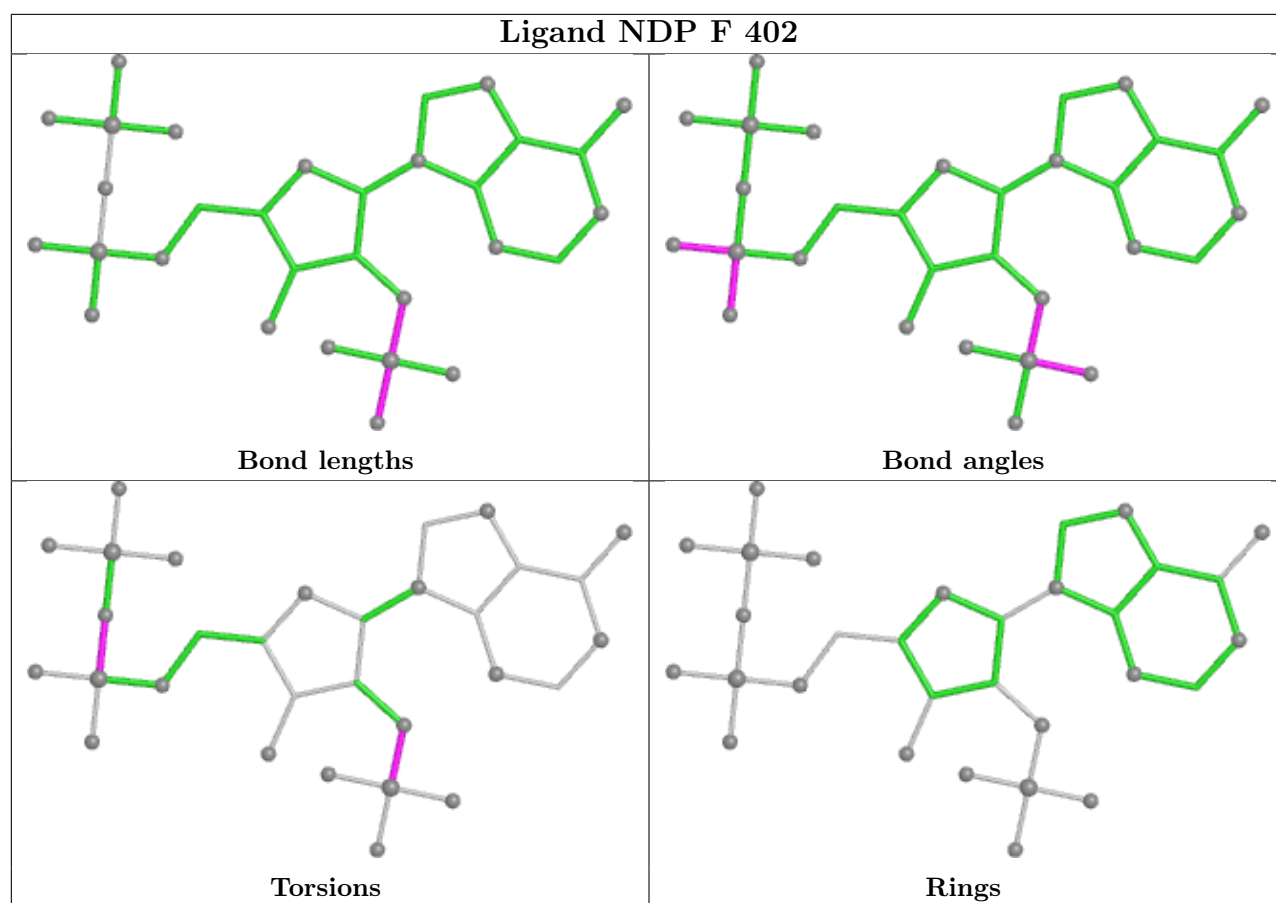
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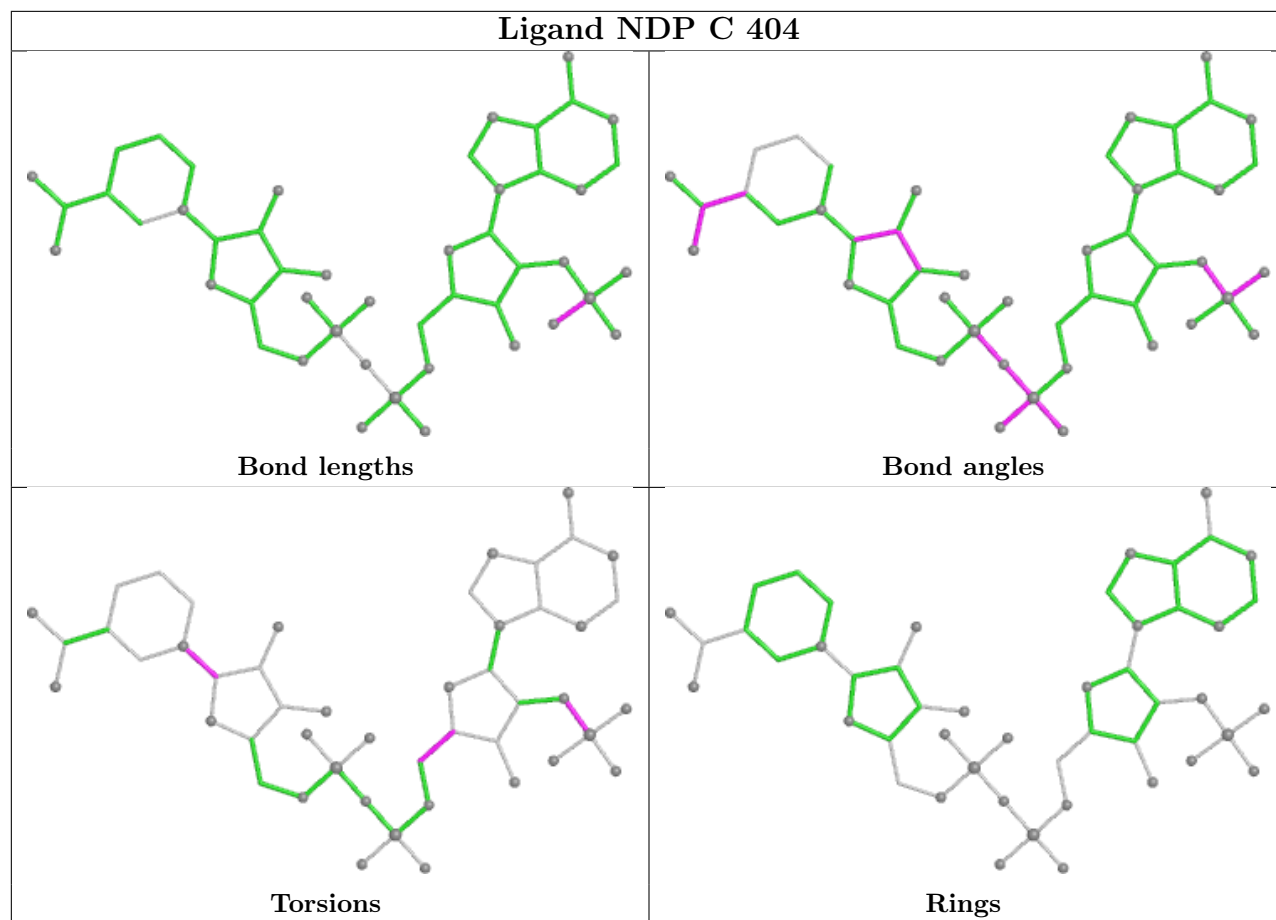
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	MRD	2	0
2	A	401	MRD	1	0
2	E	401	MRD	2	0
4	F	402	NDP	1	0
4	C	404	NDP	1	0
2	D	401	MRD	1	0

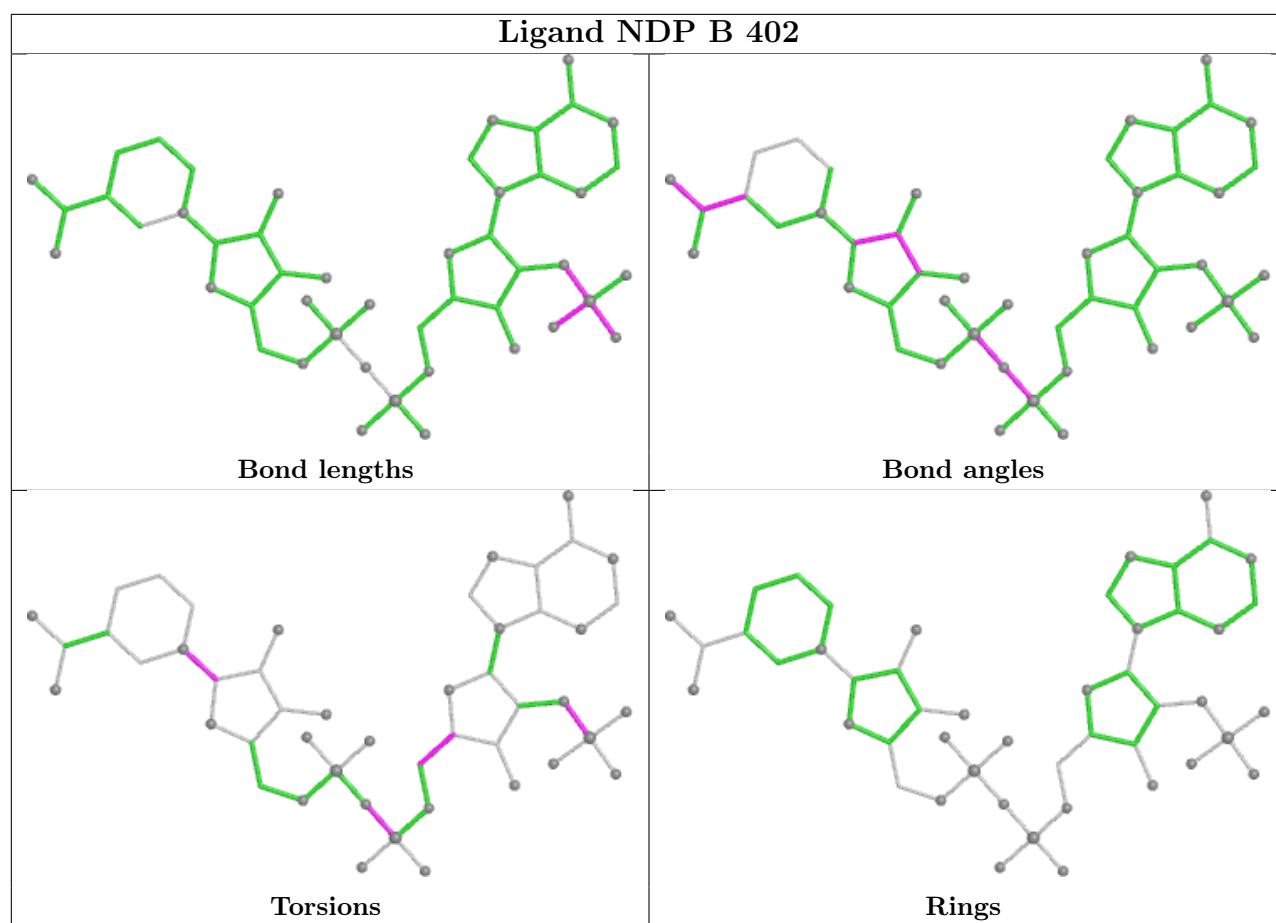
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

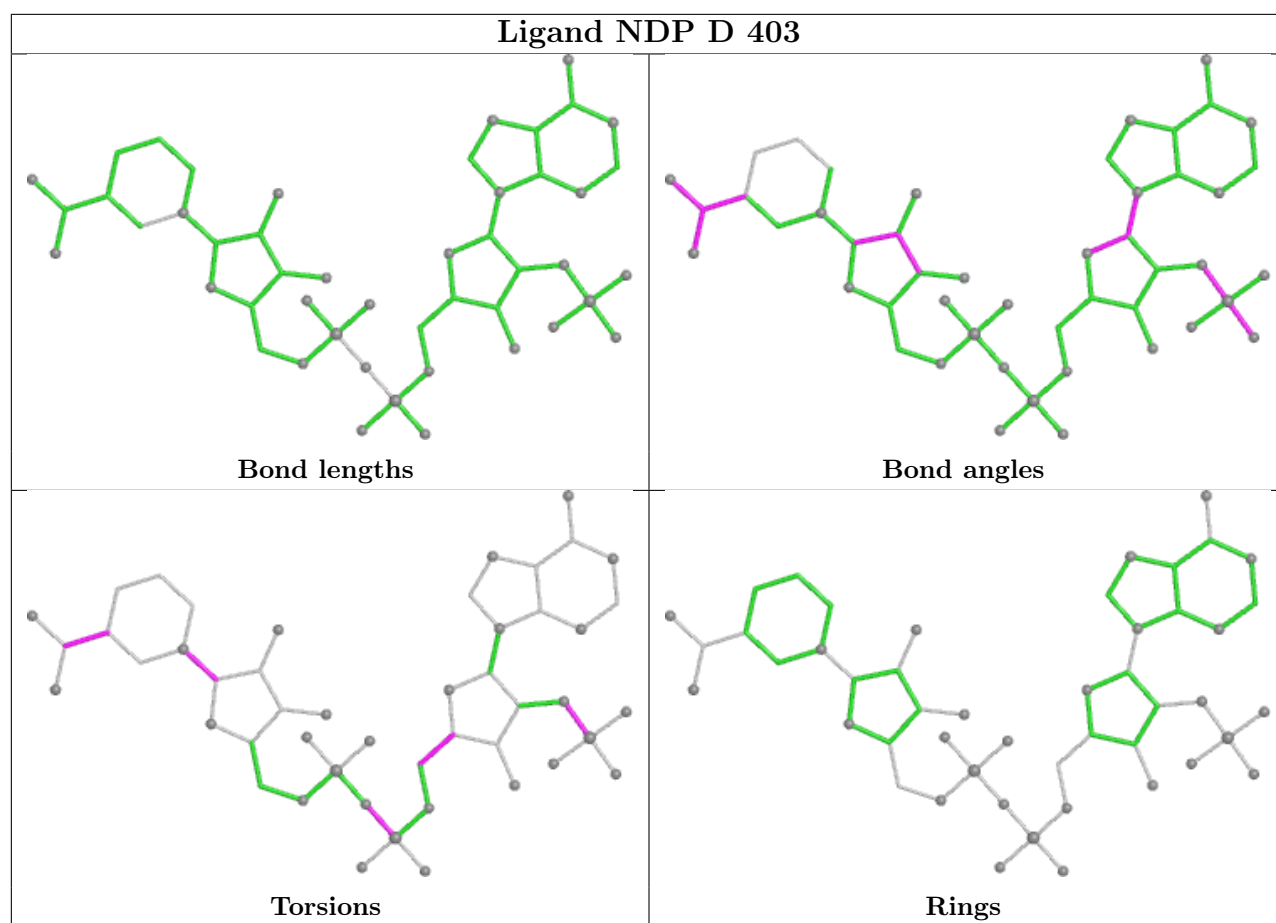












5.7 Other polymers [i](#)

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 [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	309/311 (99%)	-1.62	0 100 100	5, 13, 28, 42	7 (2%)
1	B	310/311 (99%)	-1.62	0 100 100	6, 13, 28, 41	3 (0%)
1	C	309/311 (99%)	-1.60	0 100 100	6, 15, 31, 44	0
1	D	309/311 (99%)	-1.50	0 100 100	8, 20, 38, 48	2 (0%)
1	E	308/311 (99%)	-1.41	0 100 100	6, 23, 43, 56	1 (0%)
1	F	310/311 (99%)	-1.48	0 100 100	5, 16, 58, 82	2 (0%)
All	All	1855/1866 (99%)	-1.54	0 100 100	5, 16, 39, 82	15 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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	MRD	A	402	8/8	0.98	0.05	28,35,37,38	0

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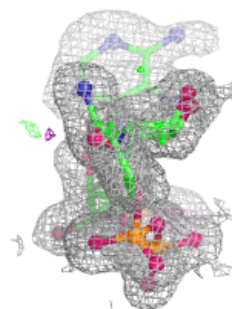
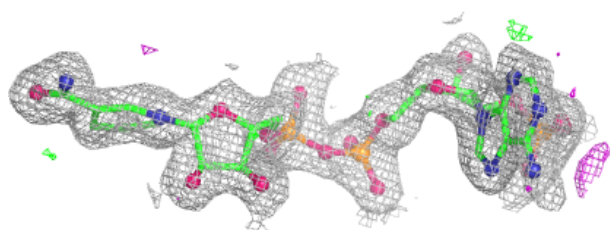
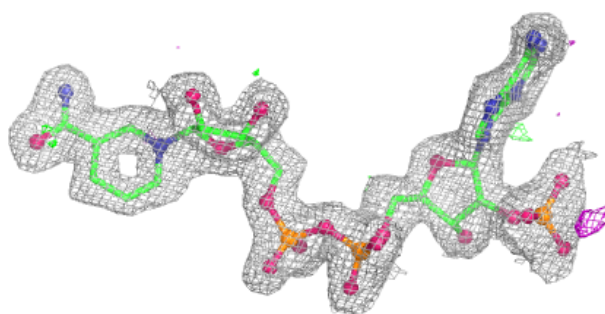
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MRD	A	405	8/8	0.98	0.04	31,36,38,41	0
2	MRD	C	403	8/8	0.98	0.04	33,37,43,46	0
2	MRD	D	401	8/8	0.98	0.04	30,34,38,40	0
2	MRD	A	401	8/8	0.99	0.04	25,26,27,29	0
2	MRD	C	401	8/8	0.99	0.04	28,32,35,35	0
2	MRD	E	401	8/8	0.99	0.05	34,37,39,43	0
3	ACT	E	402	4/4	0.99	0.03	18,18,20,23	0
4	NDP	E	403	48/48	0.99	0.03	14,20,35,38	0
4	NDP	F	402	31/48	0.99	0.02	17,21,36,42	0
3	ACT	D	402	4/4	1.00	0.02	12,13,14,14	0
3	ACT	A	403	4/4	1.00	0.02	10,10,11,12	0
4	NDP	A	404	48/48	1.00	0.02	6,11,17,19	0
4	NDP	B	402	48/48	1.00	0.01	8,12,16,17	0
4	NDP	C	404	48/48	1.00	0.02	6,12,20,21	0
4	NDP	D	403	48/48	1.00	0.02	12,17,28,32	0
3	ACT	B	401	4/4	1.00	0.02	14,15,15,16	0
3	ACT	C	402	4/4	1.00	0.01	13,13,13,14	0
5	EPE	F	401	15/15	1.00	0.03	11,15,19,19	0

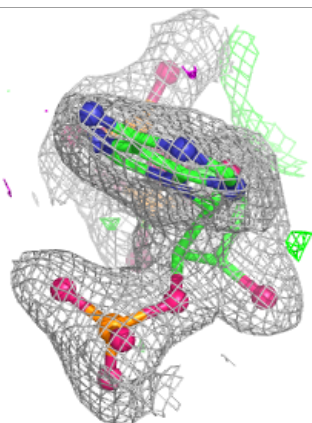
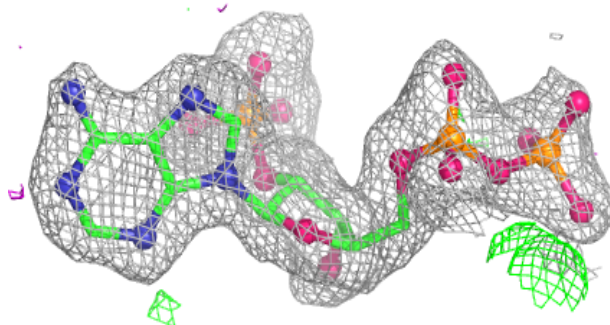
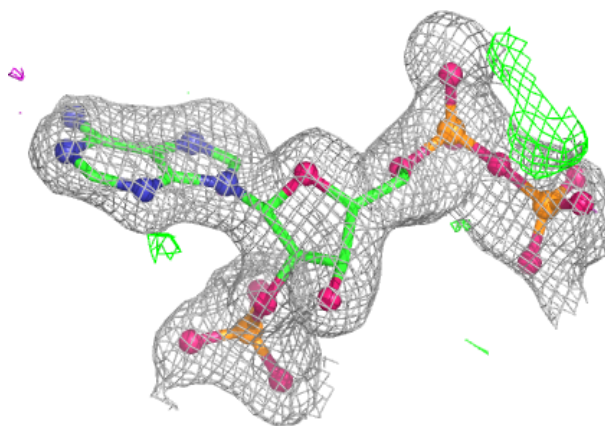
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP E 403:

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

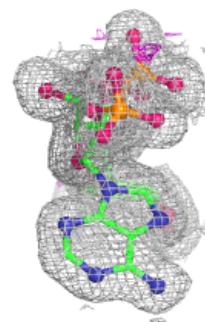
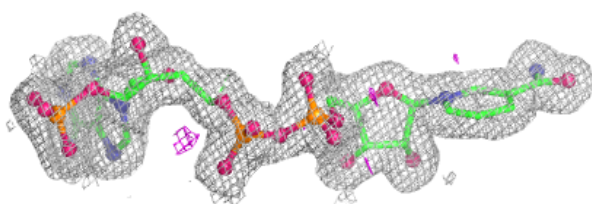
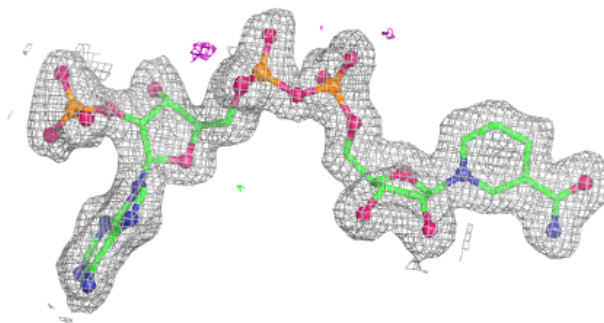
**Electron density around NDP F 402:**

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

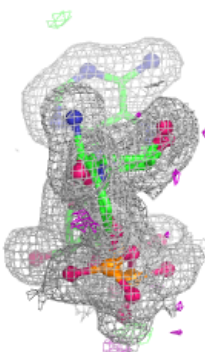
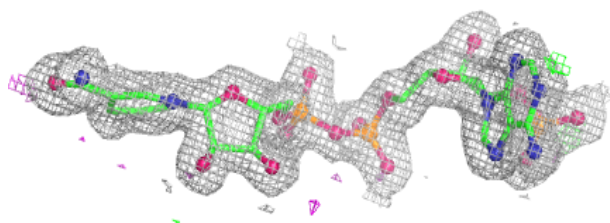
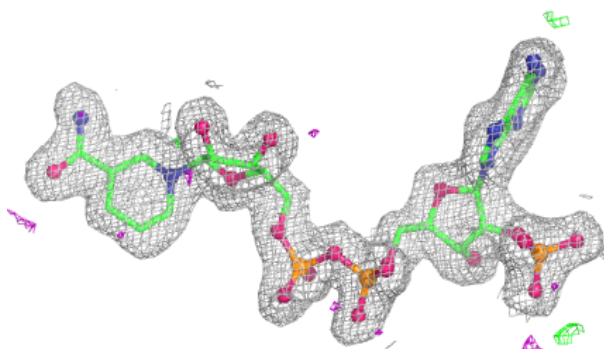


Electron density around NDP A 404:

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

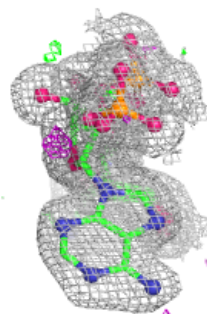
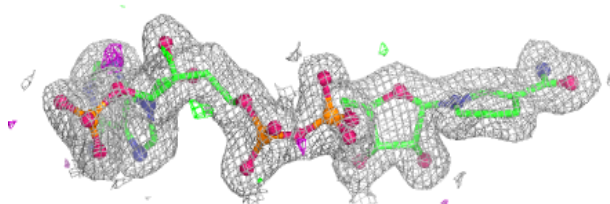
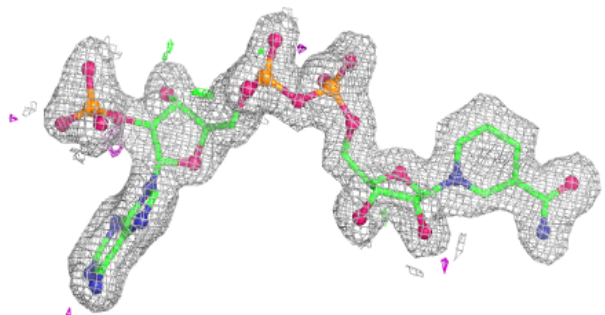
**Electron density around NDP B 402:**

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

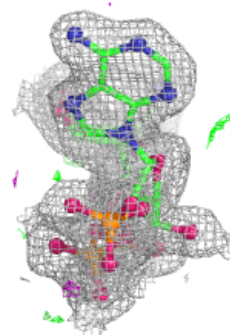
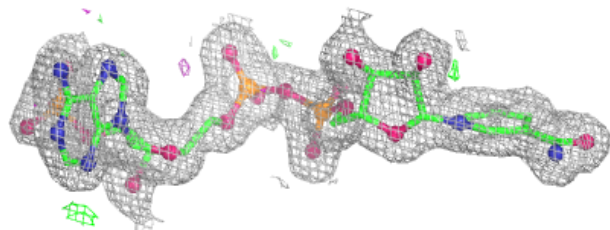
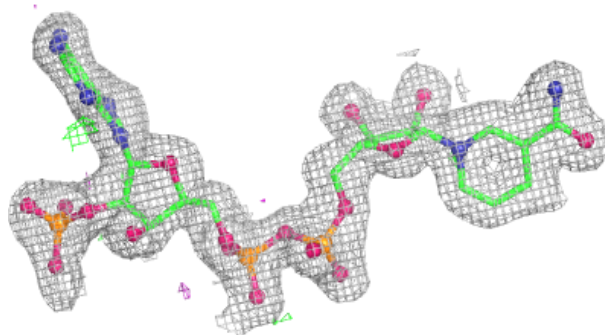


Electron density around NDP C 404:

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

**Electron density around NDP D 403:**

$2mF_o-DF_c$ (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.