



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:11 AM UTC

PDB ID : 4JAY / pdb_00004jay
Title : Crystal structure of P. aeruginosa MurB in complex with NADP+
Authors : Chen, M.W.; Lohkamp, B.; Schnell, R.; Lescar, J.; Schneider, G.
Deposited on : 2013-02-19
Resolution : 2.23 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 : 2022.3.0, CSD as543be (2022)
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

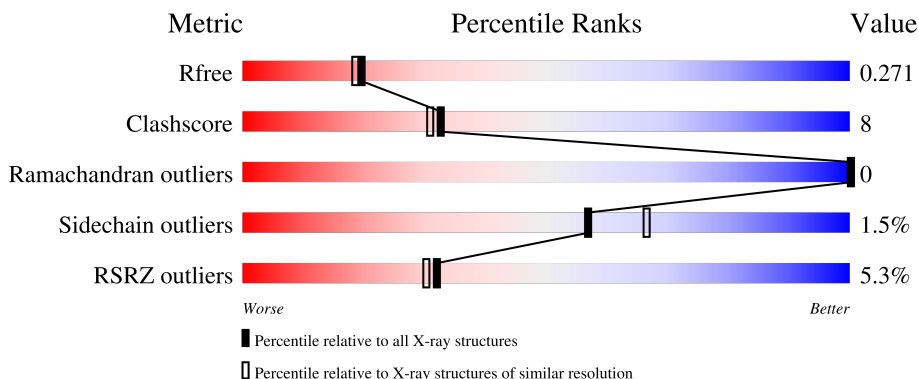
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	340	2% 84% 15% .
1	B	340	7% 85% 14% ..
1	C	340	7% 86% 13% .
1	D	340	5% 84% 15% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11404 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.

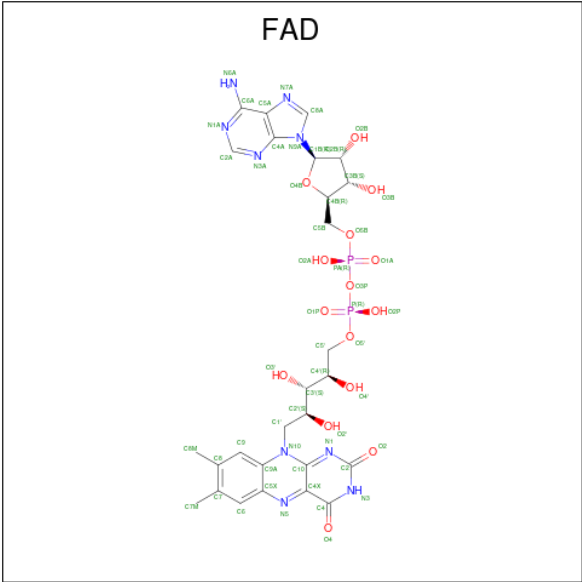
- Molecule 1 is a protein called UDP-N-acetylenolpyruvoylglucosamine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2645	1657	498	485	5			
1	B	338	Total	C	N	O	S	0	0	0
			2645	1657	498	485	5			
1	C	338	Total	C	N	O	S	0	0	0
			2645	1657	498	485	5			
1	D	338	Total	C	N	O	S	0	0	0
			2645	1657	498	485	5			

There are 4 discrepancies between the modelled and reference sequences:

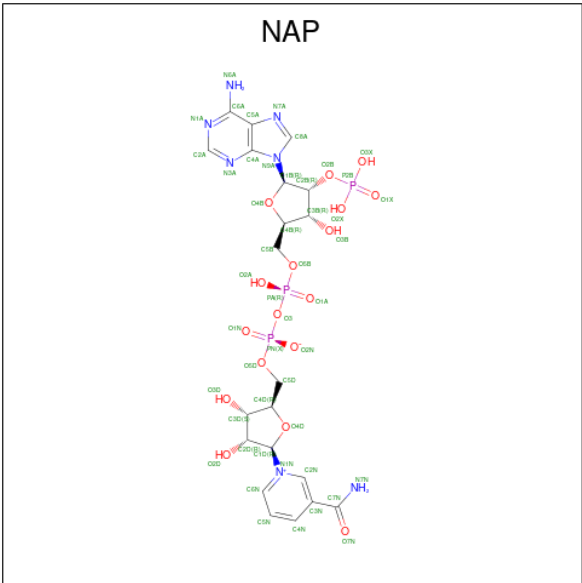
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9HZM7
B	0	SER	-	expression tag	UNP Q9HZM7
C	0	SER	-	expression tag	UNP Q9HZM7
D	0	SER	-	expression tag	UNP Q9HZM7

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



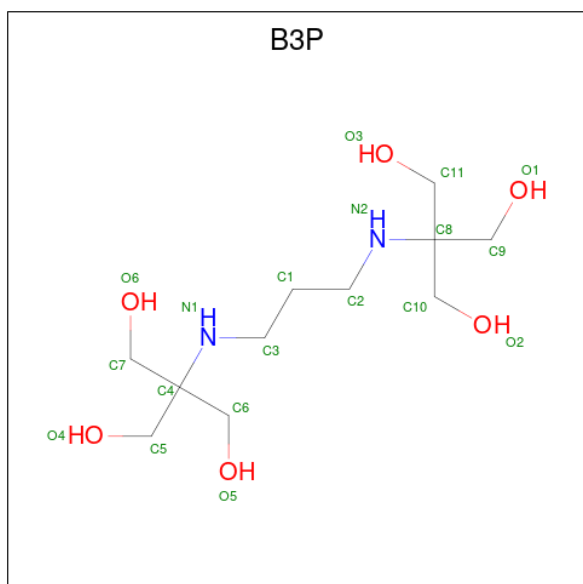
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			19	11	2	6	0	0
4	B	1	Total	C	N	O		
			19	11	2	6	0	0
4	C	1	Total	C	N	O		
			19	11	2	6	0	0
4	D	1	Total	C	N	O		
			19	11	2	6	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K		
			1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0

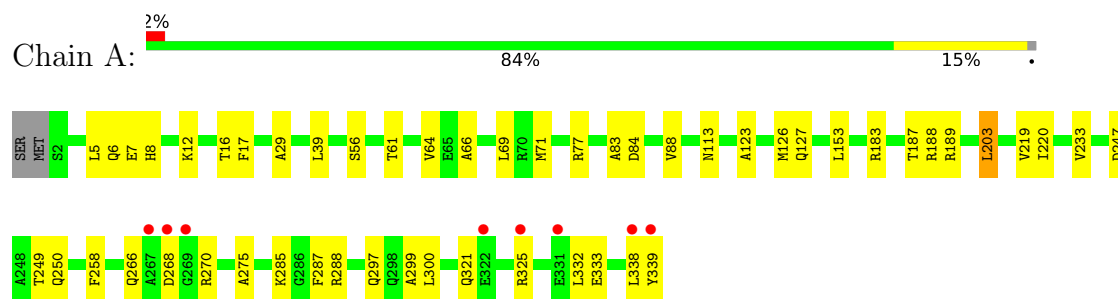
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total 98	O 98	0	0
6	B	84	Total 84	O 84	0	0
6	C	76	Total 76	O 76	0	0
6	D	82	Total 82	O 82	0	0

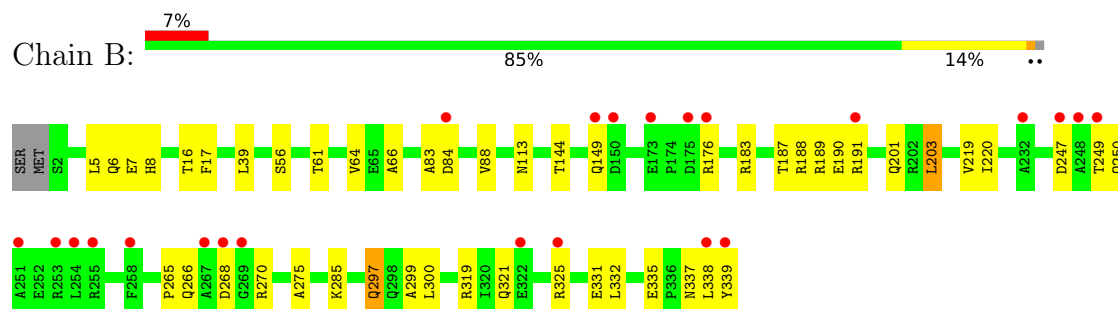
3 Residue-property plots

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.

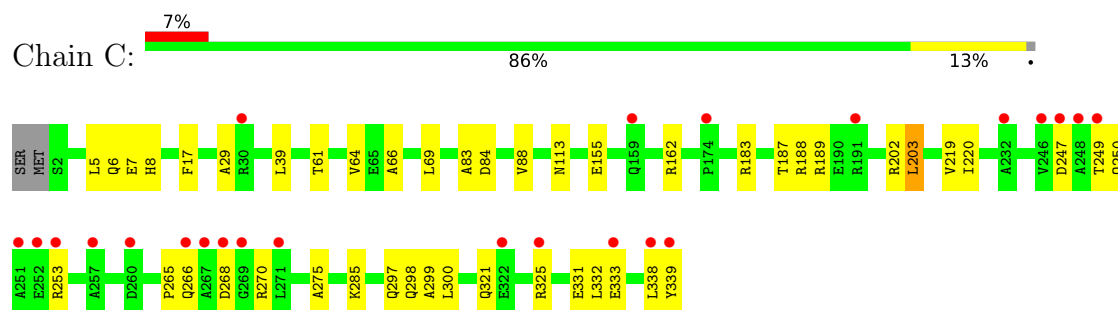
- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase



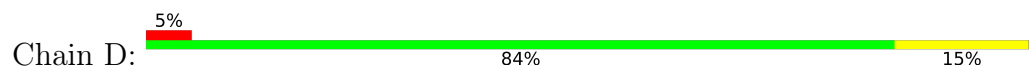
- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

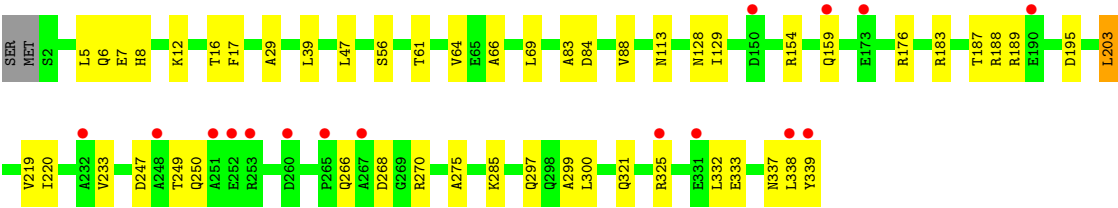


- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase



- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.70Å 154.35Å 64.47Å 90.00° 102.26° 90.00°	Depositor
Resolution (Å)	54.33 – 2.23 54.33 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.1 (54.33-2.23) 98.1 (54.33-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.258 (Not available) , 0.271	Depositor DCC
R_{free} test set	3531 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11404	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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: NAP, B3P, FAD, K

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	0.96	0/2692	0.97	2/3643 (0.1%)
1	B	0.94	0/2692	0.96	2/3643 (0.1%)
1	C	0.94	0/2692	0.97	3/3643 (0.1%)
1	D	0.96	0/2692	0.95	2/3643 (0.1%)
All	All	0.95	0/10768	0.96	9/14572 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLU	CA-C-N	-5.58	114.50	120.03
1	A	333	GLU	C-N-CA	-5.58	114.50	120.03
1	D	333	GLU	CA-C-N	-5.35	114.73	120.03
1	D	333	GLU	C-N-CA	-5.35	114.73	120.03
1	C	333	GLU	CA-C-N	-5.29	114.80	120.03
1	C	333	GLU	C-N-CA	-5.29	114.80	120.03
1	C	162	ARG	CG-CD-NE	5.19	123.42	112.00
1	B	335	GLU	CA-C-N	-5.11	114.65	119.76
1	B	335	GLU	C-N-CA	-5.11	114.65	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2657	44	0
1	B	2645	0	2657	46	4
1	C	2645	0	2657	38	0
1	D	2645	0	2657	46	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	19	0	26	0	0
4	B	19	0	26	1	0
4	C	19	0	26	0	0
4	D	19	0	26	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	98	0	0	10	1
6	B	84	0	0	14	0
6	C	76	0	0	6	0
6	D	82	0	0	10	0
All	All	11404	0	10956	174	5

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 8.

All (174) 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:B:321:GLN:HB3	1:B:325:ARG:NH1	1.64	1.12
1:A:321:GLN:HB3	1:A:325:ARG:NH1	1.63	1.12
1:D:321:GLN:HB3	1:D:325:ARG:NH1	1.64	1.10
1:C:321:GLN:HB3	1:C:325:ARG:NH1	1.67	1.08
1:D:159:GLN:HB2	6:D:519:HOH:O	1.61	1.01
1:B:265:PRO:HB3	6:B:546:HOH:O	1.61	0.99
1:A:123:ALA:HA	6:A:1111:HOH:O	1.64	0.98
1:B:187:THR:HG23	6:B:559:HOH:O	1.64	0.96
1:B:321:GLN:O	1:B:325:ARG:HD2	1.70	0.92
1:A:321:GLN:O	1:A:325:ARG:HD2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLN:O	1:D:325:ARG:HD2	1.71	0.90
1:C:321:GLN:O	1:C:325:ARG:HD2	1.72	0.88
1:B:337:ASN:HB2	6:B:557:HOH:O	1.74	0.85
1:A:321:GLN:HB3	1:A:325:ARG:CZ	2.08	0.83
1:D:321:GLN:HB3	1:D:325:ARG:CZ	2.09	0.82
1:D:337:ASN:HB2	6:D:563:HOH:O	1.78	0.82
1:B:321:GLN:HB3	1:B:325:ARG:CZ	2.11	0.81
1:C:253:ARG:HD3	6:C:549:HOH:O	1.82	0.80
1:C:321:GLN:HB3	1:C:325:ARG:CZ	2.12	0.79
1:D:154:ARG:HD2	6:D:516:HOH:O	1.84	0.78
1:B:331:GLU:C	6:B:543:HOH:O	2.31	0.71
1:B:187:THR:HG22	1:B:189:ARG:H	1.55	0.71
1:D:187:THR:HG22	1:D:189:ARG:H	1.55	0.71
1:A:187:THR:HG22	1:A:189:ARG:H	1.54	0.70
1:B:201:GLN:HB2	6:B:561:HOH:O	1.90	0.70
1:A:187:THR:HG21	1:A:189:ARG:HG2	1.73	0.70
1:B:187:THR:HG21	1:B:189:ARG:HG2	1.74	0.69
1:C:187:THR:HG21	1:C:189:ARG:HG2	1.75	0.69
1:D:187:THR:HG21	1:D:189:ARG:HG2	1.73	0.69
1:A:126:MET:CG	6:A:1111:HOH:O	2.41	0.68
1:C:187:THR:HG22	1:C:189:ARG:H	1.57	0.68
1:B:61:THR:CG2	1:B:338:LEU:HD21	2.25	0.66
1:D:61:THR:CG2	1:D:338:LEU:HD21	2.25	0.66
1:A:61:THR:CG2	1:A:338:LEU:HD21	2.26	0.65
1:C:265:PRO:HD2	6:C:530:HOH:O	1.96	0.65
1:C:61:THR:CG2	1:C:338:LEU:HD21	2.26	0.65
1:D:275:ALA:HB3	1:D:300:LEU:HD21	1.79	0.64
1:C:275:ALA:HB3	1:C:300:LEU:HD21	1.78	0.64
1:B:275:ALA:HB3	1:B:300:LEU:HD21	1.80	0.62
1:A:338:LEU:HD13	1:A:338:LEU:C	2.25	0.62
1:D:266:GLN:HB2	1:D:268:ASP:OD1	2.00	0.61
1:A:275:ALA:HB3	1:A:300:LEU:HD21	1.82	0.61
1:A:321:GLN:CB	1:A:325:ARG:NH1	2.53	0.61
1:C:266:GLN:HB2	1:C:268:ASP:OD1	2.01	0.61
1:D:154:ARG:CD	6:D:516:HOH:O	2.45	0.61
1:C:155:GLU:HG2	6:C:539:HOH:O	2.01	0.60
1:D:154:ARG:NE	6:D:516:HOH:O	2.34	0.60
1:A:266:GLN:HB2	1:A:268:ASP:OD1	2.01	0.60
1:B:339:TYR:CD2	1:B:339:TYR:C	2.80	0.60
1:B:266:GLN:HB2	1:B:268:ASP:OD1	2.01	0.59
1:B:338:LEU:C	1:B:338:LEU:HD13	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLN:CB	1:D:325:ARG:NH1	2.54	0.59
1:B:61:THR:HG21	1:B:338:LEU:HD21	1.85	0.58
1:B:191:ARG:HB2	6:B:529:HOH:O	2.03	0.58
1:C:338:LEU:C	1:C:338:LEU:HD13	2.28	0.58
1:D:187:THR:HG23	6:D:564:HOH:O	2.04	0.58
1:D:338:LEU:C	1:D:338:LEU:HD13	2.29	0.58
1:B:321:GLN:CB	1:B:325:ARG:NH1	2.55	0.58
1:C:61:THR:HG21	1:C:338:LEU:HD21	1.85	0.57
1:D:61:THR:HG21	1:D:338:LEU:HD21	1.84	0.57
1:C:321:GLN:CB	1:C:325:ARG:NH1	2.57	0.57
1:A:61:THR:HG21	1:A:338:LEU:HD21	1.85	0.56
1:C:155:GLU:CG	6:C:539:HOH:O	2.53	0.56
1:C:202:ARG:HD3	6:C:551:HOH:O	2.04	0.56
1:D:339:TYR:C	1:D:339:TYR:CD2	2.84	0.56
1:D:7:GLU:HG2	6:D:511:HOH:O	2.05	0.55
1:A:77:ARG:HD2	6:A:1115:HOH:O	2.05	0.55
1:B:61:THR:HG23	1:B:338:LEU:HD21	1.88	0.55
1:A:339:TYR:CD2	1:A:339:TYR:C	2.85	0.55
1:D:176:ARG:HA	6:D:580:HOH:O	2.06	0.55
1:D:61:THR:HG23	1:D:338:LEU:HD21	1.89	0.55
1:A:61:THR:HG23	1:A:338:LEU:HD21	1.90	0.54
1:C:61:THR:HG23	1:C:338:LEU:HD21	1.90	0.54
1:B:144:THR:HG23	6:B:527:HOH:O	2.07	0.53
1:A:288:ARG:CZ	1:B:190:GLU:HG2	2.39	0.52
1:A:71:MET:HE3	6:A:1145:HOH:O	2.08	0.52
1:C:339:TYR:C	1:C:339:TYR:CD2	2.88	0.52
1:A:12:LYS:HD3	1:D:233:VAL:HG22	1.93	0.51
1:D:195:ASP:OD2	4:D:404:B3P:O6	2.27	0.51
1:B:7:GLU:OE2	1:B:8:HIS:HD2	1.94	0.51
1:B:64:VAL:HG12	1:B:66:ALA:HB3	1.93	0.51
1:B:249:THR:HG23	1:B:250:GLN:H	1.76	0.51
1:B:285:LYS:HD3	1:B:299:ALA:HB2	1.93	0.51
1:D:7:GLU:OE2	1:D:8:HIS:HD2	1.94	0.51
1:B:247:ASP:HA	1:B:270:ARG:HG2	1.93	0.50
1:C:285:LYS:HD3	1:C:299:ALA:HB2	1.93	0.50
1:A:285:LYS:HD3	1:A:299:ALA:HB2	1.93	0.50
3:B:403:NAP:C6N	6:B:568:HOH:O	2.60	0.50
1:C:249:THR:HG23	1:C:250:GLN:H	1.76	0.50
1:D:275:ALA:CB	1:D:300:LEU:HD21	2.41	0.50
1:D:64:VAL:HG12	1:D:66:ALA:HB3	1.94	0.49
1:A:64:VAL:HG12	1:A:66:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ALA:CB	1:B:300:LEU:HD21	2.42	0.49
1:A:249:THR:HG23	1:A:250:GLN:H	1.77	0.49
1:D:285:LYS:HD3	1:D:299:ALA:HB2	1.94	0.49
1:A:233:VAL:HG22	1:D:12:LYS:HD3	1.95	0.49
1:B:5:LEU:HD13	1:B:6:GLN:N	2.28	0.49
1:C:298:GLN:HB3	6:C:572:HOH:O	2.11	0.49
1:A:275:ALA:CB	1:A:300:LEU:HD21	2.43	0.49
1:C:203:LEU:HD13	1:C:219:VAL:HG21	1.94	0.48
1:A:7:GLU:OE2	1:A:8:HIS:HD2	1.96	0.48
1:C:5:LEU:HD13	1:C:6:GLN:N	2.29	0.48
1:A:203:LEU:HD13	1:A:219:VAL:HG21	1.96	0.48
1:C:7:GLU:OE2	1:C:8:HIS:HD2	1.96	0.48
1:C:203:LEU:CD1	1:C:219:VAL:HG21	2.44	0.48
1:D:247:ASP:HA	1:D:270:ARG:HG2	1.95	0.48
2:A:1001:FAD:C5A	6:A:1111:HOH:O	2.61	0.48
1:A:153:LEU:HD13	6:A:1154:HOH:O	2.14	0.48
1:B:319:ARG:NH1	6:B:549:HOH:O	2.43	0.47
1:D:203:LEU:HD13	1:D:219:VAL:HG21	1.96	0.47
1:A:247:ASP:HA	1:A:270:ARG:HG2	1.96	0.47
1:C:247:ASP:HA	1:C:270:ARG:HG2	1.95	0.47
1:B:249:THR:HG23	1:B:250:GLN:N	2.29	0.47
1:D:47:LEU:HD23	6:D:573:HOH:O	2.14	0.47
1:D:249:THR:HG23	1:D:250:GLN:H	1.79	0.47
1:C:275:ALA:CB	1:C:300:LEU:HD21	2.42	0.47
1:D:325:ARG:NE	6:D:509:HOH:O	2.47	0.47
1:B:297:GLN:HG3	6:B:525:HOH:O	2.15	0.47
1:A:126:MET:HG3	6:A:1111:HOH:O	2.12	0.46
1:A:203:LEU:CD1	1:A:219:VAL:HG21	2.45	0.46
1:D:203:LEU:CD1	1:D:219:VAL:HG21	2.46	0.46
1:B:203:LEU:HD13	1:B:219:VAL:HG21	1.97	0.46
1:D:113:ASN:HA	1:D:220:ILE:HD12	1.97	0.46
1:A:126:MET:HG2	6:A:1111:HOH:O	2.09	0.46
1:B:331:GLU:HB3	6:B:543:HOH:O	2.16	0.46
1:C:64:VAL:HG12	1:C:66:ALA:HB3	1.96	0.46
1:D:325:ARG:NH2	1:D:332:LEU:O	2.49	0.46
1:A:325:ARG:NH2	1:A:332:LEU:O	2.49	0.46
1:A:249:THR:HG23	1:A:250:GLN:N	2.30	0.45
1:C:249:THR:HG23	1:C:250:GLN:N	2.31	0.45
1:D:5:LEU:HD13	1:D:6:GLN:N	2.31	0.45
1:B:113:ASN:HA	1:B:220:ILE:HD12	1.99	0.45
1:B:203:LEU:CD1	1:B:219:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:HG23	1:D:250:GLN:N	2.31	0.45
1:A:258:PHE:CE1	1:B:265:PRO:HG2	2.52	0.45
1:B:325:ARG:NH2	1:B:332:LEU:O	2.50	0.44
1:D:88:VAL:O	1:D:183:ARG:HA	2.18	0.44
1:A:113:ASN:HA	1:A:220:ILE:HD12	2.00	0.44
1:C:113:ASN:HA	1:C:220:ILE:HD12	1.99	0.44
1:C:187:THR:CG2	1:C:189:ARG:HG2	2.47	0.44
1:C:325:ARG:NH2	1:C:332:LEU:O	2.51	0.44
1:A:187:THR:HG22	1:A:188:ARG:N	2.32	0.44
2:A:1001:FAD:HM71	2:A:1001:FAD:HM83	1.76	0.43
1:B:88:VAL:O	1:B:183:ARG:HA	2.17	0.43
1:A:113:ASN:HA	1:A:220:ILE:CD1	2.48	0.43
1:A:88:VAL:O	1:A:183:ARG:HA	2.19	0.43
1:B:297:GLN:CG	6:B:564:HOH:O	2.66	0.43
1:D:128:ASN:O	1:D:129:ILE:C	2.62	0.43
1:B:16:THR:OG1	1:B:56:SER:HA	2.19	0.43
1:C:88:VAL:O	1:C:183:ARG:HA	2.19	0.43
1:D:321:GLN:NE2	1:D:325:ARG:HH22	2.17	0.43
1:A:287:PHE:CD1	4:B:404:B3P:H72	2.53	0.43
2:A:1001:FAD:C4A	6:A:1111:HOH:O	2.66	0.43
1:B:113:ASN:HA	1:B:220:ILE:CD1	2.49	0.43
1:A:5:LEU:HD13	1:A:6:GLN:N	2.34	0.42
1:A:83:ALA:O	1:A:84:ASP:HB2	2.18	0.42
1:B:187:THR:HG22	1:B:188:ARG:N	2.33	0.42
1:C:29:ALA:HB2	1:C:69:LEU:HD11	2.01	0.42
1:C:83:ALA:O	1:C:84:ASP:HB2	2.19	0.42
1:B:332:LEU:C	6:B:543:HOH:O	2.63	0.42
1:C:187:THR:HG22	1:C:188:ARG:N	2.34	0.42
1:D:187:THR:HG22	1:D:188:ARG:N	2.34	0.42
1:B:83:ALA:O	1:B:84:ASP:HB2	2.20	0.41
1:C:325:ARG:HE	1:C:331:GLU:HA	1.85	0.41
1:D:113:ASN:HA	1:D:220:ILE:CD1	2.49	0.41
1:B:187:THR:CG2	1:B:189:ARG:HG2	2.48	0.41
1:B:332:LEU:N	6:B:543:HOH:O	2.52	0.41
1:D:83:ALA:O	1:D:84:ASP:HB2	2.19	0.41
1:C:113:ASN:HA	1:C:220:ILE:CD1	2.50	0.41
1:A:29:ALA:HB2	1:A:69:LEU:HD11	2.03	0.40
1:A:127:GLN:HG2	6:A:1123:HOH:O	2.21	0.40
1:D:29:ALA:HB2	1:D:69:LEU:HD11	2.02	0.40
1:D:16:THR:OG1	1:D:56:SER:HA	2.20	0.40
1:A:16:THR:OG1	1:A:56:SER:HA	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:NH2	1:B:176:ARG:NH2[2_556]	1.71	0.49
1:B:149:GLN:OE1	1:B:176:ARG:NH1[2_556]	1.75	0.45
6:A:1179:HOH:O	6:A:1179:HOH:O[2_656]	1.89	0.31
1:B:176:ARG:CZ	1:B:176:ARG:NH1[2_556]	2.00	0.20
1:B:149:GLN:CD	1:B:176:ARG:NH1[2_556]	2.07	0.13

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	336/340 (99%)	330 (98%)	6 (2%)	0	100	100
1	B	336/340 (99%)	329 (98%)	7 (2%)	0	100	100
1	C	336/340 (99%)	328 (98%)	8 (2%)	0	100	100
1	D	336/340 (99%)	330 (98%)	6 (2%)	0	100	100
All	All	1344/1360 (99%)	1317 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	270/272 (99%)	266 (98%)	4 (2%)	57	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	270/272 (99%)	266 (98%)	4 (2%)	57	66
1	C	270/272 (99%)	266 (98%)	4 (2%)	57	66
1	D	270/272 (99%)	266 (98%)	4 (2%)	57	66
All	All	1080/1088 (99%)	1064 (98%)	16 (2%)	57	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	39	LEU
1	A	203	LEU
1	A	297	GLN
1	B	17	PHE
1	B	39	LEU
1	B	203	LEU
1	B	297	GLN
1	C	17	PHE
1	C	39	LEU
1	C	203	LEU
1	C	297	GLN
1	D	17	PHE
1	D	39	LEU
1	D	203	LEU
1	D	297	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	74	GLN
1	A	298	GLN
1	B	8	HIS
1	B	74	GLN
1	B	298	GLN
1	C	8	HIS
1	C	74	GLN
1	D	8	HIS
1	D	74	GLN
1	D	298	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	NAP	D	403	5	50,52,52	1.20	6 (12%)	71,80,80	1.68	17 (23%)
4	B3P	A	1003	-	18,18,18	0.67	0	23,23,23	1.52	3 (13%)
2	FAD	B	402	-	58,58,58	1.61	13 (22%)	85,89,89	1.40	11 (12%)
4	B3P	B	404	-	18,18,18	1.07	2 (11%)	23,23,23	1.47	4 (17%)
3	NAP	C	403	5	50,52,52	1.17	5 (10%)	71,80,80	1.81	17 (23%)
2	FAD	D	402	-	58,58,58	1.67	9 (15%)	85,89,89	1.68	15 (17%)
3	NAP	B	403	5	50,52,52	1.28	5 (10%)	71,80,80	1.78	18 (25%)
4	B3P	C	404	-	18,18,18	1.00	1 (5%)	23,23,23	1.46	3 (13%)
2	FAD	C	402	-	58,58,58	1.61	12 (20%)	85,89,89	1.84	24 (28%)
2	FAD	A	1001	-	58,58,58	1.66	12 (20%)	85,89,89	1.64	16 (18%)
4	B3P	D	404	-	18,18,18	0.89	1 (5%)	23,23,23	1.26	4 (17%)
3	NAP	A	1002	5	50,52,52	1.23	7 (14%)	71,80,80	1.81	18 (25%)

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	NAP	D	403	5	-	4/35/67/67	0/5/5/5
4	B3P	A	1003	-	-	13/28/28/28	-
2	FAD	B	402	-	-	3/34/50/50	0/6/6/6
4	B3P	B	404	-	-	10/28/28/28	-
3	NAP	C	403	5	-	2/35/67/67	0/5/5/5
2	FAD	D	402	-	-	2/34/50/50	0/6/6/6
3	NAP	B	403	5	-	2/35/67/67	0/5/5/5
4	B3P	C	404	-	-	15/28/28/28	-
2	FAD	C	402	-	-	3/34/50/50	0/6/6/6
2	FAD	A	1001	-	-	6/34/50/50	0/6/6/6
4	B3P	D	404	-	-	10/28/28/28	-
3	NAP	A	1002	5	-	2/35/67/67	0/5/5/5

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	FAD	C5A-N7A	-4.88	1.30	1.39
2	B	402	FAD	C9A-C5X	4.55	1.48	1.41
2	C	402	FAD	C5A-C4A	4.30	1.46	1.39
2	D	402	FAD	C5A-C4A	4.23	1.46	1.39
2	C	402	FAD	C9A-C5X	4.19	1.47	1.41
3	B	403	NAP	C5A-C4A	4.14	1.46	1.39
2	D	402	FAD	C9A-C5X	4.13	1.47	1.41
2	C	402	FAD	C5A-N7A	-4.03	1.31	1.39
3	A	1002	NAP	C5A-C4A	3.97	1.46	1.39
2	A	1001	FAD	C9A-C5X	3.88	1.47	1.41
2	A	1001	FAD	O4-C4	3.86	1.30	1.23
2	B	402	FAD	C5A-C4A	3.85	1.45	1.39
2	A	1001	FAD	C5A-C4A	3.84	1.45	1.39
3	B	403	NAP	C4A-N9A	-3.66	1.30	1.37
2	B	402	FAD	C4A-N9A	-3.58	1.30	1.37
2	B	402	FAD	C4-N3	-3.43	1.32	1.38
2	C	402	FAD	C8A-N9A	-3.41	1.31	1.37
3	C	403	NAP	C5A-C4A	3.38	1.45	1.39
2	A	1001	FAD	C5A-N7A	-3.33	1.33	1.39
3	D	403	NAP	C5A-C4A	3.27	1.44	1.39
2	A	1001	FAD	C4A-N9A	-3.21	1.31	1.37
2	D	402	FAD	C8A-N9A	-3.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	C2-N3	-3.14	1.32	1.39
3	C	403	NAP	C4A-N9A	-3.10	1.31	1.37
2	D	402	FAD	C6-C5X	-3.06	1.35	1.40
4	C	404	B3P	C3-N1	-2.93	1.43	1.46
2	B	402	FAD	C5A-N7A	-2.86	1.33	1.39
3	D	403	NAP	C5A-N7A	-2.86	1.33	1.39
2	D	402	FAD	C8-C7	2.85	1.47	1.40
3	C	403	NAP	P2B-O2B	2.84	1.64	1.59
3	B	403	NAP	C5A-N7A	-2.83	1.33	1.39
2	B	402	FAD	C8-C7	2.74	1.47	1.40
3	D	403	NAP	C4A-N9A	-2.71	1.32	1.37
3	A	1002	NAP	P2B-O2B	2.69	1.64	1.59
2	B	402	FAD	C4X-N5	2.68	1.36	1.30
3	A	1002	NAP	C4A-N9A	-2.66	1.32	1.37
2	C	402	FAD	C8A-N7A	2.66	1.36	1.31
2	C	402	FAD	C2-N3	-2.64	1.33	1.39
3	D	403	NAP	P2B-O2B	2.61	1.64	1.59
3	D	403	NAP	O4D-C1D	2.61	1.44	1.40
4	B	404	B3P	C3-N1	-2.58	1.43	1.46
3	B	403	NAP	P2B-O2B	2.55	1.64	1.59
2	A	1001	FAD	C4-N3	-2.55	1.34	1.38
2	C	402	FAD	C5X-N5	-2.53	1.34	1.39
3	B	403	NAP	PN-O3	2.49	1.62	1.59
2	C	402	FAD	C8-C7	2.48	1.46	1.40
2	A	1001	FAD	O4B-C1B	2.47	1.47	1.42
2	C	402	FAD	O4-C4	2.46	1.28	1.23
2	B	402	FAD	C2-N3	-2.43	1.33	1.39
3	C	403	NAP	C5A-C6A	2.42	1.47	1.41
3	A	1002	NAP	C5A-N7A	-2.41	1.34	1.39
2	D	402	FAD	C4A-N9A	-2.39	1.32	1.37
2	D	402	FAD	C4X-N5	2.35	1.35	1.30
2	B	402	FAD	C8A-N7A	2.33	1.36	1.31
4	D	404	B3P	C3-N1	-2.32	1.44	1.46
3	A	1002	NAP	PN-O3	2.27	1.62	1.59
2	B	402	FAD	C2'-C3'	-2.25	1.49	1.53
2	B	402	FAD	C5X-N5	-2.25	1.35	1.39
3	C	403	NAP	C5A-N7A	-2.24	1.35	1.39
3	A	1002	NAP	C5A-C6A	2.22	1.47	1.41
2	D	402	FAD	C1'-C2'	-2.21	1.49	1.52
3	A	1002	NAP	C8A-N7A	2.19	1.35	1.31
2	B	402	FAD	P-O3P	2.18	1.61	1.59
4	B	404	B3P	C6-C4	-2.17	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	NAP	O7N-C7N	-2.14	1.20	1.24
2	C	402	FAD	C1'-C2'	-2.12	1.49	1.52
2	A	1001	FAD	P-O3P	2.12	1.61	1.59
2	A	1001	FAD	PA-O3P	-2.07	1.57	1.59
2	A	1001	FAD	P-O2P	-2.06	1.45	1.55
2	C	402	FAD	C5A-C6A	2.04	1.46	1.41
2	A	1001	FAD	C8A-N9A	-2.03	1.34	1.37
2	C	402	FAD	C4A-N9A	-2.02	1.33	1.37
2	B	402	FAD	O4-C4	2.01	1.27	1.23

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FAD	N3A-C2A-N1A	-4.97	121.06	128.58
3	A	1002	NAP	N3A-C2A-N1A	-4.85	121.24	128.58
2	D	402	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	D	402	FAD	C4A-C5A-N7A	-4.76	105.13	110.58
2	C	402	FAD	C4'-C3'-C2'	-4.54	106.01	113.57
2	C	402	FAD	C2A-N1A-C6A	4.50	126.12	118.73
3	C	403	NAP	C5A-C4A-N3A	-4.50	120.53	126.72
2	A	1001	FAD	C5A-C4A-N3A	-4.46	120.58	126.72
3	C	403	NAP	N3A-C4A-N9A	4.45	134.74	127.17
4	A	1003	B3P	C3-N1-C4	4.37	122.56	116.17
3	B	403	NAP	C4A-N9A-C8A	4.32	110.27	105.74
3	D	403	NAP	N3A-C2A-N1A	-4.27	122.11	128.58
4	B	404	B3P	C3-N1-C4	4.27	122.41	116.17
3	B	403	NAP	N3A-C4A-N9A	4.19	134.29	127.17
3	B	403	NAP	N6A-C6A-N1A	4.03	127.36	118.38
2	B	402	FAD	C5A-C4A-N3A	-4.01	121.20	126.72
2	B	402	FAD	N3A-C2A-N1A	-3.97	122.57	128.58
3	D	403	NAP	O3-PN-O1N	-3.97	98.76	110.70
3	D	403	NAP	N3A-C4A-N9A	3.96	133.91	127.17
3	C	403	NAP	C4A-N9A-C8A	3.95	109.89	105.74
2	D	402	FAD	O4-C4-C4X	-3.93	116.15	126.53
3	D	403	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
3	C	403	NAP	C2B-C3B-C4B	3.91	110.40	101.99
4	C	404	B3P	C3-N1-C4	3.84	121.78	116.17
3	C	403	NAP	C4D-O4D-C1D	3.81	113.41	109.92
2	A	1001	FAD	C4A-N9A-C8A	3.80	109.73	105.74
3	B	403	NAP	N3A-C2A-N1A	-3.74	122.92	128.58
2	D	402	FAD	C5A-N7A-C8A	3.74	109.33	103.45
3	C	403	NAP	N3A-C2A-N1A	-3.73	122.93	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAP	C5A-C4A-N3A	-3.72	121.59	126.72
2	A	1001	FAD	N3A-C4A-N9A	3.72	133.49	127.17
2	C	402	FAD	C4A-C5A-N7A	-3.68	106.37	110.58
3	A	1002	NAP	C2A-N3A-C4A	3.65	120.75	111.83
3	A	1002	NAP	C4D-O4D-C1D	3.63	113.25	109.92
3	C	403	NAP	C2A-N3A-C4A	3.58	120.57	111.83
3	A	1002	NAP	N3A-C4A-N9A	3.56	133.22	127.17
3	C	403	NAP	C3N-C7N-N7N	3.50	122.05	117.74
2	C	402	FAD	C4A-N9A-C8A	3.45	109.36	105.74
3	A	1002	NAP	O2N-PN-O1N	3.45	128.51	112.44
2	A	1001	FAD	O4'-C4'-C5'	-3.44	102.40	109.99
3	A	1002	NAP	O3-PN-O1N	-3.42	100.42	110.70
2	D	402	FAD	C4'-C3'-C2'	-3.42	107.88	113.57
2	C	402	FAD	C5A-C4A-N3A	-3.40	122.03	126.72
2	A	1001	FAD	C4'-C3'-C2'	-3.40	107.91	113.57
3	B	403	NAP	C2B-C3B-C4B	3.40	109.30	101.99
2	D	402	FAD	O4-C4-N3	3.38	126.48	120.11
2	A	1001	FAD	C4A-C5A-N7A	-3.37	106.73	110.58
4	A	1003	B3P	C2-N2-C8	3.33	121.03	116.17
3	B	403	NAP	C5N-C4N-C3N	-3.32	117.10	120.36
3	D	403	NAP	C2A-N3A-C4A	3.32	119.94	111.83
3	B	403	NAP	C2A-N1A-C6A	3.26	124.09	118.73
3	D	403	NAP	O2X-P2B-O1X	3.26	123.54	110.83
2	D	402	FAD	N3A-C4A-N9A	3.25	132.70	127.17
2	B	402	FAD	N3A-C4A-N9A	3.25	132.69	127.17
3	D	403	NAP	O2N-PN-O1N	3.25	127.56	112.44
2	D	402	FAD	C2A-N1A-C6A	3.23	124.03	118.73
2	B	402	FAD	C4'-C3'-C2'	-3.20	108.24	113.57
2	A	1001	FAD	C4X-C10-N10	3.16	121.00	116.48
2	B	402	FAD	C2A-N3A-C4A	3.14	119.49	111.83
3	A	1002	NAP	C4A-N9A-C8A	3.09	108.98	105.74
2	D	402	FAD	O4'-C4'-C5'	-3.08	103.19	109.99
2	C	402	FAD	C5A-N7A-C8A	3.08	108.29	103.45
2	A	1001	FAD	N9A-C8A-N7A	-3.05	109.60	113.94
3	A	1002	NAP	O2X-P2B-O2B	-3.04	93.99	105.85
2	B	402	FAD	C9A-C5X-N5	-3.01	119.26	122.45
2	C	402	FAD	C2A-N3A-C4A	3.00	119.17	111.83
2	C	402	FAD	N3A-C4A-N9A	2.98	132.24	127.17
2	C	402	FAD	C6A-C5A-N7A	2.97	137.81	132.09
2	C	402	FAD	C4A-N9A-C1B	-2.93	119.78	126.63
2	C	402	FAD	C5'-C4'-C3'	2.93	117.74	112.22
4	A	1003	B3P	O2-C10-C8	-2.91	105.76	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAP	C2B-C3B-C4B	2.91	108.25	101.99
3	B	403	NAP	C5A-C4A-N3A	-2.87	122.77	126.72
3	B	403	NAP	O4B-C1B-N9A	-2.86	102.59	108.09
3	D	403	NAP	C4A-N9A-C8A	2.85	108.73	105.74
2	C	402	FAD	O3'-C3'-C4'	2.83	115.37	108.93
4	D	404	B3P	C3-N1-C4	2.82	120.29	116.17
4	C	404	B3P	C6-C4-C5	2.81	116.18	110.02
3	A	1002	NAP	C2A-N1A-C6A	2.80	123.33	118.73
3	B	403	NAP	C5A-C6A-N6A	-2.79	116.39	123.29
2	A	1001	FAD	C5A-N7A-C8A	2.77	107.80	103.45
3	B	403	NAP	O2B-P2B-O1X	-2.74	99.56	109.33
3	D	403	NAP	C2B-C3B-C4B	2.73	107.87	101.99
3	A	1002	NAP	O2X-P2B-O1X	2.73	121.46	110.83
4	D	404	B3P	O2-C10-C8	-2.72	106.15	111.68
2	C	402	FAD	N9A-C8A-N7A	-2.72	110.08	113.94
2	B	402	FAD	O4B-C1B-N9A	-2.66	102.97	108.09
3	D	403	NAP	N6A-C6A-N1A	2.66	124.30	118.38
3	A	1002	NAP	C5N-C4N-C3N	-2.65	117.76	120.36
3	B	403	NAP	C5A-C4A-N9A	-2.65	102.93	105.81
2	A	1001	FAD	N3A-C2A-N1A	-2.64	124.58	128.58
2	C	402	FAD	O2P-P-O3P	2.64	114.40	107.27
2	B	402	FAD	C4-C4X-N5	2.62	121.83	118.21
2	C	402	FAD	C9A-C5X-N5	-2.62	119.68	122.45
3	D	403	NAP	O2X-P2B-O2B	-2.62	95.65	105.85
2	C	402	FAD	O4B-C1B-N9A	-2.59	103.12	108.09
2	B	402	FAD	C2A-N1A-C6A	2.58	122.97	118.73
3	C	403	NAP	O2X-P2B-O2B	-2.58	95.79	105.85
2	A	1001	FAD	O2P-P-O1P	2.57	124.40	112.44
2	D	402	FAD	O2-C2-N1	-2.57	117.53	121.80
2	D	402	FAD	N3A-C2A-N1A	-2.56	124.71	128.58
3	C	403	NAP	C5N-C4N-C3N	-2.53	117.88	120.36
3	C	403	NAP	O3X-P2B-O2X	2.51	117.21	107.80
2	D	402	FAD	C2A-N3A-C4A	2.51	117.95	111.83
3	C	403	NAP	O7N-C7N-C3N	-2.49	116.55	119.60
2	A	1001	FAD	C10-C4X-N5	-2.47	119.76	124.81
3	A	1002	NAP	C3N-C7N-N7N	2.47	120.78	117.74
3	A	1002	NAP	N6A-C6A-N1A	2.43	123.78	118.38
3	B	403	NAP	C2B-C1B-N9A	2.42	117.73	113.75
4	B	404	B3P	O3-C11-C8	-2.41	106.78	111.68
4	D	404	B3P	C2-N2-C8	2.41	119.69	116.17
3	C	403	NAP	N6A-C6A-N1A	2.39	123.69	118.38
4	B	404	B3P	C1-C3-N1	-2.38	105.22	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	402	FAD	N9A-C8A-N7A	-2.36	110.58	113.94
3	D	403	NAP	C2A-N1A-C6A	2.35	122.58	118.73
3	D	403	NAP	O2A-PA-O1A	2.33	123.28	112.44
2	D	402	FAD	O3B-C3B-C2B	-2.30	104.45	111.82
3	D	403	NAP	C5A-C6A-N6A	-2.29	117.62	123.29
3	D	403	NAP	O7N-C7N-N7N	-2.29	119.31	122.62
2	A	1001	FAD	C2A-N3A-C4A	2.27	117.36	111.83
2	A	1001	FAD	C4-C4X-N5	2.26	121.33	118.21
4	B	404	B3P	O2-C10-C8	-2.26	107.09	111.68
3	B	403	NAP	C2A-N3A-C4A	2.25	117.33	111.83
3	B	403	NAP	O2N-PN-O1N	2.25	122.90	112.44
4	C	404	B3P	C1-C3-N1	-2.24	105.56	110.98
2	C	402	FAD	C2B-C1B-N9A	2.23	118.85	113.30
2	D	402	FAD	C6A-C5A-N7A	2.22	136.38	132.09
2	C	402	FAD	C4X-C10-N1	-2.22	119.16	124.59
2	B	402	FAD	C5X-N5-C4X	2.21	121.66	118.09
3	C	403	NAP	C2D-C3D-C4D	2.19	106.84	102.61
2	C	402	FAD	O2P-P-O1P	2.18	122.59	112.44
4	D	404	B3P	C3-C1-C2	-2.18	106.40	114.15
2	C	402	FAD	O4-C4-C4X	-2.16	120.83	126.53
2	B	402	FAD	C4A-N9A-C8A	2.16	108.00	105.74
2	C	402	FAD	C5X-N5-C4X	2.15	121.57	118.09
3	D	403	NAP	O3B-C3B-C4B	-2.14	104.92	111.08
3	B	403	NAP	C6N-N1N-C1D	2.14	123.94	119.73
2	C	402	FAD	C5X-C9A-N10	2.12	119.89	117.97
3	C	403	NAP	C5A-C6A-N6A	-2.09	118.12	123.29
3	A	1002	NAP	N9A-C8A-N7A	-2.08	110.99	113.94
3	D	403	NAP	C3N-C7N-N7N	2.07	120.29	117.74
3	C	403	NAP	O2N-PN-O1N	2.07	122.08	112.44
3	C	403	NAP	N9A-C8A-N7A	-2.07	111.00	113.94
3	B	403	NAP	O3X-P2B-O2X	2.06	115.54	107.80
3	A	1002	NAP	O3B-C3B-C4B	-2.06	105.16	111.08
2	A	1001	FAD	C4X-C10-N1	-2.05	119.56	124.59
3	A	1002	NAP	C6N-N1N-C1D	2.04	123.73	119.73
2	A	1001	FAD	C2A-N1A-C6A	2.01	122.03	118.73
2	C	402	FAD	C4-C4X-N5	2.01	120.98	118.21
3	B	403	NAP	O2X-P2B-O1X	2.01	118.67	110.83

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	C5B-O5B-PA-O1A
2	A	1001	FAD	N10-C1'-C2'-O2'
2	A	1001	FAD	N10-C1'-C2'-C3'
2	B	402	FAD	N10-C1'-C2'-O2'
2	B	402	FAD	N10-C1'-C2'-C3'
2	C	402	FAD	N10-C1'-C2'-O2'
2	C	402	FAD	N10-C1'-C2'-C3'
2	D	402	FAD	N10-C1'-C2'-O2'
2	D	402	FAD	N10-C1'-C2'-C3'
4	A	1003	B3P	N1-C4-C7-O6
4	A	1003	B3P	C5-C4-C7-O6
4	A	1003	B3P	C6-C4-C7-O6
4	A	1003	B3P	O3-C11-C8-N2
4	A	1003	B3P	O3-C11-C8-C9
4	A	1003	B3P	O3-C11-C8-C10
4	B	404	B3P	N1-C4-C7-O6
4	B	404	B3P	C5-C4-C7-O6
4	B	404	B3P	C6-C4-C7-O6
4	B	404	B3P	O3-C11-C8-N2
4	B	404	B3P	O3-C11-C8-C9
4	B	404	B3P	O3-C11-C8-C10
4	C	404	B3P	C5-C4-C6-O5
4	C	404	B3P	N1-C4-C7-O6
4	C	404	B3P	C6-C4-C7-O6
4	C	404	B3P	C10-C8-N2-C2
4	C	404	B3P	C11-C8-N2-C2
4	C	404	B3P	O3-C11-C8-N2
4	C	404	B3P	O3-C11-C8-C9
4	C	404	B3P	O3-C11-C8-C10
4	D	404	B3P	N1-C4-C7-O6
4	D	404	B3P	C5-C4-C7-O6
4	D	404	B3P	C6-C4-C7-O6
4	D	404	B3P	O3-C11-C8-N2
4	D	404	B3P	O3-C11-C8-C9
4	D	404	B3P	O3-C11-C8-C10
4	C	404	B3P	C3-C1-C2-N2
4	A	1003	B3P	C3-C1-C2-N2
4	B	404	B3P	C3-C1-C2-N2
4	D	404	B3P	C3-C1-C2-N2
4	C	404	B3P	C7-C4-C6-O5
4	C	404	B3P	C5-C4-C7-O6
4	D	404	B3P	C5-C4-C6-O5
4	D	404	B3P	C7-C4-C6-O5

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Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	C3B-C4B-C5B-O5B
3	C	403	NAP	PA-O3-PN-O1N
4	C	404	B3P	N1-C4-C6-O5
4	A	1003	B3P	C5-C4-C6-O5
4	B	404	B3P	C5-C4-C6-O5
3	B	403	NAP	PA-O3-PN-O2N
3	D	403	NAP	PA-O3-PN-O2N
4	C	404	B3P	C9-C8-N2-C2
4	B	404	B3P	O2-C10-C8-N2
4	A	1003	B3P	C7-C4-C5-O4
4	C	404	B3P	C11-C8-C9-O1
3	D	403	NAP	O4B-C4B-C5B-O5B
4	A	1003	B3P	C1-C3-N1-C4
4	B	404	B3P	C11-C8-C9-O1
3	A	1002	NAP	PA-O3-PN-O2N
3	C	403	NAP	PA-O3-PN-O2N
3	D	403	NAP	PA-O3-PN-O1N
4	A	1003	B3P	C7-C4-C6-O5
4	C	404	B3P	C10-C8-C9-O1
3	A	1002	NAP	PA-O3-PN-O1N
4	A	1003	B3P	N1-C4-C5-O4
4	D	404	B3P	N1-C4-C6-O5
2	A	1001	FAD	PA-O3P-P-O1P
2	B	402	FAD	PA-O3P-P-O1P
2	C	402	FAD	PA-O3P-P-O1P
3	B	403	NAP	PA-O3-PN-O1N
2	A	1001	FAD	O4B-C4B-C5B-O5B
4	A	1003	B3P	N1-C4-C6-O5
3	D	403	NAP	C3B-C4B-C5B-O5B

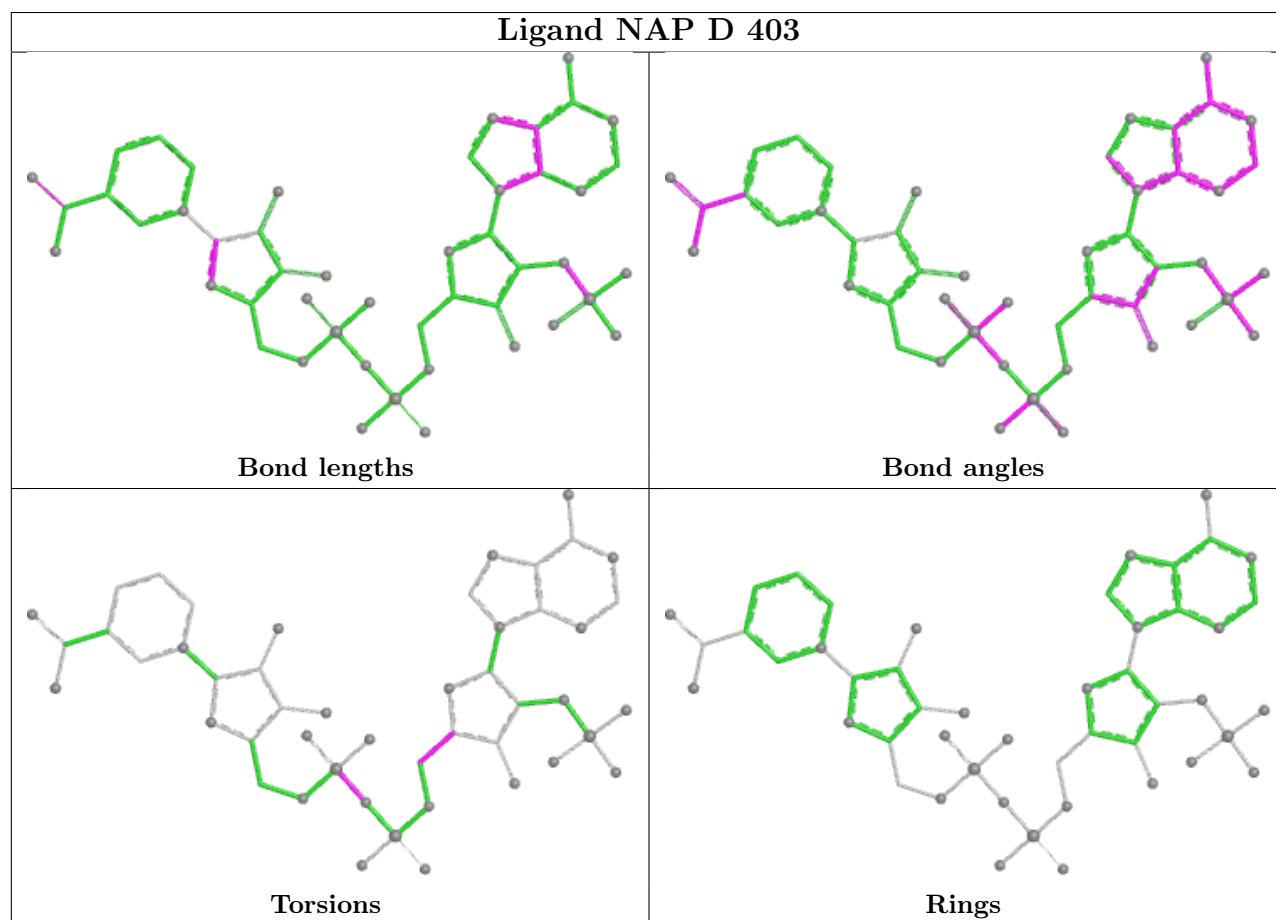
There are no ring outliers.

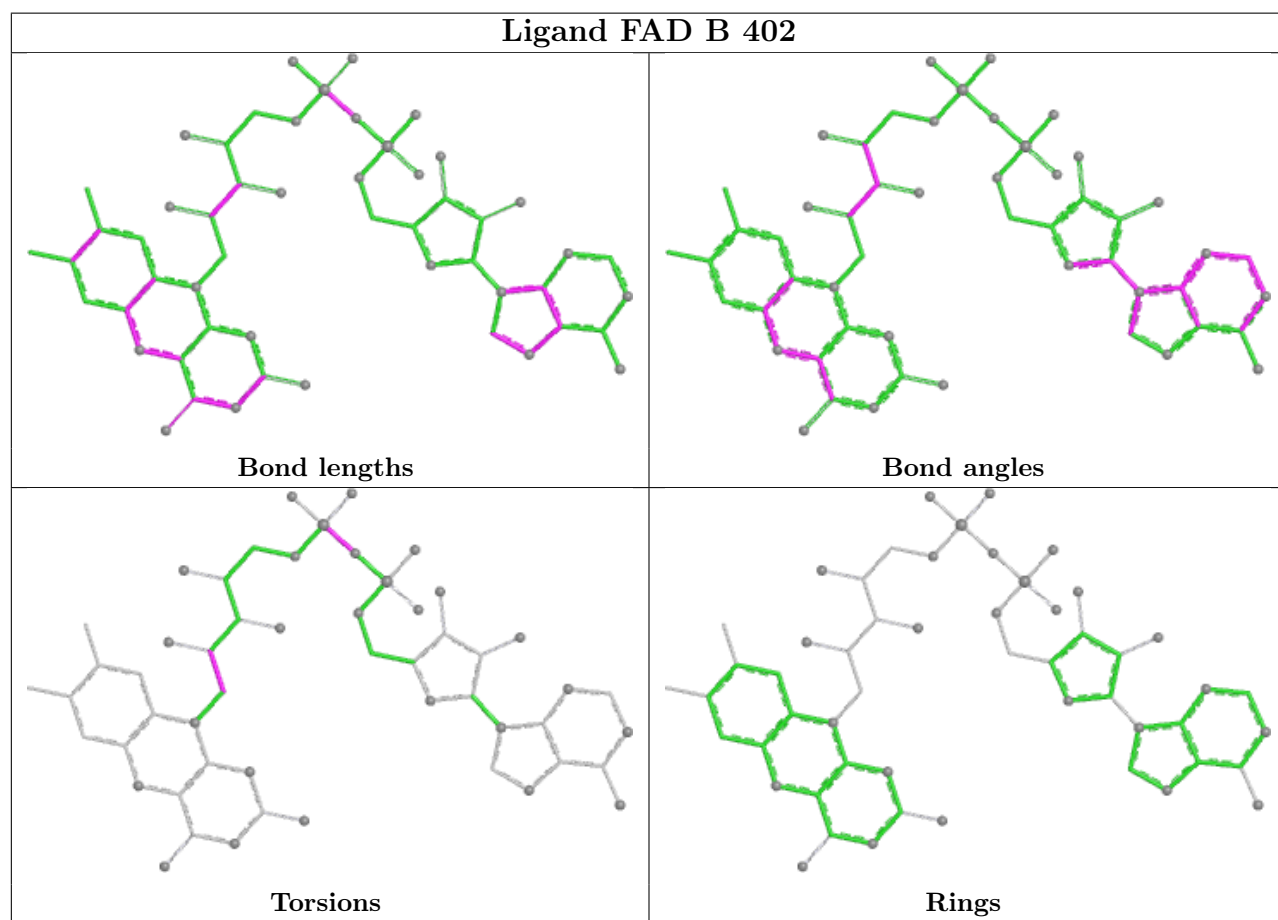
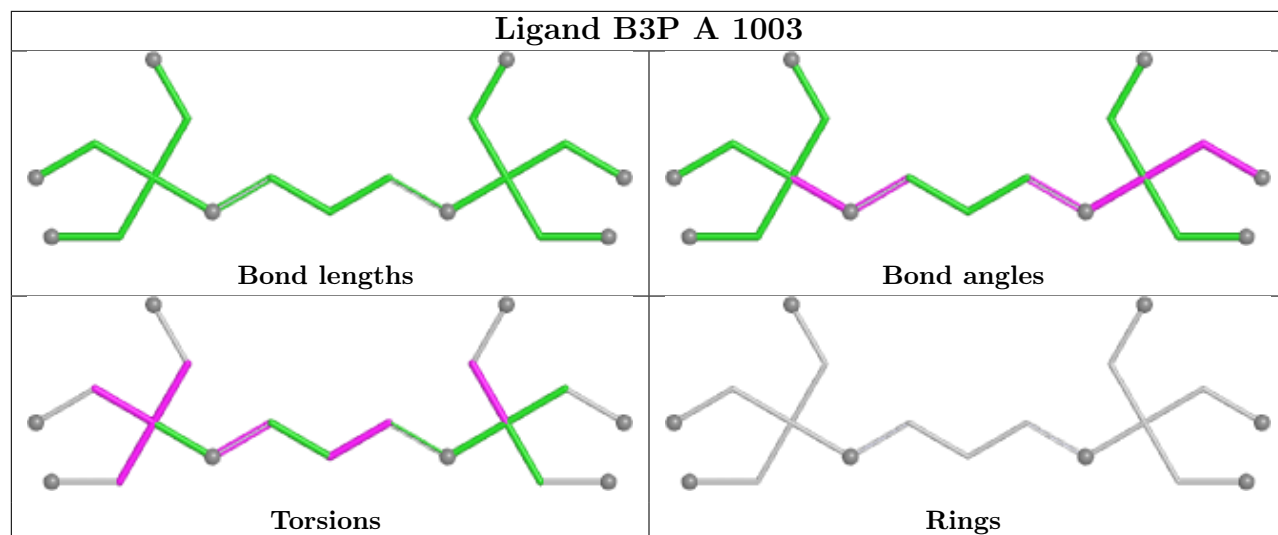
4 monomers are involved in 6 short contacts:

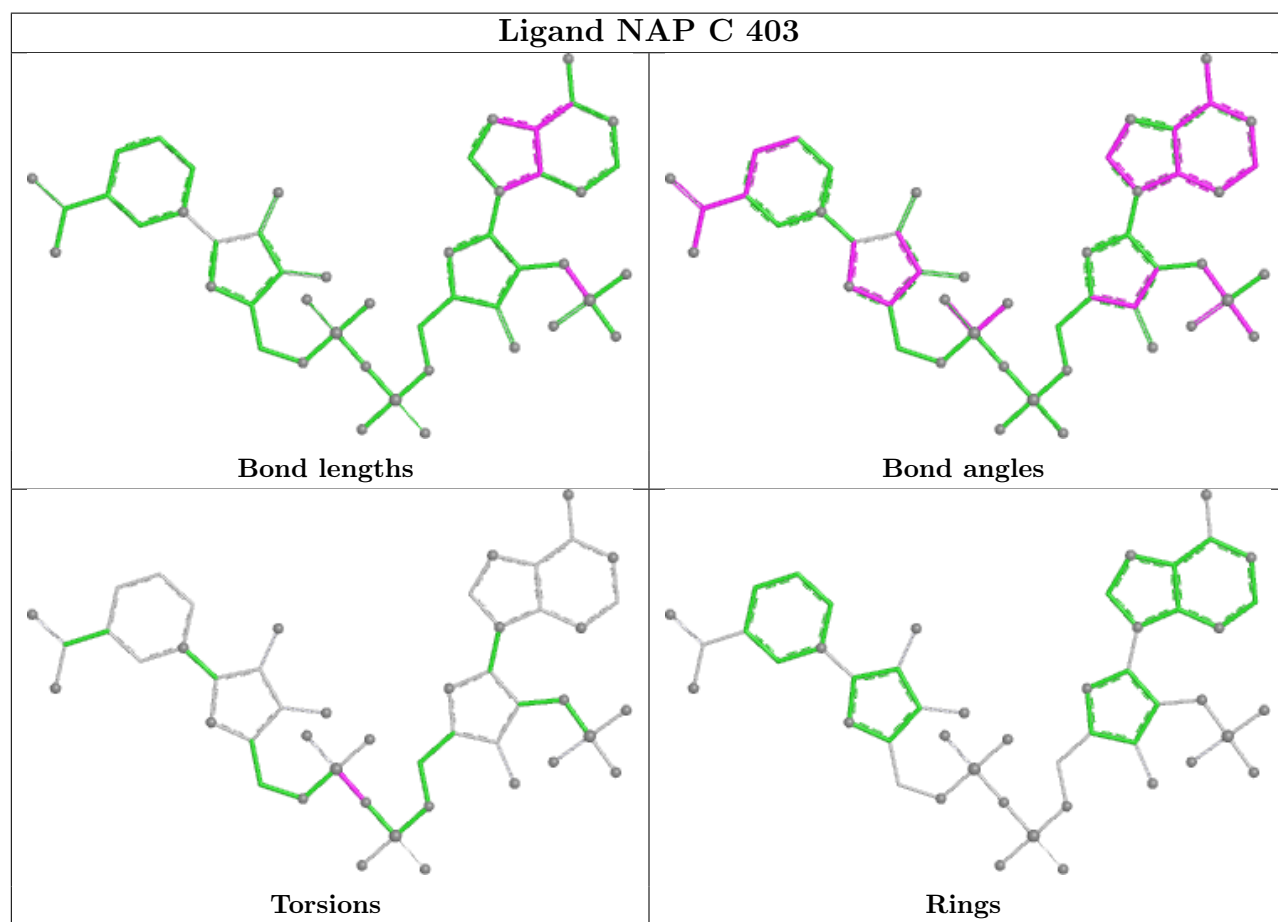
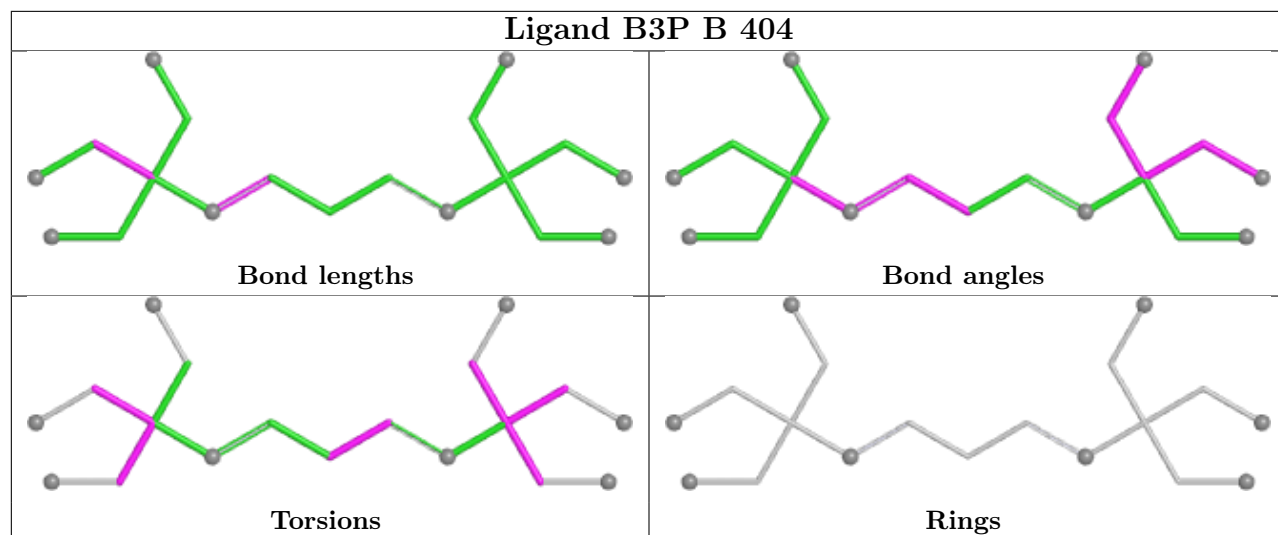
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	B3P	1	0
3	B	403	NAP	1	0
2	A	1001	FAD	3	0
4	D	404	B3P	1	0

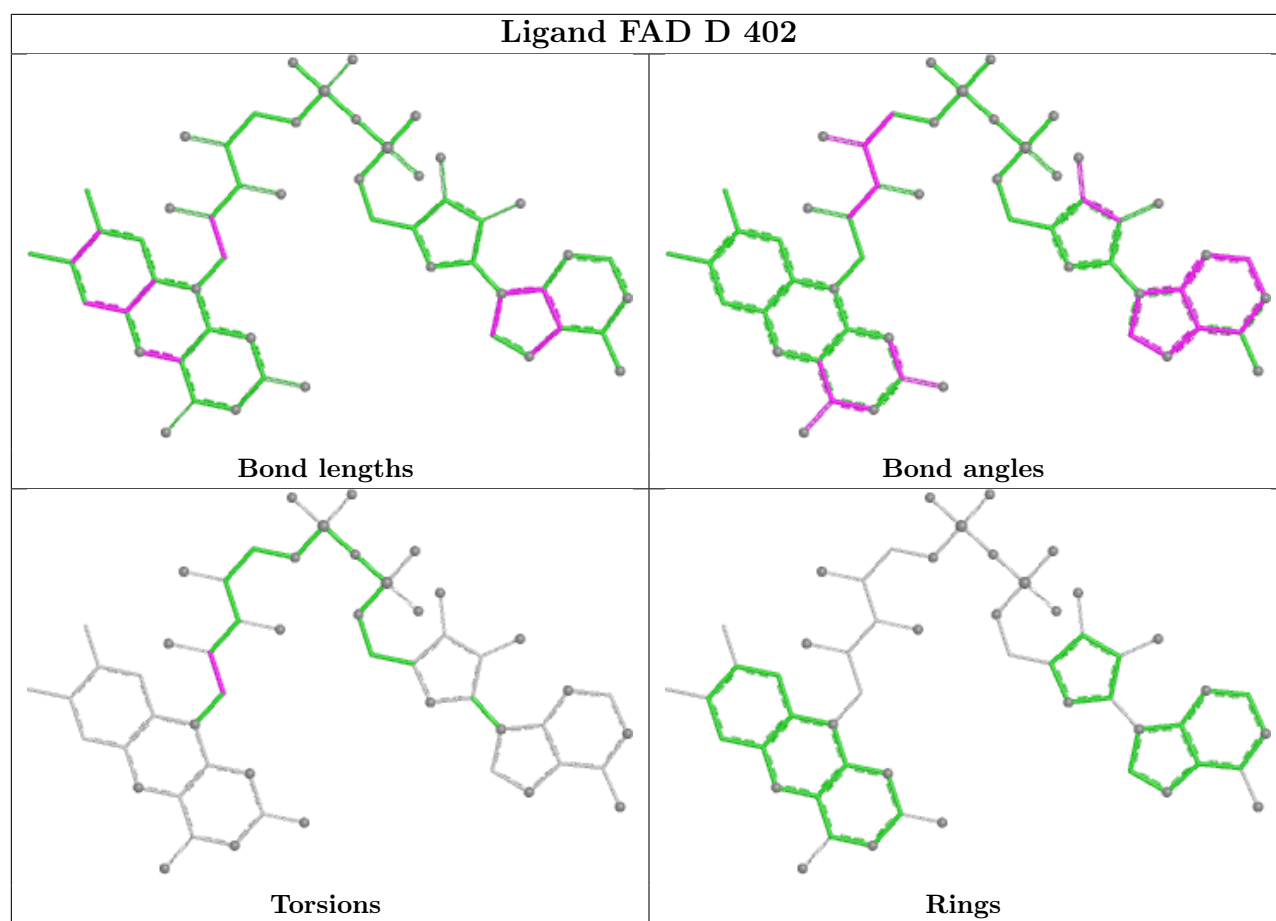
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

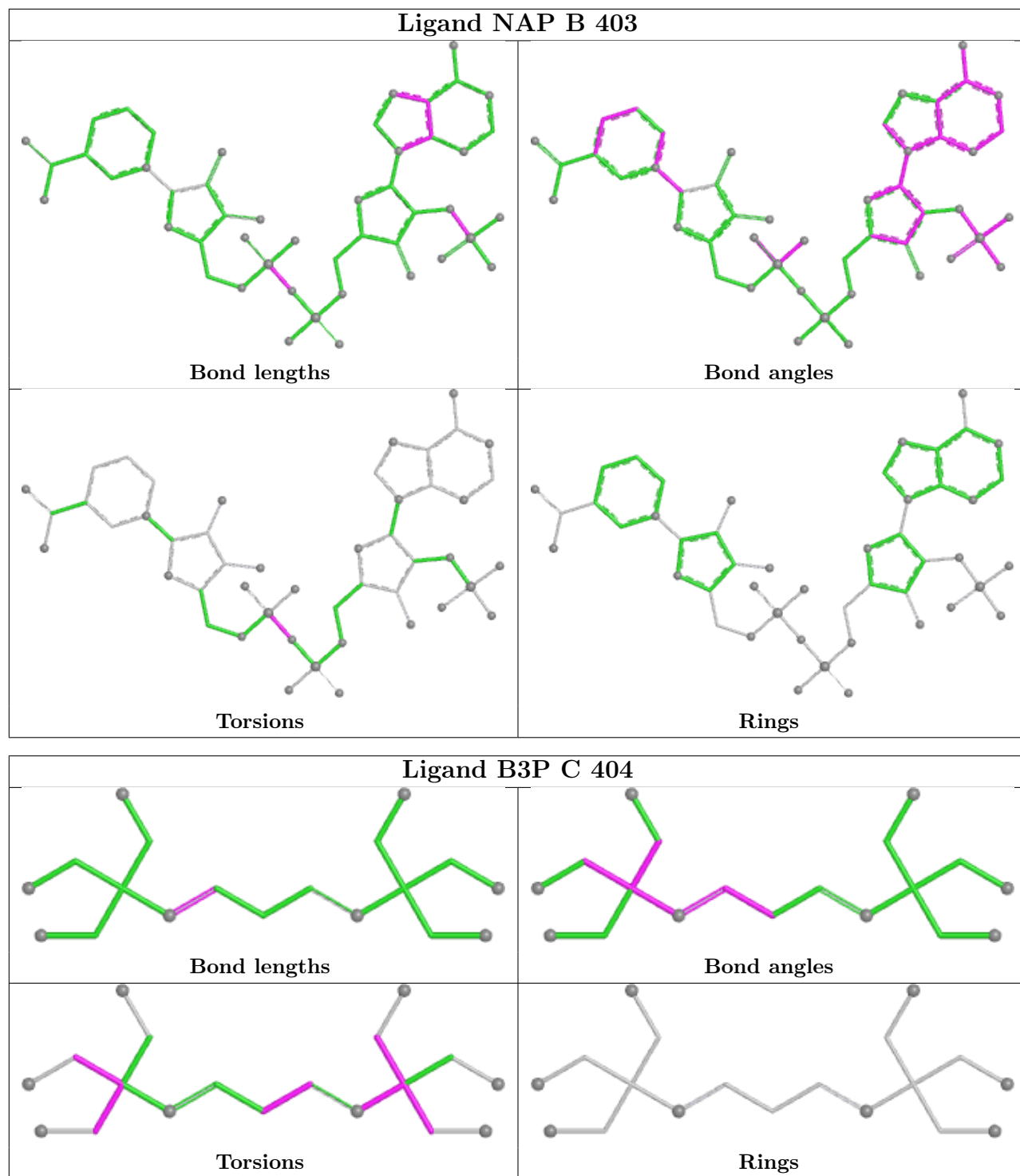
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

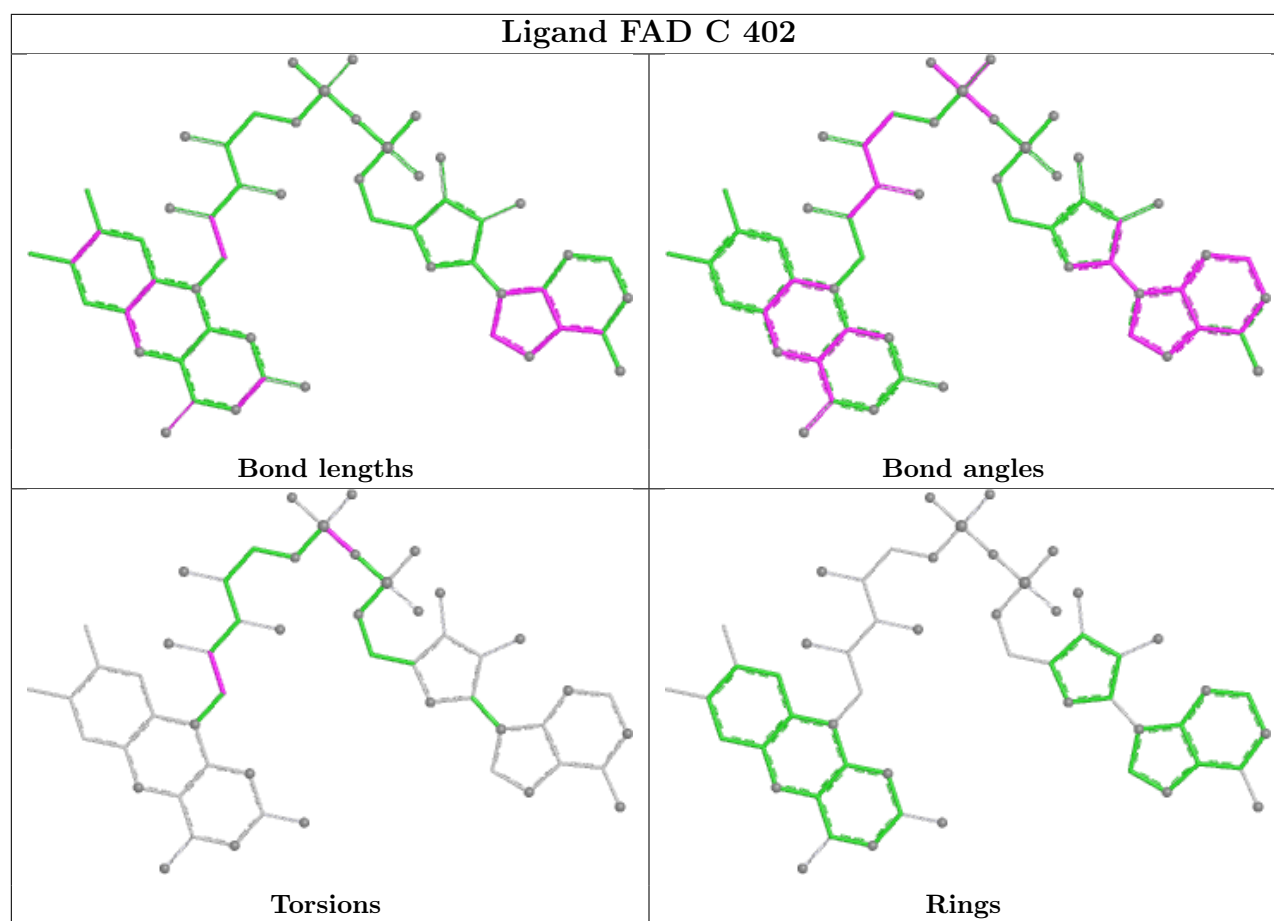


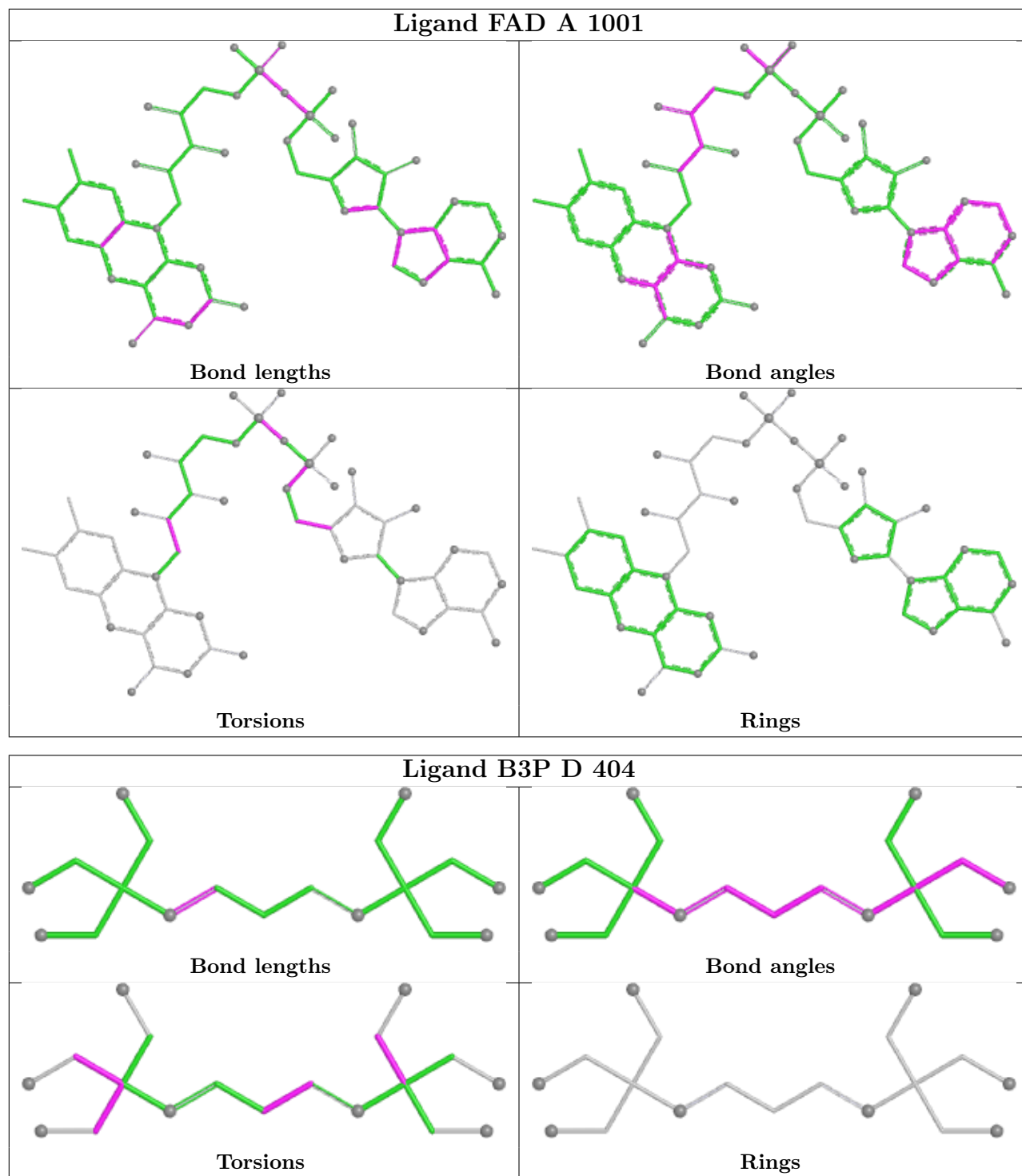


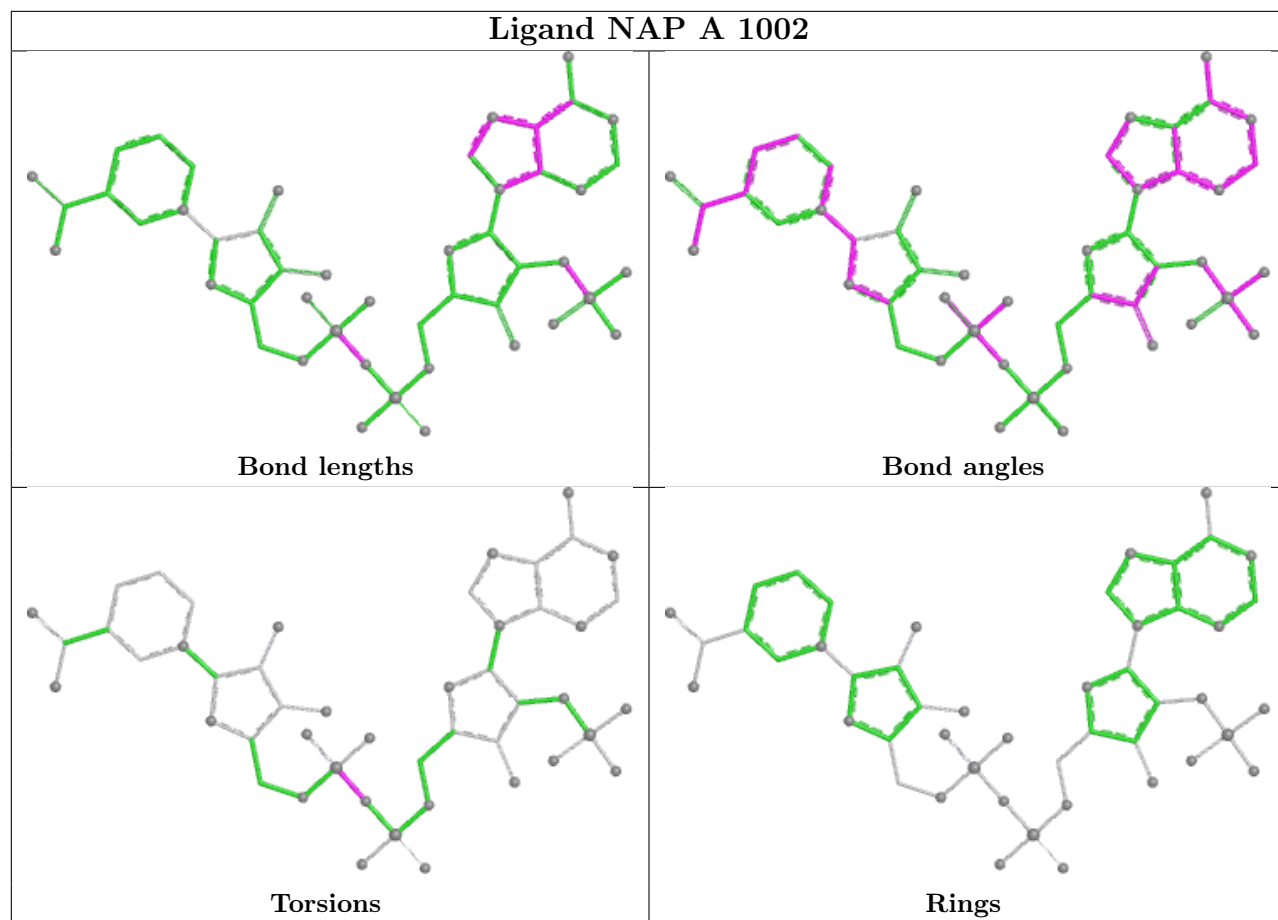












5.7 Other polymers [i](#)

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 ⓘ

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, 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	338/340 (99%)	0.14	8 (2%) 59 61	13, 28, 53, 71	0
1	B	338/340 (99%)	0.34	23 (6%) 23 21	16, 31, 61, 87	0
1	C	338/340 (99%)	0.36	24 (7%) 22 20	14, 31, 65, 97	0
1	D	338/340 (99%)	0.22	16 (4%) 36 35	14, 29, 57, 84	0
All	All	1352/1360 (99%)	0.27	71 (5%) 32 30	13, 30, 58, 97	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	TYR	5.6
1	C	267	ALA	5.0
1	C	248	ALA	4.3
1	B	339	TYR	4.2
1	C	269	GLY	4.1
1	C	247	ASP	3.8
1	B	248	ALA	3.7
1	B	149	GLN	3.7
1	B	338	LEU	3.3
1	D	338	LEU	3.3
1	C	249	THR	3.3
1	D	339	TYR	3.2
1	B	269	GLY	3.2
1	B	249	THR	3.1
1	B	268	ASP	3.1
1	D	159	GLN	3.1
1	D	251	ALA	3.1
1	B	173	GLU	3.0
1	C	322	GLU	3.0
1	A	339	TYR	3.0
1	C	268	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	251	ALA	2.9
1	C	325	ARG	2.9
1	B	150	ASP	2.9
1	D	248	ALA	2.9
1	B	247	ASP	2.8
1	A	267	ALA	2.8
1	B	84	ASP	2.8
1	D	267	ALA	2.7
1	A	268	ASP	2.6
1	B	191	ARG	2.6
1	D	325	ARG	2.6
1	A	338	LEU	2.6
1	D	253	ARG	2.5
1	D	260	ASP	2.5
1	A	325	ARG	2.4
1	B	322	GLU	2.4
1	C	253	ARG	2.4
1	D	331	GLU	2.4
1	C	252	GLU	2.4
1	D	252	GLU	2.4
1	B	325	ARG	2.4
1	B	254	LEU	2.4
1	C	251	ALA	2.3
1	B	176	ARG	2.3
1	C	266	GLN	2.3
1	C	191	ARG	2.3
1	D	150	ASP	2.3
1	D	265	PRO	2.3
1	C	159	GLN	2.3
1	C	338	LEU	2.3
1	A	269	GLY	2.3
1	D	173	GLU	2.3
1	A	331	GLU	2.2
1	B	232	ALA	2.2
1	B	267	ALA	2.2
1	B	258	PHE	2.2
1	B	255	ARG	2.1
1	B	175	ASP	2.1
1	C	246	VAL	2.1
1	C	232	ALA	2.1
1	B	253	ARG	2.1
1	C	257	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	322	GLU	2.1
1	C	174	PRO	2.1
1	C	30	ARG	2.1
1	D	232	ALA	2.1
1	C	333	GLU	2.0
1	C	260	ASP	2.0
1	D	190	GLU	2.0
1	C	271	LEU	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 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($\text{\AA}^2$)	Q<0.9
4	B3P	C	404	19/19	0.89	0.10	27,34,43,49	0
4	B3P	D	404	19/19	0.89	0.11	23,33,43,49	0
4	B3P	B	404	19/19	0.90	0.10	25,31,48,50	0
4	B3P	A	1003	19/19	0.92	0.09	23,24,40,47	0
3	NAP	B	403	48/48	0.95	0.07	14,25,34,37	0
3	NAP	C	403	48/48	0.96	0.06	17,26,37,45	0
3	NAP	D	403	48/48	0.96	0.06	15,24,31,35	0
3	NAP	A	1002	48/48	0.97	0.05	13,23,29,31	0
2	FAD	C	402	53/53	0.97	0.06	12,16,20,21	0
2	FAD	D	402	53/53	0.98	0.05	11,14,16,18	0
2	FAD	B	402	53/53	0.98	0.05	12,15,16,18	0
2	FAD	A	1001	53/53	0.98	0.05	9,11,15,16	0
5	K	C	401	1/1	0.98	0.05	19,19,19,19	0
5	K	B	401	1/1	0.99	0.07	16,16,16,16	0
5	K	A	1004	1/1	0.99	0.05	20,20,20,20	0

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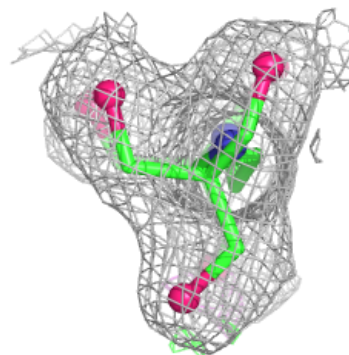
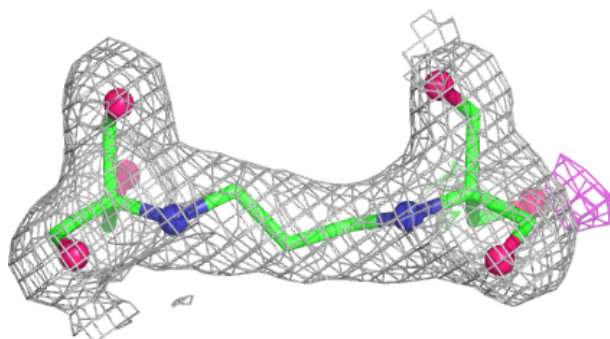
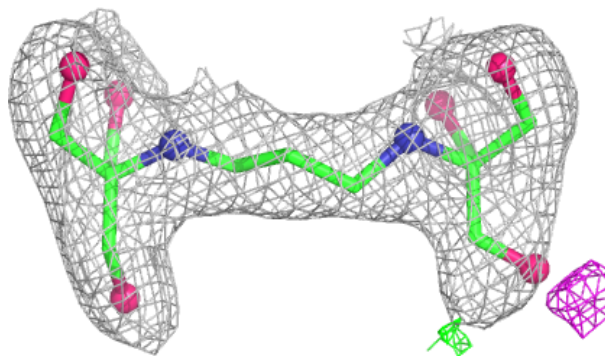
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	D	401	1/1	0.99	0.04	19,19,19,19	0

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.

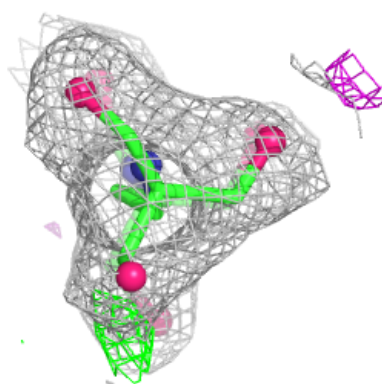
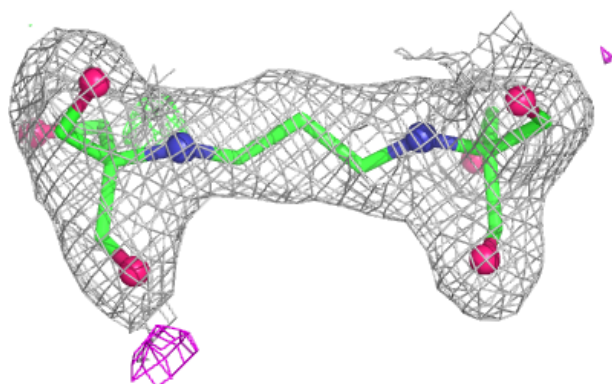
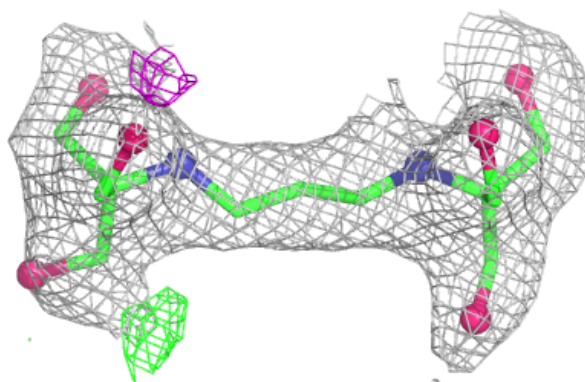
Electron density around B3P C 404:

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

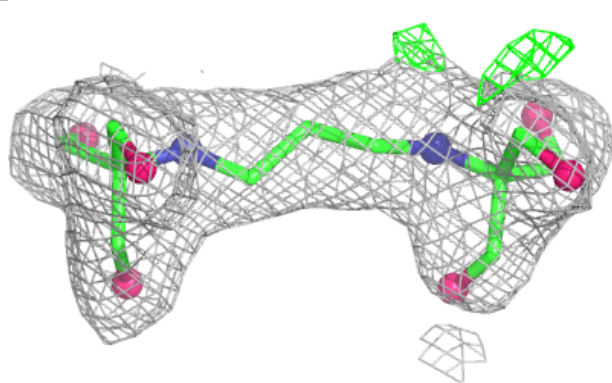
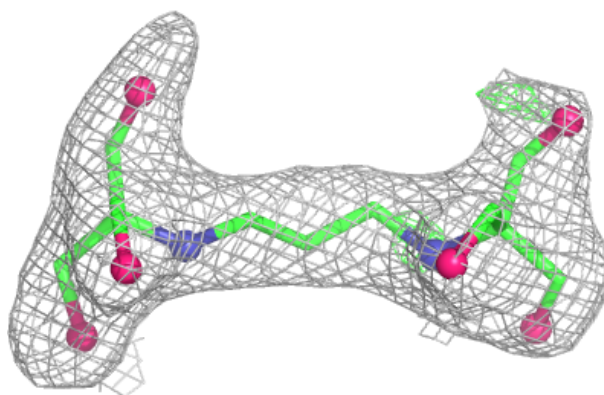


Electron density around B3P D 404:

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

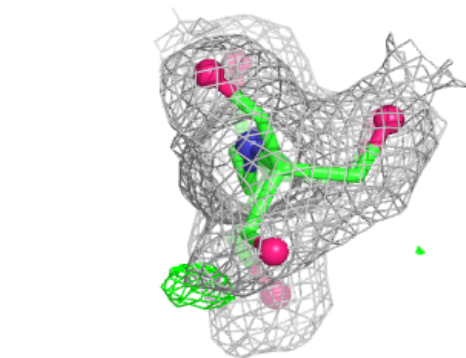
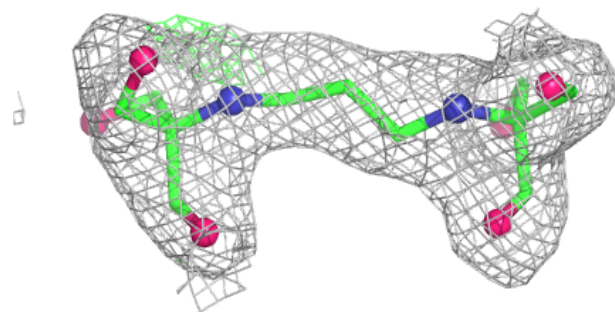
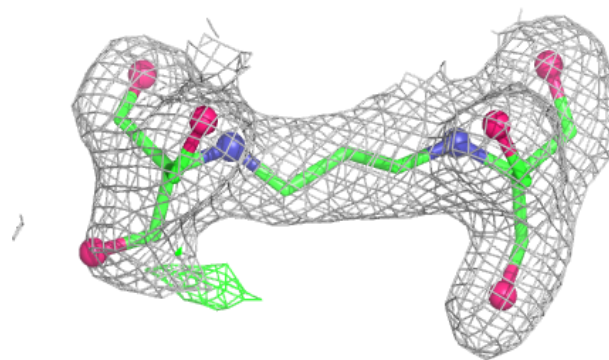
**Electron density around B3P B 404:**

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

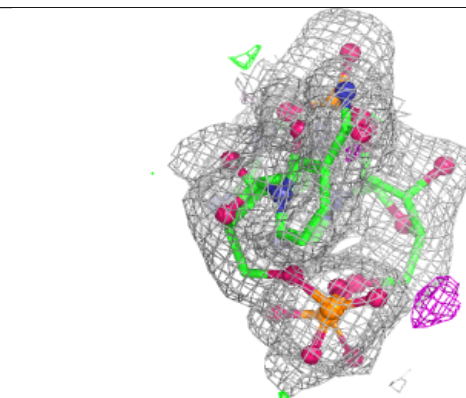
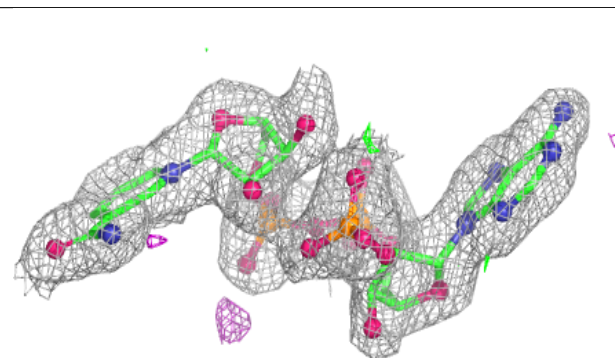
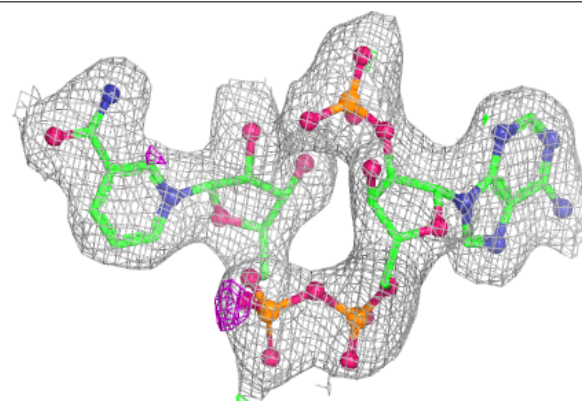


Electron density around B3P A 1003:

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and green (positive)

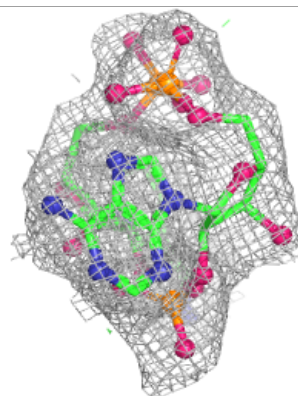
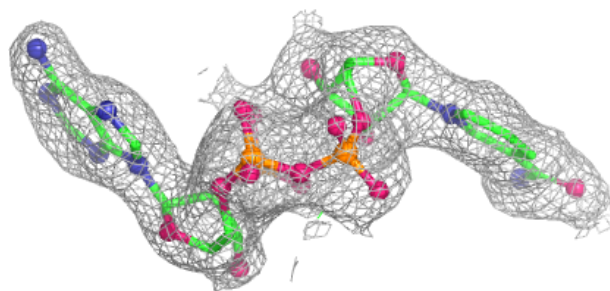
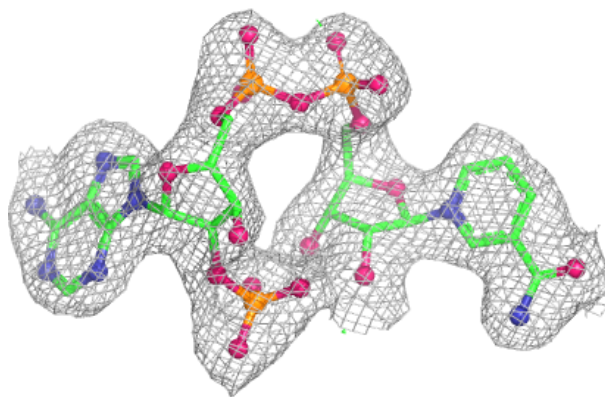
**Electron density around NAP B 403:**

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

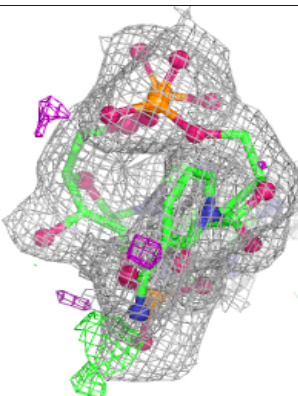
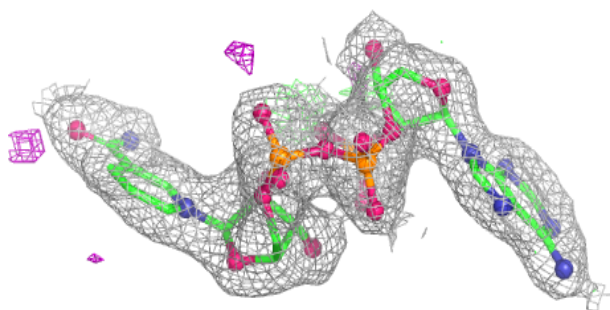
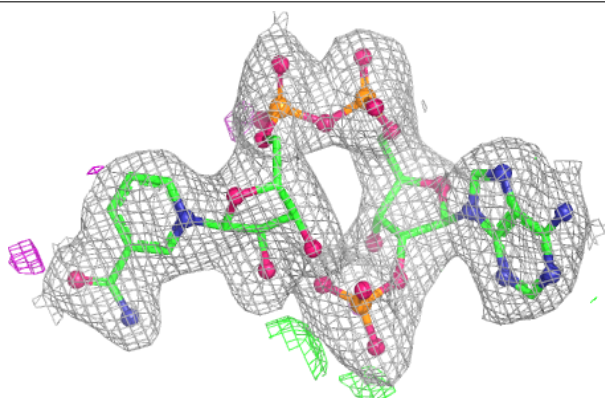


Electron density around NAP C 403:

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

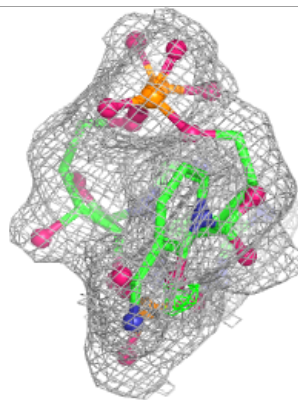
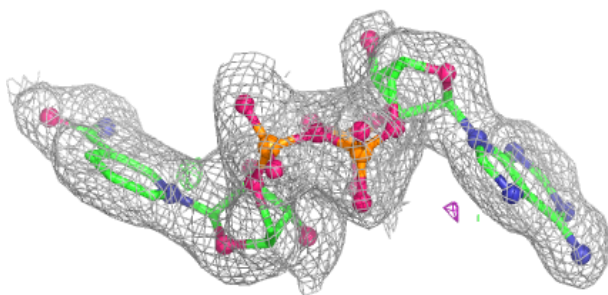
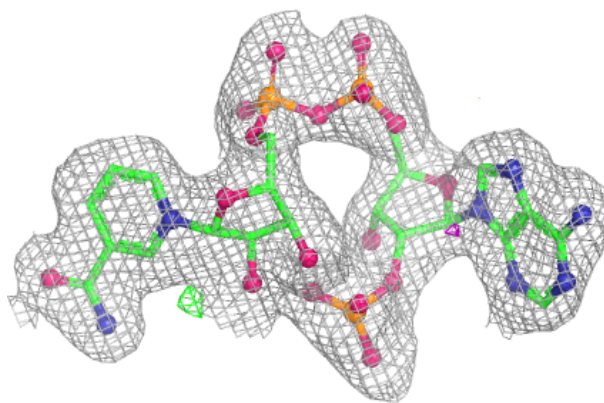
**Electron density around NAP D 403:**

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

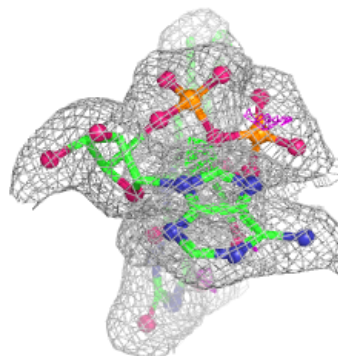
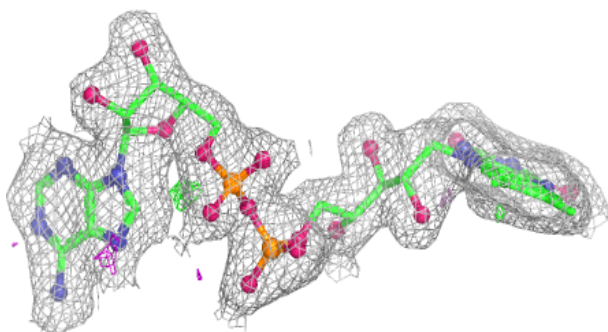
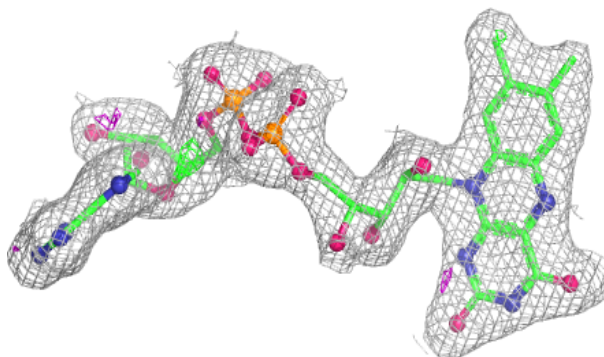


Electron density around NAP A 1002:

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

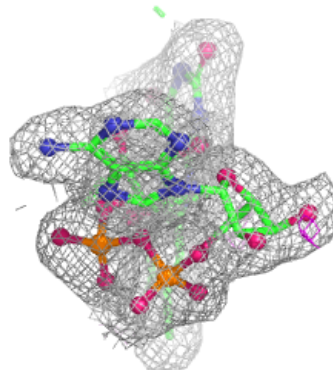
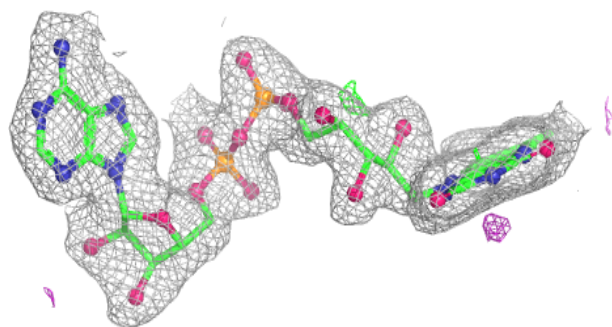
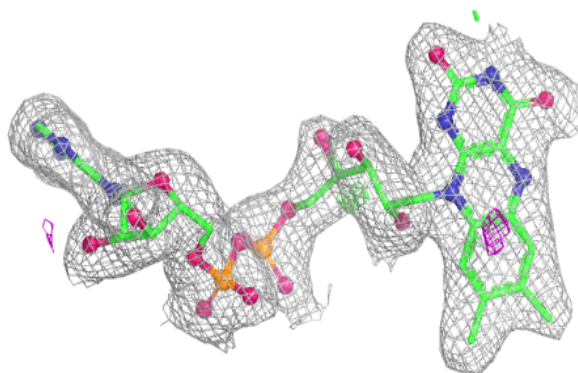
**Electron density around FAD C 402:**

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

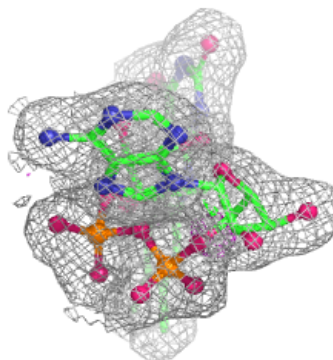
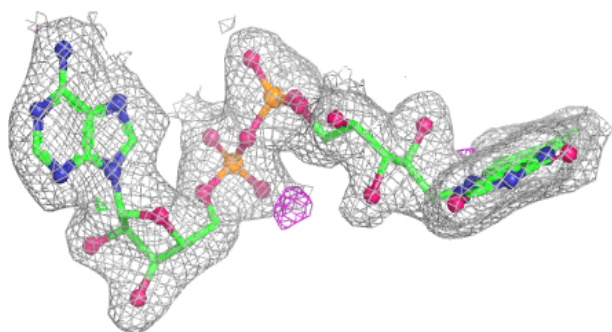
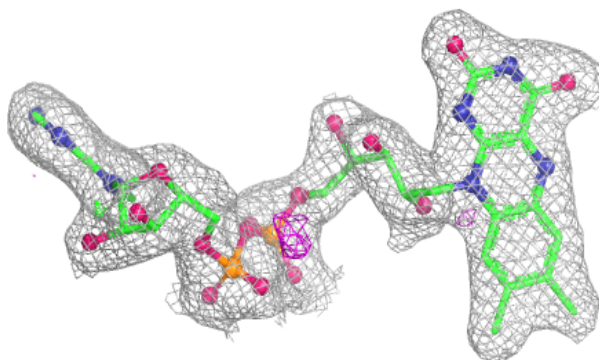


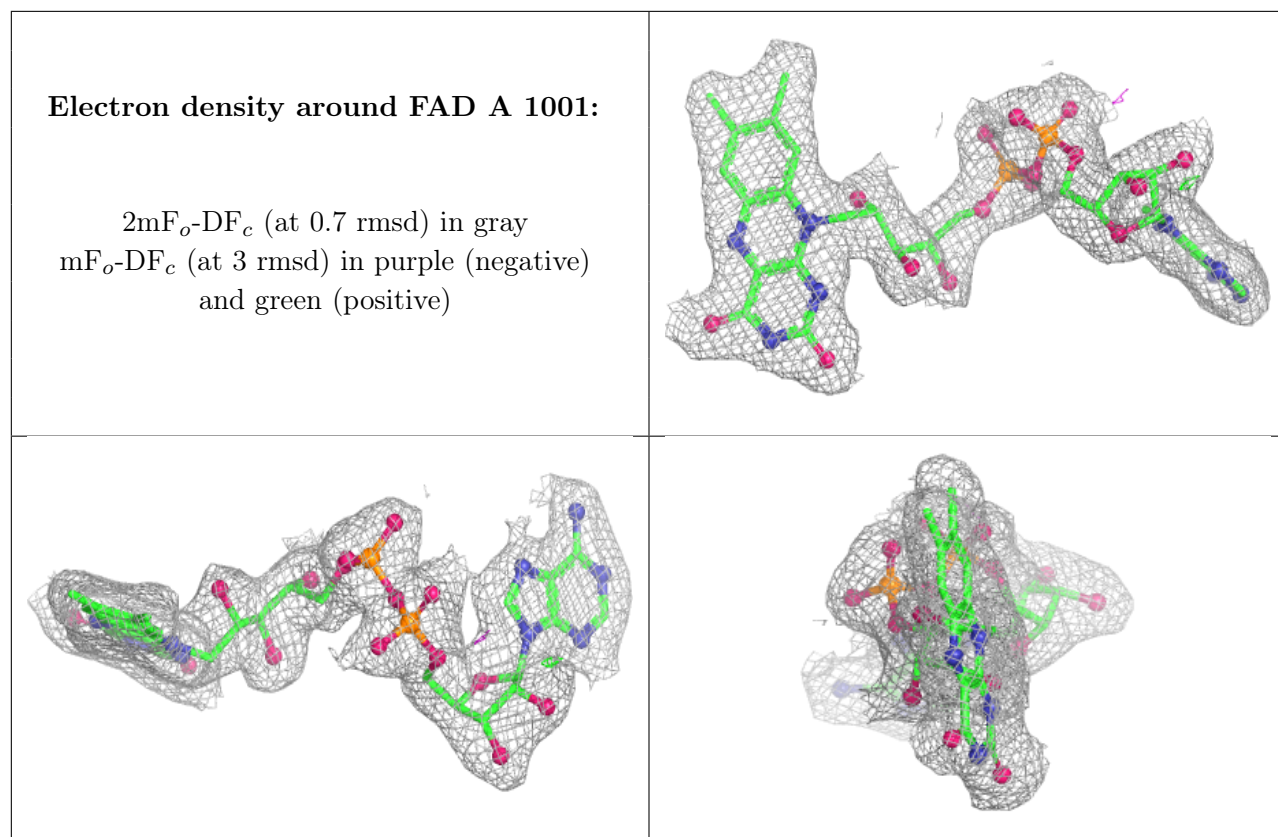
Electron density around FAD D 402:

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

**Electron density around FAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.