Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 02:17 AM EDT

PDB ID : 4JAY
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)

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

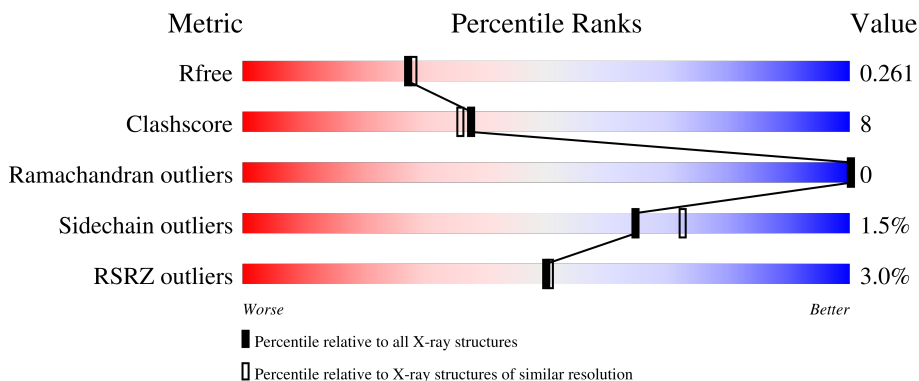|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
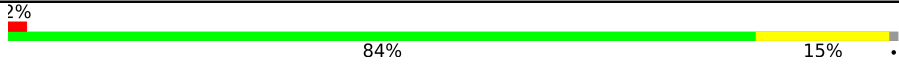*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.261
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		3.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 <=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	4% — 85% — 14% •
1	C	340	3% — 85% — 14% •
1	D	340	3% — 85% — 14% •

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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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 (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
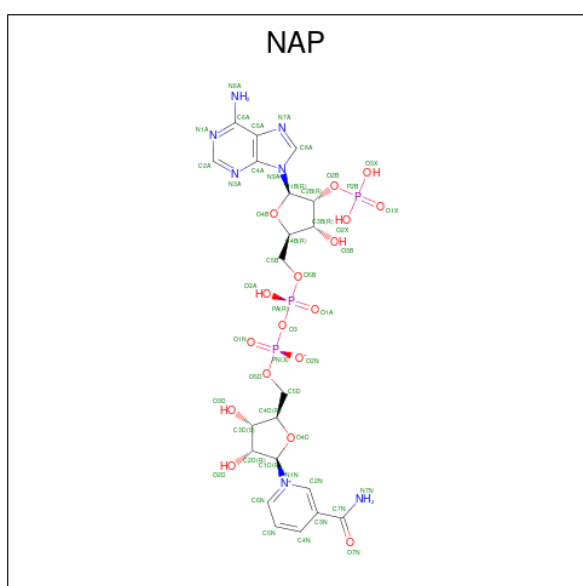
NAP

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

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).
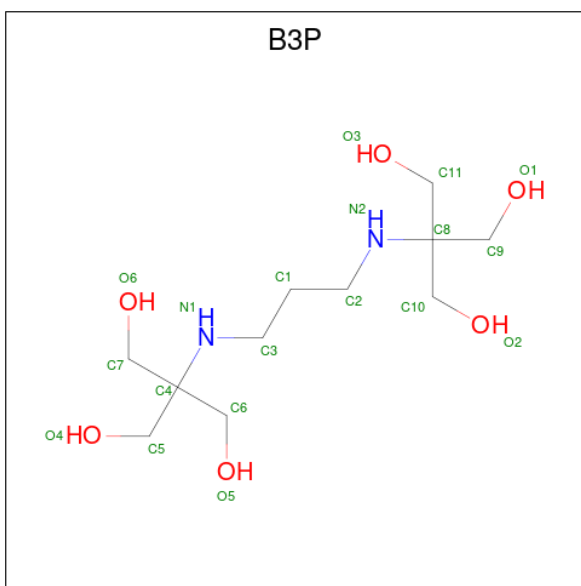
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	11	2	6		
4	B	1	Total	C	N	O	0	0
			19	11	2	6		
4	C	1	Total	C	N	O	0	0
			19	11	2	6		
4	D	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

Continued on next page...

Continued from previous page...

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.
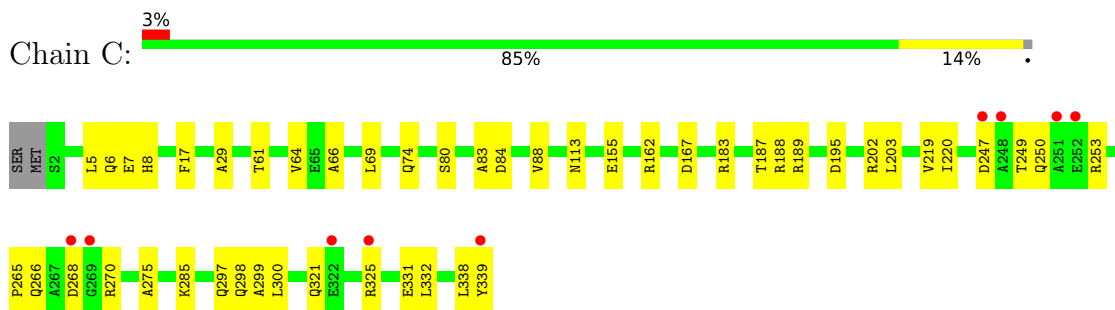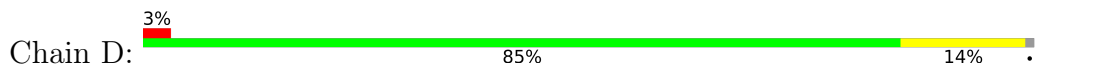
- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase
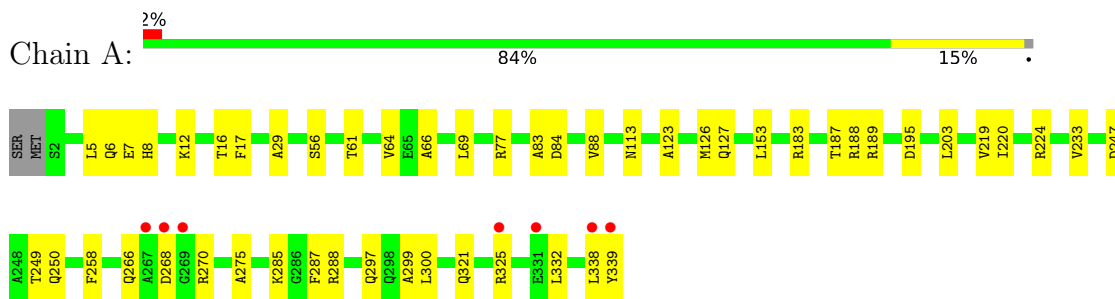
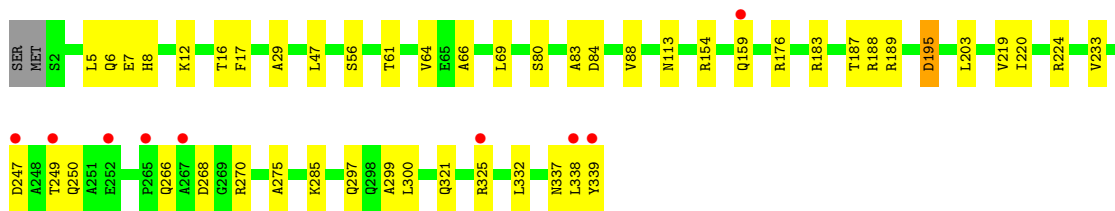- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase
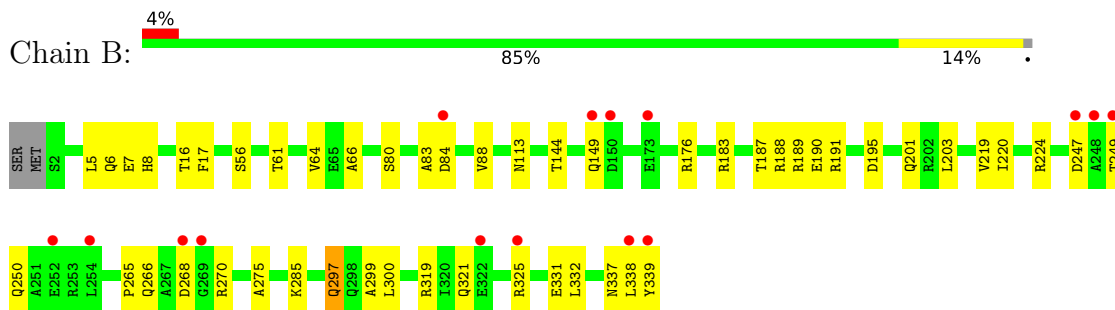
- Molecule 1: UDP-N-acetylenolpyruvoylglucosamine reductase

- 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 54.27 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.1 (54.33-2.23) 98.1 (54.27-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.258 0.227 , 0.261	Depositor DCC
R_{free} test set	3529 reflections (5.06%)	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 , 36.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, B3P, NAP, FAD

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	0.71	0/2692	0.82	1/3643 (0.0%)
1	B	0.70	0/2692	0.82	1/3643 (0.0%)
1	C	0.70	0/2692	0.83	2/3643 (0.1%)
1	D	0.72	0/2692	0.83	1/3643 (0.0%)
All	All	0.71	0/10768	0.83	5/14572 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	224	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	162	ARG	CG-CD-NE	5.53	123.42	111.80
1	A	224	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	167	ASP	CB-CG-OD1	5.02	122.82	118.30

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	2645	0	2657	43	0
1	B	2645	0	2657	45	4

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2645	0	2657	38	0
1	D	2645	0	2657	45	0
2	A	53	0	31	2	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	9	1
6	B	84	0	0	13	0
6	C	76	0	0	6	0
6	D	82	0	0	10	0
All	All	11404	0	10956	170	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 (170) 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
1:D:321:GLN:O	1:D:325:ARG:HD2	1.71	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:331:GLU:C	6:B:543:HOH:O	2.31	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: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:266:GLN:HB2	1:B:268:ASP:OD1	2.01	0.59
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:D:187:THR:HG23	6:D:564:HOH:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:338:LEU:HD13	1:A:338:LEU:C	2.25	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: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:B:339:TYR:CD2	1:B:339:TYR:C	2.80	0.55
1:D:176:ARG:HA	6:D:580:HOH:O	2.06	0.55
1:B:338:LEU:C	1:B:338:LEU:HD13	2.27	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:D:338:LEU:C	1:D:338:LEU:HD13	2.29	0.53
1:B:144:THR:HG23	6:B:527:HOH:O	2.07	0.53
1:C:338:LEU:C	1:C:338:LEU:HD13	2.28	0.53
1:A:288:ARG:CZ	1:B:190:GLU:HG2	2.39	0.52
1:D:339:TYR:C	1:D:339:TYR:CD2	2.84	0.51
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:339:TYR:CD2	1:A:339:TYR:C	2.85	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:339:TYR:C	1:C:339:TYR:CD2	2.88	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:83:ALA:O	1:C:84:ASP:HB2	2.19	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: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 ⓘ

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	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 ⓘ

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%)	267 (99%)	3 (1%)	73	80
1	B	270/272 (99%)	266 (98%)	4 (2%)	65	72
1	C	270/272 (99%)	265 (98%)	5 (2%)	57	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	270/272 (99%)	266 (98%)	4 (2%)	65	72
All	All	1080/1088 (99%)	1064 (98%)	16 (2%)	65	72

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

Mol	Chain	Res	Type
1	A	17	PHE
1	A	195	ASP
1	A	297	GLN
1	B	17	PHE
1	B	80	SER
1	B	195	ASP
1	B	297	GLN
1	C	17	PHE
1	C	74	GLN
1	C	80	SER
1	C	195	ASP
1	C	297	GLN
1	D	17	PHE
1	D	80	SER
1	D	195	ASP
1	D	297	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	266	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	C	298	GLN
1	D	8	HIS
1	D	74	GLN
1	D	101	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 monosaccharides 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	$\#|Z| > 2$
2	FAD	D	402	-	53,58,58	1.52	9 (16%)	68,89,89	1.63	14 (20%)
3	NAP	A	1002	5	45,52,52	0.98	2 (4%)	56,80,80	1.58	12 (21%)
4	B3P	B	404	-	18,18,18	1.05	2 (11%)	21,23,23	1.43	3 (14%)
4	B3P	C	404	-	18,18,18	0.98	1 (5%)	21,23,23	1.44	2 (9%)
2	FAD	A	1001	-	53,58,58	1.62	8 (15%)	68,89,89	1.50	12 (17%)
2	FAD	C	402	-	53,58,58	1.38	9 (16%)	68,89,89	1.73	14 (20%)
3	NAP	C	403	5	45,52,52	0.92	1 (2%)	56,80,80	1.56	11 (19%)
3	NAP	B	403	5	45,52,52	1.02	4 (8%)	56,80,80	1.67	13 (23%)
3	NAP	D	403	5	45,52,52	0.98	3 (6%)	56,80,80	1.45	11 (19%)
4	B3P	A	1003	-	18,18,18	0.66	0	21,23,23	1.59	3 (14%)
2	FAD	B	402	-	53,58,58	1.53	9 (16%)	68,89,89	1.30	9 (13%)
4	B3P	D	404	-	18,18,18	0.88	1 (5%)	21,23,23	1.34	4 (19%)

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	FAD	D	402	-	-	2/30/50/50	0/6/6/6
3	NAP	A	1002	5	-	2/31/67/67	0/5/5/5
4	B3P	B	404	-	-	10/28/28/28	-
4	B3P	C	404	-	-	15/28/28/28	-
2	FAD	A	1001	-	-	7/30/50/50	0/6/6/6
2	FAD	C	402	-	-	3/30/50/50	0/6/6/6
3	NAP	C	403	5	-	2/31/67/67	0/5/5/5
3	NAP	B	403	5	-	2/31/67/67	0/5/5/5
3	NAP	D	403	5	-	4/31/67/67	0/5/5/5
4	B3P	A	1003	-	-	12/28/28/28	-
2	FAD	B	402	-	-	3/30/50/50	0/6/6/6
4	B3P	D	404	-	-	10/28/28/28	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	O4B-C1B	4.75	1.47	1.41
2	B	402	FAD	C9A-C5X	4.37	1.48	1.41
2	C	402	FAD	C9A-C5X	4.03	1.47	1.41
2	D	402	FAD	C9A-C5X	3.97	1.47	1.41
2	A	1001	FAD	O4-C4	3.84	1.30	1.23
2	A	1001	FAD	C9A-C5X	3.73	1.47	1.41
2	A	1001	FAD	C2B-C1B	-3.70	1.48	1.53
2	B	402	FAD	C2B-C1B	-3.63	1.48	1.53
2	D	402	FAD	C2B-C1B	-3.48	1.48	1.53
2	B	402	FAD	C4-N3	-3.45	1.32	1.38
2	D	402	FAD	O4B-C1B	3.18	1.45	1.41
2	B	402	FAD	O4B-C1B	3.09	1.45	1.41
2	A	1001	FAD	C2-N3	-2.98	1.32	1.39
2	B	402	FAD	C4X-N5	2.98	1.36	1.30
2	D	402	FAD	C6-C5X	-2.95	1.35	1.40
4	C	404	B3P	C3-N1	-2.91	1.43	1.46
2	D	402	FAD	C8-C7	2.77	1.47	1.40
3	C	403	NAP	P2B-O2B	2.75	1.64	1.59
2	B	402	FAD	C8-C7	2.67	1.47	1.40
2	D	402	FAD	C5A-N7A	-2.63	1.30	1.39
2	D	402	FAD	C4X-N5	2.62	1.35	1.30
3	A	1002	NAP	P2B-O2B	2.61	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	B3P	C3-N1	-2.58	1.43	1.46
2	A	1001	FAD	C4-N3	-2.56	1.34	1.38
3	D	403	NAP	P2B-O2B	2.54	1.64	1.59
2	C	402	FAD	C2-N3	-2.51	1.33	1.39
3	A	1002	NAP	C2D-C1D	-2.51	1.50	1.53
3	B	403	NAP	P2B-O2B	2.48	1.64	1.59
2	C	402	FAD	O4-C4	2.45	1.28	1.23
2	C	402	FAD	C5X-N5	-2.43	1.34	1.39
2	C	402	FAD	C8-C7	2.41	1.46	1.40
2	C	402	FAD	O4B-C1B	2.40	1.44	1.41
3	B	403	NAP	O4B-C1B	2.34	1.44	1.41
4	D	404	B3P	C3-N1	-2.32	1.44	1.46
3	D	403	NAP	O4D-C1D	2.32	1.44	1.41
2	B	402	FAD	C2-N3	-2.31	1.33	1.39
2	C	402	FAD	C5A-N7A	-2.21	1.31	1.39
2	C	402	FAD	C5A-C4A	2.20	1.46	1.40
2	D	402	FAD	C1'-C2'	-2.19	1.49	1.52
2	D	402	FAD	C5A-C4A	2.16	1.46	1.40
2	B	402	FAD	C5X-N5	-2.15	1.35	1.39
3	B	403	NAP	C2A-N3A	2.15	1.35	1.32
2	B	402	FAD	C2'-C3'	-2.11	1.49	1.53
4	B	404	B3P	C6-C4	-2.11	1.51	1.53
2	C	402	FAD	C1'-C2'	-2.11	1.49	1.52
3	B	403	NAP	C5A-C4A	2.10	1.46	1.40
3	D	403	NAP	O7N-C7N	-2.09	1.20	1.24
2	A	1001	FAD	P-O2P	-2.03	1.45	1.55
2	A	1001	FAD	O2B-C2B	-2.01	1.38	1.43

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FAD	N3A-C2A-N1A	-4.87	121.06	128.68
3	A	1002	NAP	N3A-C2A-N1A	-4.76	121.24	128.68
4	A	1003	B3P	C3-N1-C4	4.57	122.56	116.08
4	B	404	B3P	C3-N1-C4	4.46	122.41	116.08
2	C	402	FAD	C2A-N1A-C6A	4.31	126.12	118.75
3	B	403	NAP	N6A-C6A-N1A	4.23	127.36	118.57
3	D	403	NAP	N3A-C2A-N1A	-4.20	122.11	128.68
2	D	402	FAD	C4A-C5A-N7A	-4.09	105.13	109.40
4	C	404	B3P	C3-N1-C4	4.02	121.78	116.08
2	D	402	FAD	O4-C4-C4X	-3.94	116.15	126.60
2	B	402	FAD	N3A-C2A-N1A	-3.91	122.57	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FAD	C1B-N9A-C4A	-3.91	119.78	126.64
3	C	403	NAP	C2B-C3B-C4B	3.87	110.40	101.99
3	B	403	NAP	N3A-C2A-N1A	-3.69	122.92	128.68
3	C	403	NAP	N3A-C2A-N1A	-3.68	122.93	128.68
3	C	403	NAP	C3N-C7N-N7N	3.58	122.05	117.75
2	D	402	FAD	P-O3P-PA	-3.56	120.61	132.83
2	C	402	FAD	C4'-C3'-C2'	-3.53	106.01	113.36
4	A	1003	B3P	C2-N2-C8	3.49	121.03	116.08
3	B	403	NAP	C2B-C3B-C4B	3.36	109.30	101.99
2	A	1001	FAD	O4'-C4'-C5'	-3.34	102.40	109.92
2	D	402	FAD	O4-C4-N3	3.32	126.48	120.12
3	A	1002	NAP	O2N-PN-O1N	3.29	128.51	112.24
3	D	403	NAP	O2X-P2B-O1X	3.28	123.54	110.68
2	C	402	FAD	P-O3P-PA	-3.16	121.99	132.83
3	B	403	NAP	C2A-N1A-C6A	3.12	124.09	118.75
3	A	1002	NAP	PN-O3-PA	-3.10	122.19	132.83
3	D	403	NAP	O2N-PN-O1N	3.10	127.56	112.24
2	A	1001	FAD	C4X-C10-N10	3.09	121.00	116.48
2	D	402	FAD	C2A-N1A-C6A	3.09	124.03	118.75
3	C	403	NAP	PN-O3-PA	-3.07	122.29	132.83
2	A	1001	FAD	P-O3P-PA	-3.02	122.46	132.83
2	D	402	FAD	O4'-C4'-C5'	-2.99	103.19	109.92
4	D	404	B3P	C3-N1-C4	2.97	120.29	116.08
2	B	402	FAD	C9A-C5X-N5	-2.92	119.26	122.43
2	C	402	FAD	C4A-C5A-N7A	-2.91	106.37	109.40
4	C	404	B3P	C6-C4-C5	2.90	116.18	110.04
4	A	1003	B3P	O2-C10-C8	-2.90	105.76	111.63
3	A	1002	NAP	C2B-C3B-C4B	2.88	108.25	101.99
2	C	402	FAD	C5'-C4'-C3'	2.87	117.74	112.20
3	B	403	NAP	PN-O3-PA	-2.83	123.13	132.83
3	D	403	NAP	N6A-C6A-N1A	2.76	124.30	118.57
3	A	1002	NAP	O2X-P2B-O1X	2.75	121.46	110.68
3	B	403	NAP	C5N-C4N-C3N	-2.74	117.10	120.34
2	C	402	FAD	O3'-C3'-C4'	2.72	115.37	108.81
4	D	404	B3P	O2-C10-C8	-2.71	106.15	111.63
3	D	403	NAP	C2B-C3B-C4B	2.71	107.87	101.99
3	A	1002	NAP	O2X-P2B-O2B	-2.68	93.99	105.99
3	A	1002	NAP	C2A-N1A-C6A	2.67	123.33	118.75
2	B	402	FAD	O4B-C1B-C2B	-2.67	103.02	106.93
2	D	402	FAD	C5A-C6A-N6A	2.66	124.39	120.35
3	B	403	NAP	C3N-C2N-N1N	2.66	123.02	120.43
2	B	402	FAD	P-O3P-PA	-2.64	123.77	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	402	FAD	C4'-C3'-C2'	-2.63	107.88	113.36
2	A	1001	FAD	N3A-C2A-N1A	-2.62	124.58	128.68
2	A	1001	FAD	C4'-C3'-C2'	-2.62	107.91	113.36
3	B	403	NAP	C5A-C6A-N6A	-2.61	116.39	120.35
2	D	402	FAD	O2-C2-N1	-2.59	117.53	121.83
3	C	403	NAP	O7N-C7N-C3N	-2.57	116.55	119.63
2	A	1001	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
3	B	403	NAP	O2B-P2B-O1X	-2.55	99.56	109.39
4	D	404	B3P	C2-N2-C8	2.55	119.69	116.08
2	D	402	FAD	N3A-C2A-N1A	-2.54	124.71	128.68
2	C	402	FAD	C9A-C5X-N5	-2.54	119.68	122.43
2	B	402	FAD	C4-C4X-N5	2.53	121.83	118.23
3	A	1002	NAP	C3N-C7N-N7N	2.52	120.78	117.75
3	A	1002	NAP	N6A-C6A-N1A	2.51	123.78	118.57
3	C	403	NAP	O3X-P2B-O2X	2.50	117.21	107.64
2	D	402	FAD	C5A-C6A-N1A	-2.49	114.70	120.35
3	C	403	NAP	N6A-C6A-N1A	2.47	123.69	118.57
2	B	402	FAD	C2A-N1A-C6A	2.47	122.97	118.75
2	B	402	FAD	C4'-C3'-C2'	-2.46	108.24	113.36
3	C	403	NAP	C3N-C2N-N1N	2.46	122.83	120.43
2	A	1001	FAD	O2P-P-O1P	2.46	124.40	112.24
2	C	402	FAD	C4X-C10-N1	-2.40	119.16	124.73
2	A	1001	FAD	C10-C4X-N5	-2.40	119.76	124.86
4	B	404	B3P	O3-C11-C8	-2.40	106.78	111.63
3	A	1002	NAP	C1B-N9A-C4A	-2.31	122.58	126.64
3	D	403	NAP	O2X-P2B-O2B	-2.31	95.65	105.99
3	D	403	NAP	O7N-C7N-N7N	-2.30	119.31	122.58
3	B	403	NAP	C1B-N9A-C4A	-2.28	122.63	126.64
2	D	402	FAD	O3B-C3B-C2B	-2.28	104.45	111.82
3	C	403	NAP	O2X-P2B-O2B	-2.28	95.79	105.99
4	B	404	B3P	O2-C10-C8	-2.24	107.09	111.63
3	D	403	NAP	C2A-N1A-C6A	2.24	122.58	118.75
3	D	403	NAP	O2A-PA-O1A	2.23	123.28	112.24
2	A	1001	FAD	C4X-C10-N1	-2.23	119.56	124.73
2	B	402	FAD	C3B-C2B-C1B	2.20	104.30	100.98
3	A	1002	NAP	C5N-C4N-C3N	-2.19	117.76	120.34
2	A	1001	FAD	C4-C4X-N5	2.18	121.33	118.23
2	C	402	FAD	O4-C4-C4X	-2.17	120.83	126.60
3	C	403	NAP	C2D-C3D-C4D	2.16	106.84	102.64
3	B	403	NAP	O2N-PN-O1N	2.16	122.90	112.24
2	B	402	FAD	C5X-N5-C4X	2.15	121.66	118.07
4	D	404	B3P	C3-C1-C2	-2.15	106.40	114.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	403	NAP	O3B-C3B-C4B	-2.12	104.92	111.05
3	D	403	NAP	C3N-C7N-N7N	2.12	120.29	117.75
2	D	402	FAD	C4X-C10-N1	-2.12	119.82	124.73
2	C	402	FAD	C5X-N5-C4X	2.10	121.57	118.07
2	C	402	FAD	O2P-P-O1P	2.09	122.59	112.24
2	A	1001	FAD	O4B-C1B-C2B	-2.09	103.88	106.93
2	D	402	FAD	C10-N1-C2	2.09	121.07	116.90
3	C	403	NAP	C5N-C4N-C3N	-2.08	117.88	120.34
3	B	403	NAP	O3X-P2B-O2X	2.07	115.54	107.64
2	A	1001	FAD	N3-C2-N1	2.05	123.40	119.38
3	B	403	NAP	O2X-P2B-O1X	2.04	118.67	110.68
3	A	1002	NAP	O3B-C3B-C4B	-2.04	105.16	111.05
2	C	402	FAD	C5A-C6A-N1A	-2.03	115.75	120.35

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	B3P	1	0
2	A	1001	FAD	2	0
3	B	403	NAP	1	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD D 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P B 404

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P C 404

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 403

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 403

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 403

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P A 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P D 404

Bond lengths

Bond angles

Torsions

Rings

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.08	7 (2%)	63	65	13, 28, 53, 71	0
1	B	338/340 (99%)	0.25	15 (4%)	34	34	16, 31, 61, 87	0
1	C	338/340 (99%)	0.16	9 (2%)	54	55	14, 31, 65, 97	0
1	D	338/340 (99%)	0.11	9 (2%)	54	55	14, 29, 57, 84	0
All	All	1352/1360 (99%)	0.15	40 (2%)	50	50	13, 30, 58, 97	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	ALA	5.4
1	C	339	TYR	5.1
1	B	149	GLN	4.4
1	B	247	ASP	4.2
1	B	248	ALA	3.7
1	C	252	GLU	3.6
1	B	339	TYR	3.5
1	C	247	ASP	3.5
1	B	269	GLY	3.3
1	A	269	GLY	3.3
1	B	338	LEU	3.2
1	B	173	GLU	3.0
1	D	252	GLU	3.0
1	B	252	GLU	3.0
1	C	268	ASP	3.0
1	D	325	ARG	3.0
1	D	339	TYR	3.0
1	B	150	ASP	3.0
1	A	339	TYR	2.9
1	D	338	LEU	2.7
1	C	269	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	267	ALA	2.7
1	B	254	LEU	2.6
1	A	325	ARG	2.6
1	D	159	GLN	2.6
1	B	325	ARG	2.5
1	A	331	GLU	2.3
1	B	268	ASP	2.3
1	B	322	GLU	2.3
1	A	338	LEU	2.3
1	C	325	ARG	2.3
1	A	268	ASP	2.2
1	D	265	PRO	2.2
1	A	267	ALA	2.1
1	C	251	ALA	2.1
1	B	84	ASP	2.1
1	D	249	THR	2.1
1	C	322	GLU	2.1
1	B	249	THR	2.1
1	D	247	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	B3P	B	404	19/19	0.93	0.14	25,31,48,50	0
4	B3P	C	404	19/19	0.93	0.14	27,34,43,49	0
4	B3P	D	404	19/19	0.93	0.13	23,33,43,49	0
4	B3P	A	1003	19/19	0.94	0.13	23,24,40,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	B	403	48/48	0.95	0.12	14,25,34,37	0
3	NAP	C	403	48/48	0.96	0.12	17,26,37,45	0
3	NAP	D	403	48/48	0.96	0.13	15,24,31,35	0
3	NAP	A	1002	48/48	0.96	0.11	13,23,29,31	0
2	FAD	C	402	53/53	0.97	0.12	12,16,20,21	0
2	FAD	A	1001	53/53	0.97	0.12	9,11,15,16	0
2	FAD	B	402	53/53	0.97	0.11	12,15,16,18	0
2	FAD	D	402	53/53	0.98	0.11	11,14,16,18	0
5	K	C	401	1/1	0.98	0.08	19,19,19,19	0
5	K	B	401	1/1	0.99	0.05	16,16,16,16	0
5	K	A	1004	1/1	0.99	0.08	20,20,20,20	0
5	K	D	401	1/1	0.99	0.09	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.
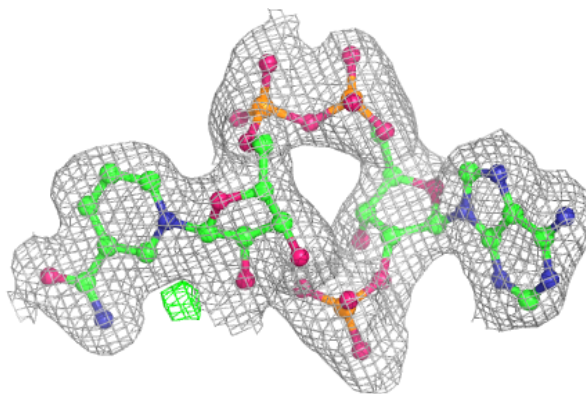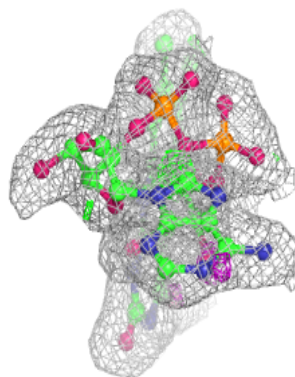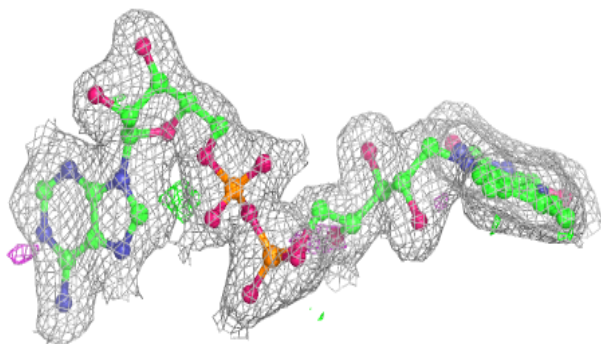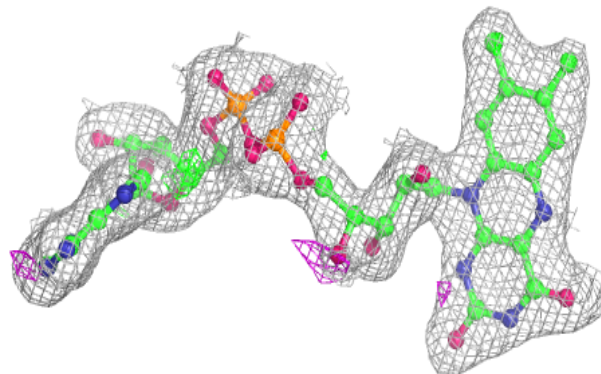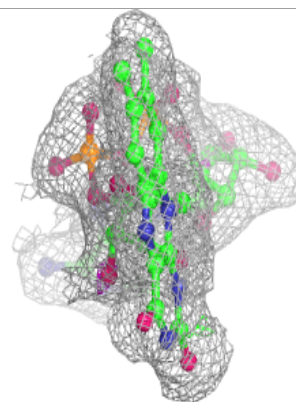

Electron density around B3P B 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
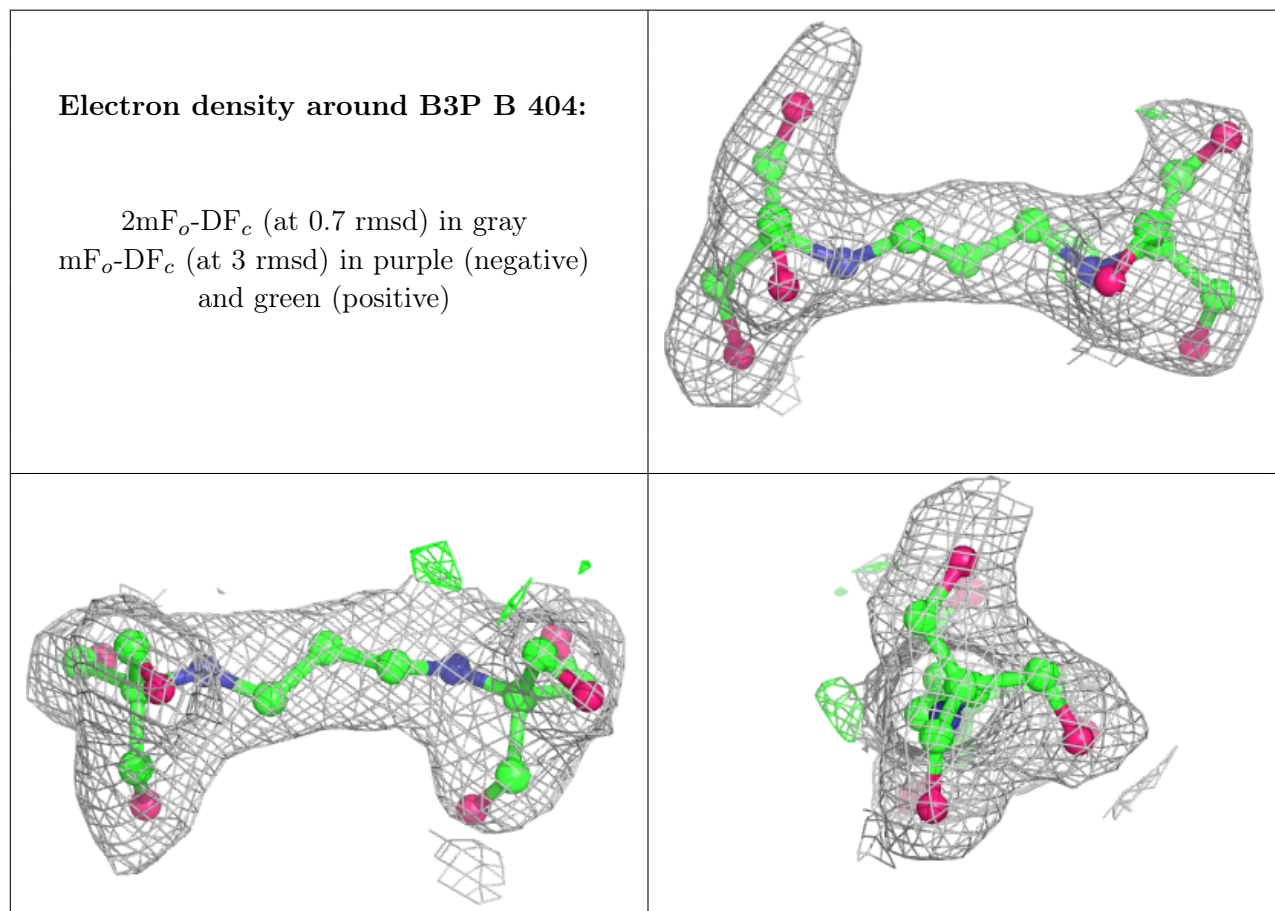
Electron density around B3P C 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
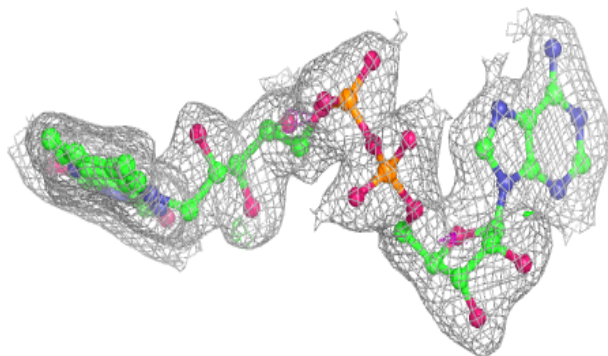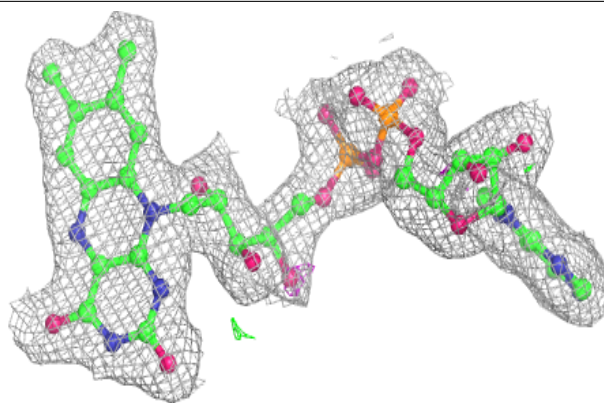and green (positive)
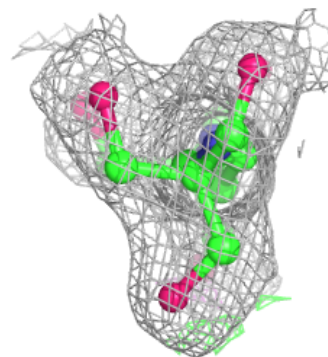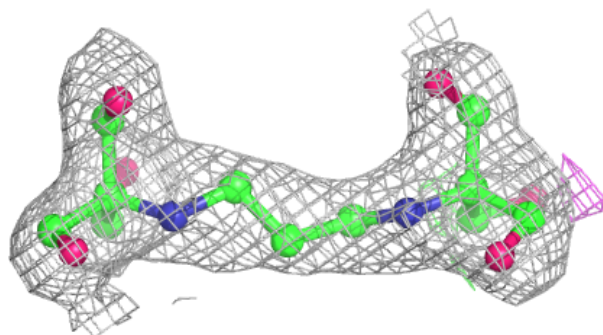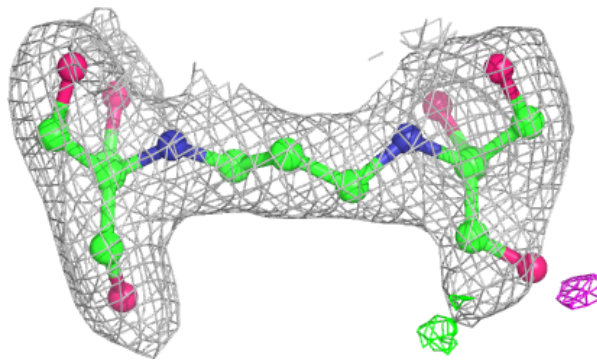
Electron density around B3P D 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
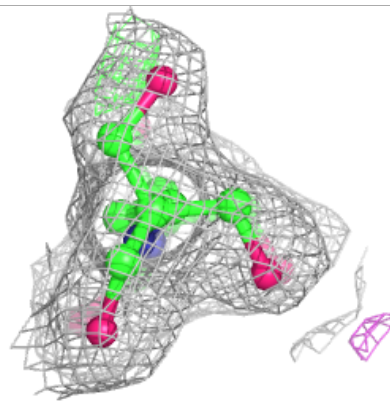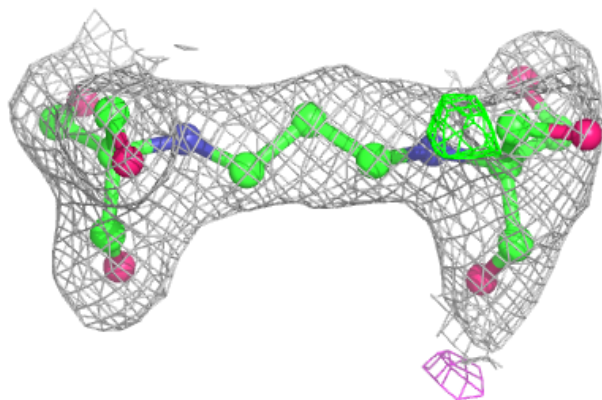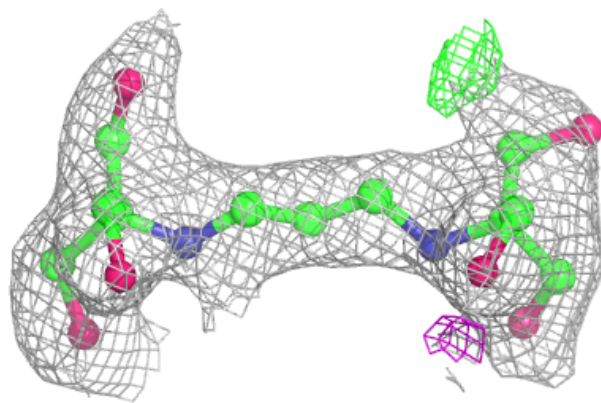
Electron density around B3P A 1003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
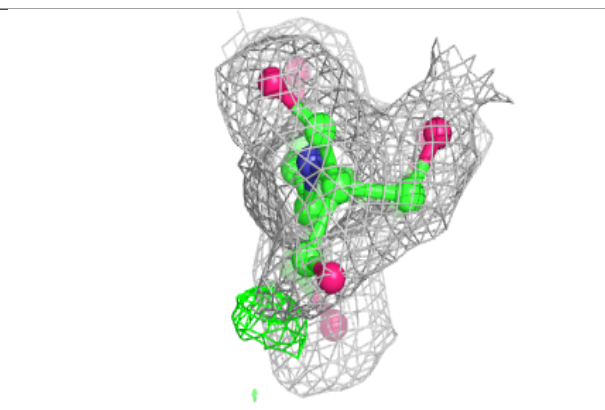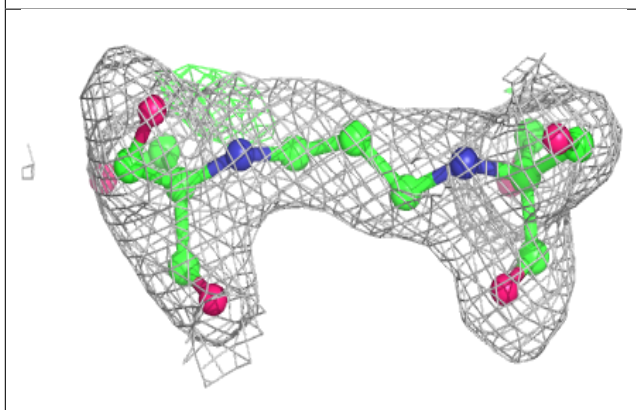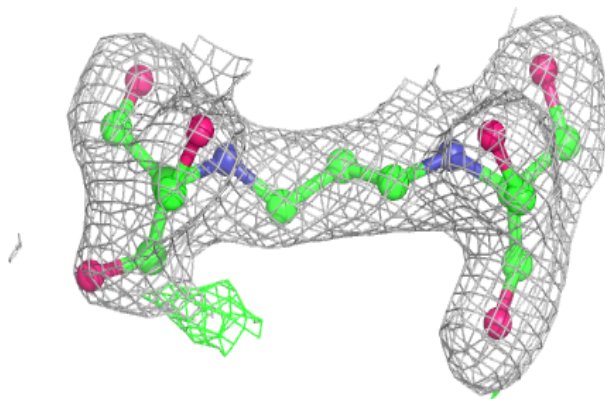
Electron density around NAP B 403:

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 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)
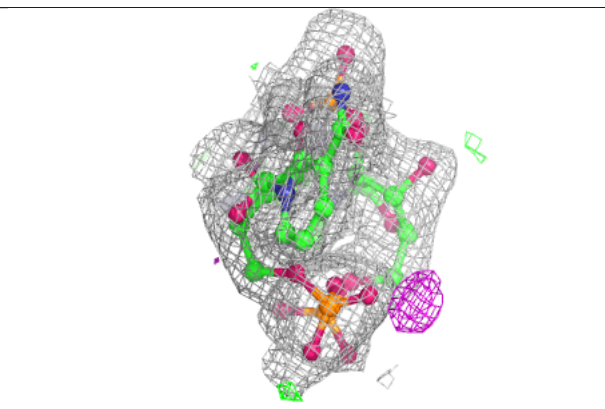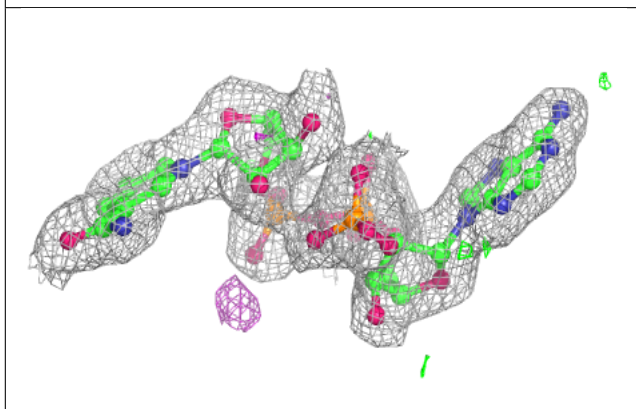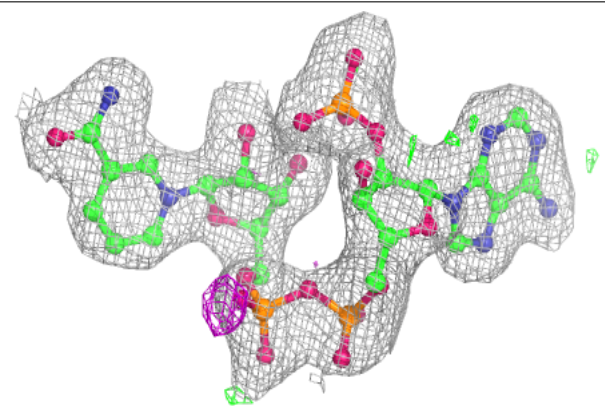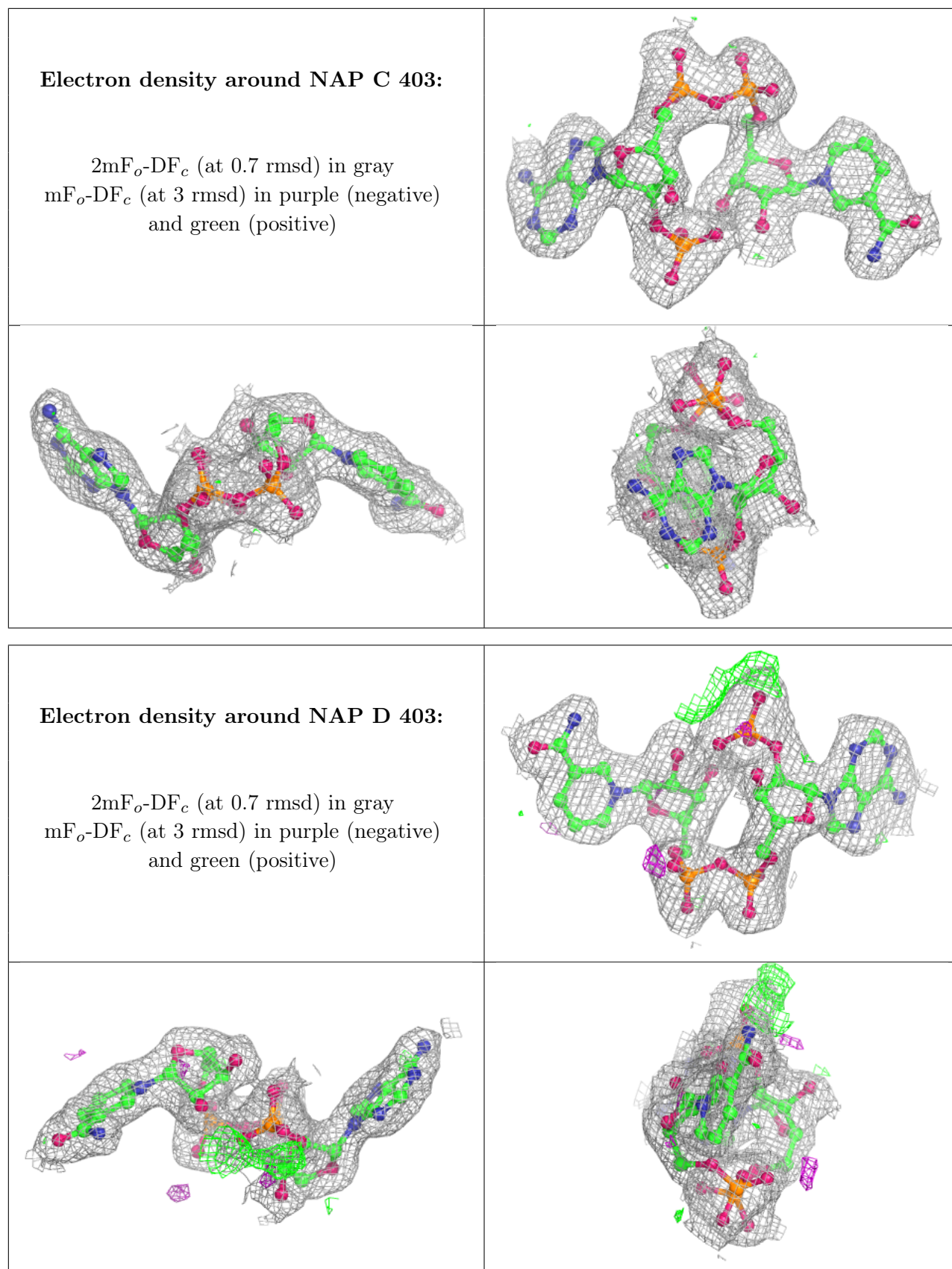
Electron density around NAP A 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
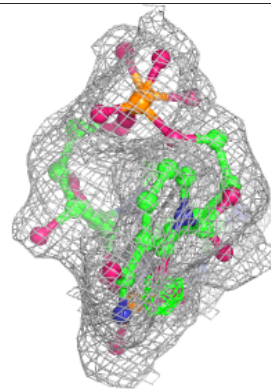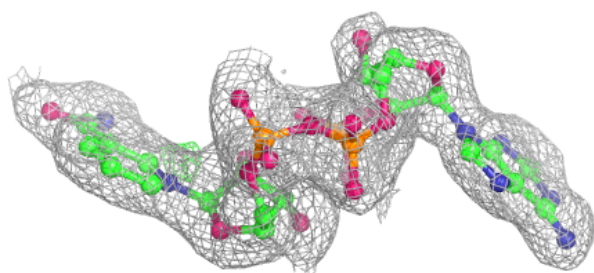
Electron density around FAD C 402:

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

Electron density around FAD A 1001:

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

Electron density around FAD B 402:

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

Electron density around FAD D 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
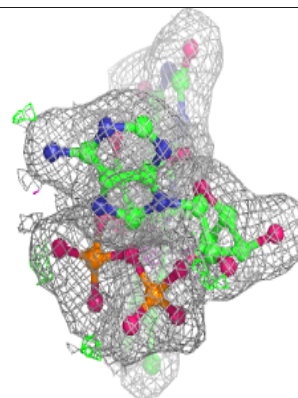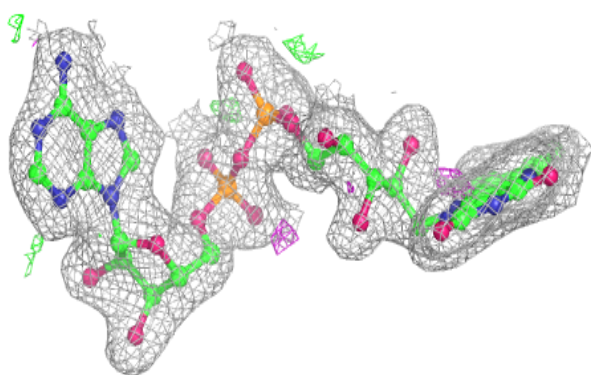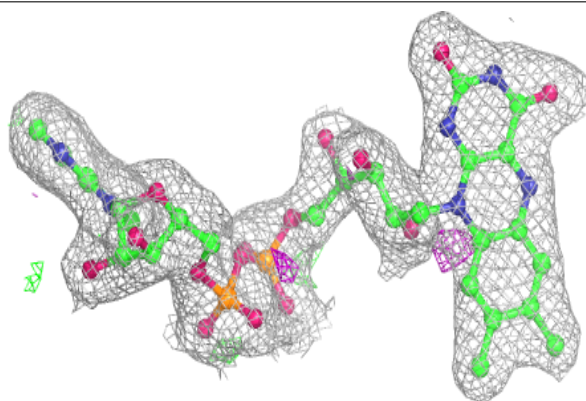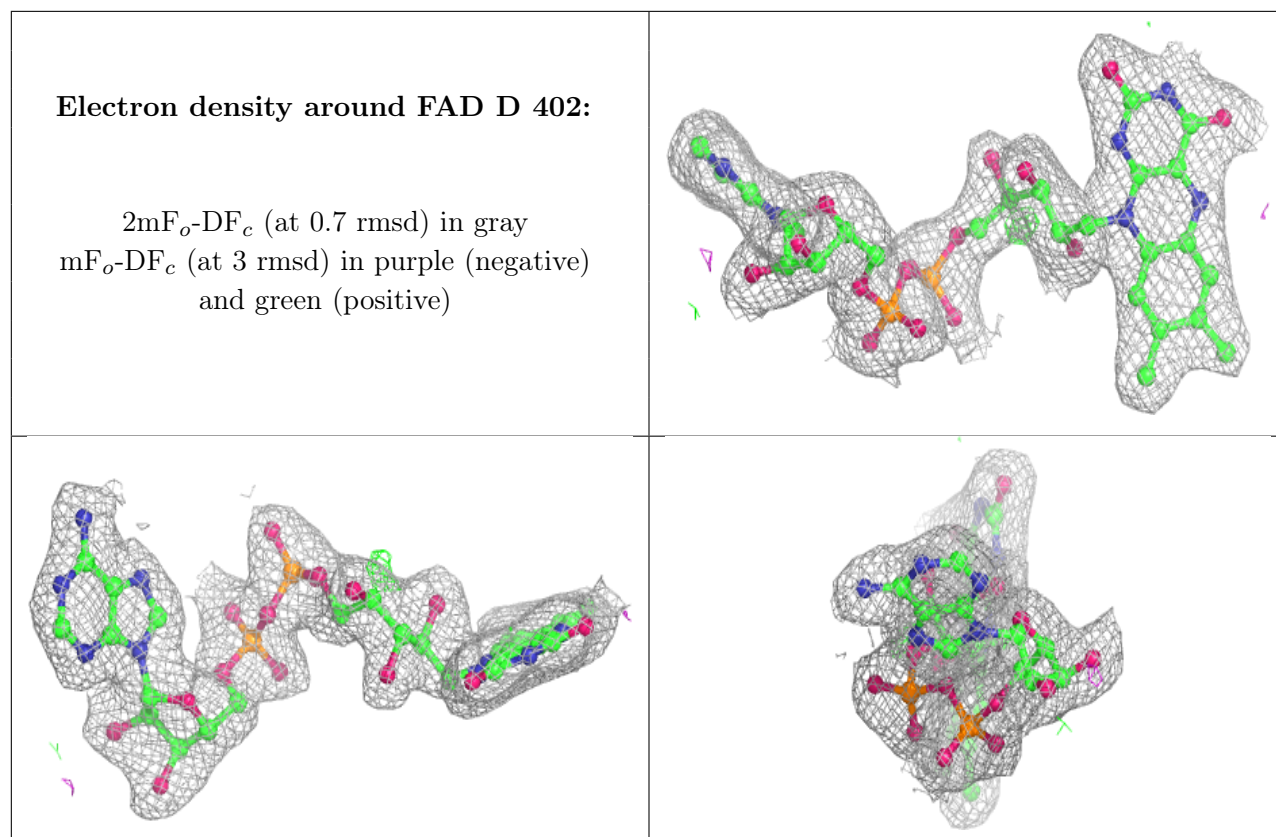
6.5 Other polymers (i)

There are no such residues in this entry.