



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:40 PM UTC

PDB ID : 4J2O / pdb_00004j2o
Title : Crystal structure of NADP-bound WbjB from *A. baumannii* community strain D1279779
Authors : Shah, B.S.; Harrop, S.J.; Paulsen, I.T.; Mabbutt, B.C.
Deposited on : 2013-02-05
Resolution : 2.65 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

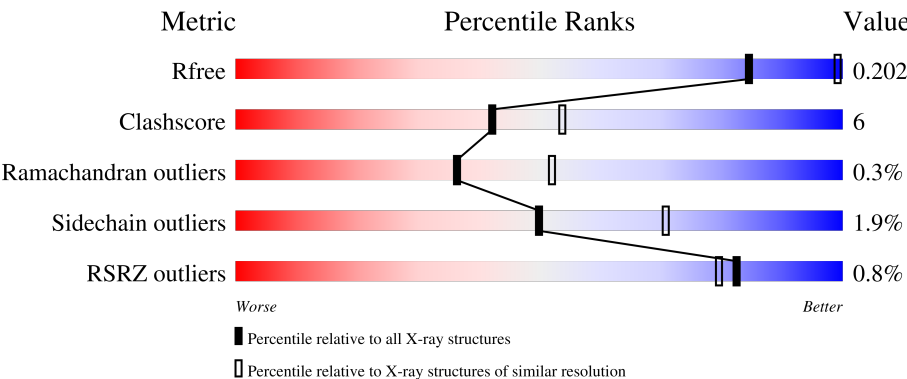
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	363	74% 12% • 13%
1	B	363	% 73% 12% • 14%
1	C	363	73% 13% • 13%
1	D	363	72% 13% • 14%
1	E	363	% 72% 11% • 17%

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Mol	Chain	Length	Quality of chain
1	F	363	 2% 69% 13% 17%

2 Entry composition [i](#)

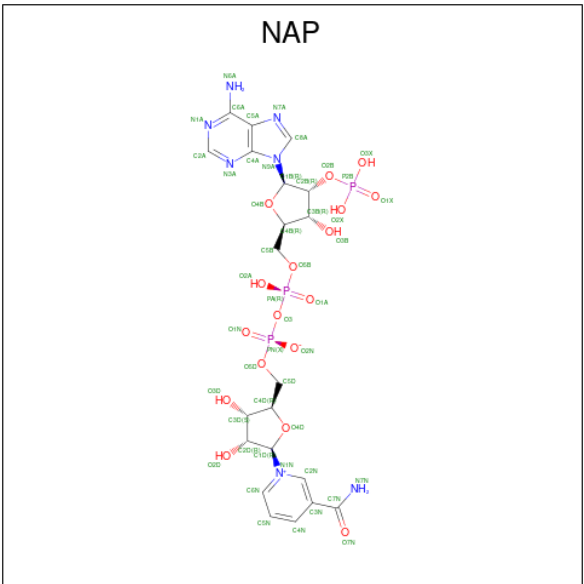
There are 3 unique types of molecules in this entry. The entry contains 15097 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-acetylglucosamine 4,6-dehydratase/5-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	Se	0	0	0
			2480	1570	431	462	3	14			
1	B	313	Total	C	N	O	S	Se	0	0	0
			2468	1565	425	462	3	13			
1	C	316	Total	C	N	O	S	Se	0	0	0
			2491	1576	434	464	3	14			
1	D	312	Total	C	N	O	S	Se	0	0	0
			2457	1556	428	456	3	14			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2389	1516	413	444	3	13			
1	F	300	Total	C	N	O	S	Se	0	0	0
			2364	1501	408	439	3	13			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

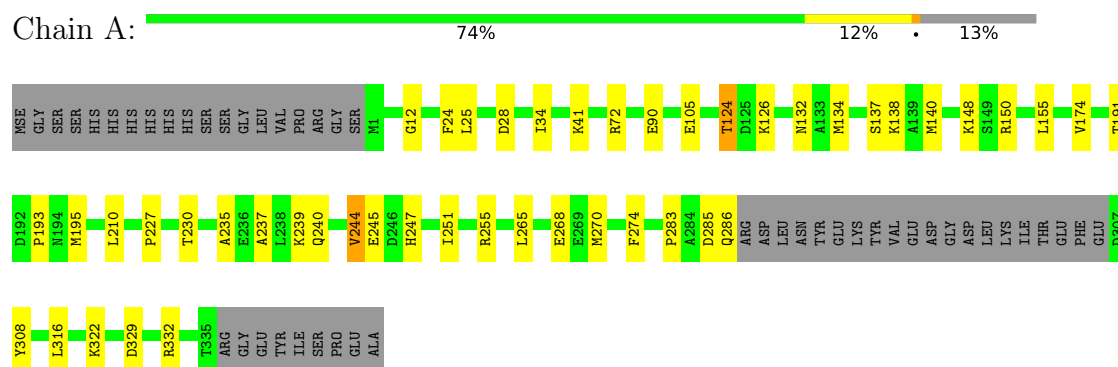
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	38	Total	O	0	0
			38	38		
3	C	25	Total	O	0	0
			25	25		
3	D	22	Total	O	0	0
			22	22		
3	E	22	Total	O	0	0
			22	22		
3	F	15	Total	O	0	0
			15	15		

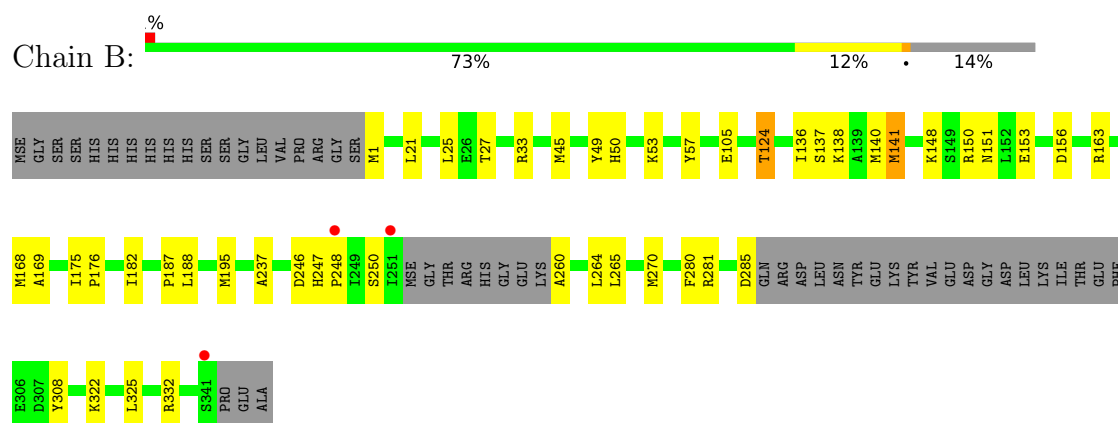
3 Residue-property plots

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.

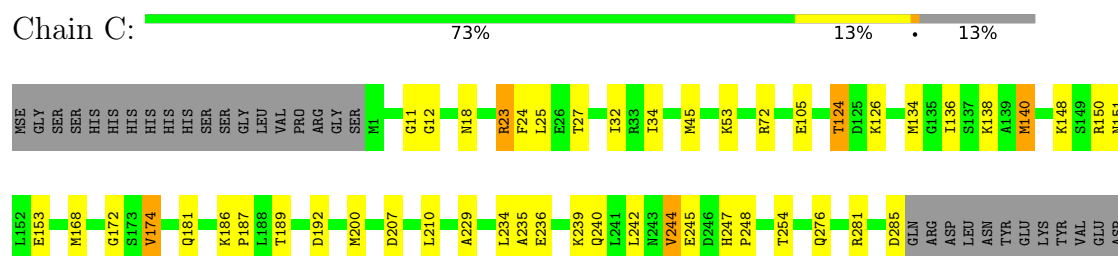
- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase



- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase



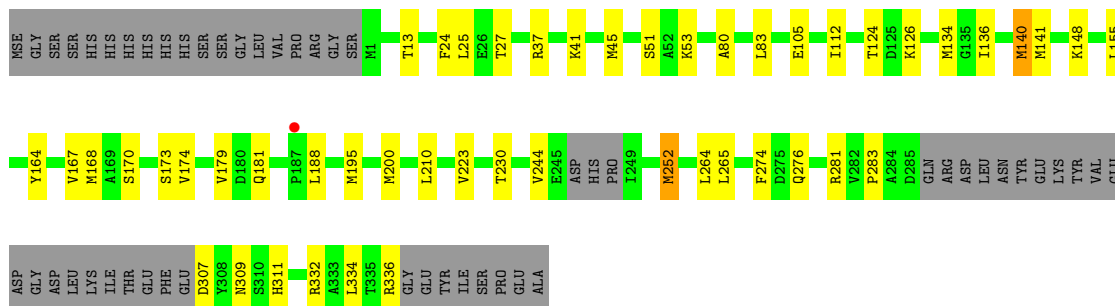
- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase





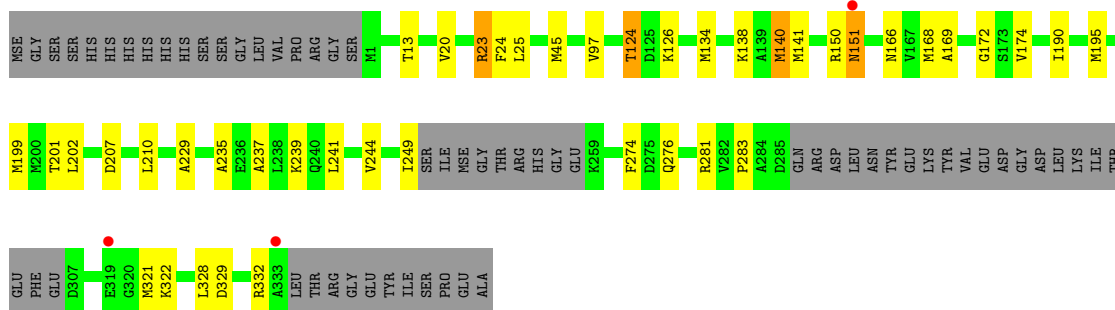
- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase

Chain D: 72% 13% 14%



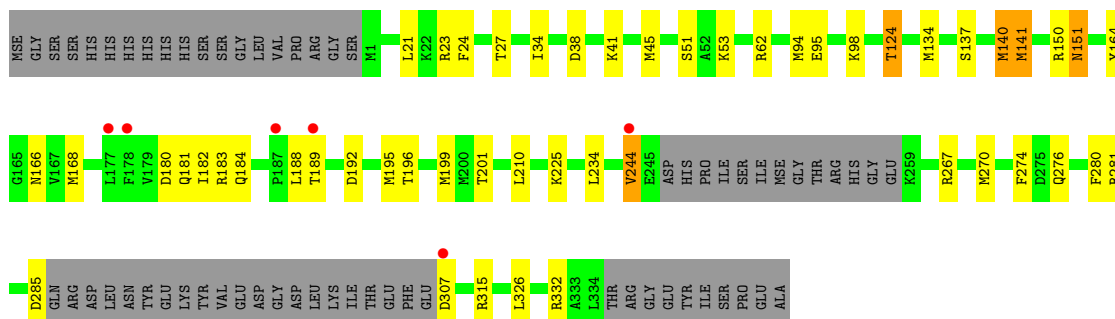
- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase

Chain E: 72% 11% 17%



- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase/5-epimerase

Chain F: 69% 13% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.93Å 114.54Å 215.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.65 24.86 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.86-2.65) 96.6 (24.86-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.160 , 0.202 0.163 , 0.202	Depositor DCC
R_{free} test set	2323 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15097	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

5.1 Standard geometry

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

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	0.65	0/2507	0.90	0/3356
1	B	0.69	0/2495	0.92	5/3342 (0.1%)
1	C	0.61	0/2518	0.89	1/3370 (0.0%)
1	D	0.61	1/2481 (0.0%)	0.89	0/3317
1	E	0.58	0/2415	0.85	1/3233 (0.0%)
1	F	0.58	0/2388	0.86	0/3195
All	All	0.62	1/14804 (0.0%)	0.88	7/19813 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	MSE	SE-CE	-5.28	1.79	1.95

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	VAL	N-CA-C	6.54	116.70	110.42
1	B	175	ILE	CA-C-N	-5.83	113.67	119.56
1	B	175	ILE	C-N-CA	-5.83	113.67	119.56
1	B	247	HIS	CA-C-N	5.81	125.81	119.89
1	B	247	HIS	C-N-CA	5.81	125.81	119.89
1	B	250	SER	N-CA-C	5.49	117.47	108.52
1	E	174	VAL	N-CA-C	5.10	115.32	110.42

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	2480	0	2513	33	0
1	B	2468	0	2496	34	0
1	C	2491	0	2524	33	0
1	D	2457	0	2499	30	0
1	E	2389	0	2422	29	0
1	F	2364	0	2404	35	0
2	A	48	0	25	2	0
2	B	48	0	25	1	0
2	C	48	0	25	2	0
2	D	48	0	25	3	0
2	E	48	0	25	3	0
2	F	48	0	25	4	0
3	A	38	0	0	2	0
3	B	38	0	0	3	0
3	C	25	0	0	0	0
3	D	22	0	0	1	0
3	E	22	0	0	0	0
3	F	15	0	0	1	0
All	All	15097	0	15008	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (188) 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:265:LEU:HD12	1:B:270:MSE:HE2	1.54	0.87
1:B:124:THR:HB	2:B:400:NAP:H6N	1.60	0.81
1:D:13:THR:HA	1:D:45:MSE:HE1	1.63	0.80
1:E:124:THR:HB	2:E:400:NAP:H6N	1.63	0.79
1:B:270:MSE:HE3	1:B:308:TYR:HB2	1.63	0.79
1:C:27:THR:O	1:C:53:LYS:NZ	2.18	0.77
1:B:27:THR:O	1:B:53:LYS:NZ	2.18	0.77
1:E:169:ALA:HB2	1:E:328:LEU:HD13	1.70	0.72
1:D:24:PHE:HZ	1:D:210:LEU:HD11	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH1	1:C:207:ASP:OD1	2.25	0.69
1:B:281:ARG:NH1	3:B:536:HOH:O	2.27	0.68
1:A:150:ARG:HG2	1:A:286:GLN:HE21	1.59	0.67
1:E:23:ARG:NH2	1:E:207:ASP:OD1	2.25	0.67
1:B:332:ARG:HD3	3:B:526:HOH:O	1.93	0.67
1:E:24:PHE:HZ	1:E:210:LEU:HD11	1.59	0.67
1:A:126:LYS:HG3	1:A:134:MSE:HE1	1.77	0.66
1:F:164:TYR:O	2:F:400:NAP:H5N	1.96	0.65
1:D:126:LYS:HD2	1:D:134:MSE:HE1	1.78	0.65
1:A:124:THR:HB	2:A:400:NAP:H6N	1.80	0.64
1:F:192:ASP:HB3	1:F:195:MSE:HE3	1.78	0.64
1:E:199:MSE:HG3	1:E:321:MSE:HE1	1.79	0.64
1:E:150:ARG:O	1:E:151:ASN:HB2	1.98	0.63
1:C:124:THR:HB	2:C:400:NAP:H6N	1.81	0.63
1:B:270:MSE:HE3	1:B:308:TYR:CB	2.28	0.62
1:C:276:GLN:NE2	1:C:281:ARG:HD3	2.16	0.61
1:C:236:GLU:OE2	1:C:240:GLN:NE2	2.29	0.61
1:A:150:ARG:NH2	1:A:285:ASP:O	2.27	0.61
1:A:237:ALA:HB1	1:A:322:LYS:HG3	1.83	0.60
1:A:274:PHE:HE2	1:A:283:PRO:HG3	1.68	0.58
1:E:229:ALA:HB2	1:E:321:MSE:HE3	1.85	0.58
1:F:27:THR:O	1:F:53:LYS:NZ	2.36	0.58
1:F:199:MSE:HE1	1:F:234:LEU:HD22	1.84	0.58
1:B:169:ALA:HA	1:B:176:PRO:HD3	1.86	0.58
1:C:24:PHE:HZ	1:C:210:LEU:HD11	1.68	0.57
1:F:150:ARG:O	1:F:151:ASN:HB2	2.03	0.57
1:E:126:LYS:HG3	1:E:134:MSE:HE1	1.86	0.57
1:F:267:ARG:HG2	1:F:307:ASP:HB2	1.86	0.57
1:B:140:MSE:HE2	1:D:136:ILE:HG22	1.86	0.56
1:A:265:LEU:HB2	1:A:270:MSE:HE1	1.87	0.56
1:A:329:ASP:OD1	1:A:332:ARG:NH1	2.38	0.56
1:A:274:PHE:CE2	1:A:283:PRO:HG3	2.41	0.56
1:C:187:PRO:HB3	1:C:248:PRO:HB2	1.89	0.55
1:E:13:THR:HA	1:E:45:MSE:HE1	1.89	0.55
1:F:181:GLN:HE22	1:F:189:THR:HB	1.73	0.54
1:B:1:MSE:N	3:B:518:HOH:O	2.23	0.54
1:D:307:ASP:OD1	1:D:309:ASN:ND2	2.41	0.54
1:F:24:PHE:HZ	1:F:210:LEU:HD11	1.73	0.54
1:B:136:ILE:HG23	1:D:136:ILE:HG23	1.90	0.54
1:C:18:ASN:ND2	1:C:45:MSE:HE3	2.23	0.53
1:F:124:THR:HG21	1:F:134:MSE:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:GLU:OE2	1:D:148:LYS:NZ	2.38	0.53
1:D:164:TYR:O	2:D:400:NAP:H5N	2.08	0.53
1:B:265:LEU:CD1	1:B:270:MSE:HE2	2.32	0.53
1:C:105:GLU:OE2	1:C:148:LYS:NZ	2.41	0.53
1:C:234:LEU:HB2	1:C:321:MSE:HE3	1.91	0.52
1:C:168:MSE:HE2	1:C:200:MSE:N	2.25	0.52
1:B:237:ALA:HB1	1:B:322:LYS:HG3	1.93	0.51
1:F:225:LYS:HE2	1:F:280:PHE:CZ	2.46	0.51
1:A:124:THR:HG22	1:A:138:LYS:HE2	1.93	0.51
1:B:265:LEU:HD12	1:B:270:MSE:CE	2.34	0.51
1:A:270:MSE:HE1	1:A:308:TYR:HB2	1.92	0.50
1:F:21:LEU:HD11	1:F:45:MSE:HE3	1.94	0.50
1:C:25:LEU:HD13	1:C:32:ILE:HD12	1.93	0.50
1:F:180:ASP:HA	1:F:183:ARG:HD3	1.92	0.50
1:B:105:GLU:OE1	1:B:148:LYS:NZ	2.44	0.49
1:F:151:ASN:ND2	3:F:511:HOH:O	2.44	0.49
1:F:23:ARG:HB3	1:F:24:PHE:CD2	2.47	0.49
1:F:94:MSE:HE3	1:F:98:LYS:HG3	1.94	0.49
1:A:24:PHE:HZ	1:A:210:LEU:HD11	1.77	0.49
1:A:28:ASP:OD1	1:A:28:ASP:N	2.44	0.49
1:A:244:VAL:HG12	1:A:247:HIS:HB2	1.95	0.49
1:F:38:ASP:OD2	1:F:41:LYS:HG3	2.12	0.49
1:C:126:LYS:HG3	1:C:134:MSE:HE1	1.94	0.48
1:C:240:GLN:HG2	1:C:245:GLU:HG2	1.95	0.48
1:D:24:PHE:CZ	1:D:210:LEU:HD11	2.42	0.48
1:B:21:LEU:CD1	1:B:45:MSE:HE3	2.43	0.48
1:E:274:PHE:HE2	1:E:283:PRO:HG3	1.78	0.48
1:D:181:GLN:OE1	1:D:188:LEU:HA	2.13	0.48
1:B:270:MSE:HE1	1:B:280:PHE:CE2	2.49	0.48
1:E:276:GLN:NE2	1:E:281:ARG:HD3	2.28	0.48
1:F:141:MSE:O	1:F:141:MSE:HG2	2.12	0.48
1:B:163:ARG:NH1	1:B:265:LEU:HD23	2.29	0.48
1:C:124:THR:HG22	1:C:138:LYS:HE2	1.95	0.48
1:D:170:SER:OG	1:D:173:SER:HB3	2.14	0.48
1:F:166:ASN:HA	2:F:400:NAP:H71N	1.79	0.48
1:B:105:GLU:CD	1:B:148:LYS:HZ3	2.21	0.47
2:F:400:NAP:H52N	2:F:400:NAP:H2N	1.96	0.47
1:C:234:LEU:HD13	1:C:321:MSE:HE3	1.95	0.47
1:E:166:ASN:HD22	2:E:400:NAP:H71N	1.61	0.47
1:E:168:MSE:HE2	1:E:201:THR:HG22	1.96	0.47
1:B:150:ARG:O	1:B:151:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:ALA:CB	1:E:321:MSE:HE3	2.44	0.47
1:D:223:VAL:HG13	1:D:264:LEU:HD13	1.95	0.47
1:F:182:ILE:HD13	1:F:244:VAL:HG21	1.96	0.46
1:F:62:ARG:NH2	1:F:95:GLU:OE1	2.41	0.46
1:C:244:VAL:HG11	1:C:247:HIS:HD2	1.80	0.46
1:F:34:ILE:HG13	1:F:45:MSE:HE1	1.97	0.46
1:E:237:ALA:HB1	1:E:322:LYS:HG3	1.98	0.46
1:D:167:VAL:CG2	1:D:170:SER:HB3	2.45	0.46
1:C:186:LYS:O	1:C:247:HIS:HE1	1.98	0.46
1:D:41:LYS:NZ	3:D:522:HOH:O	2.49	0.46
1:D:276:GLN:NE2	1:D:281:ARG:HD3	2.31	0.45
1:C:11:GLY:HA2	2:C:400:NAP:H1B	1.98	0.45
1:B:195:MSE:HG3	1:B:260:ALA:HA	1.99	0.45
1:C:181:GLN:HE22	1:C:189:THR:HG23	1.81	0.45
1:D:168:MSE:HE2	1:D:200:MSE:N	2.31	0.45
1:E:235:ALA:O	1:E:239:LYS:HG3	2.16	0.45
1:E:274:PHE:CE2	1:E:283:PRO:HG3	2.52	0.45
1:C:150:ARG:NH2	1:C:285:ASP:O	2.48	0.45
1:D:27:THR:O	1:D:53:LYS:NZ	2.49	0.45
1:C:235:ALA:O	1:C:239:LYS:HG3	2.16	0.45
1:F:182:ILE:HG13	1:F:188:LEU:HD21	1.99	0.45
1:A:150:ARG:HE	1:A:286:GLN:HG3	1.82	0.45
1:A:268:GLU:HB2	3:A:514:HOH:O	2.17	0.44
1:F:181:GLN:HA	1:F:184:GLN:HG2	1.99	0.44
1:B:141:MSE:O	1:B:141:MSE:HG2	2.17	0.44
1:D:309:ASN:OD1	1:D:311:HIS:HB3	2.16	0.44
1:B:168:MSE:HE3	1:B:325:LEU:HD23	1.98	0.44
1:F:270:MSE:HE1	1:F:280:PHE:CE1	2.52	0.44
1:F:326:LEU:O	1:F:332:ARG:NE	2.50	0.44
1:A:193:PRO:HG3	1:A:251:ILE:HD12	1.99	0.44
1:A:235:ALA:O	1:A:239:LYS:HG3	2.18	0.44
1:E:24:PHE:CZ	1:E:210:LEU:HD11	2.46	0.44
1:E:241:LEU:HG	1:E:322:LYS:HG2	2.00	0.44
1:D:25:LEU:HD12	1:D:25:LEU:HA	1.76	0.44
1:C:136:ILE:HG22	1:F:140:MSE:HE2	1.98	0.44
1:D:179:VAL:HG11	1:D:334:LEU:HD11	2.00	0.44
1:D:80:ALA:HB1	2:D:400:NAP:H51N	1.98	0.43
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.73	0.43
1:A:137:SER:HB3	1:E:140:MSE:HE3	2.00	0.43
1:E:166:ASN:HA	2:E:400:NAP:H4N	2.00	0.43
1:B:33:ARG:HD3	1:B:57:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD22	1:C:334:LEU:HB3	2.00	0.43
1:E:20:VAL:HG13	1:E:24:PHE:CD2	2.53	0.43
1:F:196:THR:CG2	1:F:315:ARG:HH11	2.30	0.43
1:A:72:ARG:NH1	3:A:511:HOH:O	2.40	0.43
1:B:21:LEU:HD11	1:B:45:MSE:HE3	1.99	0.43
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.65	0.43
1:A:270:MSE:HE2	1:A:270:MSE:HB2	1.57	0.43
1:C:234:LEU:CB	1:C:321:MSE:HE3	2.49	0.43
1:A:90:GLU:OE2	1:A:132:ASN:HB2	2.19	0.43
1:A:195:MSE:O	1:A:230:THR:HA	2.19	0.43
1:B:25:LEU:HA	1:B:25:LEU:HD23	1.73	0.43
1:D:195:MSE:O	1:D:230:THR:HA	2.18	0.43
1:D:332:ARG:HB3	1:D:336:ARG:NH2	2.33	0.43
1:C:229:ALA:CB	1:C:321:MSE:HE2	2.48	0.43
1:F:150:ARG:HH21	1:F:285:ASP:C	2.27	0.43
1:C:140:MSE:CE	1:F:137:SER:HB3	2.49	0.42
1:A:240:GLN:HG2	1:A:245:GLU:HG3	2.00	0.42
1:A:155:LEU:HD11	1:C:72:ARG:HD3	2.01	0.42
1:E:329:ASP:OD1	1:E:332:ARG:NH1	2.52	0.42
1:B:124:THR:HG22	1:B:138:LYS:HE2	2.02	0.42
1:E:124:THR:CG2	1:E:138:LYS:HE2	2.50	0.42
1:A:105:GLU:OE2	1:A:148:LYS:NZ	2.41	0.42
1:A:12:GLY:HA3	1:A:34:ILE:HG23	2.01	0.42
1:B:187:PRO:HB3	1:B:248:PRO:HB2	2.01	0.42
1:F:21:LEU:CD1	1:F:45:MSE:HE3	2.49	0.42
1:B:49:TYR:O	1:B:50:HIS:C	2.62	0.42
1:B:182:ILE:HG13	1:B:188:LEU:HD21	2.02	0.42
1:D:37:ARG:HD3	2:D:400:NAP:C6A	2.49	0.42
1:E:202:LEU:HD12	1:E:202:LEU:HA	1.80	0.42
1:F:168:MSE:HE3	1:F:201:THR:HG22	2.02	0.42
1:B:138:LYS:NZ	1:B:141:MSE:HE1	2.35	0.42
1:C:150:ARG:O	1:C:151:ASN:HB2	2.19	0.42
1:D:252:MSE:N	1:D:252:MSE:SE	3.03	0.42
1:D:274:PHE:CE2	1:D:283:PRO:HG3	2.54	0.42
1:F:274:PHE:CD2	1:F:281:ARG:NH1	2.88	0.42
1:C:12:GLY:HA3	1:C:34:ILE:HG23	2.02	0.41
1:D:112:ILE:HG23	1:D:155:LEU:HD13	2.02	0.41
1:D:264:LEU:O	1:D:265:LEU:HD23	2.20	0.41
1:C:192:ASP:HB2	1:C:254:THR:HG22	2.01	0.41
1:F:276:GLN:NE2	1:F:281:ARG:HD3	2.34	0.41
1:A:140:MSE:HE3	1:E:97:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:MSE:HE1	1:A:308:TYR:CB	2.51	0.41
1:E:229:ALA:HB2	1:E:321:MSE:CE	2.50	0.41
1:B:150:ARG:NH2	1:B:285:ASP:C	2.78	0.41
1:A:41:LYS:NZ	2:A:400:NAP:O3X	2.50	0.41
1:A:227:PRO:HB2	1:A:316:LEU:HG	2.02	0.41
1:B:137:SER:HB3	1:D:140:MSE:CE	2.50	0.41
1:F:180:ASP:O	1:F:183:ARG:HB2	2.21	0.41
1:F:274:PHE:HD2	1:F:281:ARG:NH1	2.18	0.41
2:F:400:NAP:H2N	2:F:400:NAP:H2D	1.87	0.40
1:E:190:ILE:HD12	1:E:249:ILE:HG21	2.03	0.40
1:A:191:THR:HG21	1:A:255:ARG:HG3	2.01	0.40
1:B:264:LEU:O	1:B:265:LEU:HD23	2.22	0.40
1:C:24:PHE:CZ	1:C:210:LEU:HD21	2.56	0.40
1:C:25:LEU:HD12	1:C:25:LEU:HA	1.83	0.40
1:D:83:LEU:HD23	1:D:83:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/363 (86%)	303 (97%)	8 (3%)	0	100	100
1	B	307/363 (85%)	300 (98%)	6 (2%)	1 (0%)	36	52
1	C	312/363 (86%)	304 (97%)	7 (2%)	1 (0%)	36	52
1	D	306/363 (84%)	299 (98%)	7 (2%)	0	100	100
1	E	297/363 (82%)	289 (97%)	6 (2%)	2 (1%)	18	30
1	F	294/363 (81%)	288 (98%)	5 (2%)	1 (0%)	36	52
All	All	1827/2178 (84%)	1783 (98%)	39 (2%)	5 (0%)	36	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	GLY
1	E	151	ASN
1	E	172	GLY
1	F	151	ASN
1	B	246	ASP

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	269/296 (91%)	266 (99%)	3 (1%)	65	80
1	B	268/296 (90%)	264 (98%)	4 (2%)	57	75
1	C	270/296 (91%)	264 (98%)	6 (2%)	45	67
1	D	266/296 (90%)	260 (98%)	6 (2%)	44	66
1	E	259/296 (88%)	253 (98%)	6 (2%)	44	66
1	F	256/296 (86%)	251 (98%)	5 (2%)	48	69
All	All	1588/1776 (89%)	1558 (98%)	30 (2%)	50	71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	174	VAL
1	A	244	VAL
1	B	124	THR
1	B	141	MSE
1	B	153	GLU
1	B	156	ASP
1	C	23	ARG
1	C	124	THR
1	C	140	MSE
1	C	153	GLU
1	C	174	VAL
1	C	244	VAL
1	D	51	SER

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Mol	Chain	Res	Type
1	D	124	THR
1	D	140	MSE
1	D	141	MSE
1	D	174	VAL
1	D	244	VAL
1	E	23	ARG
1	E	124	THR
1	E	140	MSE
1	E	141	MSE
1	E	195	MSE
1	E	244	VAL
1	F	51	SER
1	F	124	THR
1	F	140	MSE
1	F	141	MSE
1	F	244	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	151	ASN
1	A	286	GLN
1	C	181	GLN
1	C	215	HIS
1	C	247	HIS
1	D	50	HIS
1	D	215	HIS
1	D	276	GLN
1	E	18	ASN
1	E	50	HIS
1	E	166	ASN
1	E	247	HIS
1	F	50	HIS
1	F	272	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	400	-	50,52,52	2.47	18 (36%)	71,80,80	1.93	19 (26%)
2	NAP	F	400	-	50,52,52	2.43	16 (32%)	71,80,80	1.91	15 (21%)
2	NAP	C	400	-	50,52,52	2.50	18 (36%)	71,80,80	1.96	20 (28%)
2	NAP	A	400	-	50,52,52	2.49	17 (34%)	71,80,80	1.83	18 (25%)
2	NAP	E	400	-	50,52,52	2.45	16 (32%)	71,80,80	1.92	20 (28%)
2	NAP	D	400	-	50,52,52	2.37	17 (34%)	71,80,80	1.99	15 (21%)

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	NAP	B	400	-	-	6/35/67/67	0/5/5/5
2	NAP	F	400	-	-	8/35/67/67	0/5/5/5
2	NAP	C	400	-	-	7/35/67/67	0/5/5/5
2	NAP	A	400	-	-	2/35/67/67	0/5/5/5
2	NAP	E	400	-	-	7/35/67/67	0/5/5/5
2	NAP	D	400	-	-	4/35/67/67	0/5/5/5

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	NAP	C2N-N1N	7.79	1.43	1.35
2	B	400	NAP	C2N-N1N	7.50	1.43	1.35
2	D	400	NAP	C2N-N1N	7.46	1.43	1.35
2	F	400	NAP	C2N-N1N	7.29	1.43	1.35
2	C	400	NAP	C2N-N1N	7.20	1.42	1.35
2	A	400	NAP	C2N-N1N	6.94	1.42	1.35
2	C	400	NAP	O4D-C1D	6.43	1.49	1.40
2	F	400	NAP	O4D-C1D	6.39	1.49	1.40
2	E	400	NAP	O4D-C1D	6.18	1.49	1.40
2	B	400	NAP	O4D-C1D	6.15	1.49	1.40
2	A	400	NAP	O4D-C1D	5.94	1.48	1.40
2	A	400	NAP	C7N-N7N	5.55	1.43	1.33
2	B	400	NAP	C7N-N7N	5.49	1.43	1.33
2	C	400	NAP	C7N-N7N	5.41	1.42	1.33
2	F	400	NAP	C7N-N7N	5.34	1.42	1.33
2	D	400	NAP	C7N-N7N	5.32	1.42	1.33
2	D	400	NAP	O4D-C1D	5.21	1.47	1.40
2	E	400	NAP	C7N-N7N	5.21	1.42	1.33
2	C	400	NAP	C6A-N6A	5.02	1.47	1.34
2	D	400	NAP	C6A-N6A	5.00	1.47	1.34
2	E	400	NAP	C6A-N6A	4.97	1.46	1.34
2	A	400	NAP	C6A-N6A	4.96	1.46	1.34
2	D	400	NAP	C3B-C2B	-4.82	1.42	1.53
2	E	400	NAP	C3B-C2B	-4.57	1.43	1.53
2	F	400	NAP	C3B-C2B	-4.55	1.43	1.53
2	F	400	NAP	C6A-N6A	4.55	1.45	1.34
2	B	400	NAP	C6A-N6A	4.41	1.45	1.34
2	B	400	NAP	C3B-C2B	-4.34	1.43	1.53
2	C	400	NAP	C3B-C2B	-4.28	1.43	1.53
2	A	400	NAP	C3B-C2B	-4.22	1.43	1.53
2	F	400	NAP	C3D-C4D	-3.96	1.42	1.53
2	A	400	NAP	C3D-C4D	-3.88	1.43	1.53
2	C	400	NAP	C3N-C7N	3.88	1.56	1.50
2	B	400	NAP	C3N-C7N	3.73	1.56	1.50
2	A	400	NAP	C2D-C3D	-3.67	1.43	1.53
2	A	400	NAP	C4A-N9A	3.65	1.45	1.37
2	E	400	NAP	C3D-C4D	-3.59	1.43	1.53
2	C	400	NAP	C2D-C3D	-3.54	1.43	1.53
2	C	400	NAP	C4A-N9A	3.53	1.45	1.37
2	B	400	NAP	C3D-C4D	-3.50	1.44	1.53
2	C	400	NAP	C3D-C4D	-3.47	1.44	1.53
2	A	400	NAP	C2A-N3A	3.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NAP	C2A-N3A	3.43	1.40	1.33
2	E	400	NAP	C4A-N9A	3.42	1.44	1.37
2	E	400	NAP	C2A-N3A	3.40	1.40	1.33
2	D	400	NAP	C3D-C4D	-3.38	1.44	1.53
2	D	400	NAP	C2D-C3D	-3.38	1.44	1.53
2	A	400	NAP	C3N-C7N	3.36	1.55	1.50
2	E	400	NAP	C2D-C3D	-3.34	1.44	1.53
2	B	400	NAP	C2D-C3D	-3.33	1.44	1.53
2	B	400	NAP	C2B-C1B	-3.31	1.45	1.53
2	F	400	NAP	C2D-C3D	-3.28	1.44	1.53
2	C	400	NAP	C2A-N3A	3.27	1.39	1.33
2	E	400	NAP	C3N-C7N	3.21	1.55	1.50
2	F	400	NAP	PA-O3	-3.19	1.56	1.59
2	A	400	NAP	C1B-N9A	-3.15	1.37	1.46
2	C	400	NAP	C2B-C1B	-3.14	1.45	1.53
2	B	400	NAP	C4A-N9A	3.14	1.44	1.37
2	D	400	NAP	C2B-C1B	-3.11	1.45	1.53
2	C	400	NAP	C4A-N3A	3.09	1.40	1.34
2	D	400	NAP	C4A-N9A	3.09	1.44	1.37
2	A	400	NAP	C3B-C4B	-3.08	1.45	1.53
2	C	400	NAP	C3B-C4B	-3.06	1.45	1.53
2	A	400	NAP	C5A-C4A	3.06	1.44	1.39
2	F	400	NAP	C2A-N3A	3.02	1.39	1.33
2	E	400	NAP	C3B-C4B	-2.95	1.45	1.53
2	F	400	NAP	C2B-C1B	-2.94	1.45	1.53
2	B	400	NAP	C3B-C4B	-2.93	1.45	1.53
2	D	400	NAP	C1B-N9A	-2.91	1.38	1.46
2	F	400	NAP	C3N-C7N	2.91	1.54	1.50
2	A	400	NAP	C8A-N7A	2.89	1.37	1.31
2	E	400	NAP	C2B-C1B	-2.88	1.46	1.53
2	D	400	NAP	C3B-C4B	-2.86	1.45	1.53
2	A	400	NAP	C2B-C1B	-2.85	1.46	1.53
2	F	400	NAP	C1B-N9A	-2.85	1.38	1.46
2	D	400	NAP	C2A-N3A	2.82	1.38	1.33
2	B	400	NAP	C1B-N9A	-2.81	1.38	1.46
2	B	400	NAP	PA-O3	-2.74	1.56	1.59
2	B	400	NAP	C4A-N3A	2.68	1.39	1.34
2	D	400	NAP	C3N-C7N	2.67	1.54	1.50
2	E	400	NAP	C4A-N3A	2.63	1.39	1.34
2	F	400	NAP	C3B-C4B	-2.62	1.46	1.53
2	C	400	NAP	C1B-N9A	-2.60	1.39	1.46
2	F	400	NAP	C4A-N9A	2.57	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	NAP	C6N-N1N	2.42	1.40	1.35
2	F	400	NAP	C4A-N3A	2.31	1.38	1.34
2	E	400	NAP	C1B-N9A	-2.29	1.40	1.46
2	E	400	NAP	C5A-C4A	2.28	1.43	1.39
2	B	400	NAP	C2A-N1A	2.25	1.37	1.33
2	A	400	NAP	C4A-N3A	2.25	1.38	1.34
2	A	400	NAP	C6N-N1N	2.24	1.40	1.35
2	D	400	NAP	C4A-N3A	2.21	1.38	1.34
2	C	400	NAP	C5A-C4A	2.21	1.43	1.39
2	B	400	NAP	C6N-N1N	2.18	1.40	1.35
2	D	400	NAP	C6N-N1N	2.15	1.40	1.35
2	E	400	NAP	C6N-N1N	2.09	1.40	1.35
2	D	400	NAP	C8A-N7A	2.08	1.35	1.31
2	C	400	NAP	C2A-N1A	2.06	1.37	1.33
2	D	400	NAP	C5A-C4A	2.06	1.42	1.39
2	F	400	NAP	C5A-C4A	2.05	1.42	1.39
2	C	400	NAP	C4N-C3N	2.04	1.42	1.39
2	B	400	NAP	C5A-C4A	2.02	1.42	1.39

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	NAP	C4D-O4D-C1D	-7.97	102.63	109.92
2	F	400	NAP	C4D-O4D-C1D	-7.71	102.86	109.92
2	F	400	NAP	N3A-C2A-N1A	-6.03	119.45	128.58
2	C	400	NAP	N3A-C2A-N1A	-5.97	119.54	128.58
2	D	400	NAP	N3A-C2A-N1A	-5.94	119.59	128.58
2	B	400	NAP	N3A-C2A-N1A	-5.81	119.79	128.58
2	A	400	NAP	C4D-O4D-C1D	-5.73	104.68	109.92
2	E	400	NAP	C4D-O4D-C1D	-5.36	105.02	109.92
2	A	400	NAP	C5A-C4A-N3A	-5.18	119.58	126.72
2	C	400	NAP	N3A-C4A-N9A	5.06	135.76	127.17
2	B	400	NAP	C4D-O4D-C1D	-5.04	105.31	109.92
2	E	400	NAP	C5A-C4A-N3A	-4.97	119.88	126.72
2	E	400	NAP	N3A-C2A-N1A	-4.88	121.20	128.58
2	E	400	NAP	N3A-C4A-N9A	4.76	135.27	127.17
2	C	400	NAP	C5A-C4A-N3A	-4.69	120.26	126.72
2	D	400	NAP	C5A-C4A-N3A	-4.64	120.33	126.72
2	A	400	NAP	N3A-C2A-N1A	-4.63	121.57	128.58
2	B	400	NAP	N3A-C4A-N9A	4.63	135.04	127.17
2	C	400	NAP	C4D-O4D-C1D	-4.56	105.75	109.92
2	B	400	NAP	C5A-C4A-N3A	-4.53	120.47	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAP	N3A-C4A-N9A	4.45	134.74	127.17
2	F	400	NAP	N3A-C4A-N9A	4.45	134.74	127.17
2	D	400	NAP	N3A-C4A-N9A	4.40	134.65	127.17
2	E	400	NAP	C6N-N1N-C2N	-4.24	118.27	121.88
2	F	400	NAP	C5A-C4A-N3A	-4.20	120.94	126.72
2	F	400	NAP	C4B-O4B-C1B	-4.19	100.21	109.47
2	B	400	NAP	O2N-PN-O3	3.88	117.77	107.27
2	D	400	NAP	C4B-O4B-C1B	-3.63	101.46	109.47
2	B	400	NAP	C5A-N7A-C8A	3.61	109.12	103.45
2	A	400	NAP	C6N-N1N-C2N	-3.55	118.85	121.88
2	E	400	NAP	C5A-N7A-C8A	3.50	108.94	103.45
2	D	400	NAP	C2A-N3A-C4A	3.42	120.18	111.83
2	B	400	NAP	C2A-N3A-C4A	3.38	120.10	111.83
2	B	400	NAP	N9A-C8A-N7A	-3.38	109.14	113.94
2	C	400	NAP	C4B-O4B-C1B	-3.37	102.02	109.47
2	D	400	NAP	C5A-N7A-C8A	3.36	108.73	103.45
2	C	400	NAP	O2N-PN-O3	3.28	116.15	107.27
2	F	400	NAP	C2A-N3A-C4A	3.27	119.81	111.83
2	C	400	NAP	C2D-C3D-C4D	3.27	108.92	102.61
2	C	400	NAP	C2A-N3A-C4A	3.25	119.77	111.83
2	B	400	NAP	C3N-C7N-N7N	3.20	121.68	117.74
2	F	400	NAP	C5A-N7A-C8A	3.17	108.43	103.45
2	F	400	NAP	N9A-C8A-N7A	-3.13	109.50	113.94
2	C	400	NAP	C3N-C7N-N7N	3.12	121.58	117.74
2	C	400	NAP	C6N-N1N-C2N	-3.12	119.23	121.88
2	C	400	NAP	C5A-N7A-C8A	3.12	108.35	103.45
2	E	400	NAP	C2A-N3A-C4A	3.11	119.42	111.83
2	A	400	NAP	C5A-N7A-C8A	3.10	108.33	103.45
2	E	400	NAP	O2N-PN-O3	3.09	115.63	107.27
2	B	400	NAP	C4A-N9A-C8A	3.07	108.96	105.74
2	B	400	NAP	C4B-O4B-C1B	-3.06	102.70	109.47
2	A	400	NAP	C2A-N3A-C4A	3.04	119.27	111.83
2	E	400	NAP	C2D-C3D-C4D	3.04	108.48	102.61
2	D	400	NAP	N9A-C8A-N7A	-3.04	109.62	113.94
2	D	400	NAP	O2N-PN-O3	3.00	115.37	107.27
2	F	400	NAP	C4A-N9A-C8A	2.99	108.87	105.74
2	E	400	NAP	C3N-C7N-N7N	2.94	121.36	117.74
2	E	400	NAP	O7N-C7N-N7N	-2.93	118.38	122.62
2	B	400	NAP	C6N-N1N-C2N	-2.91	119.40	121.88
2	D	400	NAP	O2A-PA-O3	2.89	115.08	107.27
2	A	400	NAP	O2N-PN-O3	2.87	115.04	107.27
2	E	400	NAP	O2N-PN-O1N	-2.87	99.09	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAP	C2D-C3D-C4D	2.87	108.16	102.61
2	C	400	NAP	O7N-C7N-N7N	-2.86	118.48	122.62
2	A	400	NAP	C4B-O4B-C1B	-2.86	103.15	109.47
2	E	400	NAP	N9A-C8A-N7A	-2.85	109.89	113.94
2	A	400	NAP	O2N-PN-O1N	-2.83	99.27	112.44
2	C	400	NAP	N9A-C8A-N7A	-2.82	109.93	113.94
2	B	400	NAP	O7N-C7N-N7N	-2.78	118.59	122.62
2	E	400	NAP	C4B-O4B-C1B	-2.75	103.40	109.47
2	C	400	NAP	C5A-C6A-N6A	-2.65	116.73	123.29
2	C	400	NAP	C4A-N9A-C8A	2.64	108.51	105.74
2	A	400	NAP	C3N-C7N-N7N	2.60	120.94	117.74
2	F	400	NAP	C3N-C7N-N7N	2.58	120.91	117.74
2	E	400	NAP	C2B-C3B-C4B	2.53	107.43	101.99
2	D	400	NAP	C4A-N9A-C8A	2.50	108.36	105.74
2	B	400	NAP	O2A-PA-O3	2.41	113.80	107.27
2	C	400	NAP	O2A-PA-O3	2.41	113.78	107.27
2	D	400	NAP	C2B-C3B-C4B	2.41	107.17	101.99
2	B	400	NAP	O2N-PN-O1N	-2.39	101.31	112.44
2	F	400	NAP	C6N-N1N-C2N	-2.35	119.88	121.88
2	E	400	NAP	C4A-N9A-C8A	2.33	108.19	105.74
2	A	400	NAP	C3B-C2B-C1B	2.33	107.27	102.81
2	F	400	NAP	C5A-C6A-N6A	-2.31	117.56	123.29
2	A	400	NAP	N9A-C8A-N7A	-2.29	110.69	113.94
2	D	400	NAP	O4D-C4D-C3D	2.27	109.65	105.15
2	F	400	NAP	C5D-C4D-C3D	-2.26	107.09	115.21
2	E	400	NAP	C3B-C2B-C1B	2.23	107.08	102.81
2	A	400	NAP	C2B-C3B-C4B	2.21	106.74	101.99
2	A	400	NAP	C4A-C5A-N7A	-2.20	108.06	110.58
2	B	400	NAP	C2B-C3B-C4B	2.20	106.73	101.99
2	C	400	NAP	N6A-C6A-N1A	2.19	123.27	118.38
2	C	400	NAP	O2N-PN-O1N	-2.18	102.31	112.44
2	E	400	NAP	C4A-C5A-N7A	-2.15	108.12	110.58
2	E	400	NAP	O4D-C4D-C3D	2.15	109.42	105.15
2	A	400	NAP	C2D-C3D-C4D	2.14	106.74	102.61
2	C	400	NAP	C2B-C3B-C4B	2.13	106.58	101.99
2	D	400	NAP	C2A-N1A-C6A	2.11	122.20	118.73
2	C	400	NAP	C2A-N1A-C6A	2.07	122.12	118.73
2	F	400	NAP	O7N-C7N-N7N	-2.06	119.64	122.62
2	E	400	NAP	C5A-C6A-N6A	-2.04	118.23	123.29
2	D	400	NAP	C4A-C5A-N7A	-2.03	108.26	110.58
2	A	400	NAP	O4B-C1B-N9A	-2.03	104.19	108.09
2	F	400	NAP	C2A-N1A-C6A	2.03	122.06	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAP	O2A-PA-O3	2.02	112.72	107.27
2	B	400	NAP	C3B-C2B-C1B	2.01	106.66	102.81
2	B	400	NAP	C4A-C5A-N7A	-2.01	108.29	110.58

There are no chirality outliers.

All (34) torsion outliers are listed below:

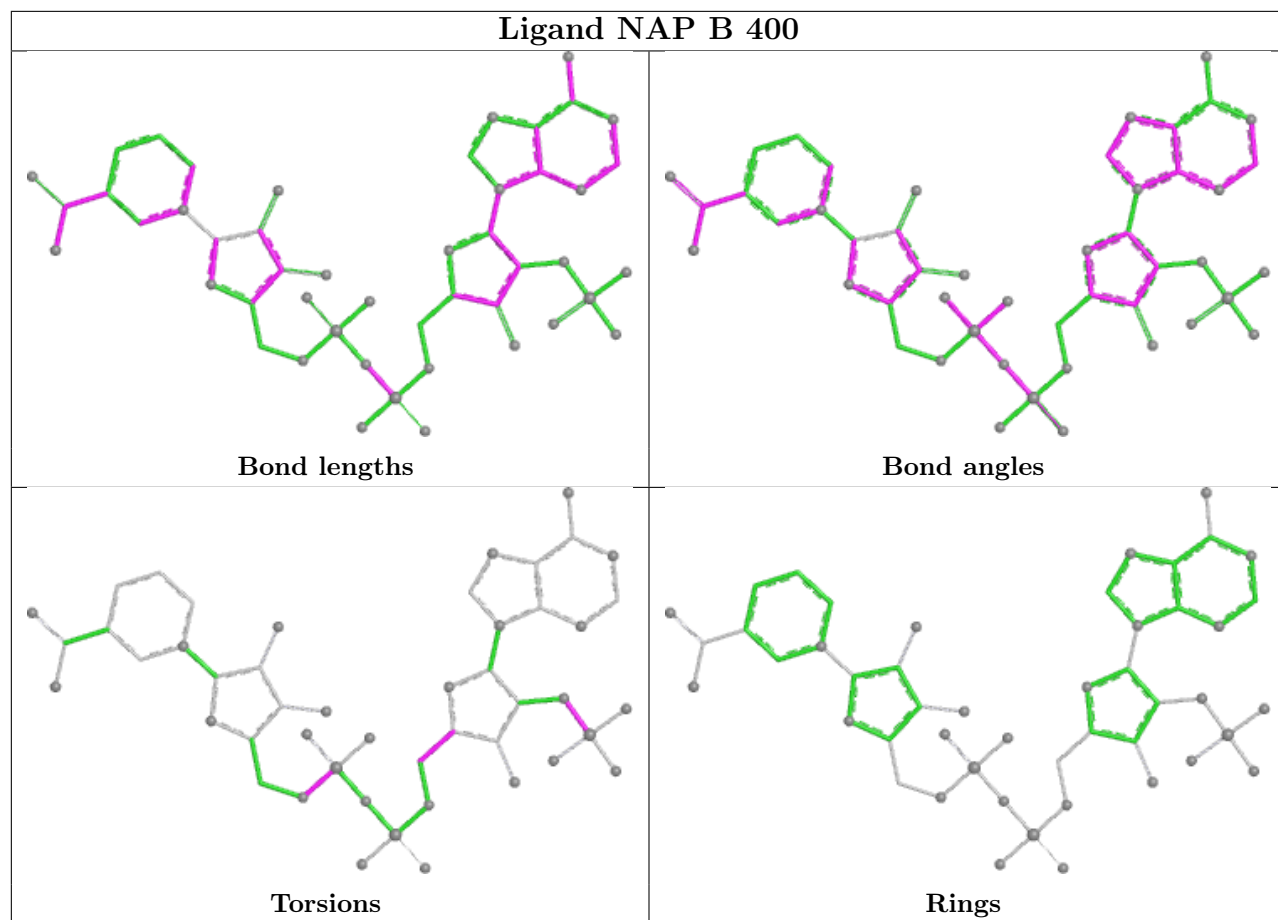
Mol	Chain	Res	Type	Atoms
2	A	400	NAP	O4D-C4D-C5D-O5D
2	B	400	NAP	C5D-O5D-PN-O3
2	B	400	NAP	C5D-O5D-PN-O1N
2	B	400	NAP	C5D-O5D-PN-O2N
2	C	400	NAP	C5D-O5D-PN-O3
2	C	400	NAP	C5D-O5D-PN-O1N
2	C	400	NAP	C5D-O5D-PN-O2N
2	D	400	NAP	O4D-C4D-C5D-O5D
2	D	400	NAP	O4D-C1D-N1N-C2N
2	E	400	NAP	C5D-O5D-PN-O3
2	E	400	NAP	O4D-C1D-N1N-C2N
2	F	400	NAP	O4D-C1D-N1N-C2N
2	F	400	NAP	O4D-C1D-N1N-C6N
2	F	400	NAP	C2D-C1D-N1N-C2N
2	F	400	NAP	C2D-C1D-N1N-C6N
2	E	400	NAP	O4D-C4D-C5D-O5D
2	E	400	NAP	C3D-C4D-C5D-O5D
2	A	400	NAP	C3D-C4D-C5D-O5D
2	D	400	NAP	C3D-C4D-C5D-O5D
2	F	400	NAP	O4B-C4B-C5B-O5B
2	B	400	NAP	C3B-C4B-C5B-O5B
2	C	400	NAP	O4D-C4D-C5D-O5D
2	B	400	NAP	O4B-C4B-C5B-O5B
2	E	400	NAP	PA-O3-PN-O2N
2	C	400	NAP	C3D-C4D-C5D-O5D
2	D	400	NAP	O4D-C1D-N1N-C6N
2	E	400	NAP	O4D-C1D-N1N-C6N
2	C	400	NAP	PN-O3-PA-O1A
2	E	400	NAP	PA-O3-PN-O1N
2	C	400	NAP	O4B-C4B-C5B-O5B
2	F	400	NAP	C3B-C4B-C5B-O5B
2	B	400	NAP	C2B-O2B-P2B-O3X
2	F	400	NAP	C2B-O2B-P2B-O2X
2	F	400	NAP	PA-O3-PN-O2N

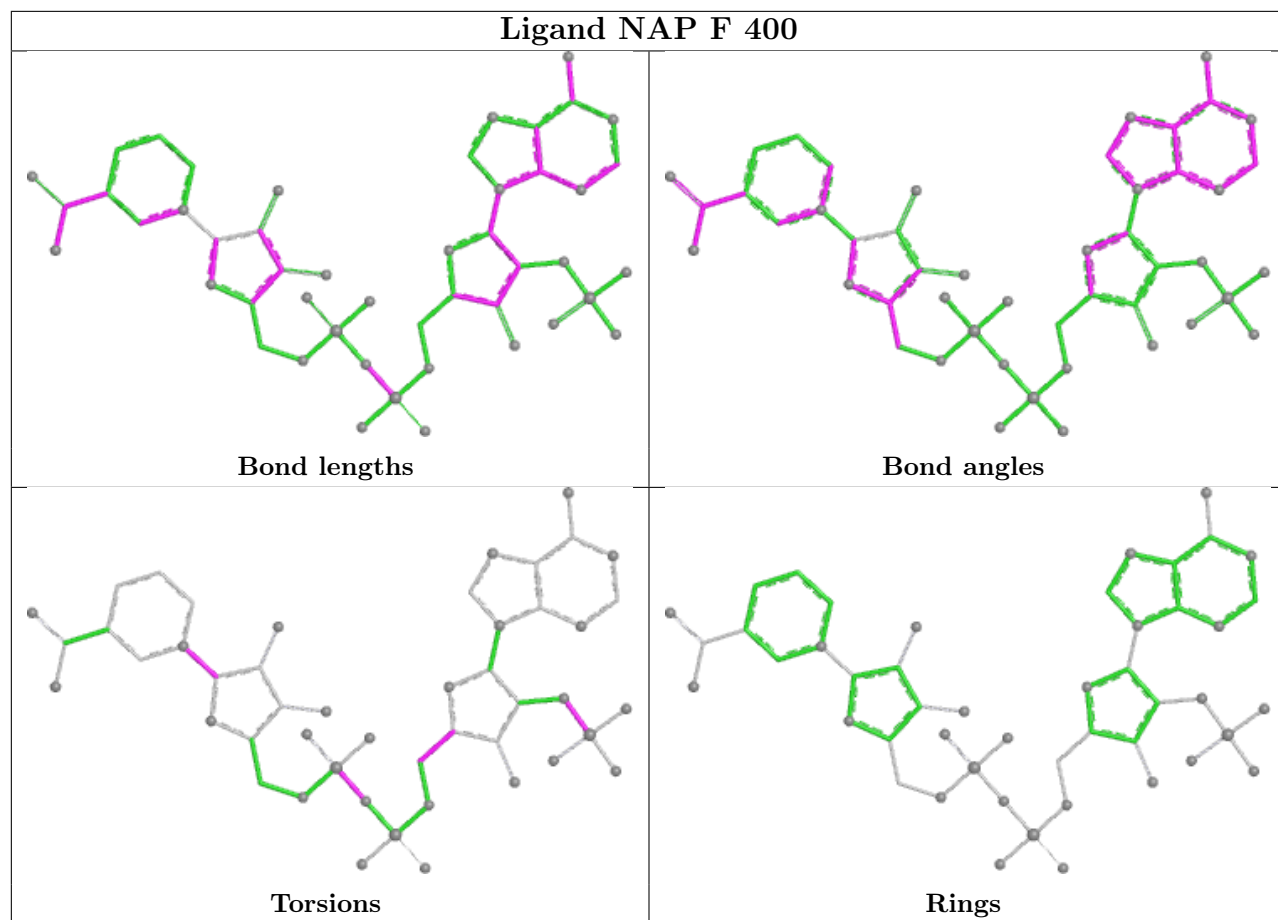
There are no ring outliers.

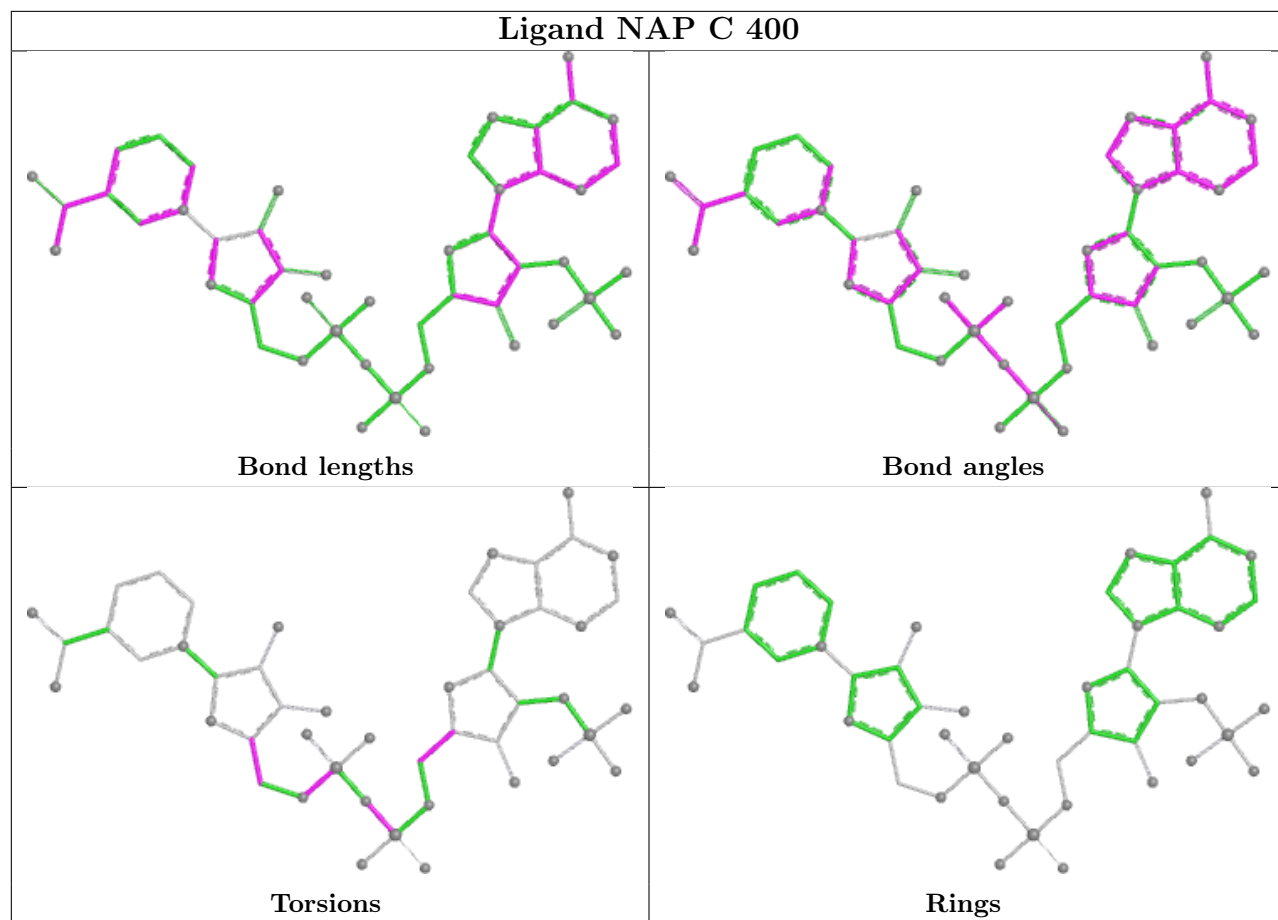
6 monomers are involved in 15 short contacts:

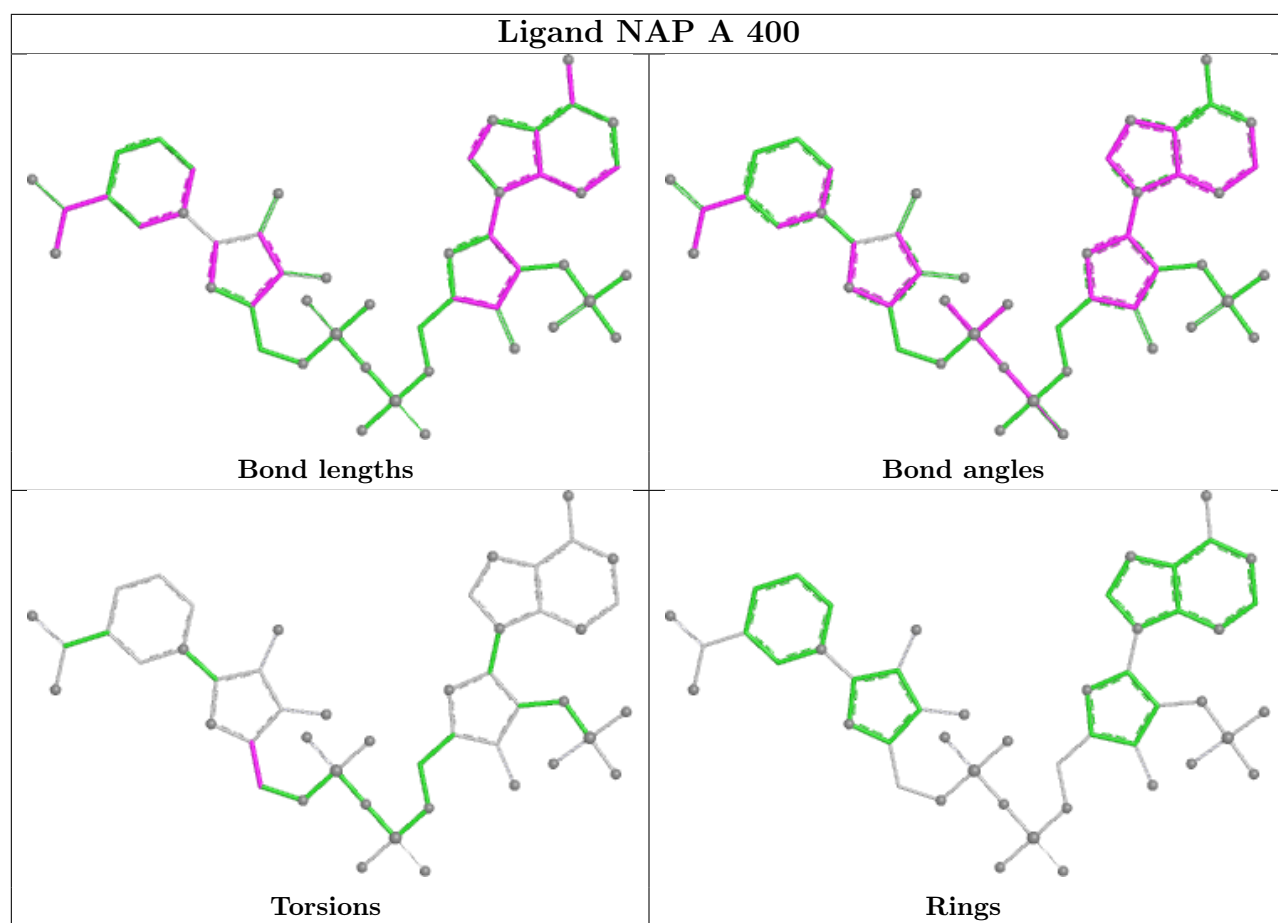
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	NAP	1	0
2	F	400	NAP	4	0
2	C	400	NAP	2	0
2	A	400	NAP	2	0
2	E	400	NAP	3	0
2	D	400	NAP	3	0

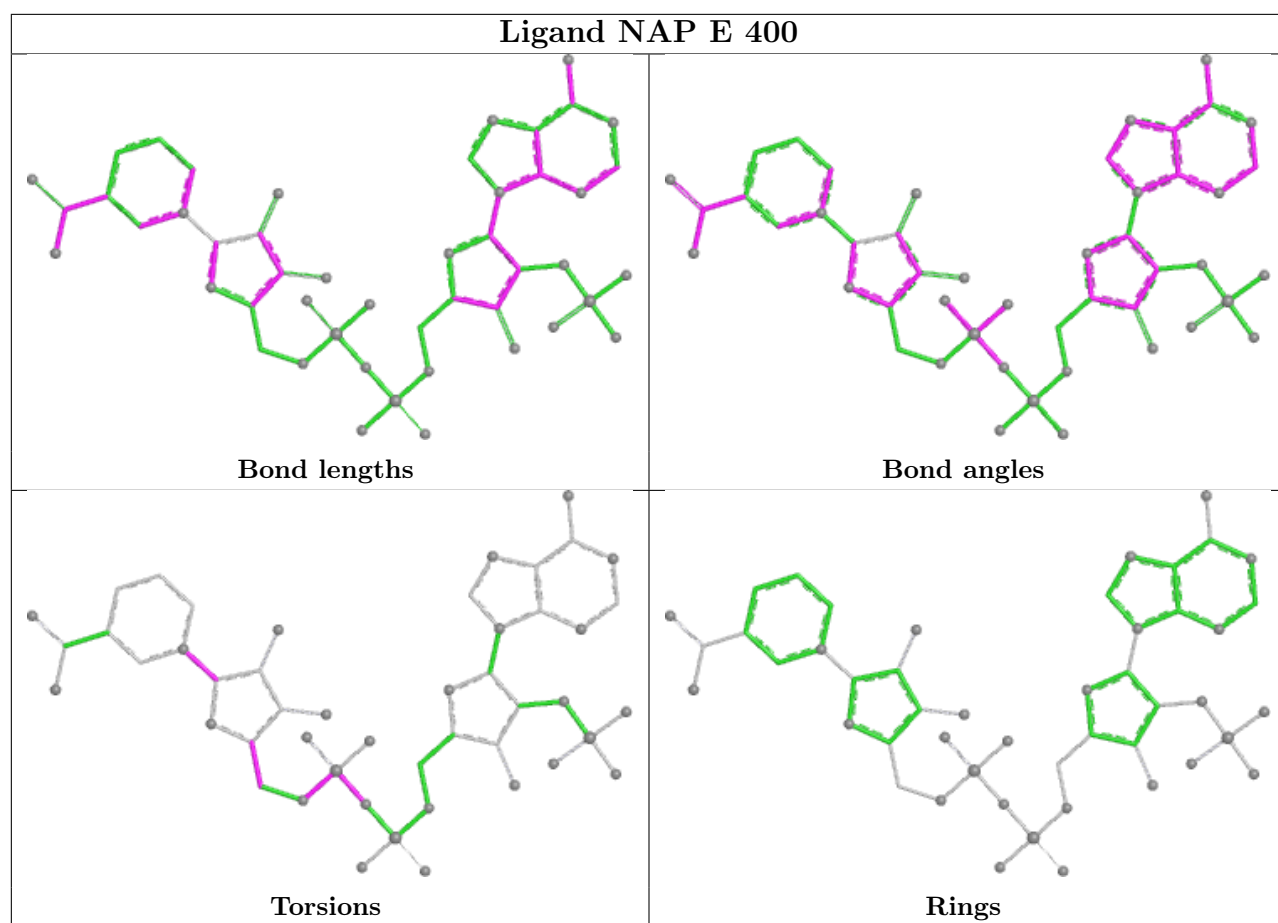
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

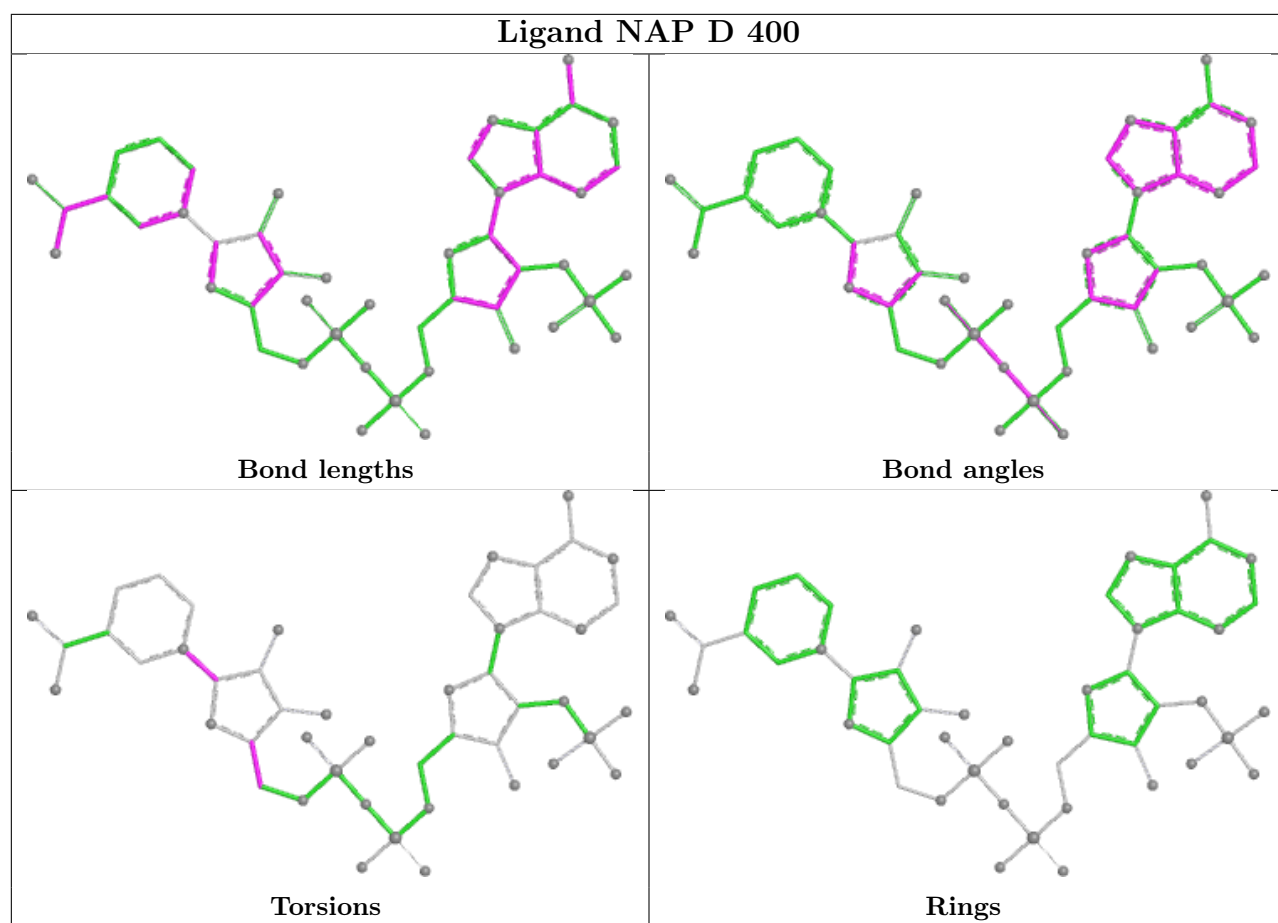












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/363 (82%)	-0.53	0 100 100	35, 58, 100, 139	0
1	B	300/363 (82%)	-0.52	3 (1%) 79 76	32, 57, 92, 138	0
1	C	302/363 (83%)	-0.39	1 (0%) 90 89	39, 68, 107, 147	0
1	D	298/363 (82%)	-0.33	1 (0%) 90 89	34, 68, 124, 149	0
1	E	290/363 (79%)	-0.22	3 (1%) 79 76	40, 71, 158, 189	0
1	F	287/363 (79%)	-0.08	6 (2%) 63 57	41, 74, 162, 183	0
All	All	1778/2178 (81%)	-0.35	14 (0%) 82 79	32, 65, 131, 189	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	333	ALA	4.0
1	F	187	PRO	3.1
1	B	251	ILE	3.1
1	F	244	VAL	3.0
1	F	178	PHE	2.4
1	B	341	SER	2.3
1	F	177	LEU	2.2
1	C	306	GLU	2.2
1	F	189	THR	2.2
1	E	319	GLU	2.2
1	F	307	ASP	2.1
1	E	151	ASN	2.1
1	D	187	PRO	2.0
1	B	248	PRO	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 [i](#)

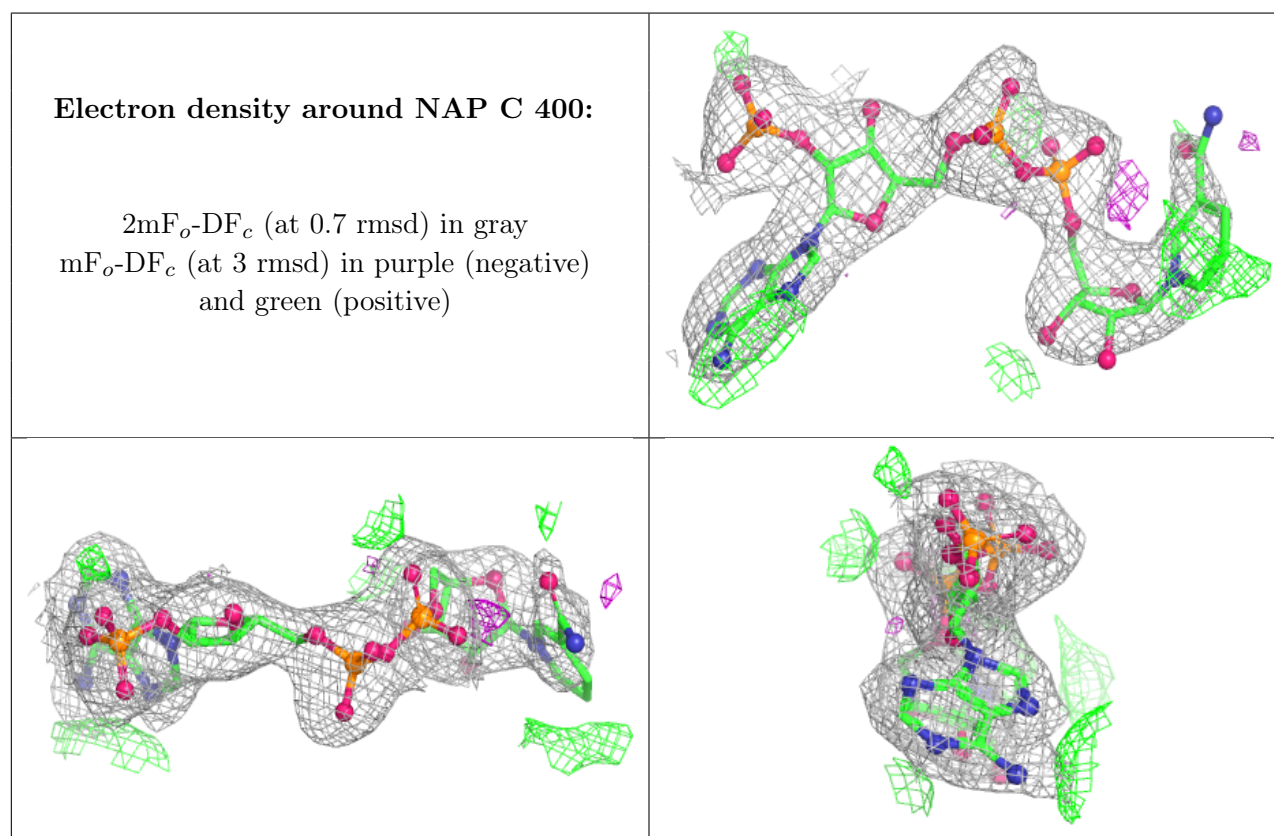
There are no oligosaccharides in this entry.

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.

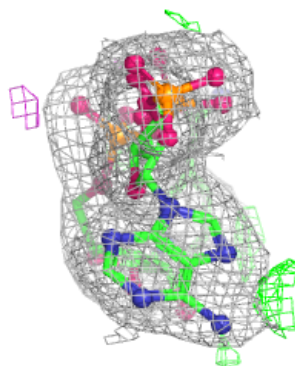
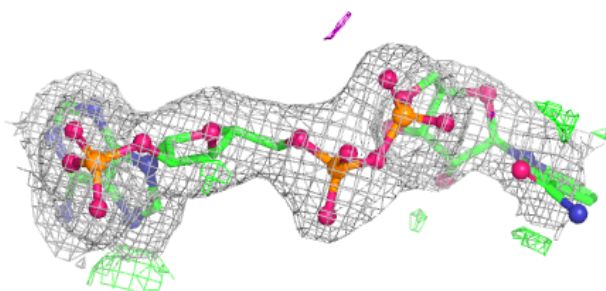
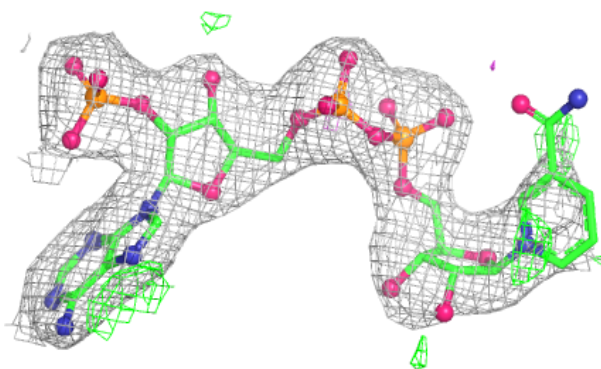
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	C	400	48/48	0.94	0.10	43,79,123,125	0
2	NAP	E	400	48/48	0.96	0.10	44,71,146,156	0
2	NAP	F	400	48/48	0.96	0.07	43,70,118,177	0
2	NAP	B	400	48/48	0.97	0.07	38,68,107,140	0
2	NAP	A	400	48/48	0.97	0.07	33,57,104,123	0
2	NAP	D	400	48/48	0.98	0.06	37,58,88,108	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.

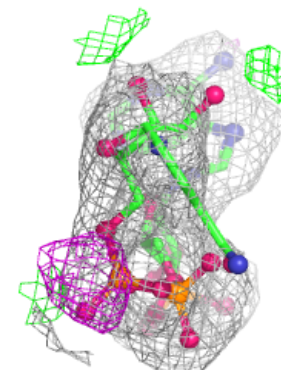
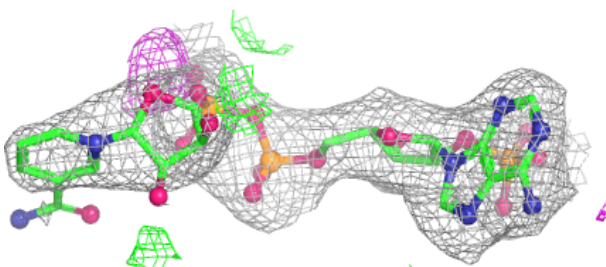
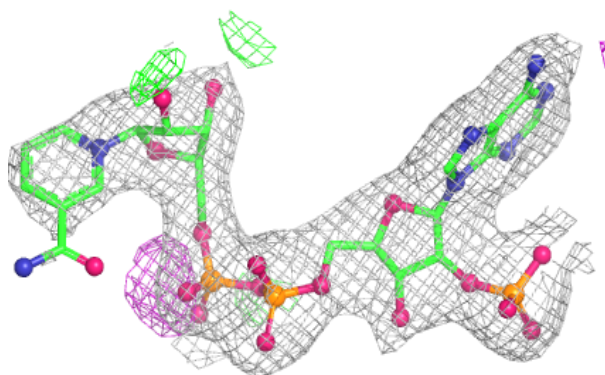


Electron density around NAP E 400:

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

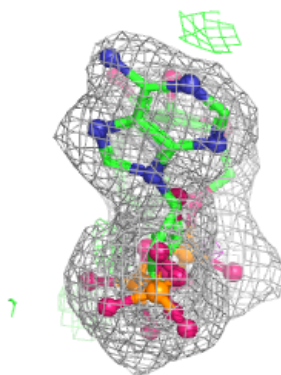
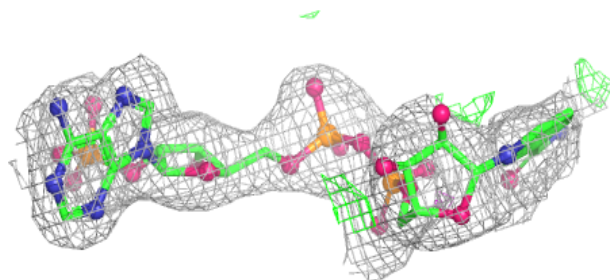
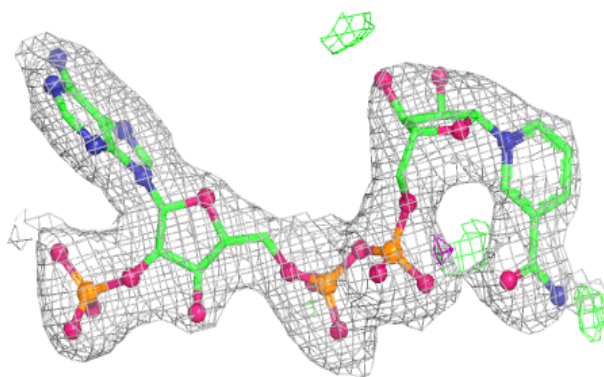
**Electron density around NAP F 400:**

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

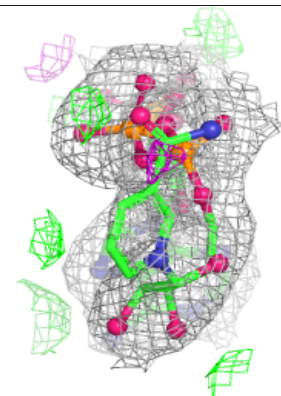
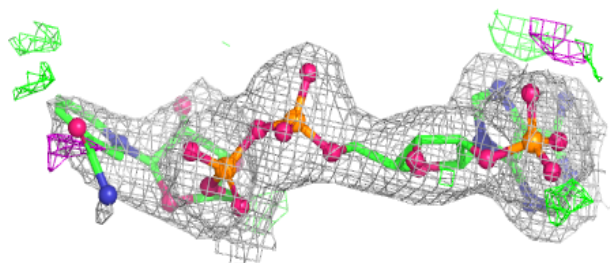
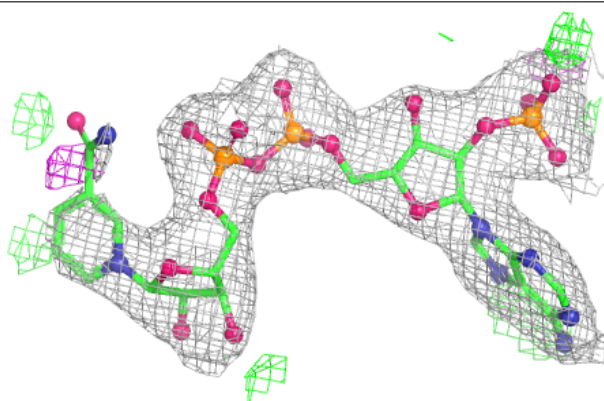


Electron density around NAP B 400:

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

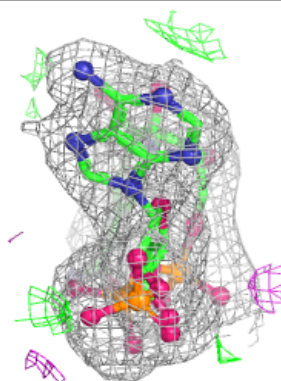
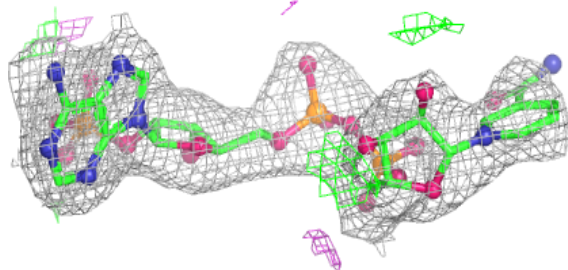
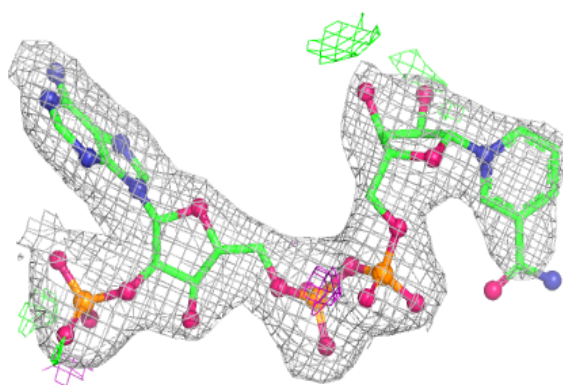
**Electron density around NAP A 400:**

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



Electron density around NAP D 400:

$2mF_o-DF_c$ (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.