



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:37 AM UTC

PDB ID : 5EK6 / pdb_00005ek6
Title : Thermostable aldehyde dehydrogenase from Pyrobaculum sp. 1860 complexed with NADP and isobutyraldehyde
Authors : Petrova, T.E.; Bezsudnova, E.Y.; Boyko, K.M.; Polyakov, K.M.; Rakitina, T.V.; Popov, V.O.
Deposited on : 2015-11-03
Resolution : 2.66 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

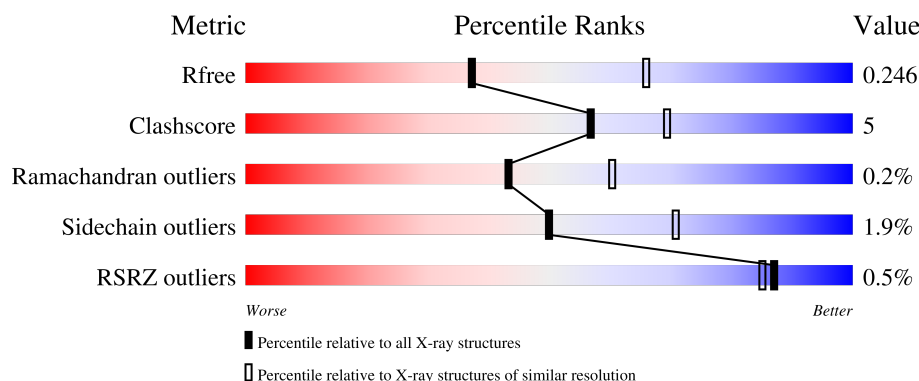
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

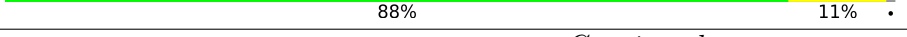
The reported resolution of this entry is 2.66 Å.

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	491	 87% 12% .
1	B	491	 84% 14% ..
1	C	491	 85% 13% .
1	D	491	 88% 11% .

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Mol	Chain	Length	Quality of chain
1	E	491	% 86% 13% .
1	F	491	% 83% 15% .
1	G	491	86% 12% ..
1	H	491	% 86% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30895 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 Aldehyde dehydrogenase.

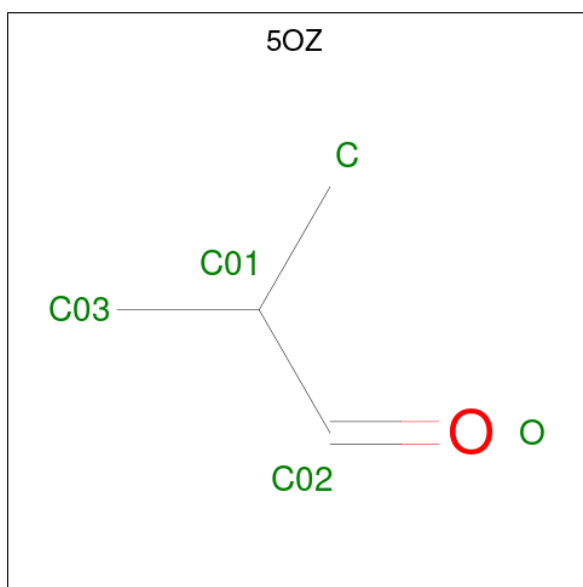
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	1
			3742	2386	651	695	10			
1	B	484	Total	C	N	O	S	0	0	0
			3761	2398	659	693	11			
1	C	485	Total	C	N	O	S	0	0	0
			3754	2393	652	698	11			
1	D	485	Total	C	N	O	S	0	0	0
			3772	2405	660	696	11			
1	E	485	Total	C	N	O	S	0	0	1
			3752	2393	657	691	11			
1	F	483	Total	C	N	O	S	0	0	1
			3747	2389	655	693	10			
1	G	484	Total	C	N	O	S	0	0	0
			3759	2398	653	697	11			
1	H	483	Total	C	N	O	S	0	1	0
			3750	2392	654	694	10			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-methylpropanal (CCD ID: 5OZ) (formula: C₄H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	4	1		
3	B	1	Total	C	O	0	0
			5	4	1		
3	C	1	Total	C	O	0	0
			5	4	1		
3	D	1	Total	C	O	0	0
			5	4	1		
3	G	1	Total	C	O	0	0
			5	4	1		
3	H	1	Total	C	O	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	59	Total	O	0	0
			59	59		
4	C	56	Total	O	0	0
			56	56		
4	D	44	Total	O	0	0
			44	44		
4	E	55	Total	O	0	0
			55	55		
4	F	56	Total	O	0	0
			56	56		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	58	Total	O	0	0
			58	58		
4	H	64	Total	O	0	0
			64	64		

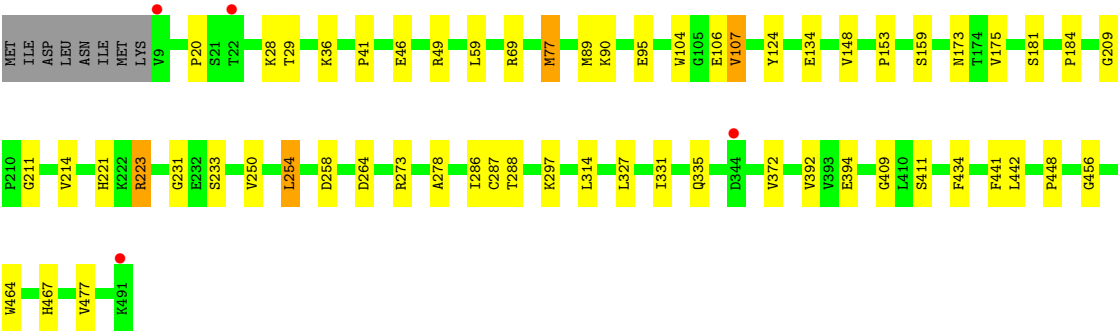
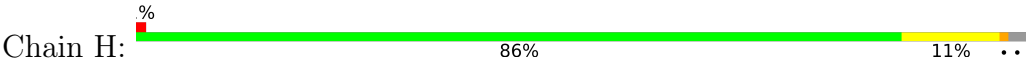
- Molecule 1: Aldehyde dehydrogenase



Chain G:



● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	183.80Å 207.85Å 166.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.14 – 2.66 59.14 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.3 (59.14-2.66) 92.7 (59.14-2.66)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.189 , 0.240 0.200 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtrriage
Anisotropy	0.588	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30895	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0316e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 5OZ

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	0.55	0/3821	0.84	2/5184 (0.0%)
1	B	0.54	0/3840	0.84	2/5206 (0.0%)
1	C	0.55	0/3833	0.85	0/5201
1	D	0.52	0/3851	0.84	4/5220 (0.1%)
1	E	0.52	0/3831	0.85	1/5196 (0.0%)
1	F	0.53	0/3826	0.84	0/5189
1	G	0.52	0/3838	0.83	1/5204 (0.0%)
1	H	0.53	0/3822	0.87	2/5183 (0.0%)
All	All	0.53	0/30662	0.84	12/41583 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	175	VAL	N-CA-C	5.78	116.21	108.11
1	A	385	GLY	CA-C-N	5.52	126.74	119.84
1	A	385	GLY	C-N-CA	5.52	126.74	119.84
1	H	59	LEU	N-CA-C	5.35	116.80	111.07
1	D	365	GLU	CA-C-N	5.32	126.49	119.84
1	D	365	GLU	C-N-CA	5.32	126.49	119.84
1	B	175	VAL	N-CA-C	5.29	115.73	108.12
1	G	332	ASN	N-CA-C	5.26	115.19	108.24
1	B	332	ASN	N-CA-C	5.23	115.26	107.88
1	E	46	GLU	N-CA-C	-5.17	106.97	113.28
1	D	212	PRO	CA-C-N	-5.04	117.81	123.16
1	D	212	PRO	C-N-CA	-5.04	117.81	123.16

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	3742	0	3733	37	0
1	B	3761	0	3767	42	0
1	C	3754	0	3733	42	0
1	D	3772	0	3777	31	0
1	E	3752	0	3752	34	0
1	F	3747	0	3749	41	0
1	G	3759	0	3757	34	0
1	H	3750	0	3745	36	0
2	A	48	0	24	4	0
2	B	48	0	24	2	0
2	C	48	0	24	2	0
2	D	48	0	24	4	0
2	E	48	0	24	3	0
2	F	48	0	24	4	0
2	G	48	0	24	3	0
2	H	48	0	24	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	52	0	0	0	0
4	B	59	0	0	1	0
4	C	56	0	0	1	0
4	D	44	0	0	0	0
4	E	55	0	0	1	0
4	F	56	0	0	0	0
4	G	58	0	0	0	0
4	H	64	0	0	0	0
All	All	30895	0	30205	280	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 5.

All (280) 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:C:222:LYS:HD2	1:C:222:LYS:H	1.40	0.84
1:D:20:PRO:HG3	1:D:41:PRO:HB3	1.63	0.81
1:G:20:PRO:HG3	1:G:41:PRO:HB3	1.68	0.75
1:C:282:HIS:O	1:C:285:GLN:HB2	1.87	0.75
1:G:178:LYS:NZ	1:G:179:PRO:O	2.21	0.73
1:B:483:ARG:NH2	1:B:490:LEU:O	2.22	0.73
1:C:178:LYS:NZ	1:C:179:PRO:O	2.22	0.72
1:F:27:VAL:HG11	1:F:36:LYS:HD3	1.73	0.70
1:F:233:SER:HA	1:F:254:LEU:HG	1.73	0.70
1:H:233:SER:HA	1:H:254:LEU:HG	1.73	0.70
1:D:226:HIS:HD1	1:D:249:THR:HG1	1.39	0.69
1:C:358:ARG:HD2	1:C:365:GLU:OE2	1.92	0.69
1:C:222:LYS:HD2	1:C:222:LYS:N	2.07	0.69
1:F:178:LYS:HE3	1:F:211:GLY:HA2	1.74	0.68
1:D:28:LYS:HE2	1:D:95:GLU:HG3	1.76	0.68
1:C:291:LYS:HE2	1:C:382:GLU:HG3	1.79	0.64
1:A:209:GLY:HA3	1:A:214:VAL:HG21	1.78	0.64
1:G:28:LYS:HE2	1:G:95:GLU:HG3	1.80	0.64
1:A:315:ARG:NH2	1:A:322:ASP:OD2	2.29	0.63
1:A:287:CYS:SG	2:A:500:NAP:C4N	2.87	0.62
1:H:221:HIS:HE1	1:H:223:ARG:HG3	1.63	0.62
1:C:178:LYS:HE2	1:C:209:GLY:O	2.01	0.61
1:H:106:GLU:HG3	1:H:159:SER:HB3	1.82	0.61
1:A:178:LYS:HE2	1:A:209:GLY:O	2.02	0.60
1:H:28:LYS:HE2	1:H:95:GLU:HG3	1.82	0.60
1:H:124:TYR:OH	1:H:467:HIS:ND1	2.30	0.60
1:B:147:VAL:HG22	1:B:224:VAL:HA	1.85	0.59
1:E:26:GLN:OE1	1:E:42:ARG:NH1	2.30	0.59
1:F:53:ASP:O	1:F:57:GLU:HG3	2.03	0.59
1:C:85:LYS:NZ	1:C:111:GLU:OE1	2.26	0.58
1:G:291:LYS:HE2	1:G:382:GLU:HG3	1.85	0.58
1:G:124:TYR:OH	1:G:467:HIS:ND1	2.30	0.58
1:B:65:ILE:HD12	1:B:69:ARG:HB3	1.86	0.58
1:B:287:CYS:SG	2:B:500:NAP:C4N	2.92	0.57
1:G:287:CYS:SG	2:G:500:NAP:C4N	2.92	0.57
1:D:287:CYS:SG	2:D:500:NAP:C4N	2.92	0.57
1:E:233:SER:HA	1:E:254:LEU:HD13	1.86	0.57
1:B:406:THR:HG22	1:B:408:TYR:H	1.70	0.57
1:D:483:ARG:NH2	1:D:490:LEU:O	2.22	0.57
1:G:253:GLU:HB3	2:G:500:NAP:N7N	2.20	0.56
1:B:318:ASP:HB3	1:B:321:LYS:HG3	1.87	0.56
1:E:155:ASN:HD21	2:E:500:NAP:H5N	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LYS:NZ	1:B:179:PRO:O	2.37	0.56
1:G:102:LYS:HE2	1:G:156:TYR:CZ	2.41	0.56
1:F:263:LEU:HD12	1:F:416:THR:HB	1.89	0.55
1:E:287:CYS:SG	2:E:500:NAP:C4N	2.94	0.55
1:H:287:CYS:SG	2:H:500:NAP:C4N	2.95	0.55
1:A:286:ILE:HG22	1:A:288:THR:H	1.73	0.54
1:H:89:MET:HG3	1:H:107:VAL:HG21	1.89	0.54
1:A:30:SER:HB2	1:A:37:ILE:HD11	1.88	0.54
1:F:287:CYS:SG	2:F:500:NAP:C4N	2.96	0.54
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.07	0.54
1:G:222:LYS:HA	1:G:246:THR:HG21	1.89	0.54
1:E:28:LYS:HE3	1:E:95:GLU:HG3	1.90	0.54
1:E:316:ILE:HD11	1:E:366:PRO:HD3	1.88	0.54
1:F:286:ILE:HG22	1:F:288:THR:H	1.73	0.53
1:D:194:VAL:HG11	1:D:204:PHE:HB3	1.89	0.53
1:G:411:SER:OG	1:G:412:GLY:N	2.41	0.53
1:C:358:ARG:HD3	1:C:360:TRP:HZ3	1.72	0.52
1:F:316:ILE:HD12	1:F:365:GLU:HG2	1.90	0.52
1:C:18:LYS:NZ	4:C:601:HOH:O	2.41	0.52
1:H:209:GLY:HA3	1:H:214:VAL:HG21	1.92	0.52
1:F:18:LYS:NZ	1:F:50:GLU:OE2	2.32	0.51
1:B:8:LYS:HE3	1:B:25:PHE:CE2	2.45	0.51
1:B:53:ASP:OD1	1:B:223:ARG:NH2	2.36	0.51
1:C:337:ALA:O	1:C:340:LYS:HG2	2.11	0.51
1:C:422:ALA:HB1	1:C:436:ILE:HD13	1.91	0.51
1:H:221:HIS:CE1	1:H:223:ARG:HG3	2.43	0.51
1:F:214:VAL:O	1:F:218:ILE:HG13	2.10	0.51
1:H:264:ASP:OD1	1:H:264:ASP:N	2.39	0.51
1:H:46:GLU:OE2	1:H:49:ARG:NH1	2.44	0.51
1:B:163:LYS:NZ	1:B:443:GLU:OE2	2.40	0.51
1:C:287:CYS:SG	2:C:500:NAP:C4N	2.99	0.51
1:A:317:ASP:OD1	1:A:318:ASP:N	2.41	0.50
1:E:9:VAL:HG13	1:E:188:TRP:CD1	2.46	0.50
1:F:95:GLU:OE2	1:F:185:VAL:N	2.40	0.50
1:F:164:LYS:NZ	1:F:228:THR:OG1	2.44	0.50
1:F:345:ASP:OD2	1:F:349:ARG:HD2	2.12	0.50
1:E:168:THR:HG22	1:E:173:ASN:HB2	1.94	0.49
1:G:173:ASN:ND2	1:G:469:THR:HB	2.27	0.49
1:G:393:VAL:HB	1:G:398:GLN:HB3	1.94	0.49
1:F:307:TYR:O	1:F:311:VAL:HG23	2.13	0.49
1:F:258:ASP:OD2	1:F:411:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:VAL:HG12	1:G:390:ILE:HB	1.94	0.49
1:C:28:LYS:NZ	1:C:182:ASP:O	2.34	0.48
1:C:397:ASP:O	1:C:401:GLU:HG3	2.13	0.48
1:D:297:LYS:NZ	1:D:394:GLU:HG2	2.28	0.48
1:E:20:PRO:HB2	1:E:22:THR:HG22	1.94	0.48
1:A:252:LEU:O	1:A:456:GLY:HA3	2.13	0.48
1:A:307:TYR:O	1:A:311:VAL:HG23	2.13	0.48
1:F:318:ASP:OD1	1:F:320:ARG:HD3	2.12	0.48
1:D:76:LYS:HD2	1:D:76:LYS:HA	1.66	0.48
1:G:61:ALA:O	1:G:65:ILE:HG23	2.13	0.48
1:A:314:LEU:HD23	1:B:487:PRO:HB3	1.94	0.48
1:D:194:VAL:HG13	1:D:199:LEU:HD22	1.95	0.48
1:F:330:LEU:HD21	1:F:386:PRO:HD3	1.94	0.48
1:B:14:ASN:HB2	1:B:54:SER:OG	2.13	0.48
1:G:414:VAL:HG12	1:G:434:PHE:HE2	1.78	0.48
1:E:278:ALA:HA	1:E:441:PHE:CE2	2.49	0.48
1:C:31:PRO:HB3	1:C:331:ILE:O	2.14	0.47
1:A:490:LEU:HD13	1:B:273:ARG:NH1	2.29	0.47
1:E:224:VAL:O	1:E:248:LYS:HE3	2.14	0.47
1:B:55:ALA:HA	1:B:202:GLY:O	2.14	0.47
1:B:100:TYR:CD2	1:B:323:GLU:HB3	2.49	0.47
1:G:490:LEU:HD13	1:H:273:ARG:NH1	2.29	0.47
1:D:228:THR:OG1	1:D:460:GLU:OE2	2.31	0.47
1:G:91:ILE:O	1:G:95:GLU:HB3	2.15	0.47
1:D:178:LYS:NZ	1:D:179:PRO:O	2.47	0.47
1:D:384:PHE:CE1	2:D:500:NAP:H2D	2.50	0.47
1:G:181:SER:O	1:G:184:PRO:HD3	2.15	0.47
1:C:91:ILE:O	1:C:95:GLU:HB3	2.14	0.47
1:E:28:LYS:NZ	1:E:29:THR:O	2.42	0.47
1:E:383:VAL:HG11	1:E:387:VAL:HB	1.97	0.46
1:G:168:THR:HG22	1:G:173:ASN:HB2	1.97	0.46
1:B:45:ARG:HH22	1:B:216:GLU:HG2	1.81	0.46
1:E:483:ARG:HG2	1:E:484:PHE:N	2.30	0.46
1:F:189:LEU:O	1:F:192:GLN:HB2	2.14	0.46
1:B:106:GLU:HG3	1:B:159:SER:HB3	1.96	0.46
1:C:224:VAL:O	1:C:248:LYS:HE3	2.15	0.46
1:F:378:ILE:HG22	1:F:383:VAL:HG21	1.97	0.46
1:H:29:THR:HG22	1:H:36:LYS:HA	1.98	0.46
1:B:415:LEU:HA	1:B:437:ASN:OD1	2.16	0.46
1:H:314:LEU:HD13	1:H:327:LEU:HD11	1.98	0.46
1:H:448:PRO:HB3	1:H:464:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:NZ	1:A:179:PRO:O	2.47	0.46
1:C:252:LEU:HB3	1:C:254:LEU:HD21	1.97	0.46
1:G:254:LEU:O	2:G:500:NAP:H2N	2.16	0.46
1:A:11:ASN:O	1:A:17:PHE:HA	2.16	0.46
1:B:414:VAL:HG12	1:B:434:PHE:HE2	1.81	0.46
1:D:352:ARG:HB3	1:D:370:VAL:HG23	1.98	0.46
1:F:384:PHE:CE1	2:F:500:NAP:H2D	2.51	0.46
1:A:137:ILE:HD12	1:C:423:PHE:CD2	2.51	0.45
1:D:210:PRO:HB2	1:D:213:VAL:HG13	1.98	0.45
1:H:448:PRO:HB3	1:H:464:TRP:CD2	2.52	0.45
1:A:485:PRO:HB2	1:B:101:ARG:HG2	1.99	0.45
1:C:219:VAL:O	1:C:248:LYS:NZ	2.33	0.45
1:F:99:THR:O	1:F:103:VAL:HG13	2.17	0.45
1:F:194:VAL:HG11	1:F:204:PHE:HB3	1.98	0.45
1:H:442:LEU:HD23	1:H:442:LEU:HA	1.80	0.45
1:H:254:LEU:HD22	1:H:456:GLY:HA2	1.99	0.45
1:A:370:VAL:HG12	1:A:390:ILE:HB	1.98	0.45
1:B:194:VAL:HG11	1:B:204:PHE:HB3	1.99	0.45
1:A:304:ILE:O	1:A:308:VAL:HG23	2.16	0.45
1:H:89:MET:HE3	1:H:104:TRP:HA	1.98	0.45
1:H:448:PRO:HB3	1:H:464:TRP:CG	2.52	0.45
1:A:91:ILE:O	1:A:95:GLU:HB3	2.17	0.45
1:F:253:GLU:HB3	2:F:500:NAP:C7N	2.47	0.45
1:H:448:PRO:HB3	1:H:464:TRP:CD1	2.52	0.45
1:D:254:LEU:O	2:D:500:NAP:H2N	2.17	0.44
1:A:178:LYS:O	1:A:178:LYS:HG3	2.15	0.44
1:C:450:GLY:HA3	1:C:459:ARG:HD3	1.99	0.44
1:G:78:LEU:HD22	1:G:115:GLN:HG3	2.00	0.44
1:A:153:PRO:HD3	1:A:230:THR:HB	1.99	0.44
1:C:270:TYR:CE1	1:D:481:THR:HB	2.52	0.44
1:E:245:GLY:O	1:F:237:ARG:HD3	2.18	0.44
1:E:253:GLU:HB3	2:E:500:NAP:C7N	2.47	0.44
1:F:27:VAL:HG22	1:F:39:GLU:HG2	1.99	0.44
1:F:178:LYS:HE2	1:F:209:GLY:O	2.18	0.44
1:B:282:HIS:O	1:B:285:GLN:HB2	2.17	0.44
1:E:61:ALA:O	1:E:65:ILE:HG23	2.17	0.44
1:B:252:LEU:O	1:B:456:GLY:HA3	2.17	0.44
1:E:258:ASP:OD2	1:E:411:SER:HB3	2.18	0.44
1:D:307:TYR:O	1:D:311:VAL:HG23	2.17	0.44
1:F:73:TYR:CE1	1:F:200:PRO:HD3	2.53	0.44
1:C:258:ASP:OD2	1:C:411:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ASP:OD1	1:E:310:TYR:OH	2.34	0.44
1:E:358:ARG:NH2	4:E:601:HOH:O	2.49	0.44
1:D:313:MET:HE2	1:D:313:MET:HB3	1.68	0.43
1:G:291:LYS:HE2	1:G:382:GLU:CG	2.48	0.43
1:H:278:ALA:HA	1:H:441:PHE:CE2	2.53	0.43
1:A:316:ILE:HG12	1:A:327:LEU:HB2	2.00	0.43
1:B:406:THR:CG2	1:B:408:TYR:H	2.31	0.43
1:C:9:VAL:O	1:C:41:PRO:HD3	2.18	0.43
1:C:9:VAL:HG13	1:C:188:TRP:CD1	2.53	0.43
1:F:355:ILE:HG12	1:F:356:GLY:N	2.33	0.43
1:H:331:ILE:HG22	1:H:335:GLN:HG3	2.00	0.43
1:A:193:MET:HE2	1:A:193:MET:HB3	1.81	0.43
1:E:316:ILE:HD12	1:E:365:GLU:HG2	2.00	0.43
1:D:463:GLU:O	1:D:466:PHE:HB2	2.18	0.43
1:E:366:PRO:HA	1:E:386:PRO:HB2	2.00	0.43
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.91	0.43
1:B:193:MET:HB3	1:B:193:MET:HE2	1.70	0.43
1:C:14:ASN:HB2	1:C:54:SER:OG	2.18	0.43
1:E:91:ILE:O	1:E:95:GLU:HB3	2.18	0.43
1:D:102:LYS:HE2	1:D:156:TYR:CZ	2.53	0.43
1:D:411:SER:HB2	1:D:433:MET:HE3	1.99	0.43
1:G:27:VAL:HG11	1:G:36:LYS:HG3	2.00	0.43
1:H:90:LYS:HA	1:H:90:LYS:HD3	1.69	0.43
1:E:273:ARG:HH11	1:F:490:LEU:HD13	1.84	0.43
1:E:318:ASP:HB3	1:E:321:LYS:HG3	2.00	0.43
1:B:306:ARG:HD2	1:B:306:ARG:HA	1.65	0.43
1:C:155:ASN:HD21	2:C:500:NAP:H5N	1.83	0.43
1:B:383:VAL:HG11	1:B:387:VAL:HB	1.99	0.43
1:D:442:LEU:HD23	1:D:442:LEU:HA	1.89	0.43
1:A:445:SER:OG	1:C:122:ARG:NH2	2.52	0.42
1:B:224:VAL:O	1:B:248:LYS:HE3	2.19	0.42
1:C:78:LEU:O	1:C:82:ARG:HG3	2.19	0.42
1:G:436:ILE:HD12	1:H:477:VAL:HG22	2.01	0.42
1:H:211:GLY:N	2:H:500:NAP:O3X	2.43	0.42
1:B:406:THR:HG23	4:B:607:HOH:O	2.18	0.42
1:F:326:ASP:O	1:F:327:LEU:HD23	2.20	0.42
1:B:255:GLY:HA2	2:B:500:NAP:O2D	2.18	0.42
1:D:160:ILE:HG23	3:D:501:5OZ:C02	2.49	0.42
1:F:81:PHE:HB2	1:F:193:MET:SD	2.59	0.42
1:B:286:ILE:HB	1:B:289:SER:HB2	2.02	0.42
1:A:306:ARG:HD3	1:A:306:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ASP:OD1	1:E:264:ASP:N	2.30	0.42
1:F:178:LYS:NZ	1:F:179:PRO:O	2.52	0.42
1:F:306:ARG:HA	1:F:309:HIS:HB3	2.01	0.42
1:B:127:ARG:HA	1:B:127:ARG:HD3	1.88	0.42
1:A:273:ARG:NH1	1:B:490:LEU:HD13	2.35	0.42
1:B:448:PRO:HD3	1:B:464:TRP:CZ3	2.55	0.42
1:G:89:MET:HG3	1:G:107:VAL:HG21	2.02	0.42
1:H:77:MET:HE3	1:H:77:MET:HB3	1.75	0.42
1:H:181:SER:O	1:H:184:PRO:HD3	2.20	0.42
1:B:378:ILE:HG22	1:B:383:VAL:HG21	2.02	0.42
1:F:253:GLU:HB3	2:F:500:NAP:N7N	2.35	0.42
1:B:154:TRP:CH2	1:B:285:GLN:HG2	2.55	0.42
1:C:414:VAL:HG12	1:C:434:PHE:HE2	1.85	0.42
1:G:383:VAL:HG11	1:G:387:VAL:HB	2.02	0.42
1:D:189:LEU:HD23	1:D:189:LEU:HA	1.84	0.42
1:H:314:LEU:HD23	1:H:314:LEU:HA	1.91	0.42
1:A:253:GLU:HB3	2:A:500:NAP:N7N	2.35	0.41
1:C:28:LYS:HE2	1:C:95:GLU:HG3	2.02	0.41
1:F:102:LYS:HE2	1:F:156:TYR:CZ	2.55	0.41
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.88	0.41
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.82	0.41
1:C:90:LYS:O	1:C:94:VAL:HG12	2.21	0.41
1:G:475:VAL:HA	1:H:434:PHE:O	2.20	0.41
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.80	0.41
1:B:258:ASP:OD2	1:B:411:SER:HB3	2.20	0.41
1:G:263:LEU:HD12	1:G:416:THR:HB	2.02	0.41
1:B:154:TRP:HH2	1:B:285:GLN:HG2	1.86	0.41
1:D:253:GLU:HB3	2:D:500:NAP:N7N	2.34	0.41
1:E:270:TYR:CE1	1:F:481:THR:HB	2.55	0.41
1:A:123:HIS:CG	1:C:120:LEU:HD21	2.55	0.41
1:E:14:ASN:O	1:E:201:LYS:HB2	2.20	0.41
1:E:230:THR:OG1	1:E:253:GLU:HB2	2.21	0.41
1:F:279:SER:HB2	1:F:388:ARG:HG3	2.02	0.41
1:C:65:ILE:HD12	1:C:69:ARG:HB3	2.03	0.41
1:D:88:PHE:CE1	1:D:189:LEU:HB3	2.55	0.41
1:E:102:LYS:HE3	1:E:282:HIS:CE1	2.55	0.41
1:E:310:TYR:HA	1:E:313:MET:HG3	2.02	0.41
1:G:153:PRO:HG3	1:G:230:THR:HG22	2.01	0.41
1:A:90:LYS:HA	1:A:90:LYS:HD3	1.87	0.41
1:F:272:ALA:HA	1:F:303:PHE:CE1	2.56	0.41
1:H:148:VAL:HG23	1:H:173:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:CD2	1:C:137:ILE:HD12	2.56	0.41
1:C:77:MET:HB2	1:C:77:MET:HE3	1.65	0.41
1:D:252:LEU:O	1:D:456:GLY:HA3	2.21	0.41
1:G:365:GLU:HA	1:G:366:PRO:HD3	1.96	0.41
1:H:286:ILE:HG22	1:H:288:THR:H	1.85	0.41
1:A:356:GLY:HA3	1:A:366:PRO:O	2.20	0.41
1:C:457:VAL:CG2	1:D:249:THR:HG22	2.51	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.76	0.41
1:D:258:ASP:OD2	1:D:411:SER:HB3	2.21	0.41
1:D:343:VAL:HG13	1:D:369:PHE:HZ	1.84	0.41
1:E:59:LEU:HD21	1:E:146:GLY:HA2	2.02	0.41
1:E:336:VAL:HG13	1:E:364:PHE:HD2	1.86	0.41
1:A:287:CYS:SG	2:A:500:NAP:C3N	3.09	0.41
1:A:255:GLY:HA2	2:A:500:NAP:O2D	2.21	0.40
1:B:68:ILE:O	1:B:72:GLU:HG3	2.21	0.40
1:B:178:LYS:HE2	1:B:211:GLY:HA2	2.02	0.40
1:C:314:LEU:HD13	1:C:327:LEU:HD11	2.03	0.40
1:F:100:TYR:CD2	1:F:323:GLU:HB3	2.57	0.40
1:G:304:ILE:O	1:G:308:VAL:HG23	2.21	0.40
1:H:20:PRO:HD3	1:H:41:PRO:HB3	2.02	0.40
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.82	0.40
1:A:137:ILE:HD12	1:C:423:PHE:HD2	1.86	0.40
1:A:444:GLU:HB2	1:A:447:VAL:HG13	2.03	0.40
1:B:268:VAL:HG11	1:B:302:LYS:HG2	2.03	0.40
1:E:102:LYS:HE3	1:E:282:HIS:CD2	2.56	0.40
1:F:366:PRO:HA	1:F:386:PRO:HB2	2.03	0.40
1:F:422:ALA:HB1	1:F:436:ILE:HD13	2.03	0.40
1:H:258:ASP:OD2	1:H:411:SER:HB3	2.22	0.40
1:A:86:GLU:O	1:A:90:LYS:HG2	2.21	0.40
1:C:487:PRO:C	1:C:489:ALA:H	2.30	0.40
1:G:331:ILE:HG22	1:G:335:GLN:HG3	2.03	0.40
1:H:231:GLY:O	1:H:254:LEU:HA	2.21	0.40
1:H:297:LYS:HD2	1:H:392:VAL:HG12	2.03	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	481/491 (98%)	456 (95%)	24 (5%)	1 (0%)	43	60
1	B	482/491 (98%)	464 (96%)	17 (4%)	1 (0%)	43	60
1	C	483/491 (98%)	464 (96%)	18 (4%)	1 (0%)	43	60
1	D	483/491 (98%)	462 (96%)	21 (4%)	0	100	100
1	E	483/491 (98%)	462 (96%)	18 (4%)	3 (1%)	21	34
1	F	481/491 (98%)	462 (96%)	19 (4%)	0	100	100
1	G	482/491 (98%)	459 (95%)	23 (5%)	0	100	100
1	H	481/491 (98%)	461 (96%)	18 (4%)	2 (0%)	30	45
All	All	3856/3928 (98%)	3690 (96%)	158 (4%)	8 (0%)	43	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	285	GLN
1	E	297	LYS
1	E	153	PRO
1	H	153	PRO
1	B	409	GLY
1	A	409	GLY
1	E	23	GLY
1	H	409	GLY

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	395/408 (97%)	389 (98%)	6 (2%)	57	75
1	B	397/408 (97%)	386 (97%)	11 (3%)	38	60
1	C	395/408 (97%)	388 (98%)	7 (2%)	51	72
1	D	398/408 (98%)	391 (98%)	7 (2%)	51	72
1	E	395/408 (97%)	388 (98%)	7 (2%)	51	72
1	F	396/408 (97%)	391 (99%)	5 (1%)	61	77
1	G	397/408 (97%)	388 (98%)	9 (2%)	44	66
1	H	394/408 (97%)	385 (98%)	9 (2%)	44	66
All	All	3167/3264 (97%)	3106 (98%)	61 (2%)	50	71

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	VAL
1	A	144	SER
1	A	171	VAL
1	A	238	GLU
1	A	295	VAL
1	A	297	LYS
1	B	9	VAL
1	B	13	ILE
1	B	40	VAL
1	B	147	VAL
1	B	285	GLN
1	B	305	GLU
1	B	352	ARG
1	B	372	VAL
1	B	401	GLU
1	B	406	THR
1	B	447	VAL
1	C	46	GLU
1	C	147	VAL
1	C	178	LYS
1	C	238	GLU
1	C	285	GLN
1	C	288	THR
1	C	295	VAL
1	D	9	VAL
1	D	107	VAL
1	D	213	VAL

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Mol	Chain	Res	Type
1	D	239	ILE
1	D	288	THR
1	D	372	VAL
1	D	482	ARG
1	E	40	VAL
1	E	144	SER
1	E	171	VAL
1	E	214	VAL
1	E	306	ARG
1	E	370	VAL
1	E	439	VAL
1	F	40	VAL
1	F	77	MET
1	F	254	LEU
1	F	372	VAL
1	F	401	GLU
1	G	107	VAL
1	G	115	GLN
1	G	139	VAL
1	G	144	SER
1	G	178	LYS
1	G	235	THR
1	G	246	THR
1	G	348	SER
1	G	372	VAL
1	H	69	ARG
1	H	77	MET
1	H	107	VAL
1	H	134	GLU
1	H	223	ARG
1	H	250	VAL
1	H	254	LEU
1	H	372	VAL
1	H	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	296	HIS
1	A	309	HIS
1	B	83	GLN

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Mol	Chain	Res	Type
1	C	192	GLN
1	C	285	GLN
1	D	205	ASN
1	D	285	GLN
1	G	285	GLN
1	H	14	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	F	500	-	50,52,52	2.24	17 (34%)	71,80,80	1.70	13 (18%)
2	NAP	E	500	-	50,52,52	2.31	18 (36%)	71,80,80	1.67	15 (21%)
3	5OZ	A	501	-	4,4,4	2.85	1 (25%)	1,4,4	1.10	0
2	NAP	A	500	-	50,52,52	2.32	17 (34%)	71,80,80	1.76	13 (18%)
2	NAP	C	500	-	50,52,52	2.29	16 (32%)	71,80,80	1.75	13 (18%)
3	5OZ	H	501	-	4,4,4	2.87	1 (25%)	1,4,4	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	D	500	-	50,52,52	2.22	15 (30%)	71,80,80	1.64	15 (21%)
3	5OZ	C	501	-	4,4,4	2.87	1 (25%)	1,4,4	0.70	0
2	NAP	H	500	-	50,52,52	2.20	19 (38%)	71,80,80	1.61	13 (18%)
3	5OZ	D	501	-	4,4,4	2.86	1 (25%)	1,4,4	1.20	0
3	5OZ	B	501	-	4,4,4	2.83	1 (25%)	1,4,4	0.60	0
2	NAP	B	500	-	50,52,52	2.25	18 (36%)	71,80,80	1.60	13 (18%)
2	NAP	G	500	-	50,52,52	2.34	17 (34%)	71,80,80	1.74	13 (18%)
3	5OZ	G	501	-	4,4,4	2.84	1 (25%)	1,4,4	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	F	500	-	-	7/35/67/67	0/5/5/5
2	NAP	E	500	-	-	6/35/67/67	0/5/5/5
3	5OZ	A	501	-	-	1/2/2/2	-
2	NAP	A	500	-	-	6/35/67/67	0/5/5/5
2	NAP	C	500	-	-	5/35/67/67	0/5/5/5
3	5OZ	H	501	-	-	2/2/2/2	-
2	NAP	D	500	-	-	5/35/67/67	0/5/5/5
3	5OZ	C	501	-	-	1/2/2/2	-
2	NAP	H	500	-	-	4/35/67/67	0/5/5/5
3	5OZ	D	501	-	-	1/2/2/2	-
3	5OZ	B	501	-	-	2/2/2/2	-
2	NAP	B	500	-	-	3/35/67/67	0/5/5/5
2	NAP	G	500	-	-	4/35/67/67	0/5/5/5
3	5OZ	G	501	-	-	1/2/2/2	-

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	NAP	P2B-O2B	6.31	1.70	1.59
2	G	500	NAP	P2B-O2B	6.08	1.70	1.59
2	C	500	NAP	P2B-O2B	6.01	1.70	1.59
2	A	500	NAP	P2B-O2B	5.90	1.69	1.59
2	B	500	NAP	P2B-O2B	5.87	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	NAP	P2B-O2B	5.74	1.69	1.59
3	H	501	5OZ	O-C02	5.73	1.41	1.20
3	C	501	5OZ	O-C02	5.72	1.41	1.20
3	D	501	5OZ	O-C02	5.72	1.41	1.20
3	A	501	5OZ	O-C02	5.67	1.41	1.20
3	G	501	5OZ	O-C02	5.66	1.41	1.20
3	B	501	5OZ	O-C02	5.65	1.41	1.20
2	D	500	NAP	P2B-O2B	5.41	1.69	1.59
2	B	500	NAP	C6A-N6A	5.40	1.48	1.34
2	C	500	NAP	C6A-N6A	5.30	1.47	1.34
2	H	500	NAP	P2B-O2B	5.24	1.68	1.59
2	A	500	NAP	O7N-C7N	-5.19	1.14	1.24
2	G	500	NAP	C6A-N6A	5.18	1.47	1.34
2	F	500	NAP	O7N-C7N	-5.17	1.14	1.24
2	E	500	NAP	C6A-N6A	5.15	1.47	1.34
2	G	500	NAP	O7N-C7N	-5.10	1.14	1.24
2	A	500	NAP	C6A-N6A	5.09	1.47	1.34
2	H	500	NAP	C6A-N6A	5.04	1.47	1.34
2	F	500	NAP	C6A-N6A	5.04	1.47	1.34
2	C	500	NAP	O7N-C7N	-4.96	1.14	1.24
2	D	500	NAP	O7N-C7N	-4.96	1.14	1.24
2	E	500	NAP	O7N-C7N	-4.93	1.14	1.24
2	D	500	NAP	C6A-N6A	4.90	1.46	1.34
2	B	500	NAP	O7N-C7N	-4.60	1.15	1.24
2	H	500	NAP	O7N-C7N	-4.49	1.15	1.24
2	G	500	NAP	C8A-N9A	-4.12	1.30	1.37
2	E	500	NAP	C8A-N9A	-4.00	1.30	1.37
2	C	500	NAP	C8A-N9A	-3.99	1.30	1.37
2	A	500	NAP	C8A-N9A	-3.96	1.30	1.37
2	A	500	NAP	C3D-C4D	-3.86	1.43	1.53
2	B	500	NAP	C8A-N7A	3.82	1.39	1.31
2	F	500	NAP	C8A-N9A	-3.82	1.31	1.37
2	B	500	NAP	C3B-C4B	-3.77	1.43	1.53
2	E	500	NAP	C3D-C4D	-3.76	1.43	1.53
2	G	500	NAP	C3D-C4D	-3.76	1.43	1.53
2	D	500	NAP	C8A-N7A	3.75	1.38	1.31
2	H	500	NAP	C8A-N9A	-3.74	1.31	1.37
2	B	500	NAP	C8A-N9A	-3.72	1.31	1.37
2	C	500	NAP	C3D-C4D	-3.70	1.43	1.53
2	A	500	NAP	PN-O3	-3.70	1.55	1.59
2	A	500	NAP	C8A-N7A	3.67	1.38	1.31
2	D	500	NAP	C8A-N9A	-3.60	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	C3D-C4D	-3.59	1.43	1.53
2	C	500	NAP	C3B-C4B	-3.53	1.44	1.53
2	B	500	NAP	C3D-C4D	-3.51	1.44	1.53
2	F	500	NAP	C8A-N7A	3.51	1.38	1.31
2	F	500	NAP	PN-O3	-3.49	1.55	1.59
2	E	500	NAP	C8A-N7A	3.44	1.38	1.31
2	A	500	NAP	C3N-C7N	3.42	1.55	1.50
2	D	500	NAP	PN-O3	-3.35	1.55	1.59
2	C	500	NAP	C8A-N7A	3.35	1.38	1.31
2	H	500	NAP	C8A-N7A	3.34	1.38	1.31
2	H	500	NAP	C3B-C4B	-3.34	1.44	1.53
2	D	500	NAP	C3B-C4B	-3.33	1.44	1.53
2	G	500	NAP	O4D-C1D	3.30	1.45	1.40
2	F	500	NAP	C1B-N9A	-3.30	1.37	1.46
2	H	500	NAP	C3D-C4D	-3.30	1.44	1.53
2	F	500	NAP	C3D-C4D	-3.28	1.44	1.53
2	G	500	NAP	PN-O3	-3.25	1.56	1.59
2	E	500	NAP	C3B-C4B	-3.22	1.44	1.53
2	C	500	NAP	C4A-N3A	3.19	1.40	1.34
2	F	500	NAP	C3B-C4B	-3.18	1.44	1.53
2	G	500	NAP	C8A-N7A	3.17	1.37	1.31
2	E	500	NAP	C1B-N9A	-3.16	1.37	1.46
2	A	500	NAP	C3B-C4B	-3.15	1.45	1.53
2	B	500	NAP	C3N-C7N	3.14	1.55	1.50
2	E	500	NAP	C3N-C7N	3.12	1.55	1.50
2	G	500	NAP	C4A-N3A	3.12	1.40	1.34
2	E	500	NAP	PN-O3	-3.10	1.56	1.59
2	C	500	NAP	PN-O3	-3.07	1.56	1.59
2	D	500	NAP	C3N-C7N	3.06	1.55	1.50
2	A	500	NAP	C1B-N9A	-3.05	1.37	1.46
2	G	500	NAP	C3B-C4B	-3.04	1.45	1.53
2	B	500	NAP	C1B-N9A	-3.03	1.38	1.46
2	G	500	NAP	C3N-C7N	2.98	1.55	1.50
2	H	500	NAP	O3B-C3B	2.95	1.50	1.43
2	C	500	NAP	C3N-C7N	2.93	1.55	1.50
2	G	500	NAP	O2D-C2D	-2.91	1.35	1.43
2	G	500	NAP	C7N-N7N	2.90	1.38	1.33
2	D	500	NAP	O2D-C2D	-2.88	1.35	1.43
2	E	500	NAP	C4N-C3N	2.87	1.43	1.39
2	G	500	NAP	C1B-N9A	-2.86	1.38	1.46
2	H	500	NAP	C1B-N9A	-2.82	1.38	1.46
2	A	500	NAP	O3B-C3B	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAP	C4N-C3N	2.77	1.43	1.39
2	E	500	NAP	C4A-N3A	2.75	1.39	1.34
2	F	500	NAP	O3B-C3B	2.74	1.49	1.43
2	F	500	NAP	O4D-C1D	2.73	1.44	1.40
2	H	500	NAP	C4A-N3A	2.71	1.39	1.34
2	C	500	NAP	O2D-C2D	-2.70	1.36	1.43
2	D	500	NAP	C1B-N9A	-2.69	1.38	1.46
2	H	500	NAP	C3N-C7N	2.69	1.54	1.50
2	H	500	NAP	PN-O1N	2.69	1.60	1.50
2	H	500	NAP	O4D-C1D	2.68	1.44	1.40
2	H	500	NAP	C7N-N7N	2.67	1.37	1.33
2	F	500	NAP	C4A-N3A	2.67	1.39	1.34
2	D	500	NAP	O3B-C3B	2.66	1.49	1.43
2	B	500	NAP	C7N-N7N	2.66	1.37	1.33
2	F	500	NAP	O2D-C2D	-2.65	1.36	1.43
2	C	500	NAP	C7N-N7N	2.63	1.37	1.33
2	A	500	NAP	C4A-N3A	2.62	1.39	1.34
2	B	500	NAP	O4D-C1D	2.61	1.44	1.40
2	E	500	NAP	O2D-C2D	-2.60	1.36	1.43
2	B	500	NAP	O2D-C2D	-2.60	1.36	1.43
2	A	500	NAP	C7N-N7N	2.59	1.37	1.33
2	C	500	NAP	C1B-N9A	-2.59	1.39	1.46
2	G	500	NAP	O3B-C3B	2.55	1.49	1.43
2	C	500	NAP	O3B-C3B	2.55	1.49	1.43
2	D	500	NAP	PN-O1N	2.55	1.59	1.50
2	B	500	NAP	PN-O1N	2.53	1.59	1.50
2	A	500	NAP	O2D-C2D	-2.52	1.36	1.43
2	H	500	NAP	O2D-C2D	-2.52	1.36	1.43
2	C	500	NAP	PN-O1N	2.51	1.59	1.50
2	D	500	NAP	C7N-N7N	2.50	1.37	1.33
2	A	500	NAP	O4D-C1D	2.48	1.44	1.40
2	B	500	NAP	C4A-N3A	2.47	1.39	1.34
2	D	500	NAP	C4A-N3A	2.47	1.39	1.34
2	C	500	NAP	C4N-C3N	2.46	1.43	1.39
2	B	500	NAP	PN-O3	-2.46	1.56	1.59
2	E	500	NAP	C7N-N7N	2.45	1.37	1.33
2	G	500	NAP	PN-O1N	2.44	1.59	1.50
2	F	500	NAP	PN-O1N	2.44	1.59	1.50
2	E	500	NAP	PN-O1N	2.43	1.59	1.50
2	E	500	NAP	O3B-C3B	2.42	1.48	1.43
2	A	500	NAP	PN-O1N	2.38	1.59	1.50
2	F	500	NAP	C7N-N7N	2.35	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	NAP	C3N-C7N	2.34	1.54	1.50
2	G	500	NAP	C4N-C3N	2.33	1.42	1.39
2	E	500	NAP	O4D-C1D	2.31	1.43	1.40
2	B	500	NAP	C4N-C3N	2.28	1.42	1.39
2	H	500	NAP	C5A-N7A	-2.27	1.34	1.39
2	H	500	NAP	PN-O3	-2.26	1.57	1.59
2	F	500	NAP	C4N-C3N	2.13	1.42	1.39
2	E	500	NAP	C3B-C2B	-2.07	1.48	1.53
2	H	500	NAP	O3D-C3D	2.04	1.48	1.43
2	B	500	NAP	O3B-C3B	2.03	1.48	1.43
2	B	500	NAP	C3B-C2B	-2.03	1.48	1.53
2	H	500	NAP	C4N-C3N	2.01	1.42	1.39

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	NAP	C3N-C7N-N7N	5.34	124.32	117.74
2	E	500	NAP	C4D-O4D-C1D	-5.19	105.17	109.92
2	C	500	NAP	C4D-O4D-C1D	-5.15	105.21	109.92
2	A	500	NAP	C5A-C4A-N3A	-4.89	119.98	126.72
2	A	500	NAP	C3N-C7N-N7N	4.86	123.73	117.74
2	F	500	NAP	C4D-O4D-C1D	-4.72	105.60	109.92
2	C	500	NAP	C5A-C4A-N3A	-4.68	120.27	126.72
2	E	500	NAP	C5A-C4A-N3A	-4.49	120.54	126.72
2	F	500	NAP	C4A-N9A-C8A	4.40	110.36	105.74
2	H	500	NAP	C5A-C4A-N3A	-4.37	120.71	126.72
2	B	500	NAP	C5A-C4A-N3A	-4.26	120.86	126.72
2	A	500	NAP	C4A-C5A-N7A	-4.25	105.72	110.58
2	G	500	NAP	C5A-C4A-N3A	-4.21	120.92	126.72
2	F	500	NAP	C5A-C4A-N3A	-4.21	120.92	126.72
2	H	500	NAP	C4D-O4D-C1D	-4.18	106.09	109.92
2	F	500	NAP	N9A-C8A-N7A	-4.17	108.01	113.94
2	C	500	NAP	N3A-C2A-N1A	-4.17	122.26	128.58
2	D	500	NAP	C4A-C5A-N7A	-4.13	105.86	110.58
2	G	500	NAP	C4A-N9A-C8A	4.11	110.05	105.74
2	A	500	NAP	C5A-N7A-C8A	4.01	109.75	103.45
2	H	500	NAP	C5A-N7A-C8A	4.00	109.73	103.45
2	H	500	NAP	C4A-C5A-N7A	-3.99	106.02	110.58
2	F	500	NAP	C4A-C5A-N7A	-3.96	106.06	110.58
2	E	500	NAP	C4A-N9A-C8A	3.94	109.87	105.74
2	D	500	NAP	C5A-C4A-N3A	-3.90	121.34	126.72
2	A	500	NAP	C4D-O4D-C1D	-3.84	106.40	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAP	N9A-C8A-N7A	-3.84	108.49	113.94
2	C	500	NAP	C5A-N7A-C8A	3.84	109.48	103.45
2	F	500	NAP	C5A-N7A-C8A	3.82	109.46	103.45
2	C	500	NAP	N3A-C4A-N9A	3.77	133.58	127.17
2	B	500	NAP	C4D-O4D-C1D	-3.76	106.48	109.92
2	G	500	NAP	N9A-C8A-N7A	-3.75	108.62	113.94
2	E	500	NAP	N3A-C4A-N9A	3.74	133.53	127.17
2	G	500	NAP	C4A-C5A-N7A	-3.70	106.35	110.58
2	C	500	NAP	C4A-C5A-N7A	-3.69	106.37	110.58
2	A	500	NAP	N3A-C4A-N9A	3.67	133.40	127.17
2	G	500	NAP	C5A-N7A-C8A	3.66	109.21	103.45
2	D	500	NAP	C3N-C7N-N7N	3.65	122.24	117.74
2	B	500	NAP	C4A-C5A-N7A	-3.65	106.41	110.58
2	H	500	NAP	N9A-C8A-N7A	-3.64	108.77	113.94
2	C	500	NAP	N9A-C8A-N7A	-3.64	108.78	113.94
2	D	500	NAP	C5A-N7A-C8A	3.63	109.16	103.45
2	D	500	NAP	N9A-C8A-N7A	-3.62	108.79	113.94
2	G	500	NAP	N3A-C4A-N9A	3.62	133.32	127.17
2	E	500	NAP	N9A-C8A-N7A	-3.56	108.89	113.94
2	F	500	NAP	N3A-C2A-N1A	-3.53	123.24	128.58
2	A	500	NAP	C4A-N9A-C8A	3.51	109.42	105.74
2	E	500	NAP	C4A-C5A-N7A	-3.48	106.61	110.58
2	D	500	NAP	C4D-O4D-C1D	-3.43	106.78	109.92
2	B	500	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	G	500	NAP	N3A-C2A-N1A	-3.42	123.40	128.58
2	F	500	NAP	N3A-C4A-N9A	3.41	132.97	127.17
2	D	500	NAP	C4A-N9A-C8A	3.41	109.32	105.74
2	B	500	NAP	N3A-C2A-N1A	-3.41	123.42	128.58
2	B	500	NAP	N9A-C8A-N7A	-3.37	109.15	113.94
2	E	500	NAP	C5A-N7A-C8A	3.35	108.71	103.45
2	C	500	NAP	C2A-N3A-C4A	3.34	119.99	111.83
2	H	500	NAP	N3A-C4A-N9A	3.33	132.84	127.17
2	G	500	NAP	C4D-O4D-C1D	-3.33	106.87	109.92
2	H	500	NAP	O4B-C1B-C2B	-3.33	100.86	106.59
2	C	500	NAP	C4A-N9A-C8A	3.32	109.22	105.74
2	A	500	NAP	N3A-C2A-N1A	-3.31	123.56	128.58
2	D	500	NAP	N3A-C2A-N1A	-3.28	123.62	128.58
2	H	500	NAP	N3A-C2A-N1A	-3.26	123.64	128.58
2	C	500	NAP	C3N-C7N-N7N	3.25	121.74	117.74
2	B	500	NAP	O4B-C1B-C2B	-3.23	101.03	106.59
2	B	500	NAP	N3A-C4A-N9A	3.22	132.65	127.17
2	B	500	NAP	P2B-O2B-C2B	-3.22	114.83	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAP	C4A-N9A-C8A	3.21	109.11	105.74
2	H	500	NAP	C4A-N9A-C8A	3.13	109.02	105.74
2	A	500	NAP	C2A-N3A-C4A	3.12	119.44	111.83
2	E	500	NAP	N3A-C2A-N1A	-3.07	123.94	128.58
2	A	500	NAP	O7N-C7N-N7N	-3.04	118.22	122.62
2	F	500	NAP	C2A-N3A-C4A	3.03	119.24	111.83
2	G	500	NAP	O7N-C7N-C3N	-2.95	116.00	119.60
2	D	500	NAP	P2B-O2B-C2B	-2.91	115.66	123.43
2	E	500	NAP	C2A-N3A-C4A	2.89	118.90	111.83
2	B	500	NAP	C2A-N3A-C4A	2.87	118.84	111.83
2	D	500	NAP	C6A-C5A-N7A	2.80	137.49	132.09
2	F	500	NAP	C6A-C5A-N7A	2.79	137.47	132.09
2	D	500	NAP	C2A-N3A-C4A	2.76	118.56	111.83
2	D	500	NAP	N3A-C4A-N9A	2.72	131.79	127.17
2	H	500	NAP	C2A-N3A-C4A	2.72	118.47	111.83
2	G	500	NAP	C2A-N3A-C4A	2.71	118.46	111.83
2	E	500	NAP	C3N-C7N-N7N	2.64	120.99	117.74
2	C	500	NAP	P2B-O2B-C2B	-2.63	116.41	123.43
2	D	500	NAP	O7N-C7N-N7N	-2.60	118.86	122.62
2	A	500	NAP	P2B-O2B-C2B	-2.53	116.67	123.43
2	A	500	NAP	C6A-C5A-N7A	2.49	136.89	132.09
2	E	500	NAP	O7N-C7N-N7N	-2.48	119.03	122.62
2	C	500	NAP	C6A-C5A-N7A	2.45	136.82	132.09
2	D	500	NAP	O4B-C1B-N9A	2.38	112.66	108.09
2	D	500	NAP	C4A-N9A-C1B	-2.36	121.11	126.63
2	F	500	NAP	P2B-O2B-C2B	-2.32	117.24	123.43
2	H	500	NAP	C3N-C7N-N7N	2.31	120.58	117.74
2	E	500	NAP	C4B-O4B-C1B	-2.28	104.43	109.47
2	E	500	NAP	C6A-C5A-N7A	2.23	136.39	132.09
2	F	500	NAP	C4A-N9A-C1B	-2.21	121.45	126.63
2	H	500	NAP	C6A-C5A-N7A	2.20	136.33	132.09
2	B	500	NAP	C6A-C5A-N7A	2.19	136.31	132.09
2	B	500	NAP	C3N-C7N-N7N	2.19	120.43	117.74
2	E	500	NAP	P2B-O2B-C2B	-2.14	117.70	123.43
2	G	500	NAP	C6A-C5A-N7A	2.06	136.06	132.09
2	C	500	NAP	O7N-C7N-N7N	-2.05	119.65	122.62
2	G	500	NAP	O7N-C7N-N7N	-2.03	119.69	122.62
2	E	500	NAP	O4B-C4B-C3B	2.03	109.17	105.15
2	H	500	NAP	P2B-O2B-C2B	-2.01	118.05	123.43
2	F	500	NAP	C3N-C7N-N7N	2.00	120.20	117.74

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	500	NAP	C5B-O5B-PA-O1A
2	F	500	NAP	C5B-O5B-PA-O3
3	A	501	5OZ	C-C01-C02-O
3	B	501	5OZ	C03-C01-C02-O
3	B	501	5OZ	C-C01-C02-O
3	D	501	5OZ	C-C01-C02-O
3	G	501	5OZ	C-C01-C02-O
3	H	501	5OZ	C03-C01-C02-O
2	B	500	NAP	PN-O3-PA-O5B
2	C	500	NAP	PN-O3-PA-O5B
2	E	500	NAP	PN-O3-PA-O5B
2	H	500	NAP	PN-O3-PA-O5B
2	A	500	NAP	C2B-C1B-N9A-C8A
2	C	500	NAP	C2B-C1B-N9A-C8A
2	D	500	NAP	C2B-C1B-N9A-C8A
2	E	500	NAP	C2B-C1B-N9A-C8A
2	F	500	NAP	C2B-C1B-N9A-C8A
2	G	500	NAP	C2B-C1B-N9A-C8A
2	H	500	NAP	C2B-C1B-N9A-C8A
2	A	500	NAP	C4D-C5D-O5D-PN
2	A	500	NAP	C5B-O5B-PA-O1A
2	D	500	NAP	C5B-O5B-PA-O1A
2	D	500	NAP	C5B-O5B-PA-O2A
2	D	500	NAP	C5B-O5B-PA-O3
2	B	500	NAP	C4D-C5D-O5D-PN
2	D	500	NAP	C4D-C5D-O5D-PN
2	E	500	NAP	C4D-C5D-O5D-PN
2	G	500	NAP	C4D-C5D-O5D-PN
2	H	500	NAP	C4D-C5D-O5D-PN
2	G	500	NAP	C2B-C1B-N9A-C4A
2	A	500	NAP	C2B-O2B-P2B-O2X
2	F	500	NAP	C2B-O2B-P2B-O2X
2	F	500	NAP	C4D-C5D-O5D-PN
2	B	500	NAP	C2B-C1B-N9A-C8A
2	F	500	NAP	C2B-C1B-N9A-C4A
2	C	500	NAP	C4D-C5D-O5D-PN
2	G	500	NAP	O4B-C1B-N9A-C8A
2	C	500	NAP	C2B-O2B-P2B-O3X
2	A	500	NAP	C2B-C1B-N9A-C4A
2	H	500	NAP	C2B-C1B-N9A-C4A
2	A	500	NAP	O4B-C1B-N9A-C8A
2	C	500	NAP	O4B-C1B-N9A-C8A

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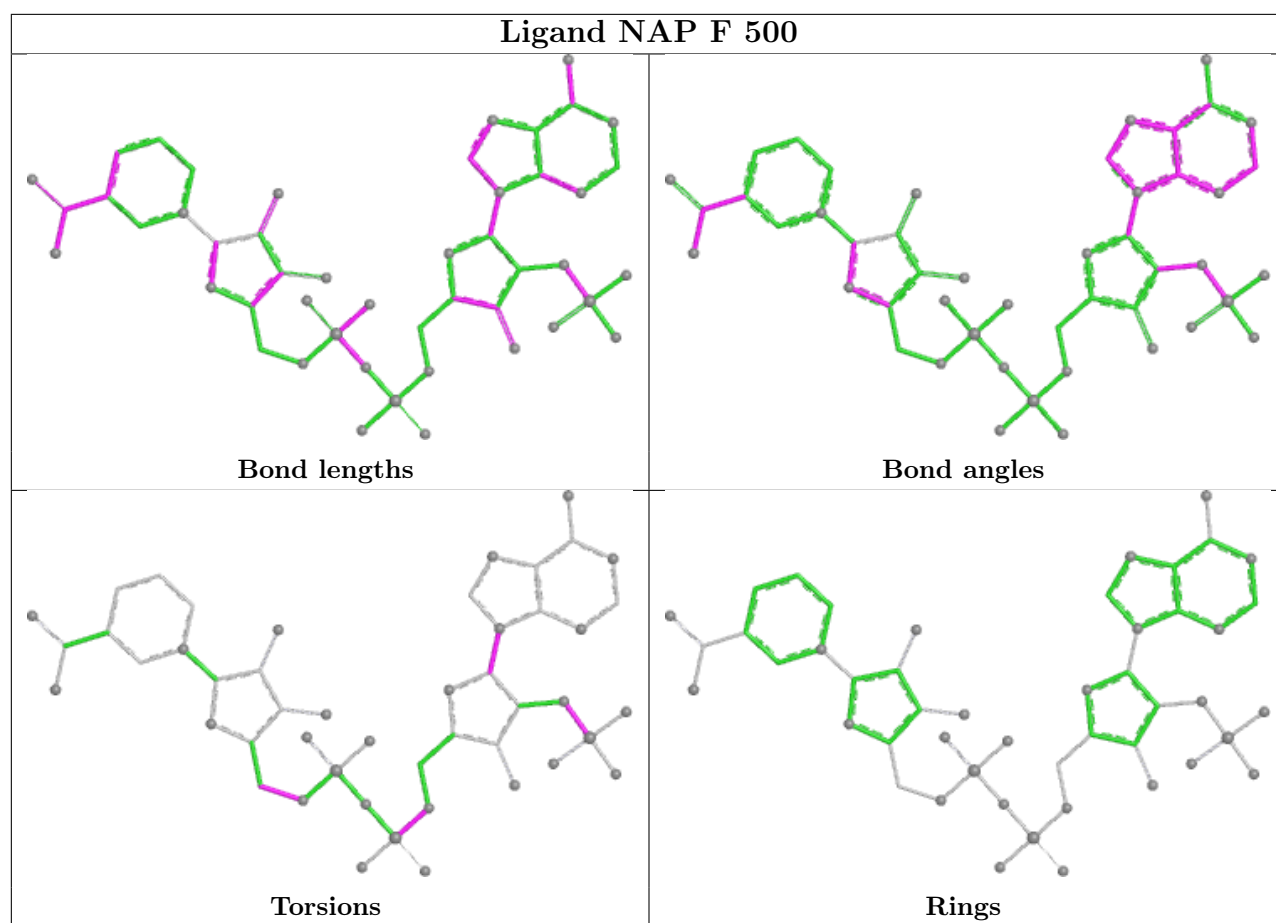
Mol	Chain	Res	Type	Atoms
2	E	500	NAP	O4B-C1B-N9A-C8A
2	F	500	NAP	O4B-C1B-N9A-C8A
3	C	501	5OZ	C-C01-C02-O
3	H	501	5OZ	C-C01-C02-O
2	E	500	NAP	C2B-C1B-N9A-C4A
2	E	500	NAP	O4D-C4D-C5D-O5D

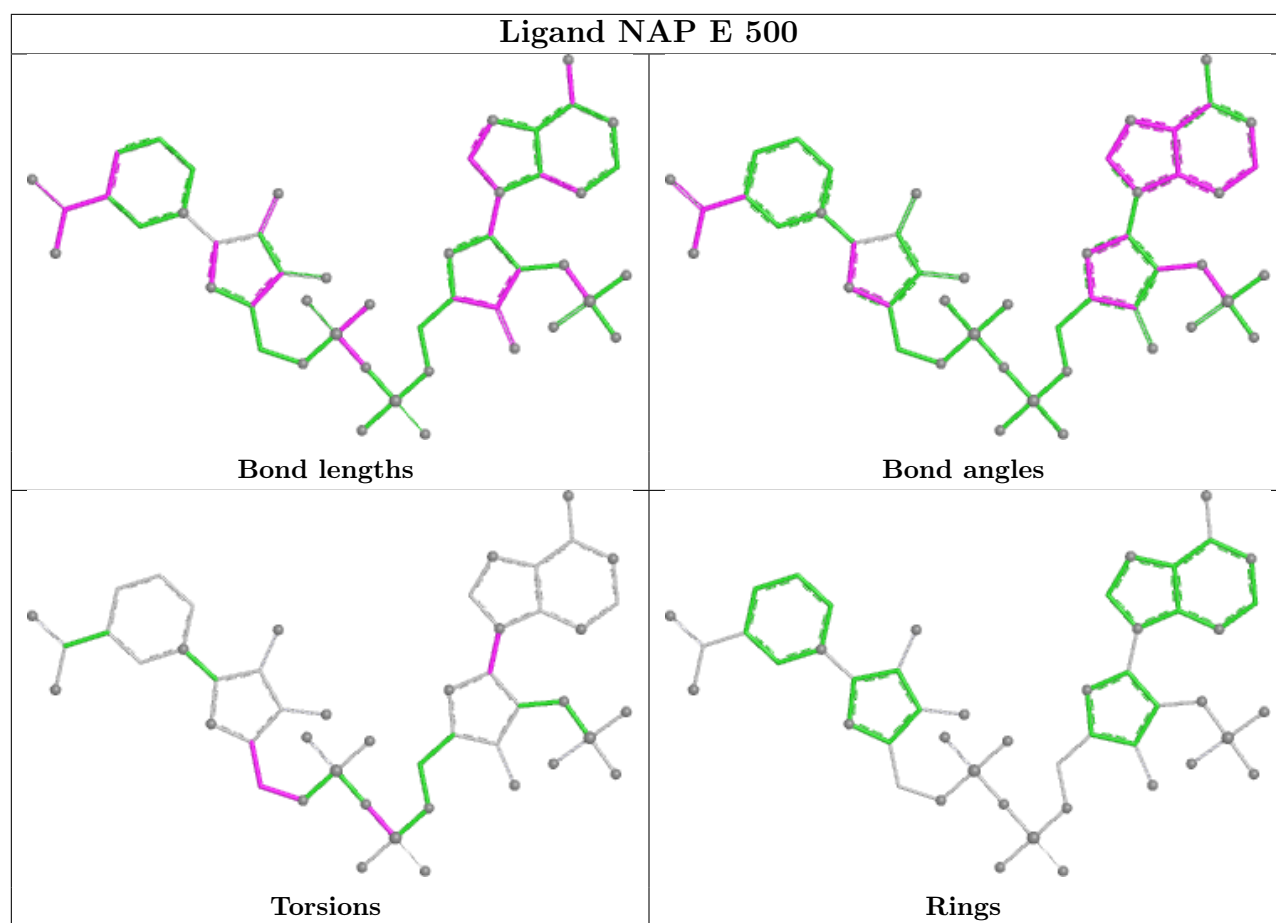
There are no ring outliers.

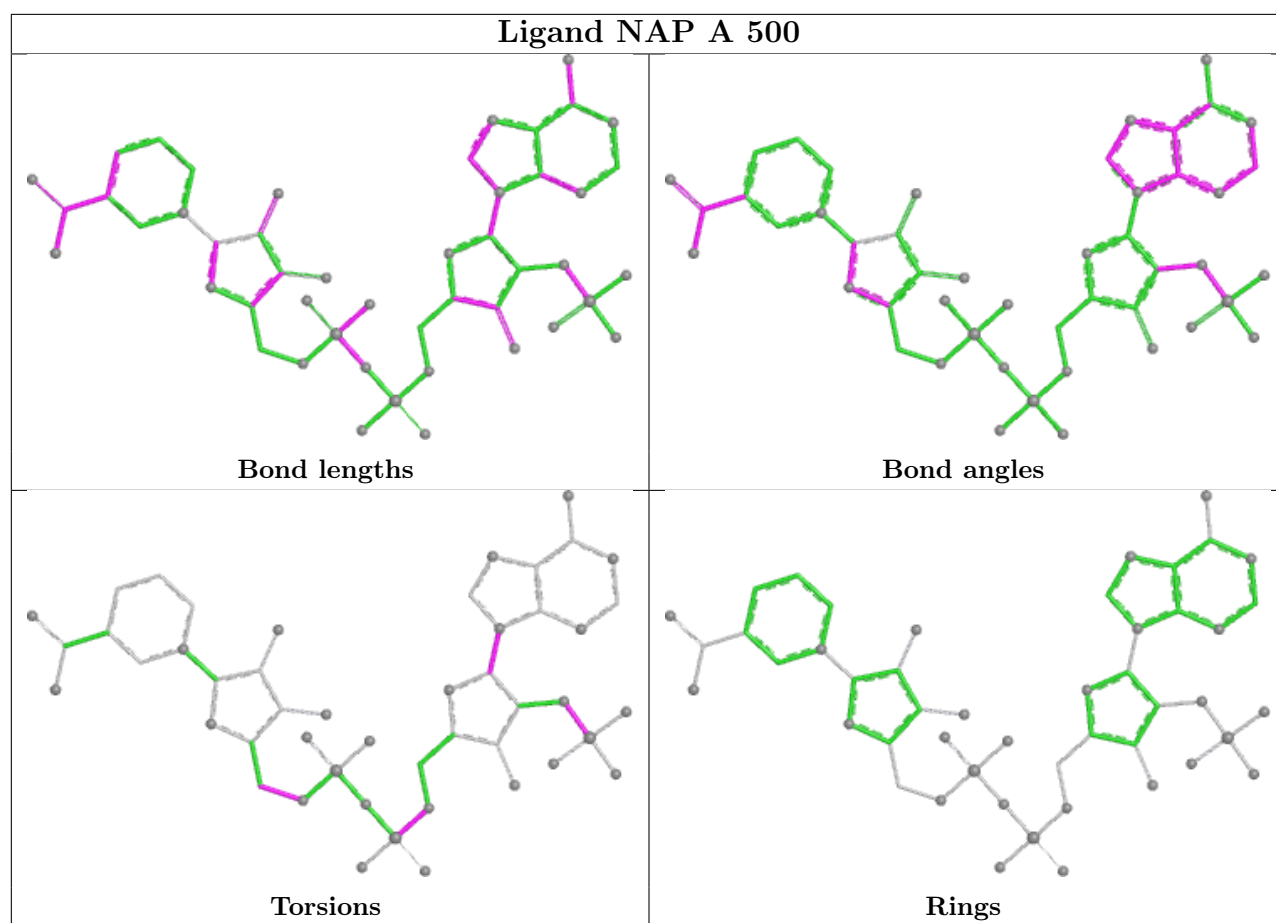
9 monomers are involved in 25 short contacts:

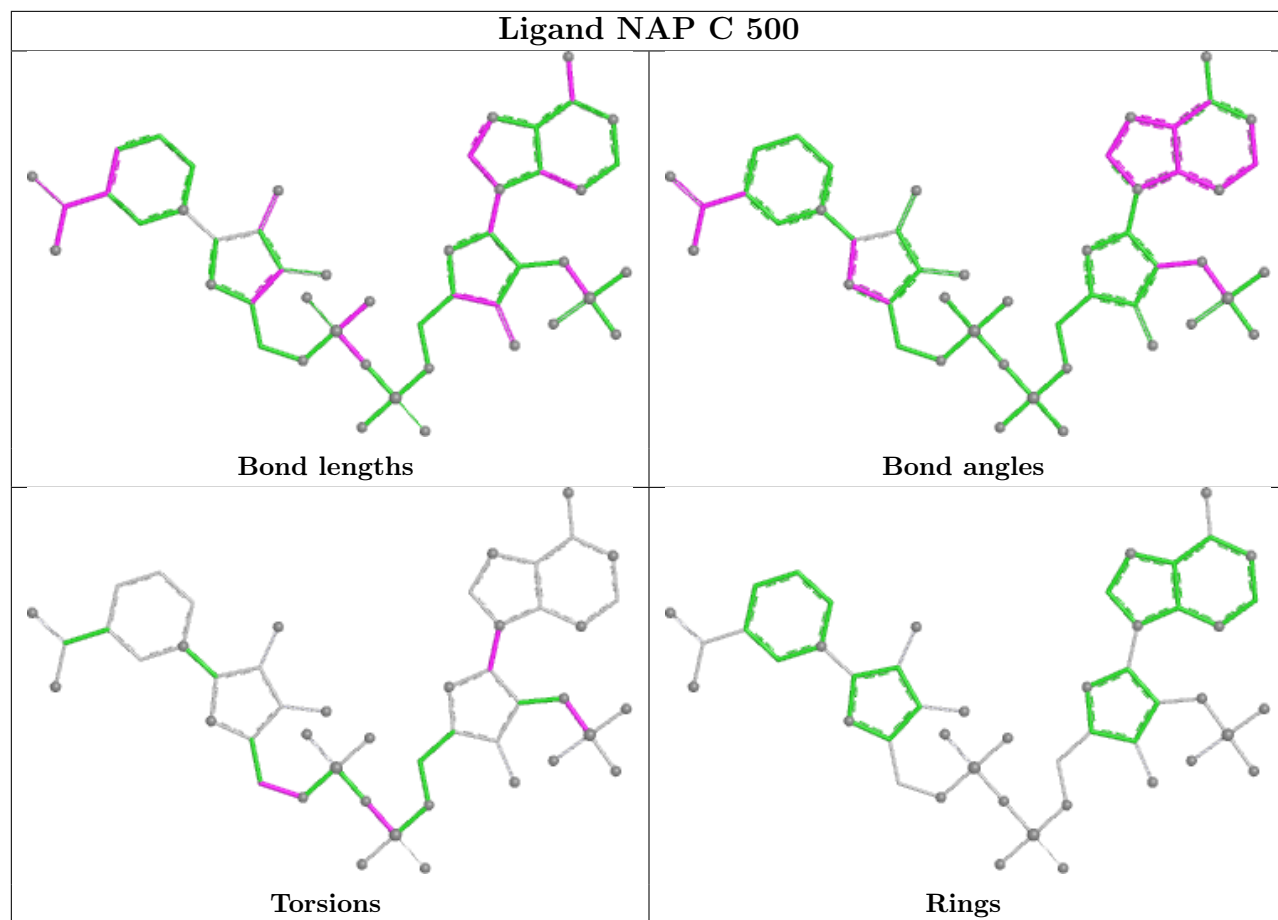
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	NAP	4	0
2	E	500	NAP	3	0
2	A	500	NAP	4	0
2	C	500	NAP	2	0
2	D	500	NAP	4	0
2	H	500	NAP	2	0
3	D	501	5OZ	1	0
2	B	500	NAP	2	0
2	G	500	NAP	3	0

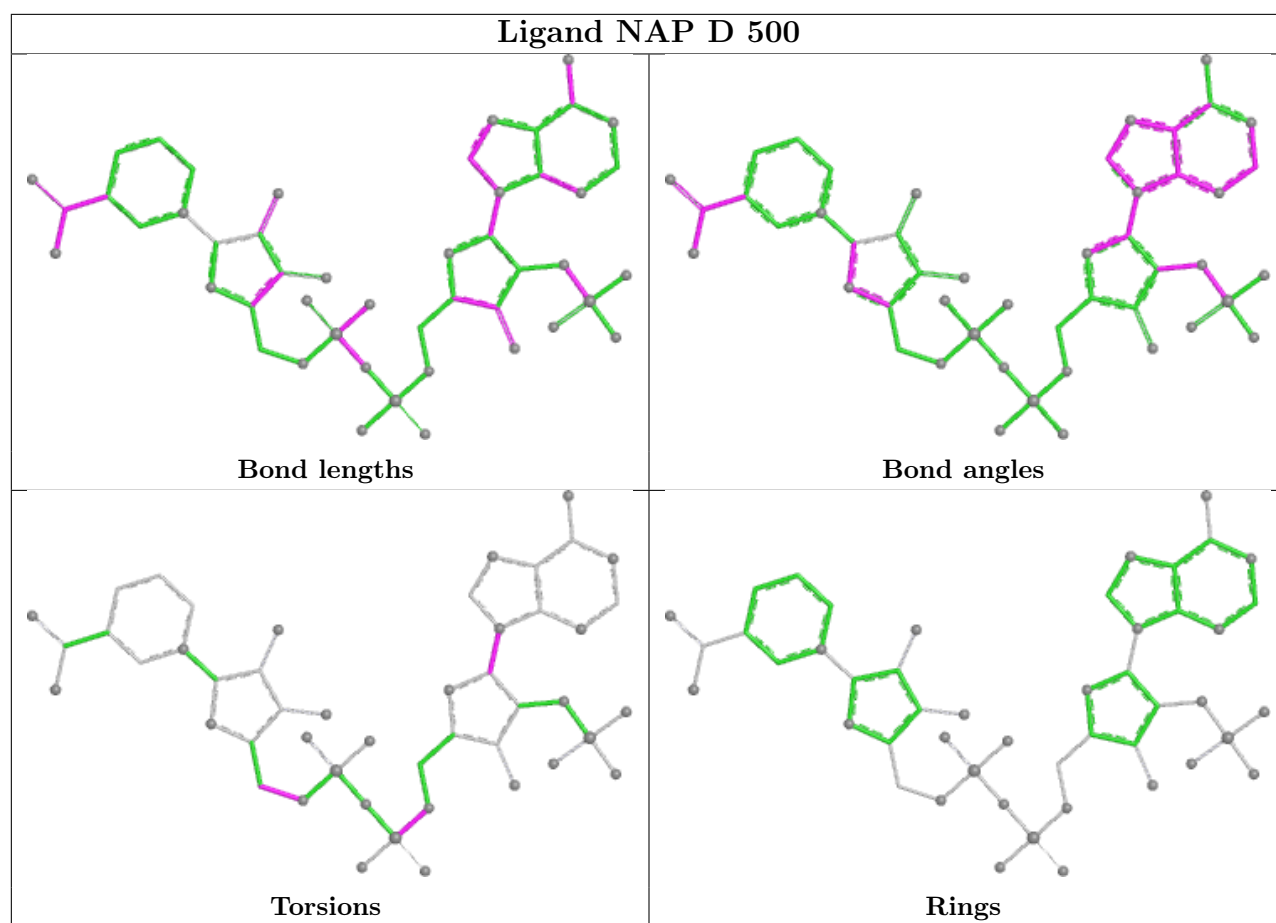
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

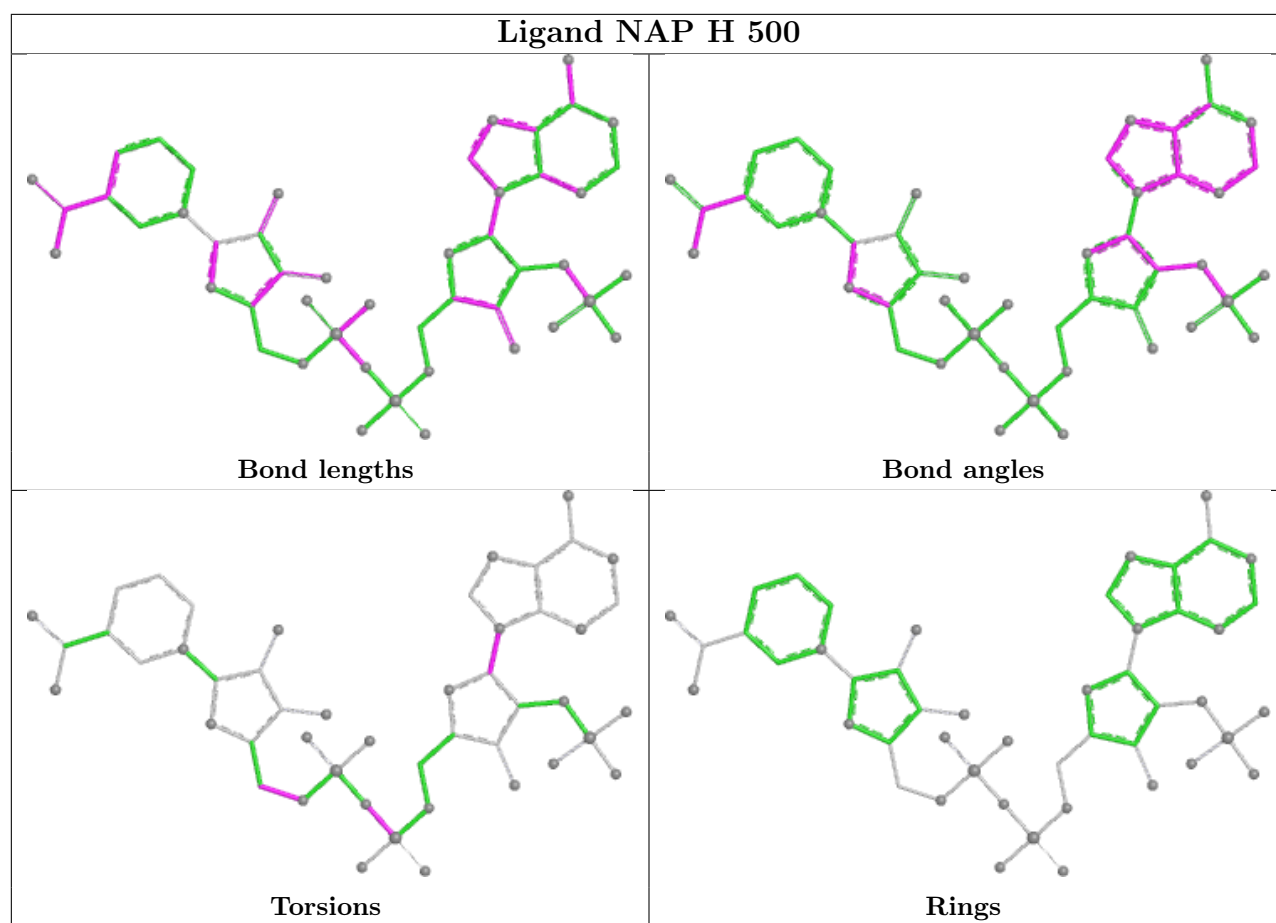


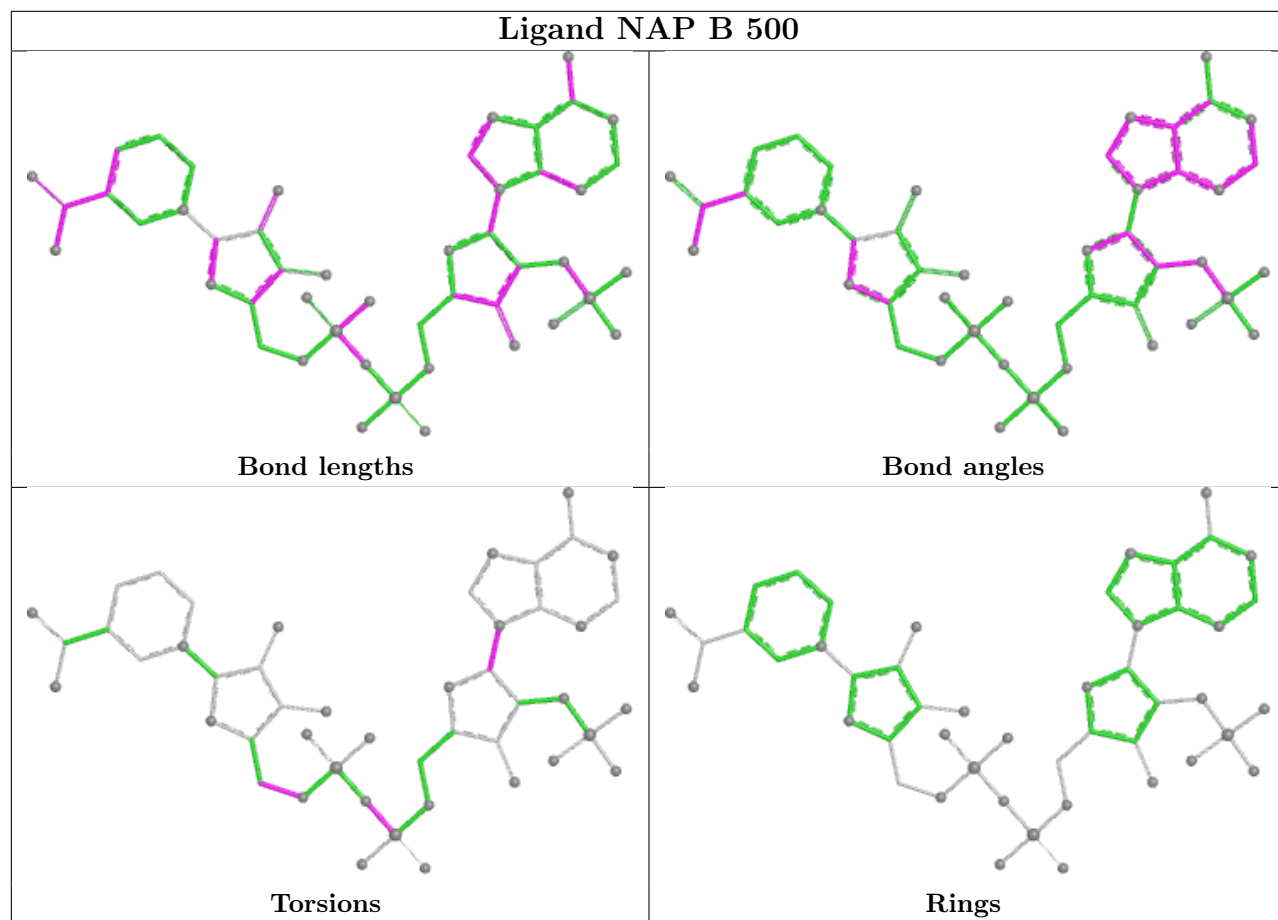


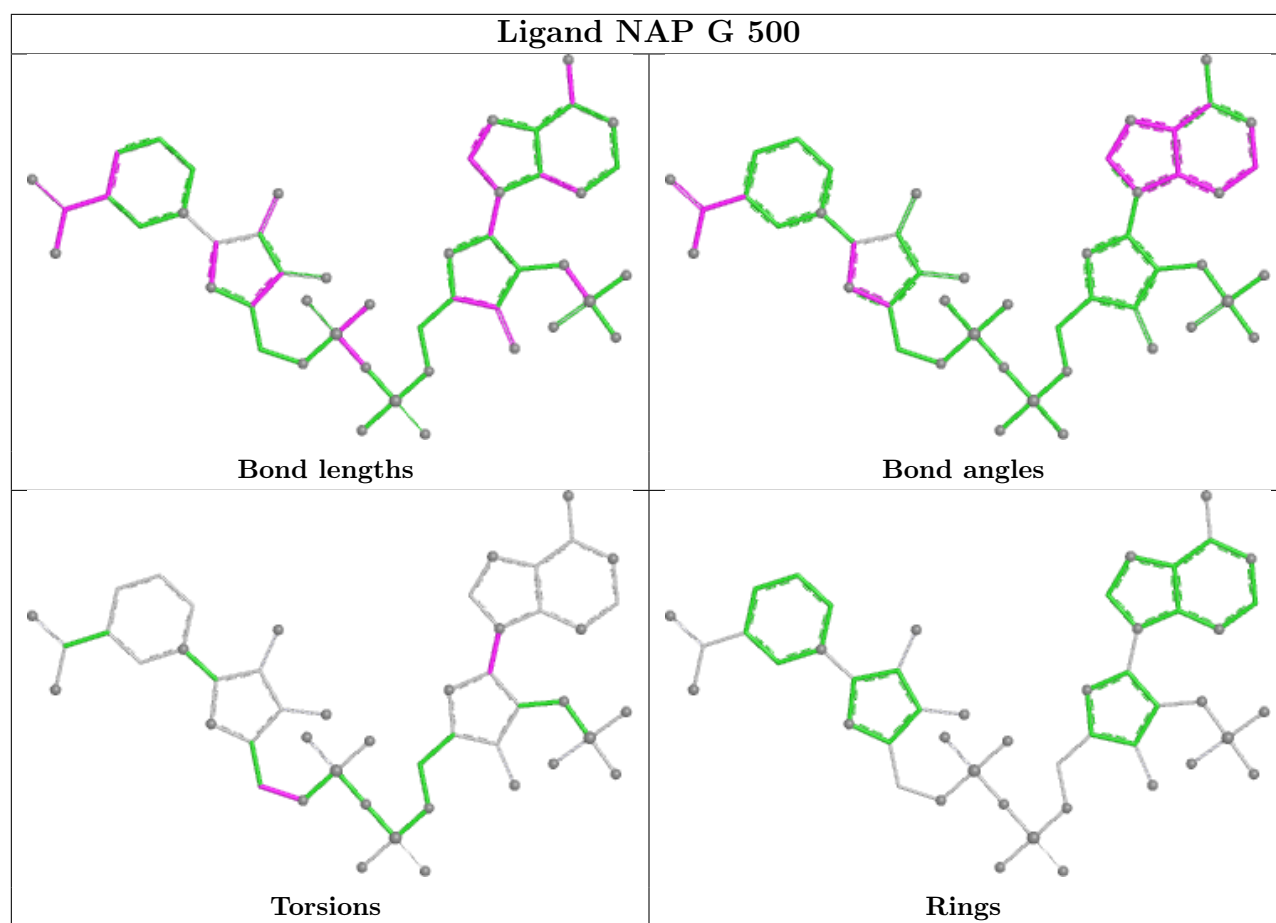












5.7 Other polymers [i](#)

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	483/491 (98%)	-0.27	1 (0%) 91 90	27, 38, 53, 81	0
1	B	484/491 (98%)	-0.30	1 (0%) 91 90	28, 38, 54, 65	0
1	C	485/491 (98%)	-0.25	3 (0%) 85 83	27, 38, 52, 85	0
1	D	485/491 (98%)	-0.21	1 (0%) 91 90	27, 39, 56, 76	0
1	E	485/491 (98%)	-0.19	5 (1%) 79 76	27, 40, 55, 76	0
1	F	483/491 (98%)	-0.17	3 (0%) 85 83	27, 40, 57, 77	0
1	G	484/491 (98%)	-0.29	2 (0%) 88 87	27, 39, 52, 59	0
1	H	483/491 (98%)	-0.23	4 (0%) 82 79	26, 38, 56, 75	0
All	All	3872/3928 (98%)	-0.24	20 (0%) 87 85	26, 39, 55, 85	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	491	LYS	5.9
1	C	491	LYS	4.2
1	D	491	LYS	3.9
1	E	46	GLU	3.2
1	F	491	LYS	2.9
1	H	9[B]	VAL	2.7
1	E	491	LYS	2.7
1	C	7	MET	2.7
1	E	483	ARG	2.6
1	H	344	ASP	2.6
1	B	21	SER	2.5
1	F	22	THR	2.5
1	E	7	MET	2.4
1	G	7	MET	2.4
1	E	86	GLU	2.3
1	A	491	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	79	GLU	2.1
1	H	22	THR	2.1
1	G	489	ALA	2.1
1	C	222	LYS	2.1

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](#)

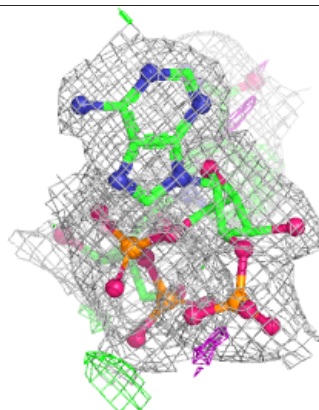
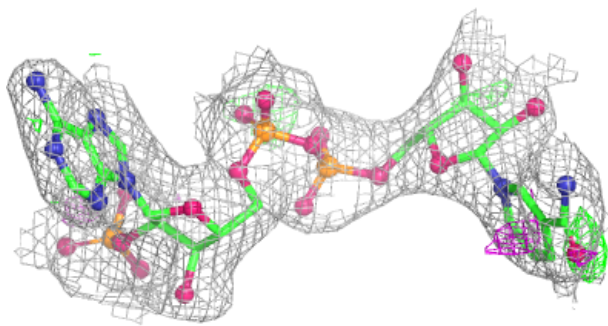
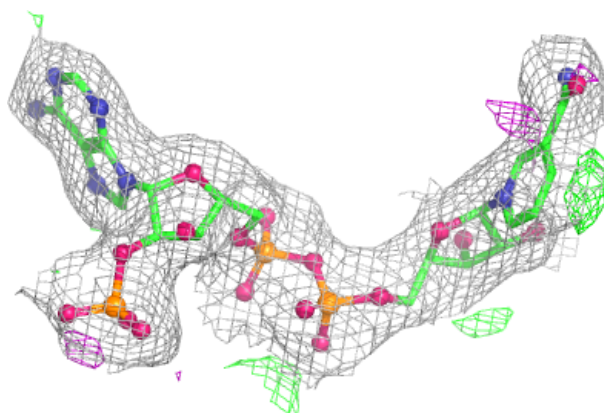
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	5OZ	A	501	5/5	0.84	0.18	33,38,45,47	0
3	5OZ	C	501	5/5	0.91	0.16	39,41,45,46	0
3	5OZ	D	501	5/5	0.92	0.15	35,40,44,49	0
3	5OZ	G	501	5/5	0.92	0.14	40,40,43,49	0
3	5OZ	H	501	5/5	0.92	0.14	30,41,47,48	0
2	NAP	F	500	48/48	0.95	0.09	38,45,52,53	0
3	5OZ	B	501	5/5	0.95	0.11	32,36,40,40	0
2	NAP	B	500	48/48	0.96	0.09	32,42,48,53	0
2	NAP	C	500	48/48	0.96	0.08	29,40,48,54	0
2	NAP	D	500	48/48	0.96	0.08	34,42,51,56	0
2	NAP	A	500	48/48	0.96	0.08	32,41,50,52	0
2	NAP	G	500	48/48	0.96	0.09	28,40,47,53	0
2	NAP	H	500	48/48	0.96	0.09	33,42,49,51	0
2	NAP	E	500	48/48	0.97	0.07	32,43,54,56	0

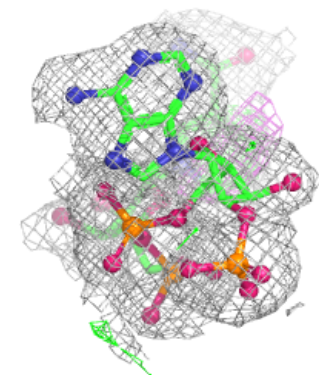
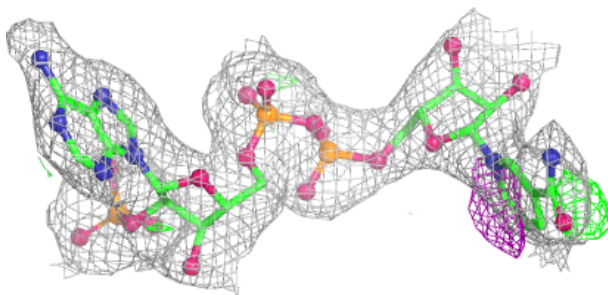
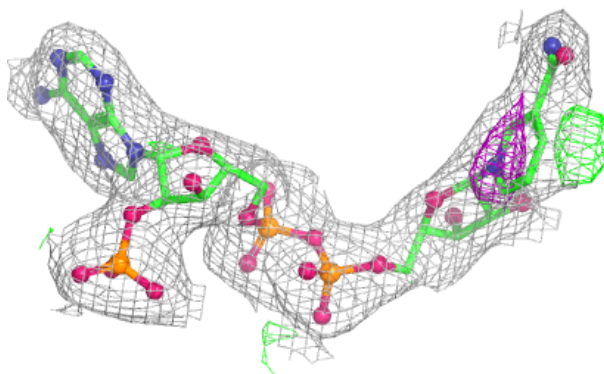
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP F 500:

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

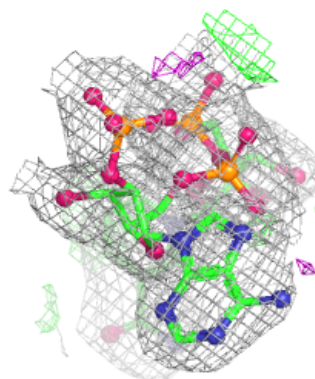
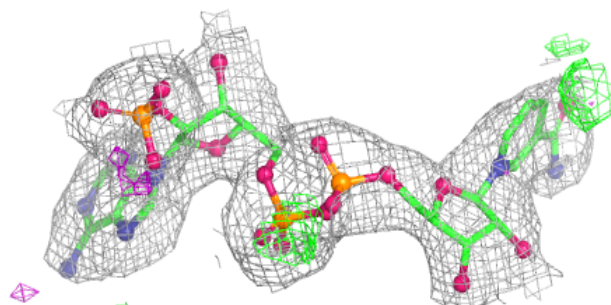
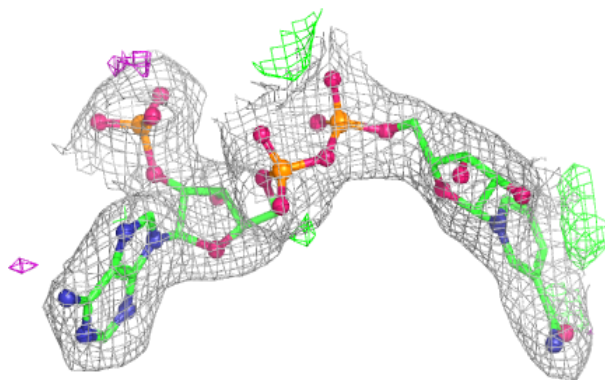
**Electron density around NAP B 500:**

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

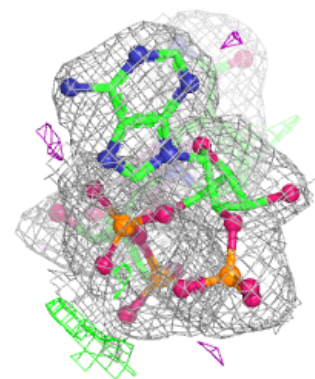
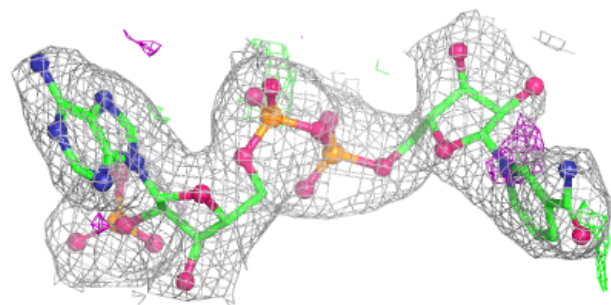
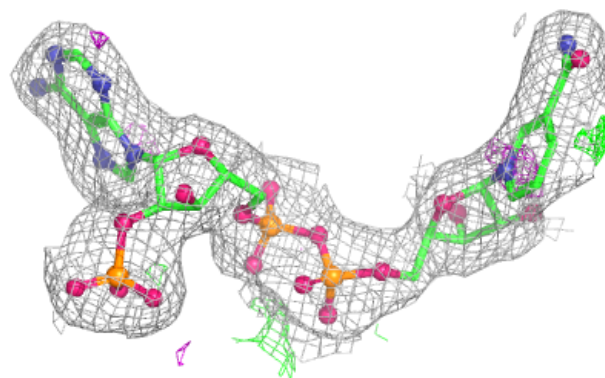


Electron density around NAP C 500:

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

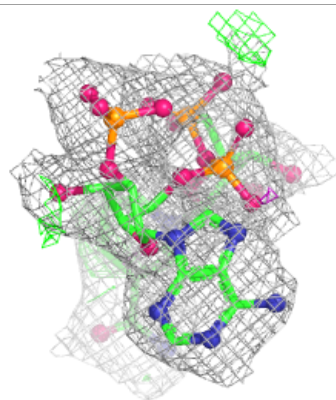
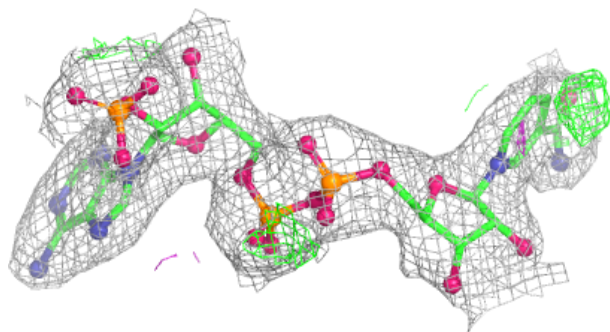
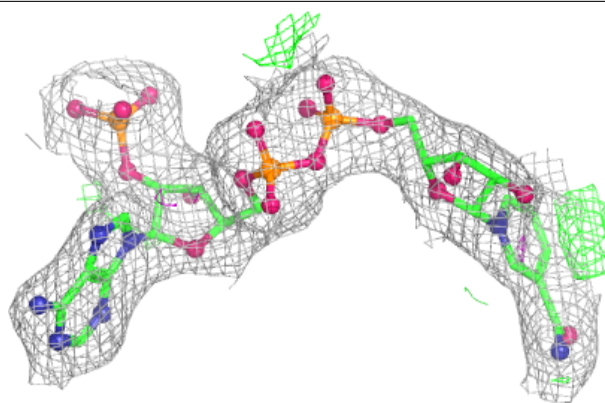
**Electron density around NAP D 500:**

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

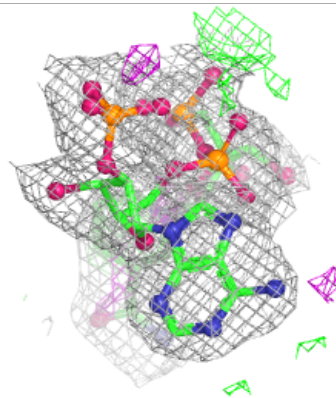
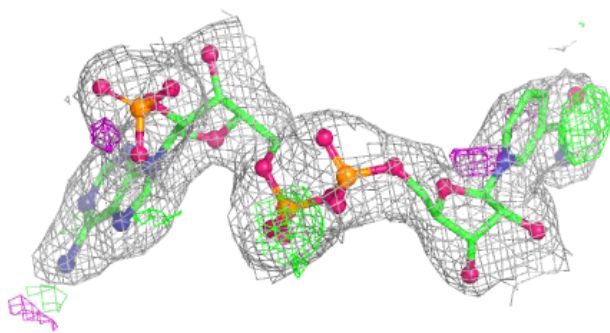
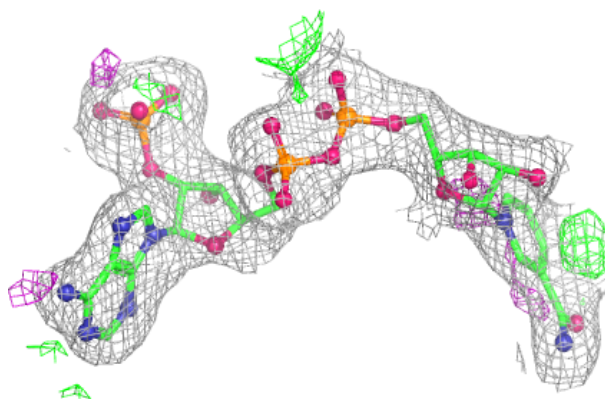


Electron density around NAP A 500:

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

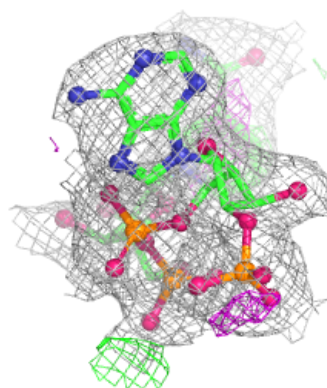
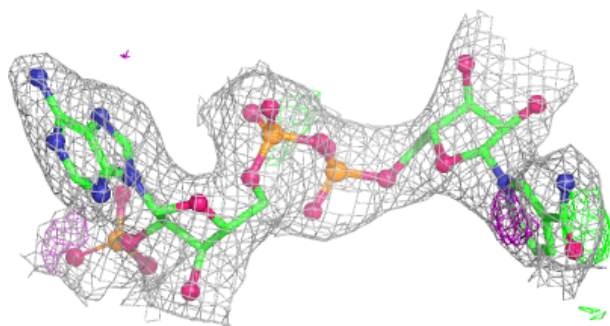
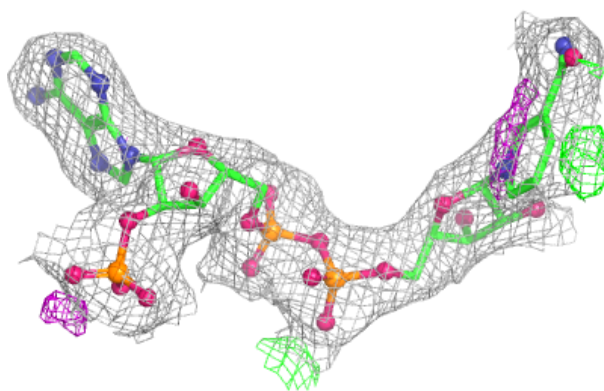
**Electron density around NAP G 500:**

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

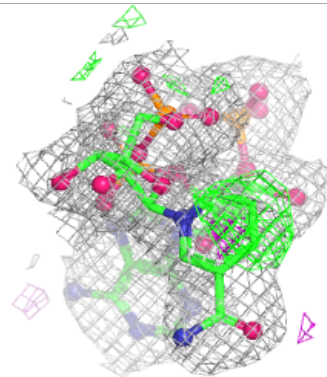
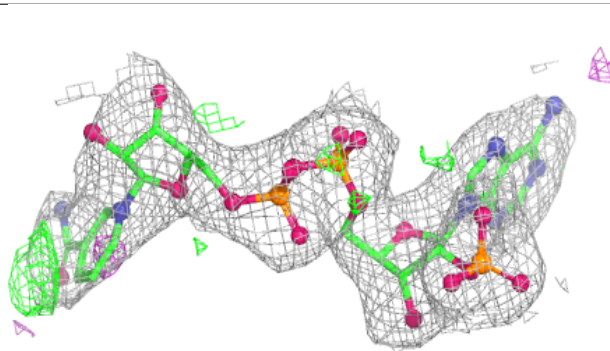
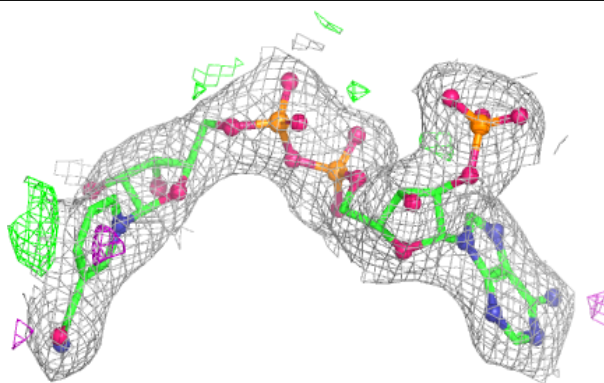


Electron density around NAP H 500:

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

**Electron density around NAP E 500:**

$2mF_o-DF_c$ (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.