



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:48 PM UTC

PDB ID : 5EKC / pdb_00005ekc
Title : Thermostable aldehyde dehydrogenase from Pyrobaculum sp.1860 complexed with NADP+
Authors : Petrova, T.; Bezsudnova, E.Y.; Boyko, K.M.; Nikolaeva, A.Y.; Rakitina, T.V.; Shabalin, I.G.; Popov, V.O.
Deposited on : 2015-11-03
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

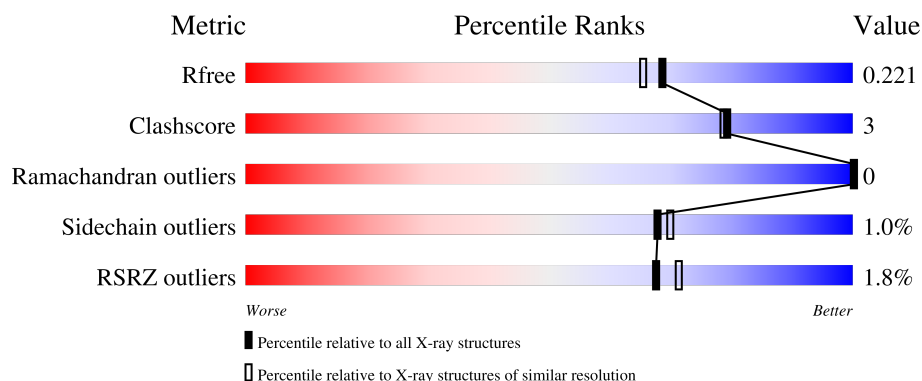
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

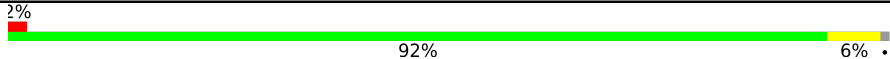
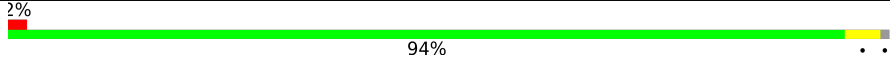
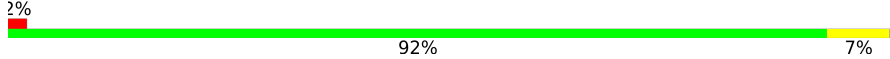
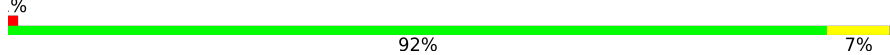
The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	
1	C	491	
1	D	491	

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Mol	Chain	Length	Quality of chain
1	E	491	 2% 92% 8%
1	F	491	 2% 92% 6% •
1	G	491	 2% 91% 7% •
1	H	491	 1% 92% 7% •

2 Entry composition

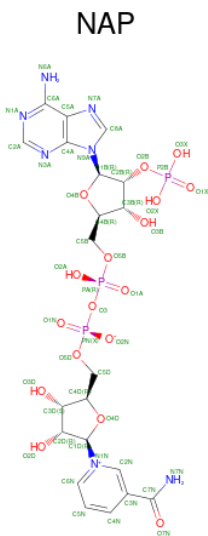
There are 3 unique types of molecules in this entry. The entry contains 33123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	485	Total	C	N	O	S	0	5	1
			3761	2398	651	700	12			
1	B	485	Total	C	N	O	S	0	4	0
			3775	2411	654	697	13			
1	C	483	Total	C	N	O	S	0	5	0
			3761	2399	658	693	11			
1	D	484	Total	C	N	O	S	0	6	0
			3755	2398	650	695	12			
1	E	490	Total	C	N	O	S	0	13	0
			3812	2433	662	704	13			
1	F	482	Total	C	N	O	S	0	5	0
			3760	2400	653	696	11			
1	G	484	Total	C	N	O	S	0	8	0
			3767	2407	653	694	13			
1	H	485	Total	C	N	O	S	0	6	0
			3781	2414	658	696	13			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	B	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	C	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	D	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	E	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	F	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	G	1	Total 39	C 15	N 5	O 16	P 3	0	0
2	H	1	Total 39	C 15	N 5	O 16	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	355	Total O 355 355	0	0
3	B	356	Total O 356 356	0	0
3	C	302	Total O 302 302	0	0
3	D	341	Total O 341 341	0	0

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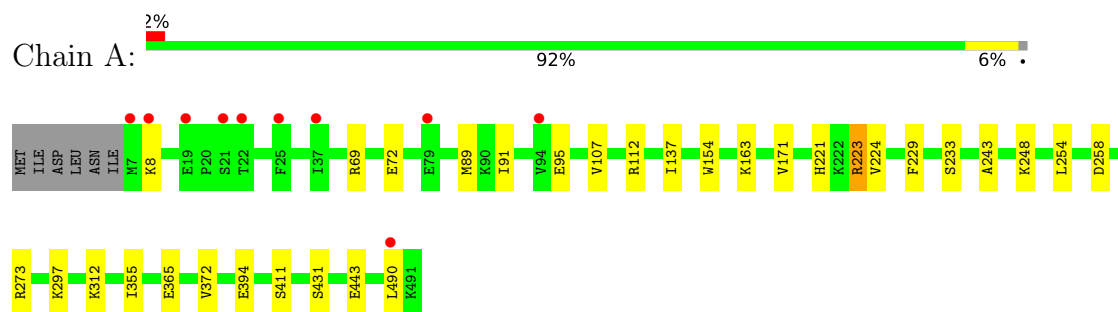
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	324	Total 324	O 324	0	0
3	F	294	Total 294	O 294	0	0
3	G	342	Total 342	O 342	0	0
3	H	325	Total 325	O 325	0	0

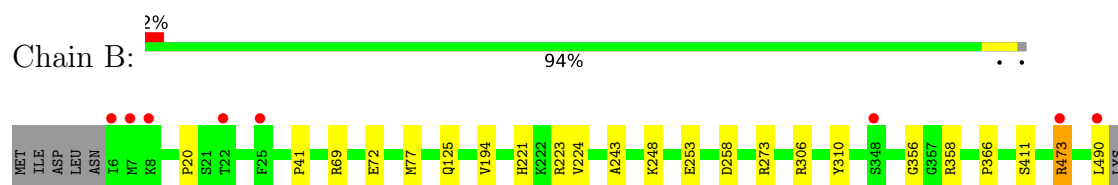
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

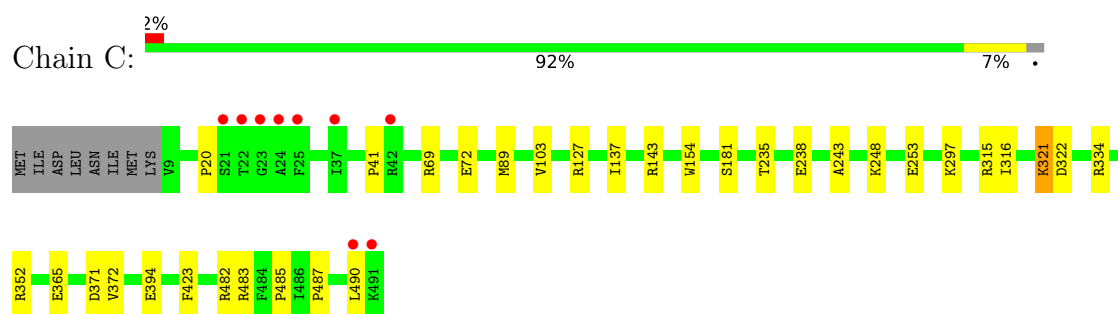
- Molecule 1: Aldehyde dehydrogenase



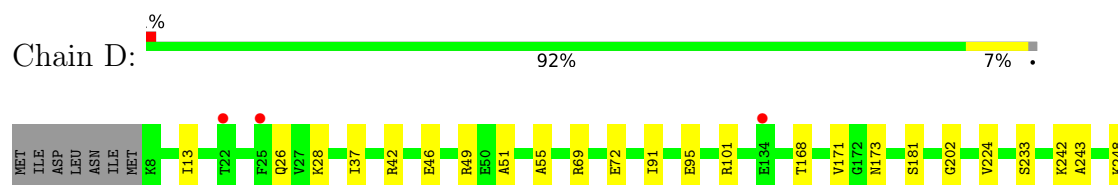
- Molecule 1: Aldehyde dehydrogenase

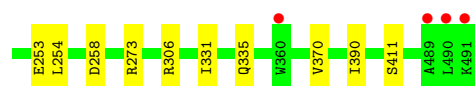


- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase

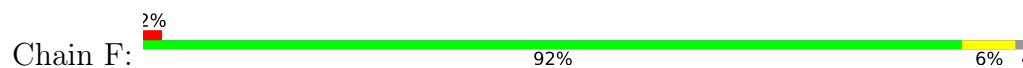




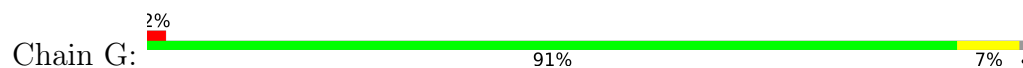
- Molecule 1: Aldehyde dehydrogenase



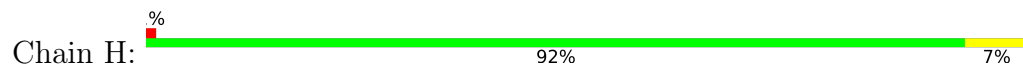
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	164.55Å 185.21Å 208.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 1.90 49.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.65-1.90) 98.6 (49.65-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.193 , 0.221 0.194 , 0.221	Depositor DCC
R_{free} test set	24753 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33123	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 44.92 % 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 1.4240e-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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/3850	0.72	0/5225
1	B	0.48	0/3865	0.74	0/5240
1	C	0.43	0/3851	0.72	0/5224
1	D	0.48	0/3851	0.74	0/5228
1	E	0.44	0/3905	0.73	0/5295
1	F	0.44	0/3851	0.73	0/5222
1	G	0.48	0/3871	0.74	0/5252
1	H	0.45	0/3877	0.72	0/5256
All	All	0.46	0/30921	0.73	0/41942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3761	0	3732	23	0
1	B	3775	0	3770	17	0
1	C	3761	0	3745	24	0
1	D	3755	0	3713	20	0
1	E	3812	0	3804	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3760	0	3755	22	0
1	G	3767	0	3752	23	0
1	H	3781	0	3779	26	0
2	A	39	0	17	3	0
2	B	39	0	17	1	0
2	C	39	0	17	5	0
2	D	39	0	17	2	0
2	E	39	0	17	3	0
2	F	39	0	17	1	0
2	G	39	0	17	1	0
2	H	39	0	17	1	0
3	A	355	0	0	1	0
3	B	356	0	0	1	0
3	C	302	0	0	2	0
3	D	341	0	0	1	0
3	E	324	0	0	0	0
3	F	294	0	0	0	0
3	G	342	0	0	2	0
3	H	325	0	0	2	0
All	All	33123	0	30186	161	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 3.

All (161) 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:H:473:ARG:HG3	1:H:473:ARG:HH11	1.45	0.81
1:B:473:ARG:HH11	1:B:473:ARG:HG3	1.49	0.77
1:C:334:ARG:HE	2:C:500:NAP:H2D	1.56	0.71
1:G:313:MET:HE1	1:H:490:LEU:HD13	1.71	0.70
1:C:315:ARG:NH2	1:C:322:ASP:OD2	2.23	0.70
1:E:426:ALA:O	1:F:473:ARG:NH2	2.25	0.70
1:C:154:TRP:HE1	2:C:500:NAP:H4D	1.57	0.69
1:H:69[A]:ARG:NH1	1:H:72[A]:GLU:OE2	2.26	0.68
1:G:7:MET:HE3	1:G:38:ALA:HB2	1.75	0.67
1:A:154:TRP:HE1	2:A:500:NAP:H4D	1.61	0.66
1:H:45:ARG:HH22	1:H:216:GLU:HG2	1.62	0.65
1:G:431:SER:O	1:H:473:ARG:NH1	2.30	0.65
1:H:473:ARG:HH11	1:H:473:ARG:CG	2.11	0.63
1:B:473:ARG:HH11	1:B:473:ARG:CG	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:OE2	1:D:49:ARG:NH1	2.30	0.63
2:B:500:NAP:O2A	2:B:500:NAP:H52N	1.99	0.63
1:C:483:ARG:NH1	1:C:490:LEU:O	2.31	0.63
1:E:424:ARG:NH2	1:G:479:LEU:O	2.35	0.59
2:D:500:NAP:O2A	2:D:500:NAP:H52N	2.03	0.58
1:E:89:MET:HG3	1:E:107:VAL:HG21	1.86	0.58
1:A:490:LEU:HD13	1:B:273:ARG:NH1	2.18	0.58
1:E:178:LYS:NZ	1:E:179:PRO:O	2.36	0.58
1:C:154:TRP:NE1	2:C:500:NAP:H4D	2.19	0.58
1:A:154:TRP:NE1	2:A:500:NAP:H4D	2.18	0.57
1:G:312:LYS:HE2	1:G:355:ILE:HD12	1.85	0.57
1:A:221:HIS:HE1	1:A:223:ARG:HG3	1.70	0.57
1:C:316:ILE:HD12	1:C:365:GLU:HG2	1.87	0.56
1:H:224:VAL:O	1:H:248:LYS:HE3	2.05	0.56
1:G:318:ASP:OD1	1:G:320:ARG:HD3	2.06	0.56
1:H:69[A]:ARG:NH2	3:H:603:HOH:O	2.39	0.55
1:E:487:PRO:HG2	1:E:490:LEU:HD12	1.89	0.54
1:A:312:LYS:HE2	1:A:355:ILE:HD12	1.88	0.54
1:C:352:ARG:NH1	1:C:371:ASP:OD2	2.39	0.54
1:C:297:LYS:HD3	1:C:394:GLU:HG2	1.90	0.53
1:C:20:PRO:HD3	1:C:41:PRO:HB3	1.90	0.53
1:D:26:GLN:OE1	1:D:42:ARG:NH1	2.41	0.53
1:G:91:ILE:O	1:G:95:GLU:HB3	2.09	0.53
1:E:431:SER:O	1:F:473:ARG:HD2	2.09	0.53
1:E:154:TRP:HE1	2:E:500:NAP:H4D	1.75	0.52
1:C:485:PRO:HB2	1:D:101:ARG:HG2	1.92	0.52
1:H:20:PRO:HD3	1:H:41:PRO:HB3	1.92	0.52
1:E:234:SER:O	1:E:238:GLU:HG3	2.10	0.52
1:F:33:ASP:CG	1:F:320:ARG:HH22	2.18	0.52
1:F:221:HIS:HE1	1:F:223:ARG:HG3	1.75	0.51
1:E:273:ARG:NH1	1:F:490:LEU:HD13	2.25	0.51
1:H:143:ARG:NH1	3:H:605:HOH:O	2.43	0.51
1:E:178:LYS:HE3	1:E:211:GLY:HA2	1.92	0.50
1:C:243:ALA:HB1	1:C:248:LYS:HG3	1.94	0.50
1:G:77[A]:MET:HE2	1:G:194:VAL:HG22	1.93	0.50
1:H:79:GLU:OE2	1:H:82:ARG:NH1	2.43	0.50
1:E:334:ARG:HH12	2:E:500:NAP:H2D	1.77	0.50
1:G:316:ILE:HD12	1:G:365[B]:GLU:HG2	1.94	0.50
1:C:482:ARG:NH1	3:C:603:HOH:O	2.40	0.50
1:B:20:PRO:HD3	1:B:41:PRO:HB3	1.94	0.49
1:F:243:ALA:HB1	1:F:248:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:O	1:B:473:ARG:NH1	2.46	0.49
1:F:163:LYS:NZ	1:F:443:GLU:OE2	2.37	0.49
1:F:137:ILE:HD12	1:H:423:PHE:CD2	2.48	0.49
1:E:7[A]:MET:HE3	1:E:38:ALA:HB2	1.94	0.49
1:D:28:LYS:HE2	1:D:95:GLU:HG3	1.93	0.49
1:B:243:ALA:HB1	1:B:248:LYS:HG3	1.95	0.49
1:D:242:LYS:NZ	3:D:610:HOH:O	2.47	0.48
1:D:168:THR:HG22	1:D:173:ASN:HB2	1.96	0.48
1:G:490:LEU:HD13	1:H:273:ARG:NH1	2.28	0.48
1:E:221:HIS:HE1	1:E:223:ARG:HG3	1.79	0.48
1:H:19:GLU:HB2	1:H:20:PRO:HD2	1.96	0.48
1:F:479:LEU:O	1:H:424[A]:ARG:NH2	2.41	0.48
1:F:487:PRO:HD2	1:F:490:LEU:HD12	1.95	0.48
1:F:224:VAL:O	1:F:248:LYS:HE3	2.14	0.47
1:H:221:HIS:HE1	1:H:223:ARG:HG3	1.78	0.47
1:A:243:ALA:HB1	1:A:248:LYS:HG3	1.97	0.47
1:E:258:ASP:OD2	1:E:411:SER:HB3	2.14	0.47
1:C:143:ARG:NH1	3:C:606:HOH:O	2.47	0.47
1:C:490:LEU:HD13	1:D:273:ARG:NH1	2.30	0.47
1:G:115:GLN:O	1:G:119:GLU:HG3	2.15	0.47
1:D:258:ASP:OD2	1:D:411:SER:HB3	2.15	0.46
1:E:4[A]:LEU:HA	1:E:7[A]:MET:HE2	1.97	0.46
1:E:154:TRP:NE1	2:E:500:NAP:H4D	2.30	0.46
1:H:243:ALA:HB1	1:H:248:LYS:HG3	1.97	0.46
1:D:224:VAL:O	1:D:248:LYS:HE3	2.15	0.46
2:G:500:NAP:O2A	2:G:500:NAP:H52N	2.15	0.46
1:C:321:LYS:HG2	1:C:322:ASP:OD2	2.16	0.46
1:B:77[A]:MET:HE2	1:B:194:VAL:HG22	1.98	0.46
1:D:181:SER:OG	2:D:500:NAP:O3X	2.33	0.46
1:E:55:ALA:HA	1:E:202:GLY:O	2.16	0.46
1:A:233:SER:HA	1:A:254:LEU:HB3	1.98	0.46
1:A:297:LYS:HB3	1:A:297:LYS:HE3	1.76	0.46
1:E:490:LEU:HD13	1:F:273:ARG:NH1	2.30	0.46
1:E:243:ALA:HB1	1:E:248:LYS:HG3	1.98	0.45
1:A:137:ILE:HD12	1:C:423:PHE:CE2	2.52	0.45
1:F:262:ILE:HG12	1:F:415:LEU:HD12	1.98	0.45
1:F:233:SER:HA	1:F:254:LEU:HB3	1.99	0.45
1:A:221:HIS:CE1	1:A:223:ARG:HG3	2.52	0.45
1:C:69[B]:ARG:HD2	1:C:72[B]:GLU:OE1	2.16	0.45
1:B:224:VAL:O	1:B:248:LYS:HE3	2.17	0.45
1:D:370:VAL:HG12	1:D:390:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ARG:HG2	1:H:485:PRO:HB2	1.99	0.45
1:C:334:ARG:HH21	2:C:500:NAP:C1D	2.30	0.44
1:E:28:LYS:HE3	1:E:37:ILE:HD12	1.99	0.44
2:F:500:NAP:O2A	2:F:500:NAP:H52N	2.17	0.44
1:G:365[A]:GLU:HG2	3:G:733:HOH:O	2.17	0.44
1:G:221:HIS:HE1	1:G:223:ARG:HG3	1.83	0.44
1:G:331:ILE:HG22	1:G:335:GLN:HG3	1.99	0.44
1:G:485:PRO:HB2	1:H:101:ARG:HG2	1.98	0.44
1:G:360:TRP:HZ3	1:G:365[B]:GLU:HG3	1.82	0.44
1:B:358:ARG:NH2	3:B:601:HOH:O	2.28	0.44
1:E:490:LEU:HD22	1:F:273:ARG:HH12	1.83	0.44
1:F:30:SER:HB2	1:F:37:ILE:HD11	1.99	0.44
1:C:487:PRO:HD2	1:C:490:LEU:HD12	1.98	0.44
1:C:235:THR:O	1:C:238:GLU:HB3	2.18	0.44
1:F:137:ILE:HD12	1:H:423:PHE:CE2	2.53	0.44
1:G:243:ALA:HB1	1:G:248:LYS:HG3	1.98	0.44
1:A:163:LYS:NZ	1:A:443:GLU:OE2	2.43	0.43
1:A:224:VAL:O	1:A:248:LYS:HE3	2.18	0.43
1:D:13:ILE:HG23	1:D:51:ALA:HA	2.00	0.43
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.18	0.43
1:A:112:ARG:HH22	1:C:69[A]:ARG:HH22	1.65	0.43
1:D:243:ALA:HB1	1:D:248:LYS:HG3	1.99	0.43
1:E:101:ARG:HG2	1:F:485:PRO:HB2	2.01	0.43
1:A:273:ARG:NH1	1:B:490:LEU:HD13	2.34	0.43
1:B:258:ASP:OD2	1:B:411:SER:HB3	2.19	0.43
1:D:69[A]:ARG:HD2	1:D:72[A]:GLU:OE1	2.17	0.43
1:E:316:ILE:HD12	1:E:365:GLU:HG2	1.99	0.43
1:G:306:ARG:HA	1:G:306:ARG:HD2	1.71	0.43
1:D:331:ILE:HG22	1:D:335:GLN:HG3	2.01	0.43
1:A:297:LYS:HE2	1:A:394:GLU:HG2	2.01	0.43
1:A:258:ASP:OD2	1:A:411:SER:HB3	2.19	0.42
1:B:306:ARG:HA	1:B:306:ARG:HD2	1.80	0.42
1:F:258:ASP:OD2	1:F:411:SER:HB3	2.20	0.42
1:H:229:PHE:HE1	2:H:500:NAP:O4B	2.02	0.42
1:D:55:ALA:HA	1:D:202:GLY:O	2.20	0.42
1:H:473:ARG:NH1	1:H:473:ARG:CG	2.79	0.42
1:D:91:ILE:O	1:D:95:GLU:HB3	2.19	0.42
1:E:313:MET:HE1	1:F:490:LEU:HG	2.01	0.42
1:H:233:SER:HA	1:H:254:LEU:HB3	2.02	0.42
1:A:89:MET:HG3	1:A:107:VAL:HG21	2.01	0.42
1:F:221:HIS:CE1	1:F:223:ARG:HG3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:LEU:HD23	1:G:189:LEU:HA	1.92	0.41
1:H:370:VAL:HG12	1:H:390:ILE:HB	2.03	0.41
1:B:356:GLY:HA3	1:B:366:PRO:O	2.21	0.41
1:B:69:ARG:HD2	1:B:72[B]:GLU:OE1	2.20	0.41
1:A:91:ILE:O	1:A:95:GLU:HB3	2.20	0.41
1:E:69:ARG:NE	1:E:72[A]:GLU:OE1	2.53	0.41
1:E:224:VAL:O	1:E:248:LYS:HE3	2.19	0.41
1:G:352:ARG:HD2	3:G:603:HOH:O	2.21	0.41
1:A:490:LEU:HD11	1:B:310:TYR:CD1	2.56	0.41
1:A:229:PHE:HE1	2:A:500:NAP:O4B	2.04	0.41
1:E:233:SER:HA	1:E:254:LEU:HB3	2.02	0.41
1:H:115:GLN:O	1:H:119:GLU:HG3	2.21	0.41
1:H:102:LYS:HE2	1:H:156:TYR:CZ	2.56	0.41
1:B:125:GLN:OE1	1:C:127:ARG:HD2	2.20	0.41
1:C:181:SER:OG	2:C:500:NAP:O3X	2.38	0.41
1:D:28:LYS:HE3	1:D:37:ILE:HD12	2.02	0.41
1:D:233:SER:HA	1:D:254:LEU:HB3	2.02	0.41
1:B:221:HIS:HE1	1:B:223:ARG:HG3	1.85	0.41
1:C:89:MET:HE3	1:C:103:VAL:HG23	2.04	0.41
1:D:306:ARG:HA	1:D:306:ARG:HD2	1.85	0.41
1:A:69:ARG:HH11	1:A:72[A]:GLU:HB3	1.86	0.40
1:A:365[B]:GLU:HG2	3:A:706:HOH:O	2.20	0.40
1:E:423:PHE:CD2	1:G:137:ILE:HD12	2.56	0.40
1:F:356:GLY:HA3	1:F:366:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	487/491 (99%)	474 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	486/491 (99%)	475 (98%)	11 (2%)	0	100	100
1	C	485/491 (99%)	474 (98%)	11 (2%)	0	100	100
1	D	487/491 (99%)	474 (97%)	13 (3%)	0	100	100
1	E	492/491 (100%)	479 (97%)	13 (3%)	0	100	100
1	F	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
1	G	489/491 (100%)	477 (98%)	12 (2%)	0	100	100
1	H	488/491 (99%)	475 (97%)	13 (3%)	0	100	100
All	All	3898/3928 (99%)	3799 (98%)	99 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/408 (97%)	390 (99%)	4 (1%)	68	70
1	B	398/408 (98%)	396 (100%)	2 (0%)	81	84
1	C	394/408 (97%)	390 (99%)	4 (1%)	68	70
1	D	390/408 (96%)	388 (100%)	2 (0%)	81	84
1	E	402/408 (98%)	399 (99%)	3 (1%)	76	78
1	F	397/408 (97%)	392 (99%)	5 (1%)	61	61
1	G	395/408 (97%)	390 (99%)	5 (1%)	61	61
1	H	398/408 (98%)	393 (99%)	5 (1%)	61	61
All	All	3168/3264 (97%)	3138 (99%)	30 (1%)	68	73

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

Mol	Chain	Res	Type
1	A	8	LYS
1	A	171	VAL

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Mol	Chain	Res	Type
1	A	223	ARG
1	A	372	VAL
1	B	253[B]	GLU
1	B	473	ARG
1	C	137	ILE
1	C	253[B]	GLU
1	C	321	LYS
1	C	372	VAL
1	D	171	VAL
1	D	253[B]	GLU
1	E	178	LYS
1	E	253[B]	GLU
1	E	372	VAL
1	F	171	VAL
1	F	253[B]	GLU
1	F	355	ILE
1	F	358	ARG
1	F	372	VAL
1	G	39	GLU
1	G	238	GLU
1	G	253[B]	GLU
1	G	320	ARG
1	G	372	VAL
1	H	137	ILE
1	H	171	VAL
1	H	216	GLU
1	H	253[B]	GLU
1	H	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	285	GLN
1	B	14	ASN
1	B	285	GLN
1	C	285	GLN
1	C	375	ASN
1	D	285	GLN
1	D	362	ASN
1	F	14	ASN
1	F	192	GLN

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Mol	Chain	Res	Type
1	F	285	GLN
1	F	335	GLN
1	G	192	GLN
1	H	115	GLN

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](#)

8 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	D	500	-	42,42,52	2.01	12 (28%)	60,65,80	1.91	11 (18%)
2	NAP	A	500	-	42,42,52	2.00	12 (28%)	60,65,80	1.95	14 (23%)
2	NAP	G	500	-	42,42,52	2.02	12 (28%)	60,65,80	1.92	13 (21%)
2	NAP	H	500	-	42,42,52	2.01	12 (28%)	60,65,80	1.90	13 (21%)
2	NAP	C	500	-	42,42,52	2.02	12 (28%)	60,65,80	1.92	14 (23%)
2	NAP	B	500	-	42,42,52	2.02	12 (28%)	60,65,80	1.96	14 (23%)
2	NAP	F	500	-	42,42,52	2.00	12 (28%)	60,65,80	1.92	14 (23%)
2	NAP	E	500	-	42,42,52	2.02	13 (30%)	60,65,80	1.97	14 (23%)

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	D	500	-	-	9/27/56/67	0/4/4/5
2	NAP	A	500	-	-	7/27/56/67	0/4/4/5
2	NAP	G	500	-	-	8/27/56/67	0/4/4/5
2	NAP	H	500	-	-	7/27/56/67	0/4/4/5
2	NAP	C	500	-	-	6/27/56/67	0/4/4/5
2	NAP	B	500	-	-	10/27/56/67	0/4/4/5
2	NAP	F	500	-	-	8/27/56/67	0/4/4/5
2	NAP	E	500	-	-	7/27/56/67	0/4/4/5

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	C6A-N6A	6.08	1.49	1.34
2	H	500	NAP	C6A-N6A	6.03	1.49	1.34
2	C	500	NAP	C6A-N6A	6.03	1.49	1.34
2	A	500	NAP	C6A-N6A	5.99	1.49	1.34
2	E	500	NAP	C6A-N6A	5.99	1.49	1.34
2	G	500	NAP	C6A-N6A	5.98	1.49	1.34
2	F	500	NAP	C6A-N6A	5.93	1.49	1.34
2	B	500	NAP	C6A-N6A	5.83	1.49	1.34
2	B	500	NAP	C3B-C2B	-5.26	1.41	1.53
2	C	500	NAP	C3B-C2B	-5.25	1.41	1.53
2	G	500	NAP	C3B-C2B	-5.23	1.41	1.53
2	D	500	NAP	C3B-C2B	-5.20	1.41	1.53
2	E	500	NAP	C3B-C2B	-5.18	1.41	1.53
2	A	500	NAP	C3B-C2B	-5.17	1.41	1.53
2	F	500	NAP	C3B-C2B	-5.15	1.41	1.53
2	H	500	NAP	C3B-C2B	-4.95	1.42	1.53
2	B	500	NAP	C2D-C3D	-4.41	1.46	1.53
2	F	500	NAP	C2D-C3D	-4.16	1.46	1.53
2	G	500	NAP	C2D-C3D	-4.08	1.46	1.53
2	H	500	NAP	C2D-C3D	-4.05	1.46	1.53
2	E	500	NAP	C2D-C3D	-4.05	1.46	1.53
2	D	500	NAP	C2D-C3D	-4.04	1.46	1.53
2	A	500	NAP	C2D-C3D	-3.90	1.47	1.53
2	C	500	NAP	C2D-C3D	-3.87	1.47	1.53
2	B	500	NAP	O3D-C3D	-3.25	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	O3D-C3D	-3.23	1.35	1.43
2	E	500	NAP	O3D-C3D	-3.19	1.35	1.43
2	C	500	NAP	PN-O3	3.17	1.62	1.59
2	H	500	NAP	O3D-C3D	-3.17	1.35	1.43
2	F	500	NAP	O3D-C3D	-3.04	1.35	1.43
2	G	500	NAP	O3D-C3D	-3.01	1.35	1.43
2	A	500	NAP	O3D-C3D	-2.97	1.35	1.43
2	E	500	NAP	C5D-C4D	-2.94	1.42	1.51
2	C	500	NAP	O3D-C3D	-2.93	1.35	1.43
2	C	500	NAP	C5D-C4D	-2.89	1.42	1.51
2	G	500	NAP	C5D-C4D	-2.88	1.42	1.51
2	A	500	NAP	C5D-C4D	-2.87	1.42	1.51
2	E	500	NAP	C2B-C1B	-2.82	1.46	1.53
2	D	500	NAP	C5D-C4D	-2.80	1.43	1.51
2	F	500	NAP	PN-O3	2.79	1.62	1.59
2	B	500	NAP	PN-O3	2.78	1.62	1.59
2	B	500	NAP	C5D-C4D	-2.77	1.43	1.51
2	D	500	NAP	C2B-C1B	-2.77	1.46	1.53
2	G	500	NAP	PN-O3	2.77	1.62	1.59
2	A	500	NAP	C2B-C1B	-2.74	1.46	1.53
2	C	500	NAP	C2B-C1B	-2.72	1.46	1.53
2	B	500	NAP	C2B-C1B	-2.72	1.46	1.53
2	F	500	NAP	C5D-C4D	-2.70	1.43	1.51
2	H	500	NAP	C2B-C1B	-2.70	1.46	1.53
2	E	500	NAP	C3D-C4D	-2.67	1.46	1.53
2	G	500	NAP	O2D-C2D	-2.66	1.37	1.43
2	H	500	NAP	C5D-C4D	-2.66	1.43	1.51
2	G	500	NAP	C2B-C1B	-2.65	1.46	1.53
2	D	500	NAP	C3D-C4D	-2.62	1.46	1.53
2	A	500	NAP	PN-O3	2.61	1.62	1.59
2	C	500	NAP	C3D-C4D	-2.60	1.46	1.53
2	C	500	NAP	O2D-C2D	-2.60	1.37	1.43
2	F	500	NAP	C2B-C1B	-2.59	1.46	1.53
2	B	500	NAP	C3D-C4D	-2.59	1.46	1.53
2	E	500	NAP	O2D-C2D	-2.58	1.37	1.43
2	G	500	NAP	C3D-C4D	-2.58	1.46	1.53
2	F	500	NAP	O2D-C2D	-2.57	1.38	1.43
2	H	500	NAP	PN-O3	2.56	1.62	1.59
2	H	500	NAP	C3D-C4D	-2.50	1.46	1.53
2	A	500	NAP	O2D-C2D	-2.48	1.38	1.43
2	D	500	NAP	PN-O3	2.46	1.62	1.59
2	H	500	NAP	O2D-C2D	-2.45	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAP	O2D-C2D	-2.42	1.38	1.43
2	F	500	NAP	C3D-C4D	-2.41	1.46	1.53
2	H	500	NAP	O4B-C4B	-2.40	1.39	1.45
2	E	500	NAP	PN-O3	2.38	1.62	1.59
2	G	500	NAP	O4B-C4B	-2.37	1.39	1.45
2	B	500	NAP	O4B-C4B	-2.36	1.39	1.45
2	D	500	NAP	O4B-C4B	-2.32	1.39	1.45
2	F	500	NAP	O4B-C4B	-2.32	1.39	1.45
2	A	500	NAP	C3D-C4D	-2.30	1.47	1.53
2	D	500	NAP	O2D-C2D	-2.27	1.38	1.43
2	C	500	NAP	C3B-C4B	-2.26	1.47	1.53
2	B	500	NAP	P2B-O2X	-2.23	1.46	1.54
2	E	500	NAP	O4B-C4B	-2.22	1.40	1.45
2	C	500	NAP	O4B-C4B	-2.22	1.40	1.45
2	A	500	NAP	O4B-C4B	-2.22	1.40	1.45
2	H	500	NAP	C3B-C4B	-2.22	1.47	1.53
2	E	500	NAP	C3B-C4B	-2.22	1.47	1.53
2	B	500	NAP	C3B-C4B	-2.13	1.47	1.53
2	A	500	NAP	P2B-O2X	-2.11	1.47	1.54
2	H	500	NAP	P2B-O2X	-2.10	1.47	1.54
2	F	500	NAP	C3B-C4B	-2.10	1.47	1.53
2	A	500	NAP	C3B-C4B	-2.08	1.47	1.53
2	E	500	NAP	P2B-O3X	-2.06	1.47	1.54
2	C	500	NAP	P2B-O2X	-2.06	1.47	1.54
2	G	500	NAP	P2B-O2X	-2.05	1.47	1.54
2	F	500	NAP	P2B-O2X	-2.04	1.47	1.54
2	D	500	NAP	P2B-O2X	-2.02	1.47	1.54
2	E	500	NAP	O5D-C5D	-2.01	1.37	1.44
2	G	500	NAP	C3B-C4B	-2.01	1.47	1.53
2	D	500	NAP	C3B-C4B	-2.01	1.47	1.53

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAP	C5A-C4A-N3A	-5.82	118.70	126.72
2	F	500	NAP	C5A-C4A-N3A	-5.50	119.14	126.72
2	A	500	NAP	C5A-C4A-N3A	-5.49	119.15	126.72
2	H	500	NAP	C5A-C4A-N3A	-5.42	119.25	126.72
2	D	500	NAP	C4A-N9A-C8A	5.28	111.28	105.74
2	G	500	NAP	C5A-C4A-N3A	-5.25	119.48	126.72
2	B	500	NAP	N3A-C4A-N9A	5.21	136.03	127.17
2	E	500	NAP	C4A-N9A-C8A	5.13	111.12	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAP	C5A-C4A-N3A	-5.12	119.66	126.72
2	D	500	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
2	E	500	NAP	C4A-N9A-C1B	-5.12	114.66	126.63
2	D	500	NAP	N3A-C4A-N9A	4.88	135.47	127.17
2	C	500	NAP	C4A-N9A-C8A	4.85	110.83	105.74
2	C	500	NAP	C4A-N9A-C1B	-4.83	115.33	126.63
2	B	500	NAP	C4A-N9A-C8A	4.83	110.81	105.74
2	A	500	NAP	N3A-C4A-N9A	4.82	135.37	127.17
2	F	500	NAP	N3A-C4A-N9A	4.81	135.34	127.17
2	H	500	NAP	N3A-C4A-N9A	4.78	135.30	127.17
2	D	500	NAP	N9A-C8A-N7A	-4.76	107.18	113.94
2	E	500	NAP	C5A-C4A-N3A	-4.76	120.16	126.72
2	A	500	NAP	C4A-N9A-C8A	4.75	110.73	105.74
2	G	500	NAP	C4A-N9A-C8A	4.74	110.72	105.74
2	G	500	NAP	N3A-C4A-N9A	4.74	135.23	127.17
2	A	500	NAP	N9A-C8A-N7A	-4.72	107.24	113.94
2	E	500	NAP	N9A-C8A-N7A	-4.67	107.31	113.94
2	B	500	NAP	N9A-C8A-N7A	-4.66	107.32	113.94
2	H	500	NAP	C4A-N9A-C8A	4.65	110.62	105.74
2	F	500	NAP	C4A-N9A-C8A	4.61	110.58	105.74
2	C	500	NAP	N3A-C4A-N9A	4.56	134.92	127.17
2	C	500	NAP	N9A-C8A-N7A	-4.56	107.47	113.94
2	D	500	NAP	C4A-N9A-C1B	-4.54	116.02	126.63
2	G	500	NAP	C4A-N9A-C1B	-4.54	116.02	126.63
2	F	500	NAP	C4A-N9A-C1B	-4.53	116.05	126.63
2	F	500	NAP	N9A-C8A-N7A	-4.50	107.55	113.94
2	G	500	NAP	N9A-C8A-N7A	-4.49	107.56	113.94
2	A	500	NAP	C4A-N9A-C1B	-4.45	116.23	126.63
2	H	500	NAP	N9A-C8A-N7A	-4.43	107.66	113.94
2	E	500	NAP	N3A-C4A-N9A	4.35	134.57	127.17
2	H	500	NAP	C4A-N9A-C1B	-4.22	116.77	126.63
2	E	500	NAP	N3A-C2A-N1A	-4.20	122.23	128.58
2	D	500	NAP	N3A-C2A-N1A	-4.05	122.45	128.58
2	B	500	NAP	C4A-N9A-C1B	-4.04	117.17	126.63
2	G	500	NAP	N3A-C2A-N1A	-4.00	122.53	128.58
2	H	500	NAP	N3A-C2A-N1A	-3.90	122.67	128.58
2	B	500	NAP	N3A-C2A-N1A	-3.74	122.91	128.58
2	C	500	NAP	N3A-C2A-N1A	-3.74	122.93	128.58
2	A	500	NAP	C5A-N7A-C8A	3.68	109.24	103.45
2	B	500	NAP	C2A-N3A-C4A	3.58	120.58	111.83
2	F	500	NAP	N3A-C2A-N1A	-3.57	123.17	128.58
2	B	500	NAP	C5A-N7A-C8A	3.54	109.01	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAP	N3A-C2A-N1A	-3.53	123.24	128.58
2	D	500	NAP	C5A-N7A-C8A	3.49	108.94	103.45
2	F	500	NAP	C5A-N7A-C8A	3.47	108.91	103.45
2	H	500	NAP	C5A-N7A-C8A	3.44	108.85	103.45
2	C	500	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	G	500	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	H	500	NAP	C2A-N3A-C4A	3.39	120.12	111.83
2	G	500	NAP	C2A-N3A-C4A	3.39	120.11	111.83
2	E	500	NAP	C5A-N7A-C8A	3.38	108.77	103.45
2	F	500	NAP	C2A-N3A-C4A	3.33	119.97	111.83
2	A	500	NAP	C2A-N3A-C4A	3.27	119.82	111.83
2	D	500	NAP	C2A-N3A-C4A	3.27	119.81	111.83
2	E	500	NAP	C2A-N3A-C4A	3.25	119.77	111.83
2	C	500	NAP	C2A-N3A-C4A	3.24	119.75	111.83
2	E	500	NAP	C1B-N9A-C8A	3.21	134.21	127.09
2	A	500	NAP	C1D-O4D-C4D	-3.14	101.12	108.06
2	C	500	NAP	C1D-O4D-C4D	-3.12	101.16	108.06
2	E	500	NAP	C1D-O4D-C4D	-3.10	101.22	108.06
2	C	500	NAP	C1B-N9A-C8A	3.04	133.84	127.09
2	A	500	NAP	C4A-C5A-N7A	-2.86	107.31	110.58
2	F	500	NAP	C1B-N9A-C8A	2.83	133.37	127.09
2	F	500	NAP	C1D-C2D-C3D	2.81	106.12	101.63
2	G	500	NAP	C1D-C2D-C3D	2.79	106.09	101.63
2	G	500	NAP	C1B-N9A-C8A	2.78	133.26	127.09
2	H	500	NAP	C4A-C5A-N7A	-2.76	107.43	110.58
2	C	500	NAP	C4A-C5A-N7A	-2.75	107.44	110.58
2	F	500	NAP	C4A-C5A-N7A	-2.74	107.45	110.58
2	H	500	NAP	O4B-C1B-C2B	-2.72	101.91	106.59
2	A	500	NAP	C1B-N9A-C8A	2.68	133.04	127.09
2	H	500	NAP	C1D-C2D-C3D	2.68	105.91	101.63
2	E	500	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
2	D	500	NAP	C1D-C2D-C3D	2.64	105.84	101.63
2	G	500	NAP	C4A-C5A-N7A	-2.62	107.59	110.58
2	B	500	NAP	C1D-C2D-C3D	2.62	105.81	101.63
2	B	500	NAP	C4A-C5A-N7A	-2.60	107.61	110.58
2	B	500	NAP	O2D-C2D-C3D	-2.59	106.33	111.43
2	A	500	NAP	C1D-C2D-C3D	2.53	105.67	101.63
2	D	500	NAP	C1B-N9A-C8A	2.53	132.71	127.09
2	E	500	NAP	C1D-C2D-C3D	2.51	105.65	101.63
2	G	500	NAP	C1D-O4D-C4D	-2.49	102.55	108.06
2	H	500	NAP	C1B-N9A-C8A	2.49	132.61	127.09
2	A	500	NAP	O2A-PA-O3	2.48	113.98	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAP	C4A-C5A-N7A	-2.48	107.75	110.58
2	F	500	NAP	O4B-C1B-C2B	-2.45	102.37	106.59
2	C	500	NAP	C1D-C2D-C3D	2.45	105.54	101.63
2	E	500	NAP	O2A-PA-O3	2.41	113.79	107.27
2	H	500	NAP	O5D-C5D-C4D	2.37	117.08	108.99
2	A	500	NAP	O4B-C1B-C2B	-2.33	102.57	106.59
2	B	500	NAP	C1B-N9A-C8A	2.22	132.02	127.09
2	G	500	NAP	O2A-PA-O3	2.20	113.22	107.27
2	B	500	NAP	O4B-C1B-C2B	-2.19	102.82	106.59
2	C	500	NAP	O2A-PA-O3	2.18	113.16	107.27
2	B	500	NAP	C1D-O4D-C4D	-2.14	103.33	108.06
2	E	500	NAP	O5D-C5D-C4D	2.13	116.25	108.99
2	F	500	NAP	C1D-O4D-C4D	-2.07	103.48	108.06
2	C	500	NAP	O4B-C1B-C2B	-2.03	103.09	106.59
2	F	500	NAP	O2D-C2D-C3D	-2.02	107.45	111.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAP	C5B-O5B-PA-O1A
2	A	500	NAP	C5B-O5B-PA-O3
2	B	500	NAP	PN-O3-PA-O5B
2	F	500	NAP	PN-O3-PA-O5B
2	F	500	NAP	C5D-O5D-PN-O1N
2	G	500	NAP	C5D-O5D-PN-O1N
2	H	500	NAP	PN-O3-PA-O5B
2	C	500	NAP	O4D-C4D-C5D-O5D
2	B	500	NAP	C3D-C4D-C5D-O5D
2	C	500	NAP	C3D-C4D-C5D-O5D
2	D	500	NAP	C3D-C4D-C5D-O5D
2	G	500	NAP	C3D-C4D-C5D-O5D
2	A	500	NAP	O4D-C4D-C5D-O5D
2	A	500	NAP	C3D-C4D-C5D-O5D
2	B	500	NAP	O4D-C4D-C5D-O5D
2	D	500	NAP	O4D-C4D-C5D-O5D
2	F	500	NAP	O4D-C4D-C5D-O5D
2	F	500	NAP	C3D-C4D-C5D-O5D
2	G	500	NAP	O4D-C4D-C5D-O5D
2	E	500	NAP	C3D-C4D-C5D-O5D
2	C	500	NAP	PN-O3-PA-O5B
2	D	500	NAP	PN-O3-PA-O5B

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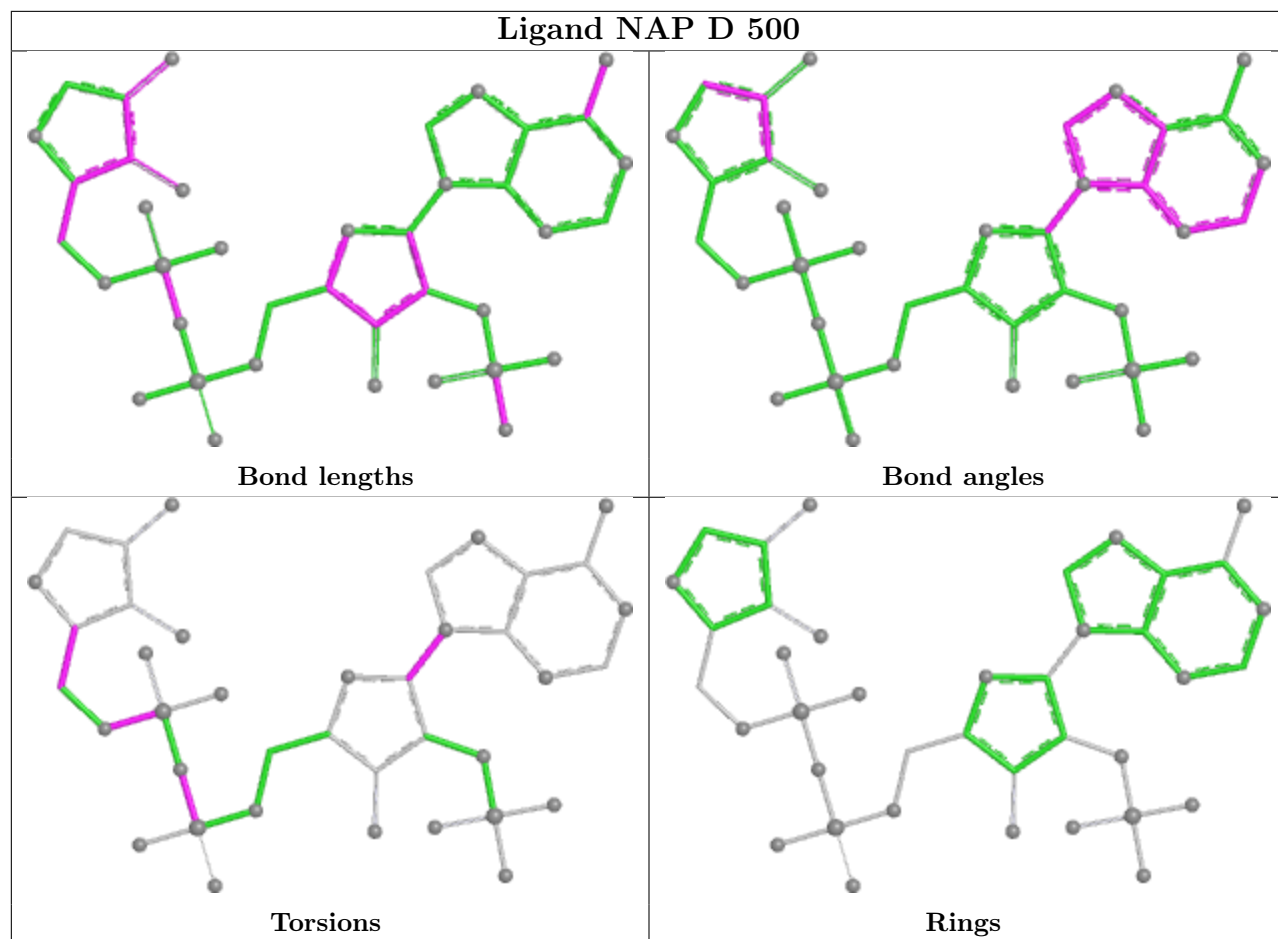
Mol	Chain	Res	Type	Atoms
2	G	500	NAP	PN-O3-PA-O5B
2	E	500	NAP	O4D-C4D-C5D-O5D
2	A	500	NAP	C2B-C1B-N9A-C8A
2	B	500	NAP	C2B-C1B-N9A-C8A
2	C	500	NAP	C2B-C1B-N9A-C8A
2	D	500	NAP	C2B-C1B-N9A-C8A
2	E	500	NAP	C2B-C1B-N9A-C8A
2	F	500	NAP	C2B-C1B-N9A-C8A
2	G	500	NAP	C2B-C1B-N9A-C8A
2	H	500	NAP	C2B-C1B-N9A-C8A
2	B	500	NAP	C5B-O5B-PA-O1A
2	B	500	NAP	C5D-O5D-PN-O3
2	B	500	NAP	C5D-O5D-PN-O1N
2	B	500	NAP	C5D-O5D-PN-O2N
2	D	500	NAP	C5D-O5D-PN-O3
2	D	500	NAP	C5D-O5D-PN-O1N
2	D	500	NAP	C5D-O5D-PN-O2N
2	E	500	NAP	C5B-O5B-PA-O1A
2	G	500	NAP	C5B-O5B-PA-O1A
2	H	500	NAP	C5D-O5D-PN-O1N
2	E	500	NAP	C2B-C1B-N9A-C4A
2	H	500	NAP	C3D-C4D-C5D-O5D
2	B	500	NAP	C2B-C1B-N9A-C4A
2	E	500	NAP	O4B-C1B-N9A-C8A
2	E	500	NAP	PN-O3-PA-O5B
2	H	500	NAP	O4D-C4D-C5D-O5D
2	A	500	NAP	C2B-C1B-N9A-C4A
2	D	500	NAP	C2B-C1B-N9A-C4A
2	C	500	NAP	O4B-C1B-N9A-C8A
2	G	500	NAP	O4B-C1B-N9A-C8A
2	A	500	NAP	O4B-C1B-N9A-C8A
2	B	500	NAP	O4B-C1B-N9A-C8A
2	D	500	NAP	O4B-C1B-N9A-C8A
2	F	500	NAP	O4B-C1B-N9A-C8A
2	F	500	NAP	C2B-O2B-P2B-O2X
2	C	500	NAP	C2B-C1B-N9A-C4A
2	F	500	NAP	C2B-C1B-N9A-C4A
2	G	500	NAP	C2B-C1B-N9A-C4A
2	H	500	NAP	C2B-C1B-N9A-C4A
2	H	500	NAP	O4B-C1B-N9A-C8A

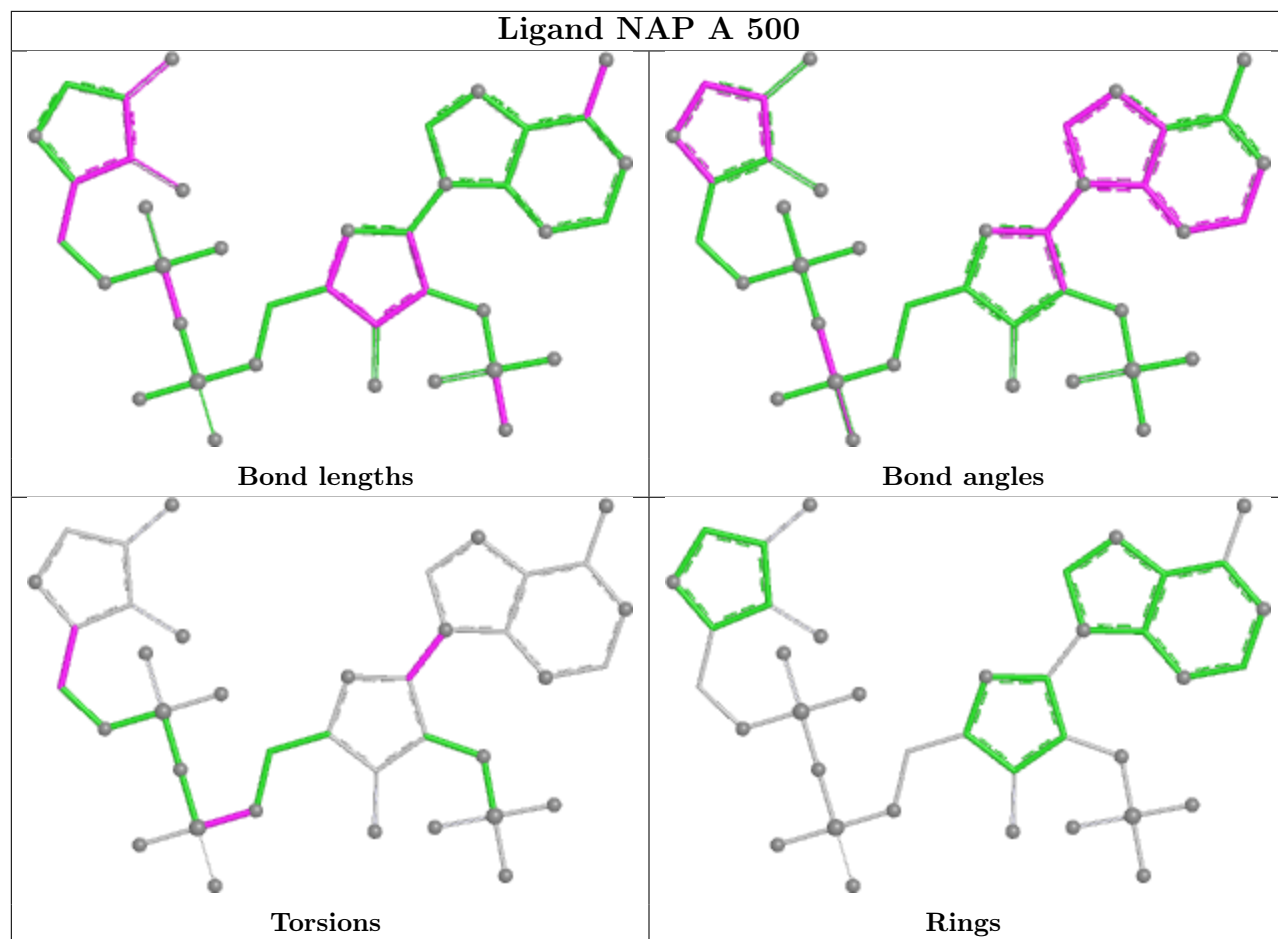
There are no ring outliers.

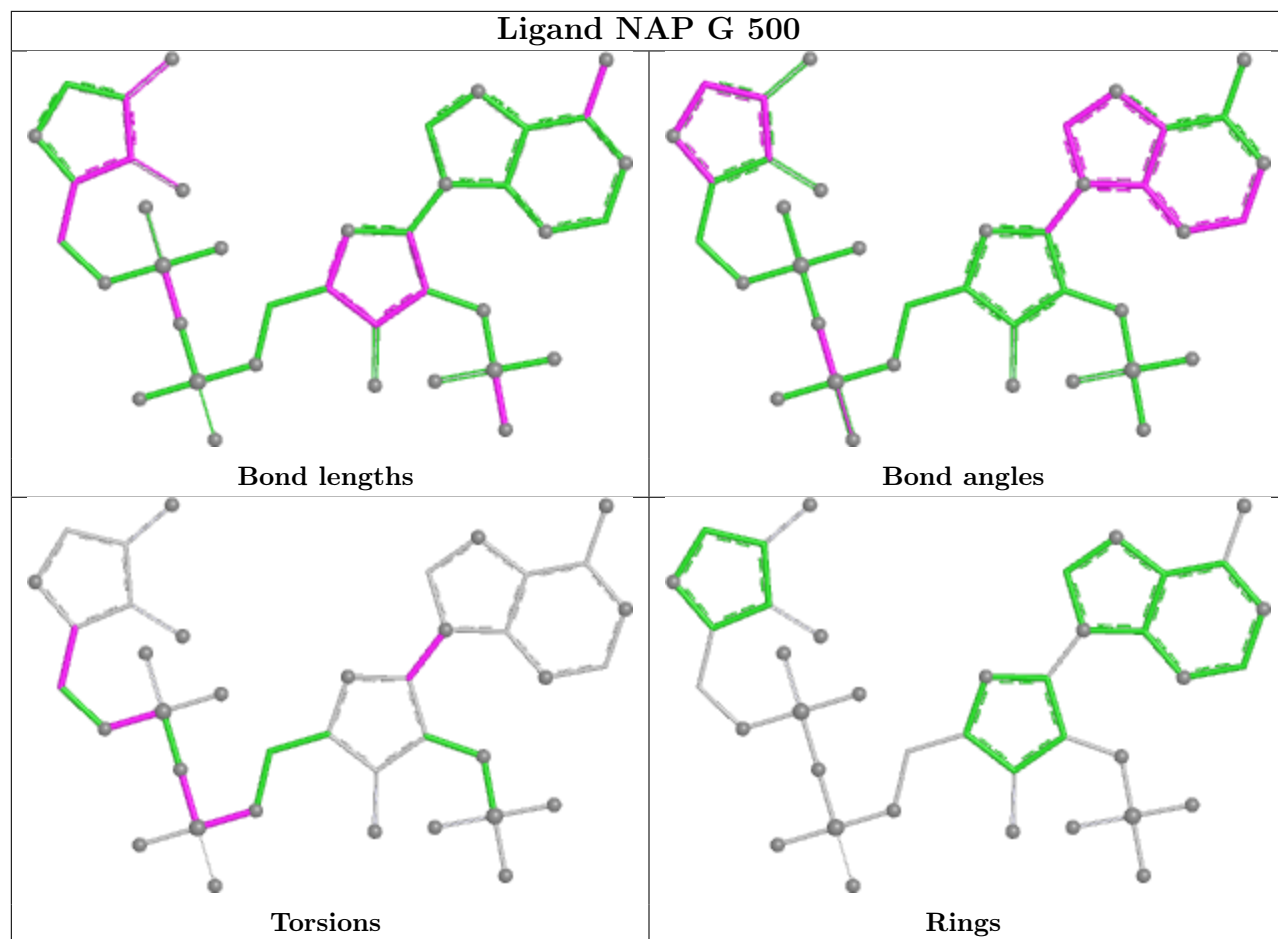
8 monomers are involved in 17 short contacts:

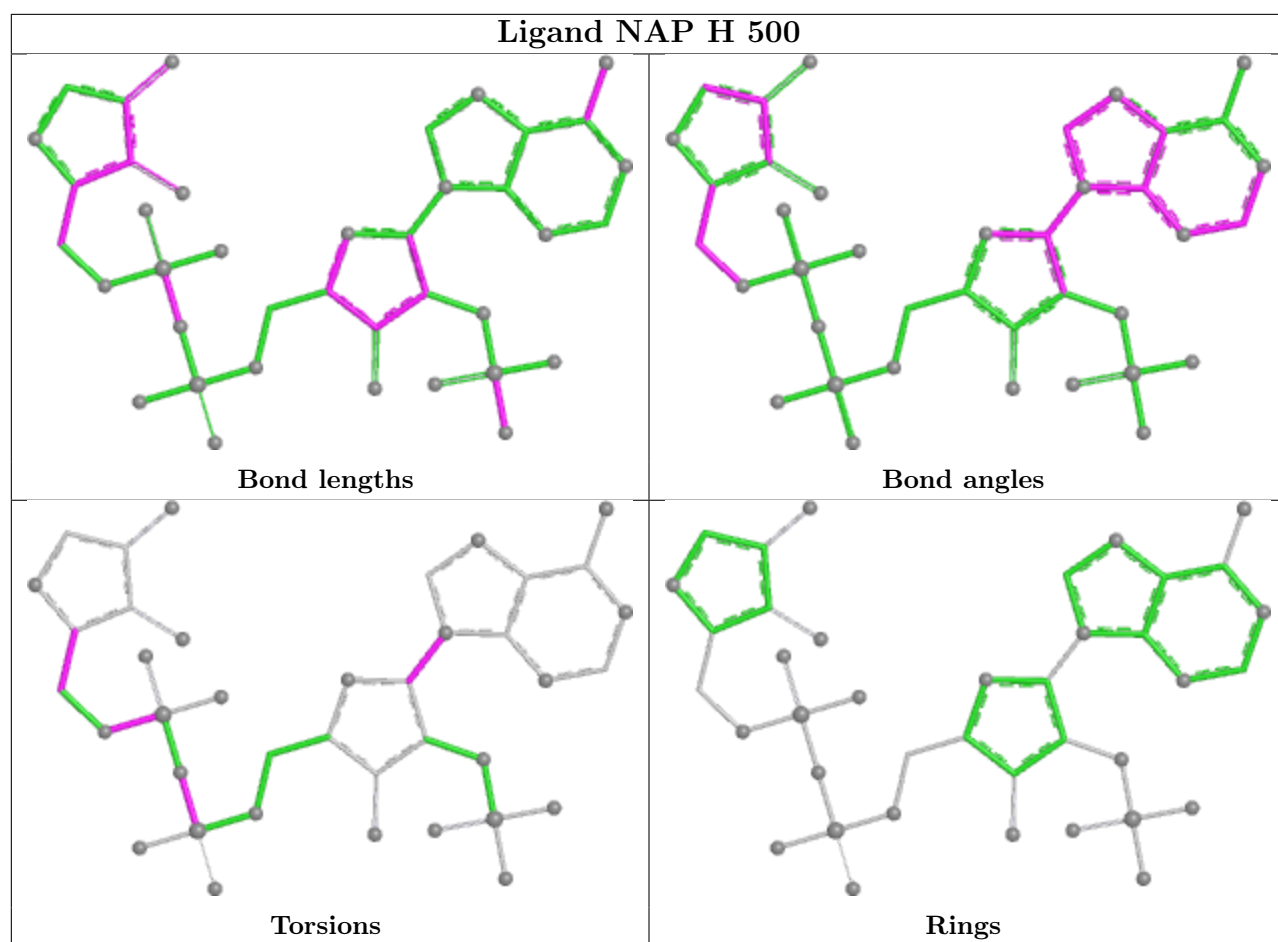
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	NAP	2	0
2	A	500	NAP	3	0
2	G	500	NAP	1	0
2	H	500	NAP	1	0
2	C	500	NAP	5	0
2	B	500	NAP	1	0
2	F	500	NAP	1	0
2	E	500	NAP	3	0

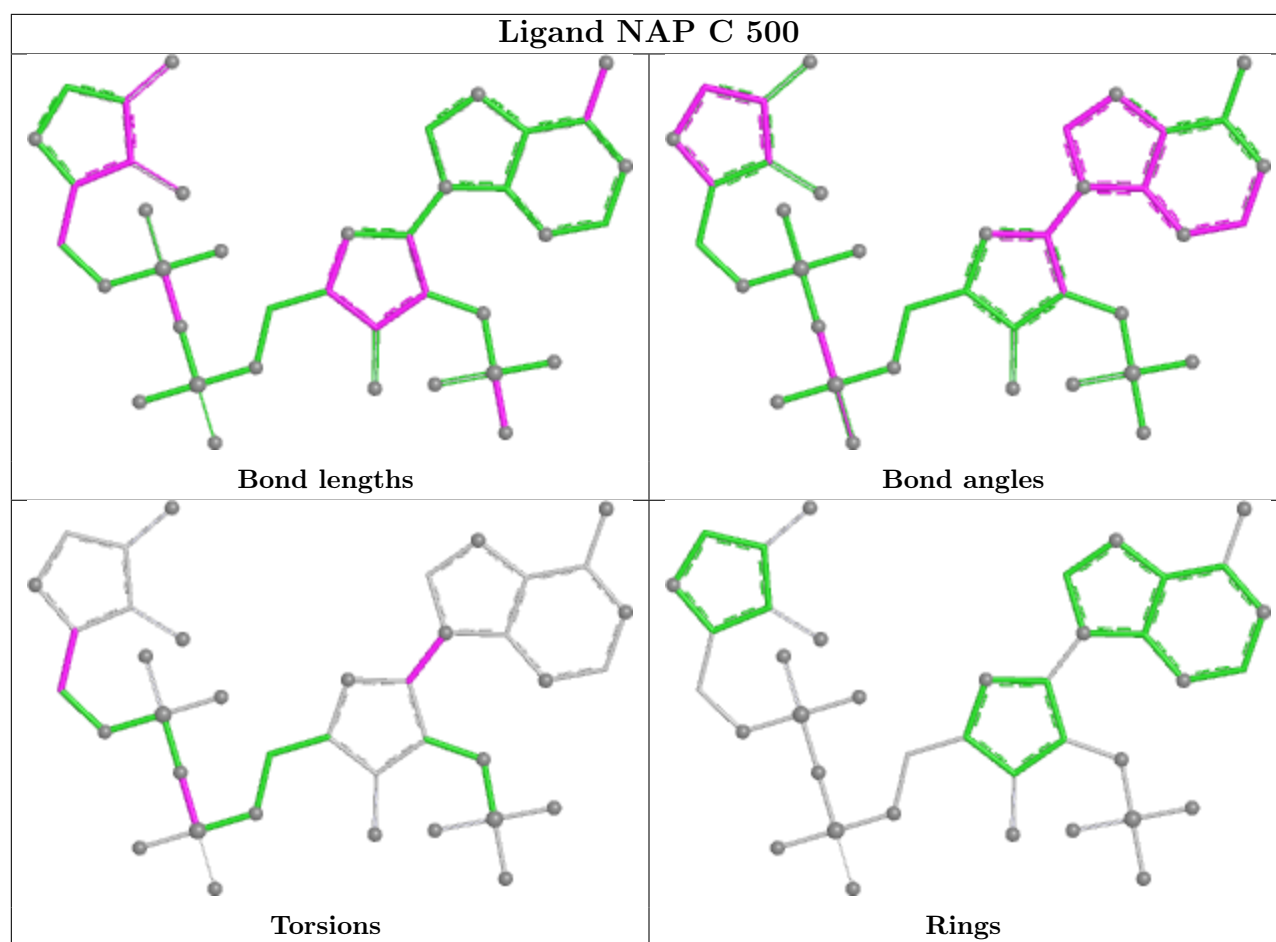
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

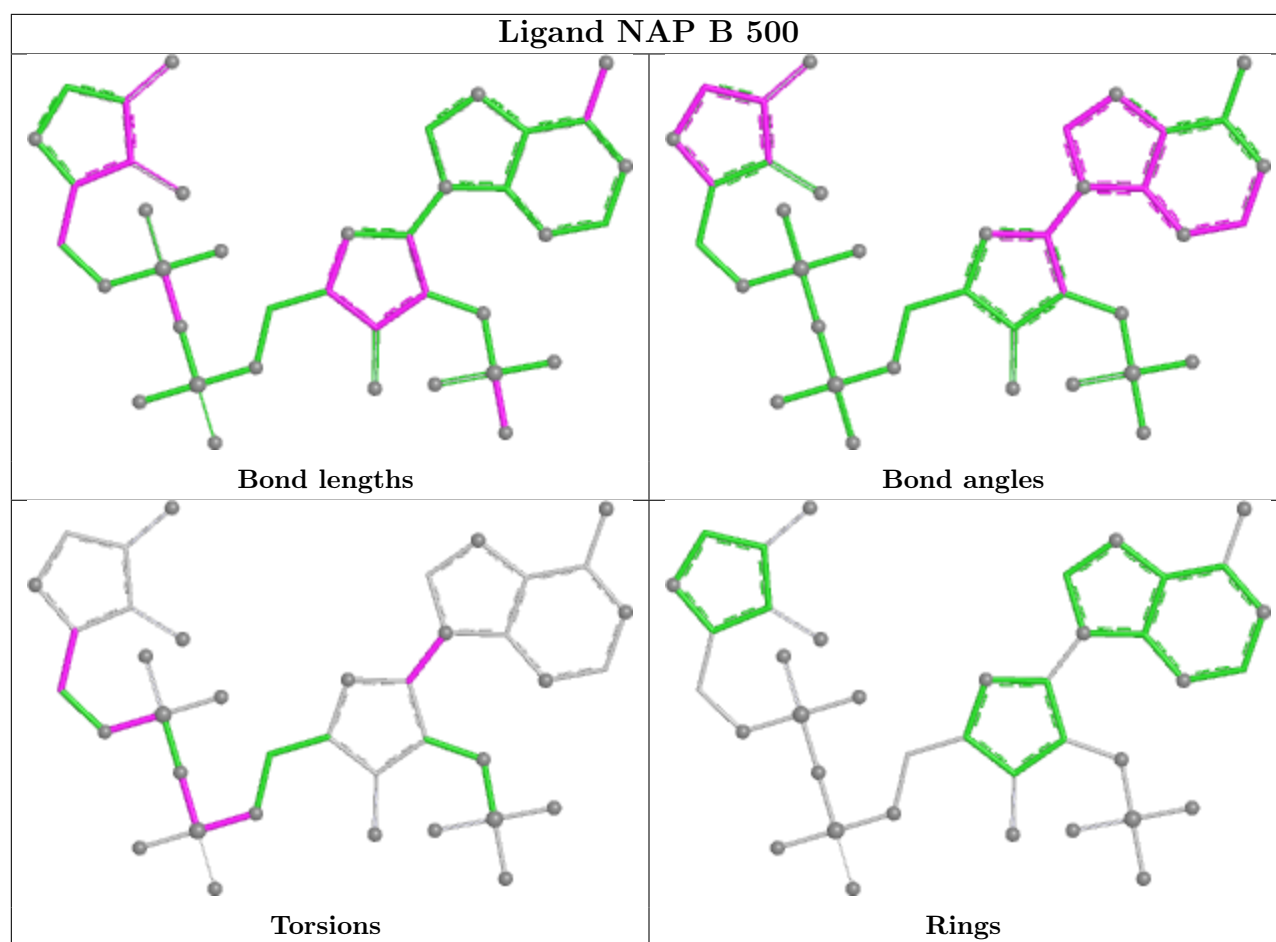


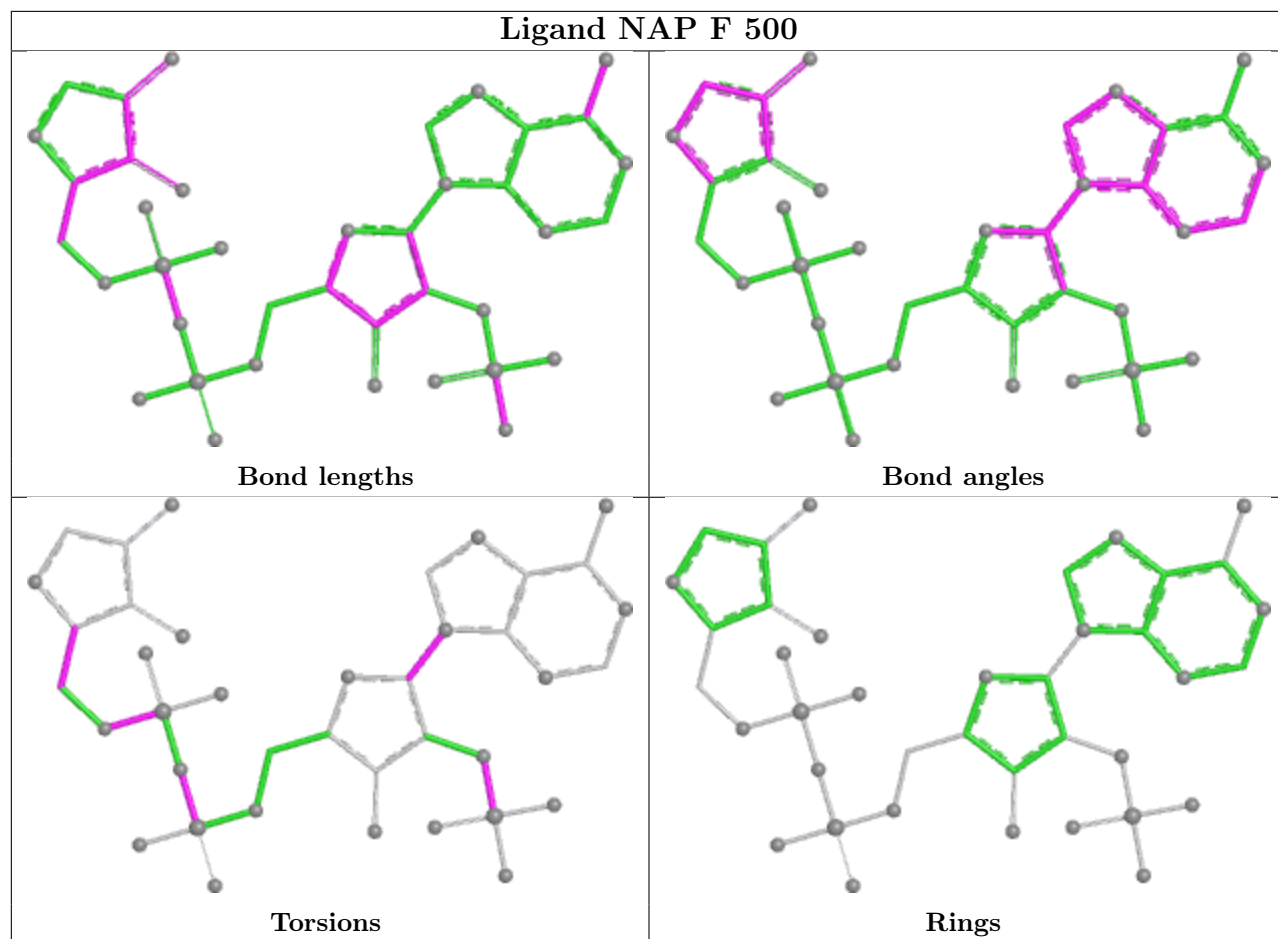


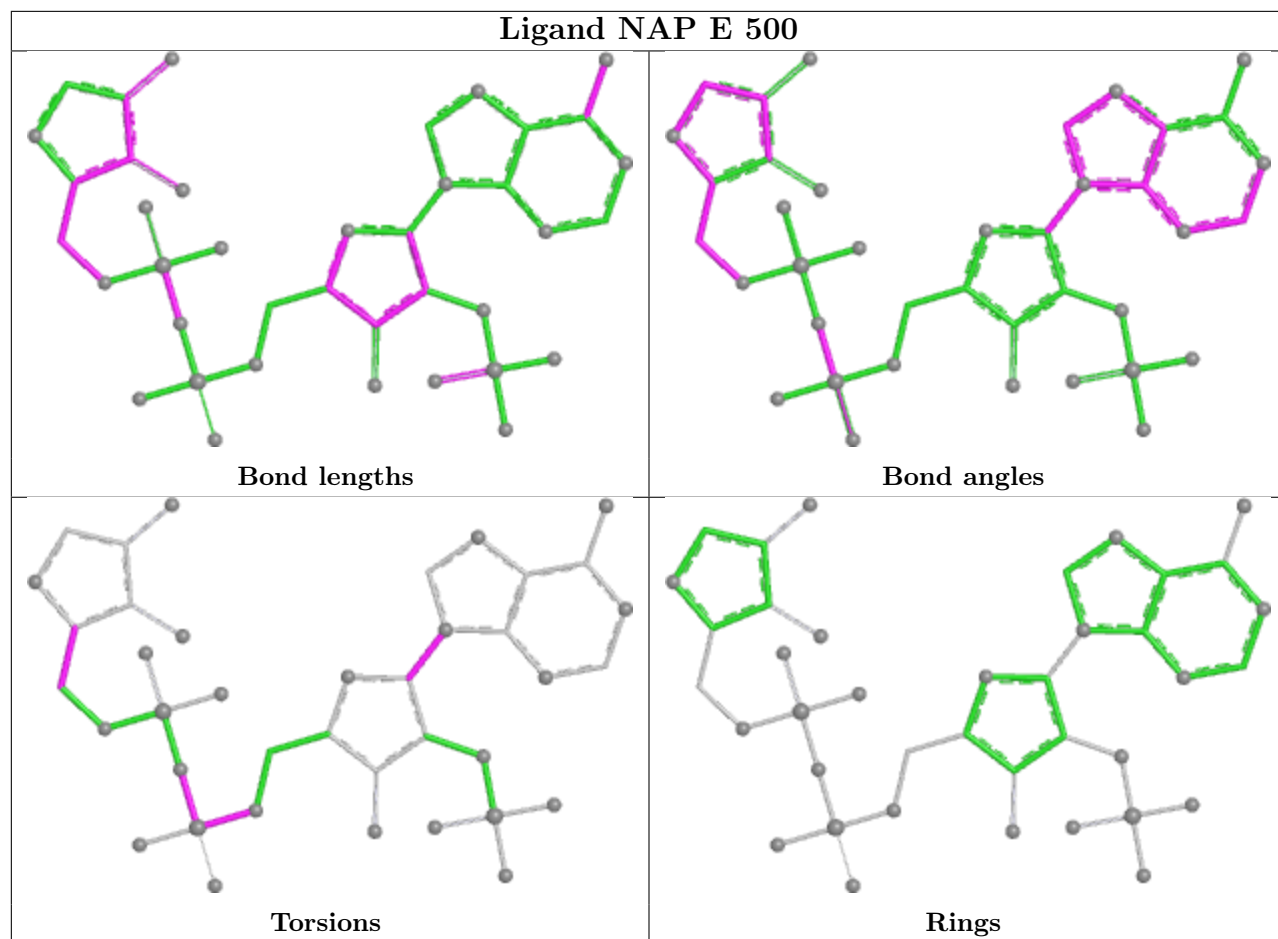












5.7 Other polymers [i](#)

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	485/491 (98%)	-0.09	10 (2%) 63 67	9, 19, 35, 53	5 (1%)
1	B	485/491 (98%)	-0.26	8 (1%) 70 74	9, 17, 32, 44	4 (0%)
1	C	483/491 (98%)	0.16	9 (1%) 66 70	10, 22, 40, 63	5 (1%)
1	D	484/491 (98%)	0.01	7 (1%) 73 76	10, 19, 33, 65	6 (1%)
1	E	490/491 (99%)	-0.11	8 (1%) 70 74	9, 19, 34, 51	13 (2%)
1	F	482/491 (98%)	-0.04	11 (2%) 61 65	10, 21, 38, 55	5 (1%)
1	G	484/491 (98%)	-0.07	11 (2%) 61 65	9, 18, 35, 51	8 (1%)
1	H	485/491 (98%)	-0.11	6 (1%) 76 79	9, 20, 33, 63	6 (1%)
All	All	3878/3928 (98%)	-0.06	70 (1%) 67 71	9, 19, 36, 65	52 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	25	PHE	5.3
1	F	25	PHE	5.2
1	D	491	LYS	4.8
1	C	491	LYS	4.7
1	E	2[A]	ILE	4.7
1	H	491	LYS	4.6
1	C	25	PHE	4.4
1	E	491	LYS	4.2
1	E	25	PHE	4.2
1	E	6[A]	ILE	3.9
1	G	7	MET	3.7
1	B	6	ILE	3.5
1	E	490	LEU	3.5
1	G	490	LEU	3.4
1	F	22	THR	3.4
1	E	4[A]	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	24	ALA	3.2
1	C	490	LEU	3.2
1	D	25	PHE	3.2
1	A	7	MET	3.2
1	C	22	THR	3.1
1	C	37	ILE	3.1
1	B	490	LEU	3.1
1	E	344	ASP	3.0
1	G	24	ALA	3.0
1	A	37	ILE	3.0
1	H	8	LYS	2.9
1	D	22	THR	2.9
1	G	8	LYS	2.9
1	G	22	THR	2.9
1	D	489	ALA	2.9
1	A	490	LEU	2.8
1	B	8	LYS	2.7
1	H	25	PHE	2.7
1	C	42	ARG	2.7
1	F	27	VAL	2.7
1	G	42	ARG	2.6
1	B	25	PHE	2.6
1	D	490	LEU	2.6
1	H	42	ARG	2.6
1	B	22	THR	2.5
1	G	489	ALA	2.5
1	E	5[A]	ASN	2.5
1	B	7	MET	2.5
1	F	38	ALA	2.4
1	H	7	MET	2.4
1	C	21	SER	2.4
1	F	26	GLN	2.3
1	A	21	SER	2.2
1	F	490	LEU	2.2
1	H	490	LEU	2.2
1	A	19	GLU	2.2
1	G	21	SER	2.2
1	A	25	PHE	2.2
1	A	79	GLU	2.1
1	A	22	THR	2.1
1	C	23	GLY	2.1
1	F	46	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	297	LYS	2.1
1	F	24	ALA	2.1
1	A	8	LYS	2.0
1	F	333	GLU	2.0
1	D	360	TRP	2.0
1	G	320	ARG	2.0
1	D	134	GLU	2.0
1	B	348	SER	2.0
1	F	37	ILE	2.0
1	A	94	VAL	2.0
1	B	473	ARG	2.0
1	F	9	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

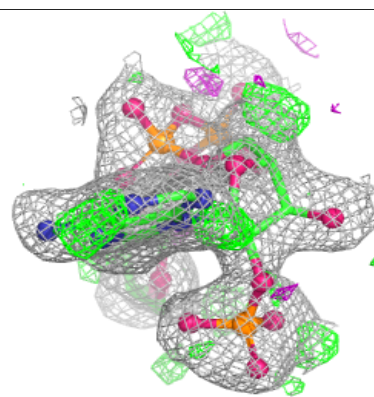
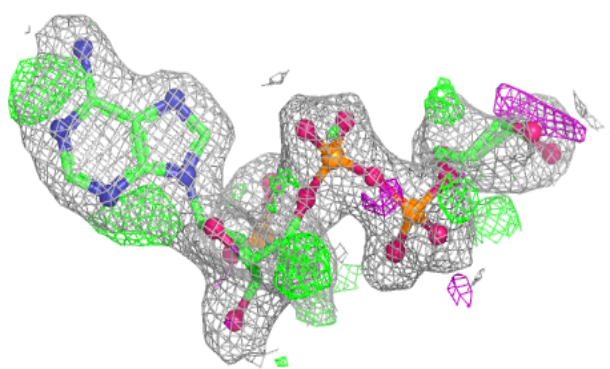
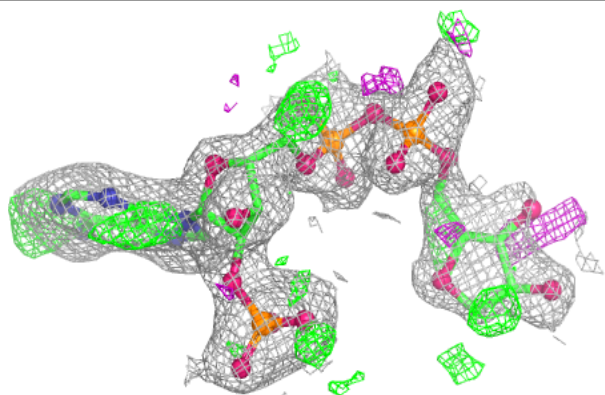
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	C	500	39/48	0.89	0.14	23,29,43,44	39
2	NAP	F	500	39/48	0.90	0.13	21,28,42,43	39
2	NAP	A	500	39/48	0.91	0.14	18,24,39,41	39
2	NAP	D	500	39/48	0.92	0.13	19,26,41,45	39
2	NAP	H	500	39/48	0.92	0.12	17,24,42,45	39
2	NAP	G	500	39/48	0.93	0.12	18,22,36,42	39
2	NAP	E	500	39/48	0.93	0.11	16,22,39,42	39
2	NAP	B	500	39/48	0.95	0.10	15,20,38,43	39

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.

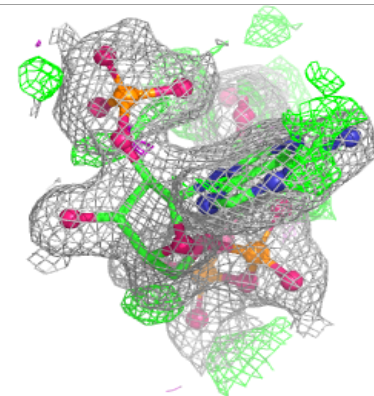
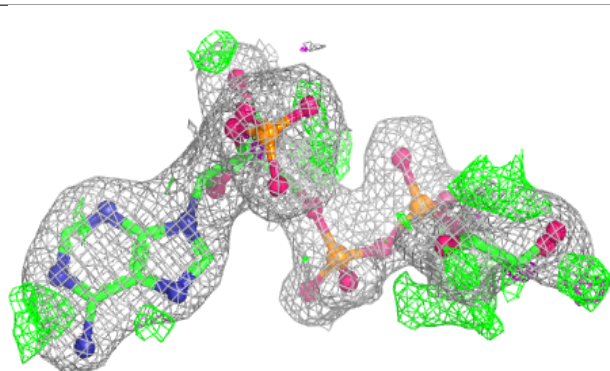
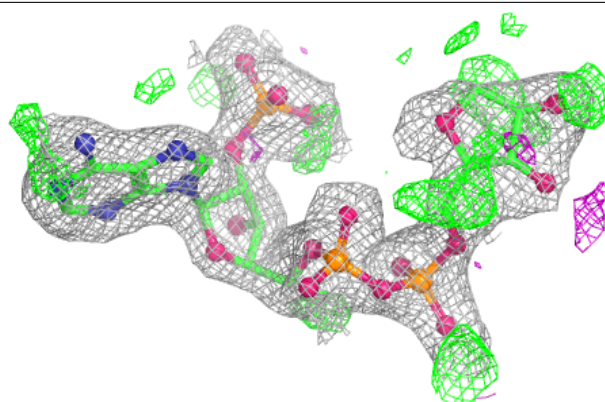
Electron density around NAP C 500:

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



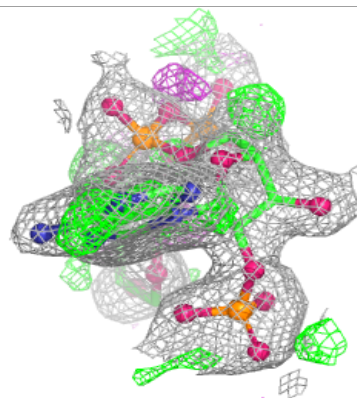
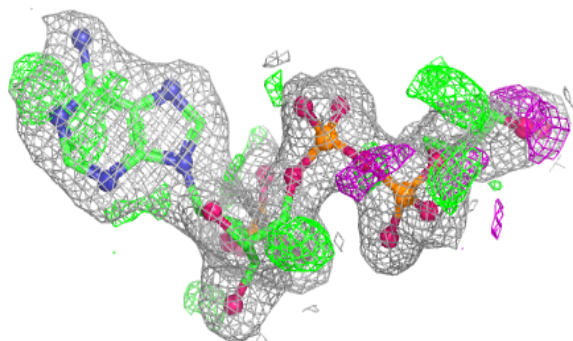
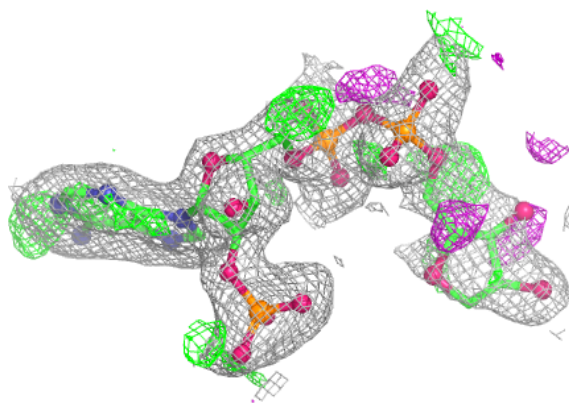
Electron density around NAP F 500:

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

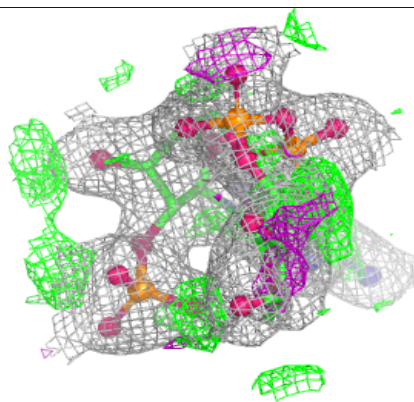
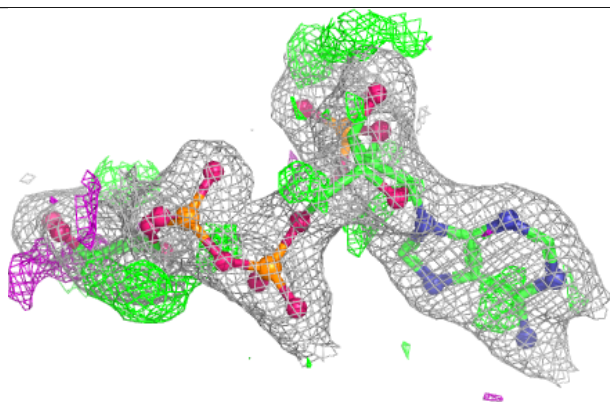
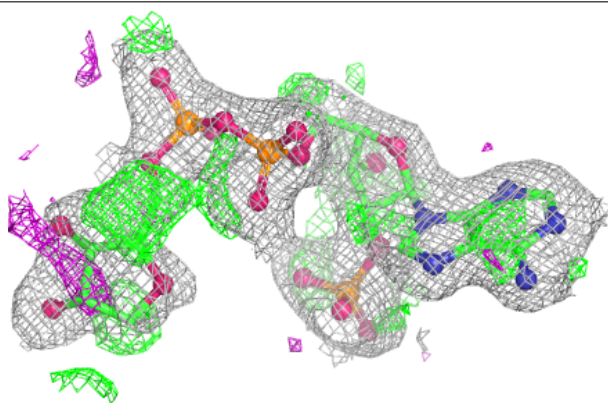


Electron density around NAP A 500:

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

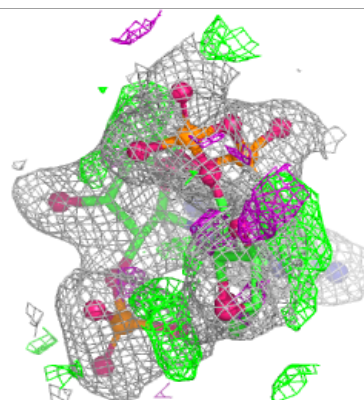
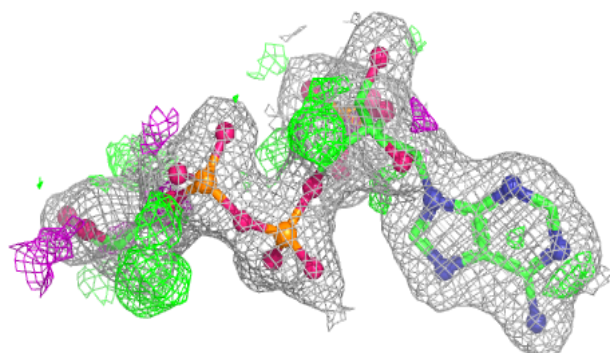
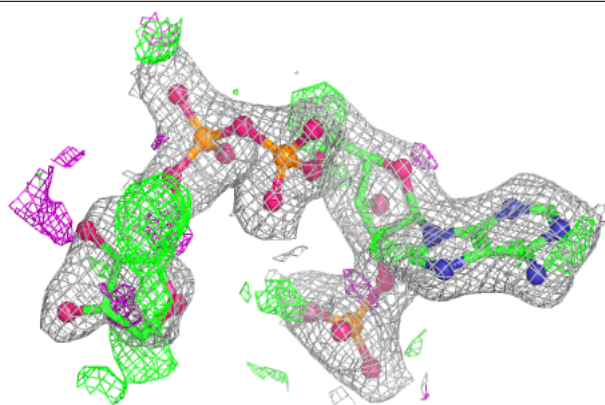
**Electron density around NAP D 500:**

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

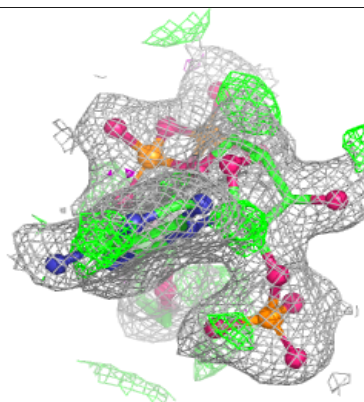
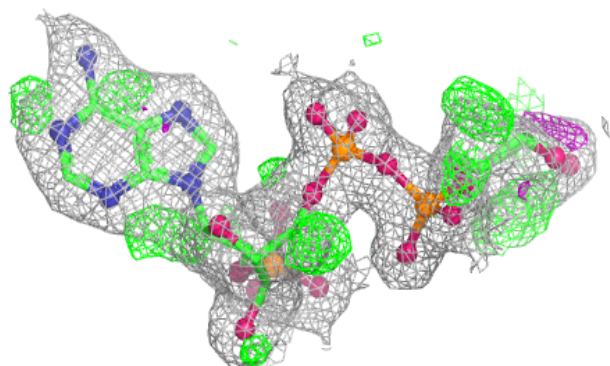
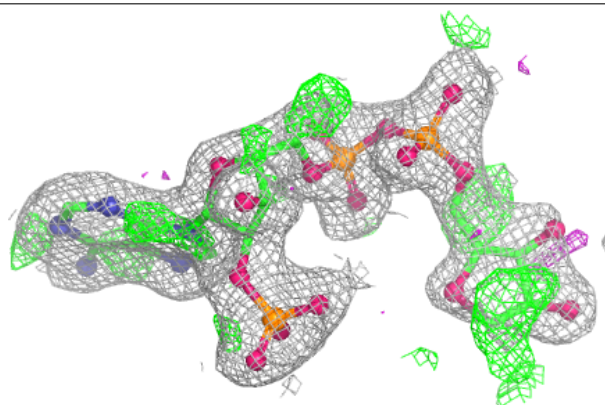


Electron density around NAP H 500:

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

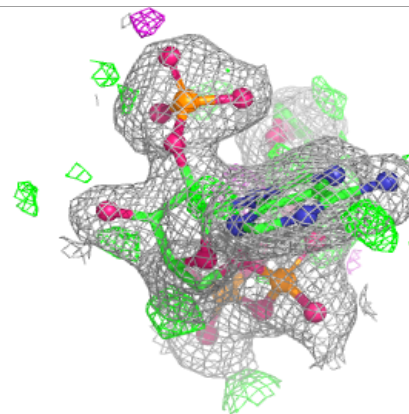
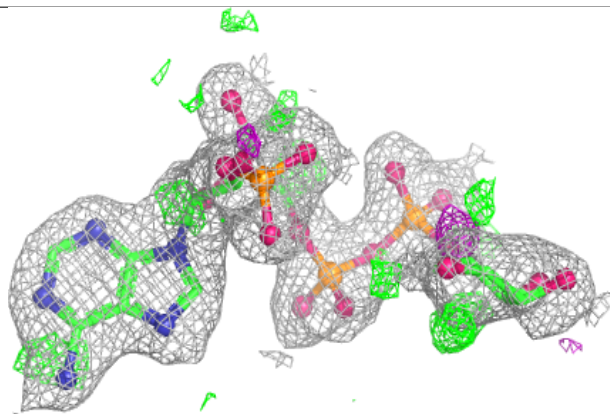
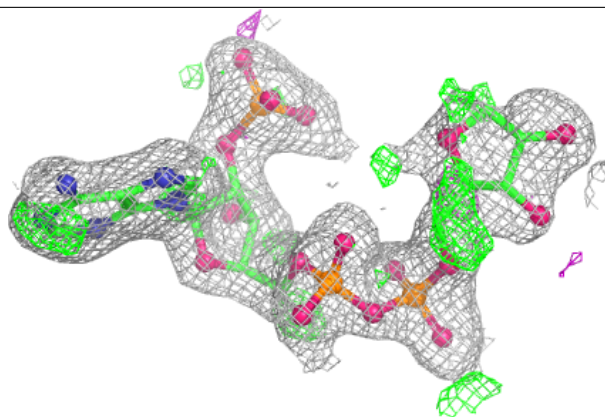
**Electron density around NAP G 500:**

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

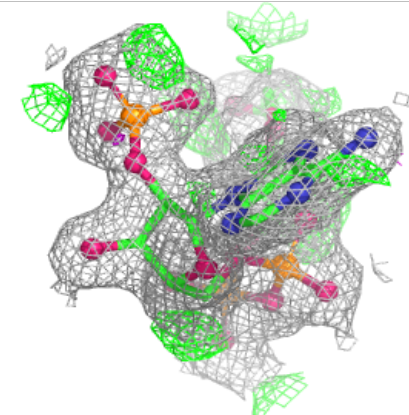
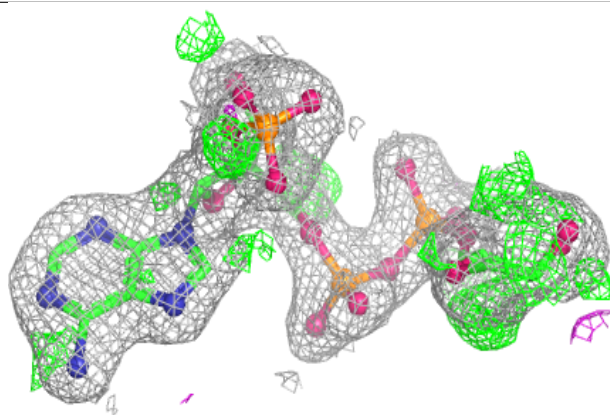
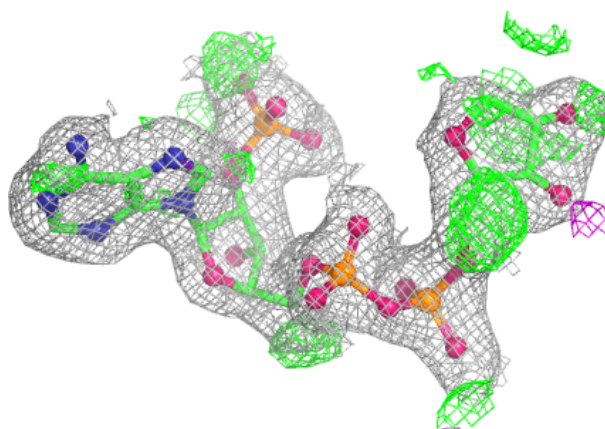


Electron density around NAP E 500:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.