Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 10:59 PM EDT

PDB ID	:	1EZ0
Title	:	CRYSTAL STRUCTURE OF THE NADP+ DEPENDENT ALDEHYDE DEHYDROGENASE FROM VIBRIO HARVEYI.
Authors	:	Ahvazi, B.; Coulombe, R.; Delarge, M.; Vedadi, M.; Zhang, L.; Meighen, E.; Vrielink, A.
Deposited on	:	2000-05-09
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

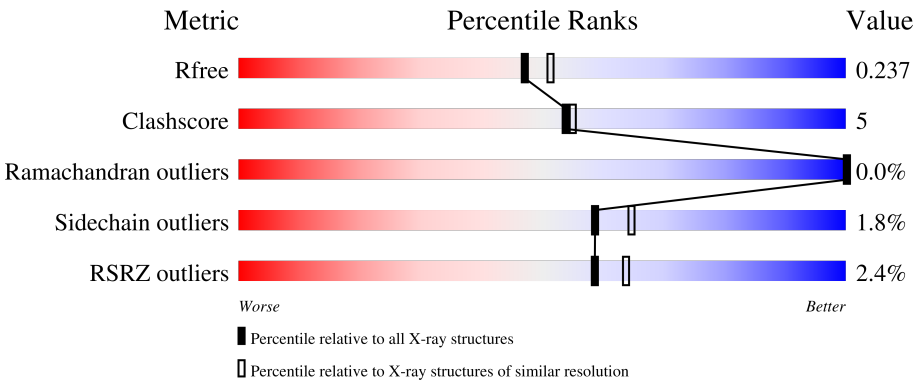
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	510	2% 88% 10% ••
1	B	510	3% 85% 13% •
1	C	510	2% 86% 12% ••
1	D	510	2% 84% 14% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15951 atoms, of which 0 are hydrogens and 0 are deuteriums.

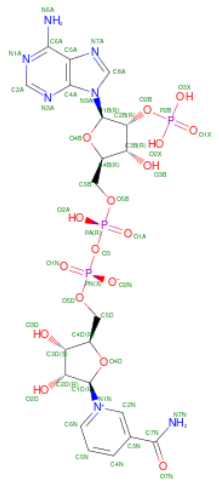
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	3788	2386	664	726	12	0	0	0
1	B	502	3773	2378	662	721	12	0	0	0
1	C	502	3773	2378	662	721	12	0	0	0
1	D	502	3773	2378	662	721	12	0	0	0

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

NAP



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

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

- Molecule 3 is water.

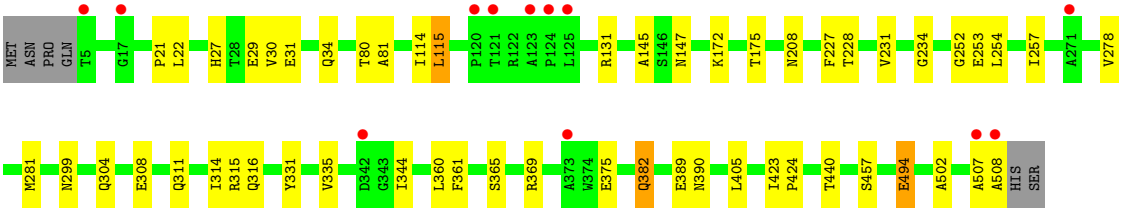
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	164	164	164	0	0
			Total	O		
3	B	164	164	164	0	0
			Total	O		
3	C	163	163	163	0	0
			Total	O		
3	D	161	161	161	0	0

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.

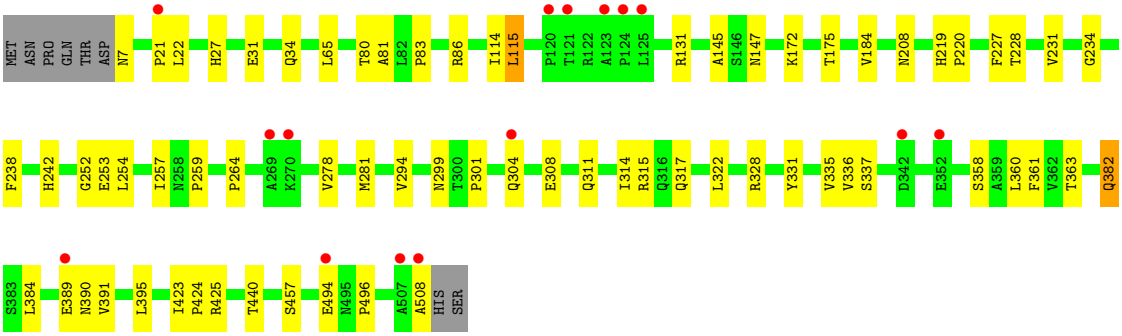
• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain A:



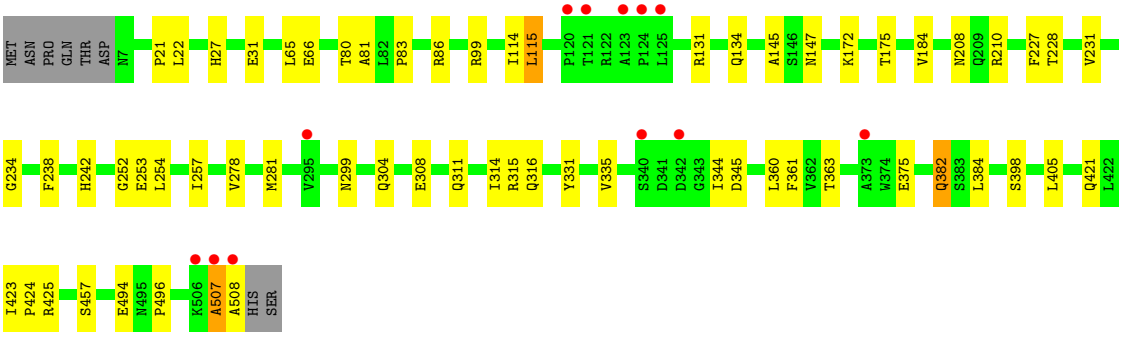
• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain B:



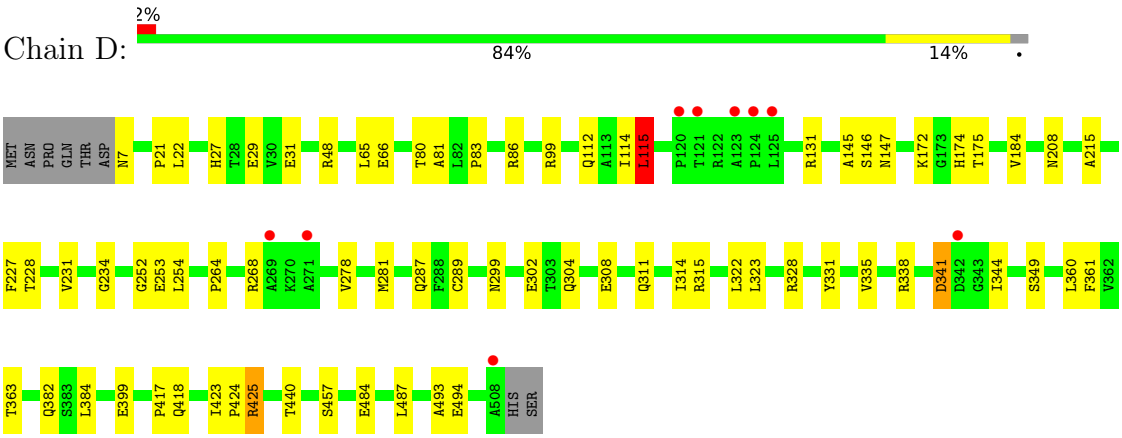
• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain C:



• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.38Å 131.18Å 92.54Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	26.44 – 2.10 26.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.8 (26.44-2.10) 83.9 (26.44-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.34 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.215 , 0.246 0.207 , 0.237	Depositor DCC
R_{free} test set	9248 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15951	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (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	0.34	0/3872	0.59	0/5283
1	B	0.34	0/3857	0.57	0/5262
1	C	0.34	0/3857	0.60	0/5262
1	D	0.34	0/3857	0.59	1/5262 (0.0%)
All	All	0.34	0/15443	0.59	1/21069 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	115	LEU	CA-CB-CG	5.11	127.06	115.30

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	3788	0	3743	34	0
1	B	3773	0	3732	44	0
1	C	3773	0	3732	43	0
1	D	3773	0	3732	47	0
2	A	48	0	25	4	0
2	B	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	6	0
2	D	48	0	25	5	0
3	A	164	0	0	0	0
3	B	164	0	0	1	0
3	C	163	0	0	1	0
3	D	161	0	0	1	0
All	All	15951	0	15039	162	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 (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ALA:HB3	1:C:508:ALA:HB1	1.32	1.08
1:B:508:ALA:HB3	1:C:508:ALA:CB	2.06	0.85
1:A:424:PRO:HG3	1:D:48:ARG:NH2	1.93	0.83
1:D:83:PRO:HG2	1:D:86:ARG:HB3	1.70	0.73
1:A:253:GLU:HB3	2:A:650:NAP:N7N	2.05	0.72
1:D:484:GLU:OE2	1:D:493:ALA:HB2	1.92	0.68
1:D:147:ASN:OD1	2:D:950:NAP:H5N	1.92	0.68
1:D:484:GLU:OE2	1:D:493:ALA:CB	2.41	0.68
1:C:253:GLU:HB3	2:C:850:NAP:N7N	2.09	0.67
1:D:289:CYS:HB3	2:D:950:NAP:C4N	2.24	0.67
1:B:301:PRO:HA	1:B:304:GLN:HG2	1.76	0.67
1:B:253:GLU:HB3	2:B:750:NAP:N7N	2.13	0.64
1:D:484:GLU:OE1	1:D:484:GLU:HA	1.98	0.64
1:B:391:VAL:HG12	1:B:395:LEU:HD12	1.80	0.63
1:C:147:ASN:OD1	2:C:850:NAP:H6N	1.99	0.63
1:C:494:GLU:HG3	1:C:496:PRO:HD3	1.83	0.61
1:B:257:ILE:HD12	1:B:259:PRO:HD3	1.83	0.60
1:D:29:GLU:HG2	1:D:215:ALA:CB	2.31	0.60
1:A:30:VAL:O	1:A:34:GLN:HG3	2.00	0.60
1:A:253:GLU:HB3	2:A:650:NAP:C7N	2.31	0.60
1:D:231:VAL:HA	1:D:254:LEU:HB3	1.84	0.60
1:B:83:PRO:HG2	1:B:86:ARG:HB3	1.84	0.59
1:A:344:ILE:HD11	1:A:361:PHE:HB3	1.85	0.59
1:B:253:GLU:HB3	2:B:750:NAP:C7N	2.31	0.59
1:D:29:GLU:HG2	1:D:215:ALA:HB2	1.86	0.58
1:A:424:PRO:HG3	1:D:48:ARG:HH21	1.66	0.58
1:C:253:GLU:HB3	2:C:850:NAP:C7N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:HD21	1:D:184:VAL:HG13	1.87	0.56
1:B:27:HIS:CD2	1:B:31:GLU:HG2	2.41	0.56
1:A:21:PRO:O	1:A:22:LEU:HB2	2.06	0.56
1:D:289:CYS:HB3	2:D:950:NAP:H4N	1.87	0.56
1:C:21:PRO:O	1:C:22:LEU:HB2	2.07	0.55
1:B:252:GLY:O	1:B:457:SER:HA	2.07	0.54
1:C:27:HIS:CD2	1:C:31:GLU:HG2	2.43	0.54
1:C:405:LEU:HD11	2:C:850:NAP:N7N	2.23	0.54
1:D:27:HIS:CD2	1:D:31:GLU:HG2	2.43	0.54
1:B:231:VAL:HA	1:B:254:LEU:HB3	1.90	0.54
1:B:494:GLU:HG3	1:B:496:PRO:HD3	1.90	0.54
1:A:405:LEU:HD11	2:A:650:NAP:N7N	2.23	0.53
1:B:21:PRO:O	1:B:22:LEU:HB2	2.08	0.53
1:D:21:PRO:O	1:D:22:LEU:HB2	2.09	0.53
1:D:112:GLN:HG2	1:D:112:GLN:O	2.09	0.53
1:A:27:HIS:CD2	1:A:31:GLU:HG2	2.44	0.53
1:B:317:GLN:HG2	1:B:358:SER:OG	2.09	0.52
1:C:231:VAL:HA	1:C:254:LEU:HB3	1.91	0.52
1:C:175:THR:HG21	1:C:208:ASN:HA	1.91	0.51
1:B:257:ILE:CD1	1:B:259:PRO:HD3	2.40	0.51
1:B:257:ILE:HD13	1:B:294:VAL:HG12	1.93	0.50
1:D:175:THR:HG21	1:D:208:ASN:HA	1.92	0.50
1:C:145:ALA:HB2	1:C:228:THR:CG2	2.42	0.50
1:B:314:ILE:HG13	1:B:360:LEU:HB2	1.94	0.50
1:A:316:GLN:O	1:A:316:GLN:HG3	2.12	0.49
1:A:145:ALA:HB2	1:A:228:THR:CG2	2.43	0.49
1:C:316:GLN:O	1:C:316:GLN:HG3	2.12	0.49
1:B:304:GLN:O	1:B:308:GLU:HG3	2.13	0.49
1:C:361:PHE:HE1	1:C:382:GLN:HG2	1.78	0.49
1:A:175:THR:HG21	1:A:208:ASN:HA	1.94	0.48
1:B:361:PHE:HE1	1:B:382:GLN:HG2	1.77	0.48
1:B:389:GLU:HG2	1:B:390:ASN:ND2	2.28	0.48
1:C:83:PRO:HG2	1:C:86:ARG:HB3	1.96	0.48
1:A:361:PHE:HE1	1:A:382:GLN:HG2	1.78	0.48
1:B:322:LEU:HD12	1:B:328:ARG:HA	1.95	0.48
1:D:314:ILE:HG13	1:D:360:LEU:HB2	1.96	0.48
1:C:421:GLN:O	1:C:425:ARG:NH1	2.46	0.48
1:A:389:GLU:HG2	1:A:390:ASN:ND2	2.28	0.48
1:B:301:PRO:O	1:B:304:GLN:HG2	2.14	0.47
1:B:363:THR:HG22	1:B:384:LEU:HD11	1.95	0.47
1:A:314:ILE:HG13	1:A:360:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:C	1:B:115:LEU:HD22	2.34	0.47
1:C:145:ALA:HB2	1:C:228:THR:HG21	1.96	0.47
1:A:311:GLN:O	1:A:315:ARG:HG3	2.14	0.47
1:A:80:THR:O	1:A:81:ALA:HB3	2.15	0.47
1:A:145:ALA:HB2	1:A:228:THR:HG21	1.96	0.47
1:C:257:ILE:CD1	1:C:375:GLU:HG3	2.44	0.47
1:D:344:ILE:HD11	1:D:361:PHE:HB3	1.97	0.47
1:D:363:THR:HG22	1:D:384:LEU:HD11	1.96	0.47
1:A:115:LEU:CD1	1:A:131:ARG:HD3	2.45	0.47
1:B:175:THR:HG21	1:B:208:ASN:HA	1.96	0.47
1:B:238:PHE:HZ	1:C:242:HIS:HD2	1.63	0.47
1:D:484:GLU:OE1	1:D:487:LEU:HD12	2.15	0.46
1:D:304:GLN:O	1:D:308:GLU:HG3	2.15	0.46
1:A:231:VAL:HA	1:A:254:LEU:HB3	1.96	0.46
1:B:242:HIS:HD2	1:C:238:PHE:HZ	1.62	0.46
1:C:507:ALA:O	1:C:508:ALA:HB3	2.15	0.46
1:A:114:ILE:C	1:A:115:LEU:HD22	2.36	0.46
1:C:311:GLN:O	1:C:315:ARG:HG3	2.16	0.46
1:C:114:ILE:C	1:C:115:LEU:HD22	2.37	0.45
1:D:264:PRO:HD2	3:D:1527:HOH:O	2.14	0.45
1:D:114:ILE:C	1:D:115:LEU:HD22	2.36	0.45
1:B:145:ALA:HB2	1:B:228:THR:CG2	2.46	0.45
1:D:311:GLN:O	1:D:315:ARG:HG3	2.16	0.45
1:D:145:ALA:HB2	1:D:228:THR:CG2	2.46	0.45
1:A:257:ILE:HD13	1:A:375:GLU:HG3	1.98	0.45
1:A:494:GLU:H	1:A:494:GLU:HG3	1.45	0.45
1:D:227:PHE:O	1:D:252:GLY:HA2	2.17	0.45
1:A:365:SER:O	1:A:369:ARG:HG3	2.17	0.45
1:A:502:ALA:HA	1:A:508:ALA:HA	1.99	0.45
1:B:395:LEU:HB3	1:B:425:ARG:NH1	2.32	0.45
1:C:344:ILE:HD11	1:C:361:PHE:HB3	1.98	0.45
1:D:331:TYR:O	1:D:335:VAL:HG22	2.17	0.45
1:B:278:VAL:HA	1:B:281:MET:HG2	1.99	0.45
1:C:331:TYR:O	1:C:335:VAL:HG22	2.18	0.44
1:D:268:ARG:NE	1:D:302:GLU:OE2	2.47	0.44
1:D:399:GLU:OE2	1:D:425:ARG:CZ	2.66	0.44
1:C:234:GLY:HA3	1:C:254:LEU:HD22	1.99	0.44
1:A:234:GLY:HA3	1:A:254:LEU:HD22	1.99	0.44
1:B:65:LEU:HD21	1:B:184:VAL:HG13	1.99	0.44
1:B:227:PHE:O	1:B:252:GLY:HA2	2.18	0.44
1:C:80:THR:O	1:C:81:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ILE:HG13	1:C:360:LEU:HB2	2.00	0.44
1:B:80:THR:O	1:B:81:ALA:HB3	2.18	0.44
1:D:115:LEU:CD1	1:D:131:ARG:HD3	2.48	0.43
1:C:252:GLY:O	1:C:457:SER:HA	2.19	0.43
1:C:227:PHE:O	1:C:252:GLY:HA2	2.19	0.43
1:C:494:GLU:HG2	3:C:1462:HOH:O	2.19	0.43
1:D:278:VAL:HA	1:D:281:MET:HG2	2.00	0.43
1:C:363:THR:HG22	1:C:384:LEU:HD11	2.01	0.43
1:A:304:GLN:O	1:A:308:GLU:HG3	2.18	0.43
1:B:257:ILE:HD12	1:B:257:ILE:C	2.39	0.43
1:D:322:LEU:HD12	1:D:328:ARG:HA	2.01	0.43
1:D:234:GLY:HA3	1:D:254:LEU:HD22	2.00	0.43
1:D:484:GLU:OE2	1:D:493:ALA:HB3	2.19	0.43
1:A:227:PHE:O	1:A:252:GLY:HA2	2.19	0.42
1:B:311:GLN:O	1:B:315:ARG:HG3	2.19	0.42
1:D:253:GLU:HB3	2:D:950:NAP:O7N	2.20	0.42
1:C:210:ARG:HE	2:C:850:NAP:P2B	2.42	0.42
1:B:145:ALA:HB2	1:B:228:THR:HG21	2.01	0.42
1:B:147:ASN:OD1	2:B:750:NAP:H6N	2.19	0.42
1:B:219:HIS:HA	1:B:220:PRO:HD3	1.86	0.42
1:A:147:ASN:OD1	2:A:650:NAP:H6N	2.20	0.42
1:B:331:TYR:O	1:B:335:VAL:HG22	2.20	0.42
1:B:336:VAL:HG23	1:B:337:SER:N	2.34	0.42
1:B:423:ILE:HB	1:B:424:PRO:HD3	2.00	0.42
1:B:264:PRO:HD2	3:B:1204:HOH:O	2.19	0.42
1:C:423:ILE:HB	1:C:424:PRO:HD3	2.02	0.42
1:D:423:ILE:HB	1:D:424:PRO:HD3	2.01	0.42
1:A:278:VAL:HA	1:A:281:MET:HG2	2.02	0.41
1:C:278:VAL:HA	1:C:281:MET:HG2	2.02	0.41
1:D:80:THR:O	1:D:81:ALA:HB3	2.20	0.41
1:C:134:GLN:HE21	1:C:134:GLN:HB3	1.68	0.41
1:D:253:GLU:HB3	2:D:950:NAP:C7N	2.50	0.41
1:C:304:GLN:O	1:C:308:GLU:HG3	2.20	0.41
1:D:338:ARG:O	1:D:341:ASP:HB2	2.20	0.41
1:A:423:ILE:HB	1:A:424:PRO:HD3	2.02	0.41
1:D:66:GLU:CD	1:D:99:ARG:HH22	2.24	0.41
1:D:252:GLY:O	1:D:457:SER:HA	2.20	0.41
1:B:234:GLY:HA3	1:B:254:LEU:HD22	2.02	0.41
1:D:417:PRO:HB2	1:D:418:GLN:NE2	2.35	0.41
1:A:331:TYR:O	1:A:335:VAL:HG22	2.21	0.41
1:C:65:LEU:HD21	1:C:184:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:OD1	2:C:850:NAP:C6N	2.68	0.41
1:C:257:ILE:HD13	1:C:375:GLU:HG3	2.03	0.41
1:D:145:ALA:HB2	1:D:228:THR:HG21	2.03	0.41
1:C:66:GLU:CD	1:C:99:ARG:HH22	2.25	0.41
1:D:287:GLN:OE1	1:D:323:LEU:HG	2.21	0.41
1:D:314:ILE:O	1:D:349:SER:HB3	2.22	0.41
1:B:115:LEU:CD1	1:B:131:ARG:HD3	2.51	0.40
1:C:398:SER:OG	1:C:425:ARG:HD3	2.22	0.40
1:D:146:SER:HB3	1:D:174:HIS:NE2	2.36	0.40
1:A:507:ALA:O	1:A:508:ALA:C	2.60	0.40
1:C:115:LEU:CD1	1:C:131:ARG:HD3	2.52	0.40
1:A:252:GLY:O	1:A:457:SER:HA	2.22	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	502/510 (98%)	490 (98%)	12 (2%)	0	100	100
1	B	500/510 (98%)	485 (97%)	15 (3%)	0	100	100
1	C	500/510 (98%)	487 (97%)	12 (2%)	1 (0%)	47	49
1	D	500/510 (98%)	486 (97%)	14 (3%)	0	100	100
All	All	2002/2040 (98%)	1948 (97%)	53 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	507	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/405 (98%)	392 (98%)	7 (2%)	59	65
1	B	397/405 (98%)	390 (98%)	7 (2%)	59	65
1	C	397/405 (98%)	392 (99%)	5 (1%)	69	75
1	D	397/405 (98%)	388 (98%)	9 (2%)	50	55
All	All	1590/1620 (98%)	1562 (98%)	28 (2%)	59	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	115	LEU
1	A	172	LYS
1	A	299	ASN
1	A	382	GLN
1	A	440	THR
1	A	494	GLU
1	B	7	ASN
1	B	34	GLN
1	B	115	LEU
1	B	172	LYS
1	B	299	ASN
1	B	382	GLN
1	B	440	THR
1	C	115	LEU
1	C	172	LYS
1	C	299	ASN
1	C	345	ASP
1	C	382	GLN
1	D	7	ASN
1	D	115	LEU
1	D	172	LYS
1	D	299	ASN
1	D	341	ASP

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Mol	Chain	Res	Type
1	D	382	GLN
1	D	425	ARG
1	D	440	THR
1	D	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	112	GLN
1	A	134	GLN
1	A	209	GLN
1	A	299	ASN
1	A	311	GLN
1	A	334	GLN
1	A	367	ASN
1	A	382	GLN
1	A	418	GLN
1	A	459	HIS
1	B	7	ASN
1	B	51	ASN
1	B	134	GLN
1	B	209	GLN
1	B	299	ASN
1	B	311	GLN
1	B	334	GLN
1	B	367	ASN
1	B	382	GLN
1	B	418	GLN
1	B	459	HIS
1	C	7	ASN
1	C	51	ASN
1	C	112	GLN
1	C	134	GLN
1	C	209	GLN
1	C	242	HIS
1	C	299	ASN
1	C	311	GLN
1	C	334	GLN
1	C	367	ASN
1	C	382	GLN
1	C	418	GLN

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Mol	Chain	Res	Type
1	C	459	HIS
1	C	471	HIS
1	D	51	ASN
1	D	134	GLN
1	D	209	GLN
1	D	299	ASN
1	D	311	GLN
1	D	316	GLN
1	D	317	GLN
1	D	334	GLN
1	D	367	ASN
1	D	382	GLN
1	D	418	GLN
1	D	459	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	C	850	-	45,52,52	2.31	11 (24%)	56,80,80	2.06	11 (19%)
2	NAP	D	950	-	45,52,52	2.18	12 (26%)	56,80,80	2.07	13 (23%)
2	NAP	B	750	-	45,52,52	2.31	13 (28%)	56,80,80	2.03	11 (19%)
2	NAP	A	650	-	45,52,52	2.29	12 (26%)	56,80,80	2.01	11 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	850	-	-	8/31/67/67	0/5/5/5
2	NAP	D	950	-	-	14/31/67/67	0/5/5/5
2	NAP	B	750	-	-	7/31/67/67	0/5/5/5
2	NAP	A	650	-	-	8/31/67/67	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	850	NAP	C2N-N1N	7.79	1.44	1.35
2	A	650	NAP	C2N-N1N	7.74	1.44	1.35
2	B	750	NAP	C2N-N1N	7.69	1.44	1.35
2	C	850	NAP	P2B-O2B	7.40	1.73	1.59
2	A	650	NAP	P2B-O2B	6.96	1.72	1.59
2	D	950	NAP	C2N-N1N	6.92	1.43	1.35
2	B	750	NAP	P2B-O2B	6.83	1.72	1.59
2	D	950	NAP	P2B-O2B	6.45	1.71	1.59
2	B	750	NAP	C3N-C7N	4.77	1.57	1.50
2	D	950	NAP	C3N-C7N	4.63	1.57	1.50
2	C	850	NAP	C4N-C3N	4.31	1.46	1.39
2	D	950	NAP	C4N-C3N	4.27	1.46	1.39
2	C	850	NAP	C3N-C7N	4.20	1.56	1.50
2	A	650	NAP	C4N-C3N	4.19	1.46	1.39
2	B	750	NAP	C4N-C3N	4.18	1.46	1.39
2	A	650	NAP	C3N-C7N	4.15	1.56	1.50
2	A	650	NAP	C2A-N1A	3.39	1.40	1.33
2	D	950	NAP	C2A-N1A	3.24	1.39	1.33
2	C	850	NAP	C2A-N1A	3.18	1.39	1.33
2	B	750	NAP	C2A-N1A	3.15	1.39	1.33
2	A	650	NAP	C5N-C4N	3.01	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	NAP	C5N-C4N	3.00	1.45	1.38
2	D	950	NAP	C5N-C4N	2.89	1.45	1.38
2	A	650	NAP	C3B-C2B	2.79	1.59	1.52
2	A	650	NAP	C7N-N7N	2.78	1.38	1.33
2	B	750	NAP	C3B-C2B	2.76	1.59	1.52
2	D	950	NAP	C6N-N1N	2.74	1.42	1.35
2	C	850	NAP	C3B-C2B	2.73	1.59	1.52
2	C	850	NAP	C5N-C4N	2.72	1.44	1.38
2	B	750	NAP	C7N-N7N	2.71	1.38	1.33
2	A	650	NAP	C6N-N1N	2.68	1.41	1.35
2	B	750	NAP	C6N-N1N	2.64	1.41	1.35
2	D	950	NAP	C7N-N7N	2.62	1.38	1.33
2	C	850	NAP	C7N-N7N	2.60	1.37	1.33
2	C	850	NAP	C6N-N1N	2.53	1.41	1.35
2	B	750	NAP	P2B-O3X	-2.51	1.45	1.54
2	D	950	NAP	C3B-C2B	2.49	1.58	1.52
2	D	950	NAP	P2B-O3X	-2.47	1.45	1.54
2	A	650	NAP	P2B-O3X	-2.46	1.45	1.54
2	C	850	NAP	P2B-O3X	-2.40	1.45	1.54
2	B	750	NAP	C2N-C3N	2.40	1.42	1.39
2	B	750	NAP	C4A-N3A	2.38	1.38	1.35
2	B	750	NAP	C5B-C4B	2.32	1.58	1.51
2	C	850	NAP	C2N-C3N	2.32	1.42	1.39
2	D	950	NAP	C5B-C4B	2.29	1.58	1.51
2	A	650	NAP	C5B-C4B	2.29	1.58	1.51
2	D	950	NAP	C4A-N3A	2.27	1.38	1.35
2	A	650	NAP	C2N-C3N	2.21	1.42	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	850	NAP	C5N-C4N-C3N	-7.48	111.49	120.34
2	B	750	NAP	C5N-C4N-C3N	-7.31	111.69	120.34
2	A	650	NAP	C5N-C4N-C3N	-7.30	111.70	120.34
2	D	950	NAP	C5N-C4N-C3N	-7.14	111.90	120.34
2	D	950	NAP	C3N-C2N-N1N	-6.14	114.42	120.43
2	C	850	NAP	C2N-C3N-C4N	6.13	125.20	118.26
2	A	650	NAP	C2N-C3N-C4N	6.06	125.13	118.26
2	B	750	NAP	C2N-C3N-C4N	6.01	125.08	118.26
2	D	950	NAP	C2N-C3N-C4N	5.53	124.53	118.26
2	A	650	NAP	C3N-C2N-N1N	-4.90	115.64	120.43
2	C	850	NAP	C3N-C2N-N1N	-4.86	115.68	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	850	NAP	O4D-C1D-C2D	-4.69	100.07	106.93
2	B	750	NAP	C3N-C2N-N1N	-4.60	115.93	120.43
2	B	750	NAP	C6N-C5N-C4N	4.55	126.05	119.44
2	B	750	NAP	O4D-C1D-C2D	-4.48	100.37	106.93
2	A	650	NAP	C6N-C5N-C4N	4.40	125.84	119.44
2	C	850	NAP	C6N-C5N-C4N	4.39	125.82	119.44
2	D	950	NAP	C6N-C5N-C4N	4.38	125.80	119.44
2	A	650	NAP	O4D-C1D-C2D	-4.00	101.08	106.93
2	B	750	NAP	O2B-P2B-O1X	-3.45	96.08	109.39
2	D	950	NAP	O4D-C1D-C2D	-3.38	101.98	106.93
2	D	950	NAP	O2B-P2B-O1X	-3.34	96.51	109.39
2	D	950	NAP	C5N-C6N-N1N	-3.32	115.64	120.40
2	A	650	NAP	O2B-P2B-O1X	-3.29	96.68	109.39
2	B	750	NAP	PN-O3-PA	3.29	144.12	132.83
2	C	850	NAP	O2B-P2B-O1X	-3.17	97.17	109.39
2	D	950	NAP	PN-O3-PA	3.13	143.55	132.83
2	C	850	NAP	C4A-C5A-N7A	3.06	112.58	109.40
2	C	850	NAP	PN-O3-PA	3.01	143.15	132.83
2	A	650	NAP	PN-O3-PA	2.99	143.08	132.83
2	D	950	NAP	C4A-C5A-N7A	2.63	112.14	109.40
2	A	650	NAP	C5N-C6N-N1N	-2.49	116.83	120.40
2	D	950	NAP	C2N-N1N-C1D	-2.43	113.71	119.14
2	B	750	NAP	C5N-C6N-N1N	-2.39	116.98	120.40
2	C	850	NAP	O7N-C7N-C3N	-2.36	116.81	119.63
2	C	850	NAP	N6A-C6A-N1A	2.36	123.47	118.57
2	A	650	NAP	N6A-C6A-N1A	2.35	123.45	118.57
2	A	650	NAP	C4A-C5A-N7A	2.29	111.78	109.40
2	A	650	NAP	O7N-C7N-C3N	-2.24	116.96	119.63
2	B	750	NAP	C4A-C5A-N7A	2.21	111.70	109.40
2	B	750	NAP	O7N-C7N-C3N	-2.17	117.03	119.63
2	C	850	NAP	C5N-C6N-N1N	-2.11	117.38	120.40
2	B	750	NAP	N6A-C6A-N1A	2.10	122.94	118.57
2	D	950	NAP	O7N-C7N-C3N	-2.08	117.15	119.63
2	D	950	NAP	N6A-C6A-N1A	2.07	122.87	118.57
2	D	950	NAP	O3X-P2B-O2X	2.00	115.30	107.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	650	NAP	C5D-O5D-PN-O2N
2	A	650	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	B	750	NAP	PN-O3-PA-O5B
2	B	750	NAP	C5D-O5D-PN-O1N
2	B	750	NAP	C5D-O5D-PN-O2N
2	B	750	NAP	O4D-C4D-C5D-O5D
2	B	750	NAP	C3D-C4D-C5D-O5D
2	C	850	NAP	C5D-O5D-PN-O2N
2	D	950	NAP	PN-O3-PA-O5B
2	D	950	NAP	C5D-O5D-PN-O1N
2	D	950	NAP	C5D-O5D-PN-O2N
2	D	950	NAP	C2N-C3N-C7N-N7N
2	A	650	NAP	O4D-C4D-C5D-O5D
2	C	850	NAP	O4D-C4D-C5D-O5D
2	C	850	NAP	C3D-C4D-C5D-O5D
2	D	950	NAP	C3D-C4D-C5D-O5D
2	D	950	NAP	O4D-C4D-C5D-O5D
2	D	950	NAP	C4N-C3N-C7N-N7N
2	D	950	NAP	C2N-C3N-C7N-O7N
2	A	650	NAP	C5D-O5D-PN-O3
2	B	750	NAP	C5D-O5D-PN-O3
2	C	850	NAP	C5D-O5D-PN-O3
2	D	950	NAP	C4D-C5D-O5D-PN
2	A	650	NAP	C5D-O5D-PN-O1N
2	C	850	NAP	C5D-O5D-PN-O1N
2	B	750	NAP	C4D-C5D-O5D-PN
2	A	650	NAP	C3B-C2B-O2B-P2B
2	D	950	NAP	C2B-O2B-P2B-O1X
2	A	650	NAP	C1B-C2B-O2B-P2B
2	C	850	NAP	C1B-C2B-O2B-P2B
2	C	850	NAP	C3B-C2B-O2B-P2B
2	A	650	NAP	C2B-O2B-P2B-O2X
2	C	850	NAP	C2B-O2B-P2B-O2X
2	D	950	NAP	C2B-O2B-P2B-O2X
2	D	950	NAP	C5D-O5D-PN-O3
2	D	950	NAP	C1B-C2B-O2B-P2B
2	D	950	NAP	C3B-C2B-O2B-P2B

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	850	NAP	6	0
2	D	950	NAP	5	0

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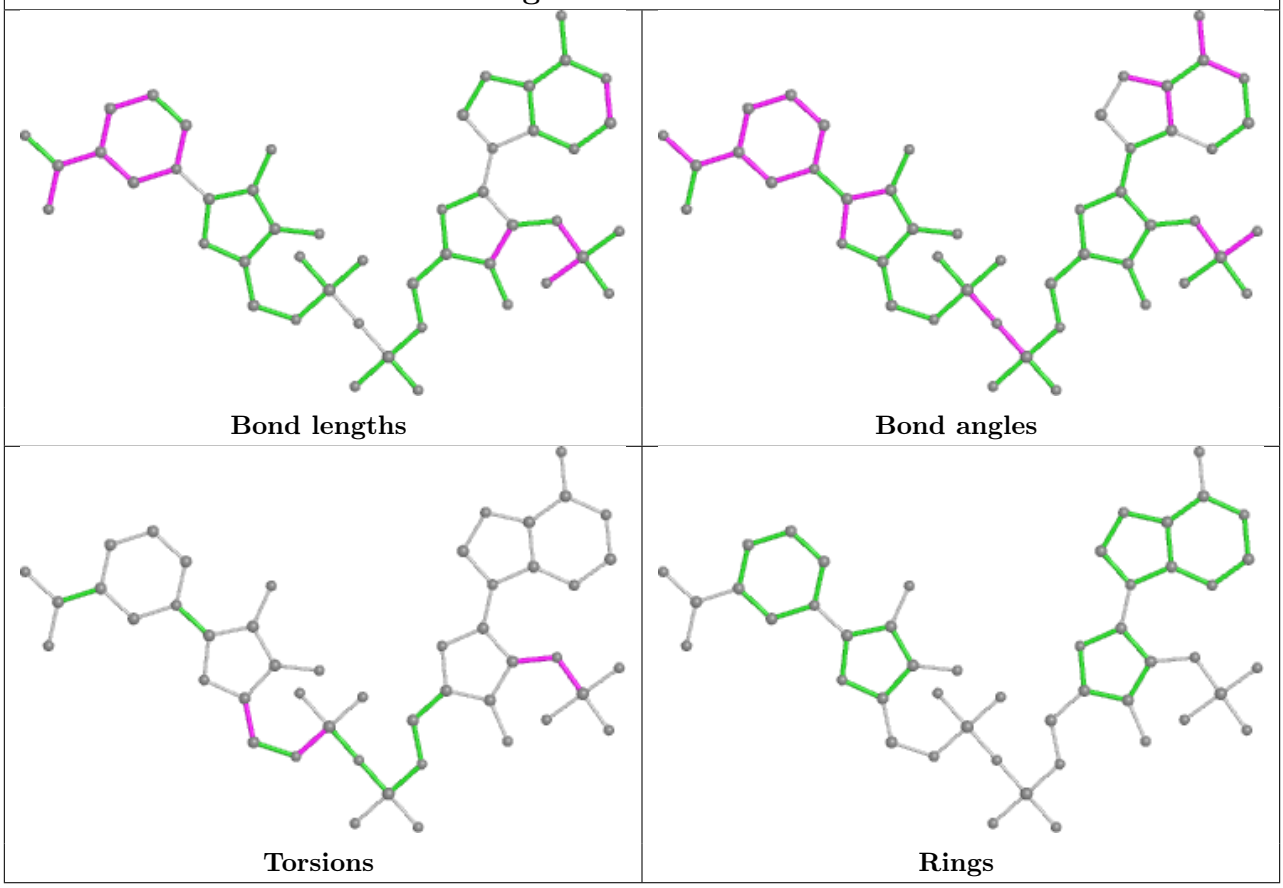
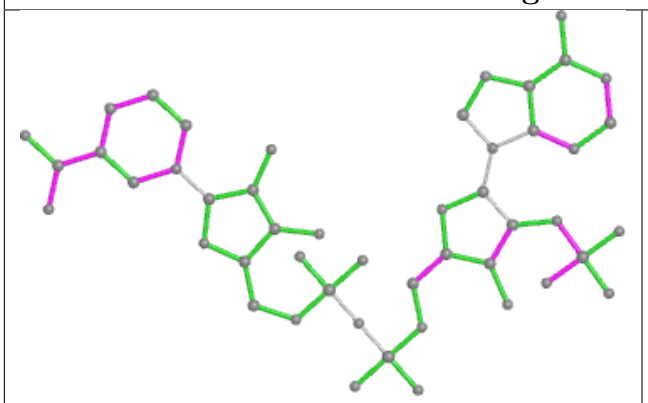
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	NAP	3	0
2	A	650	NAP	4	0

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

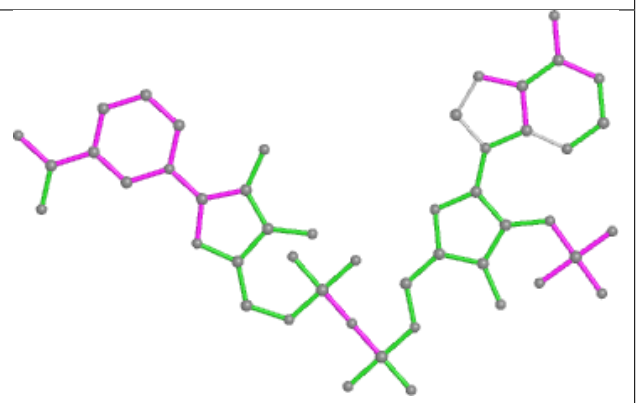
Ligand NAP C 850



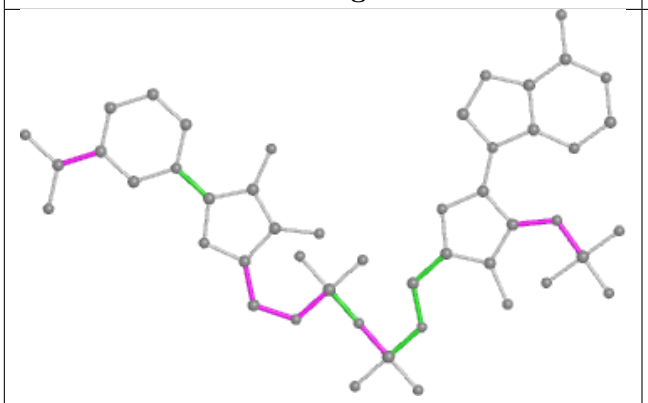
Ligand NAP D 950



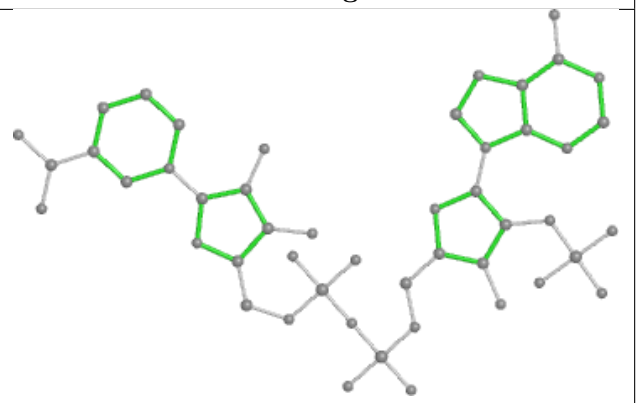
Bond lengths



Bond angles

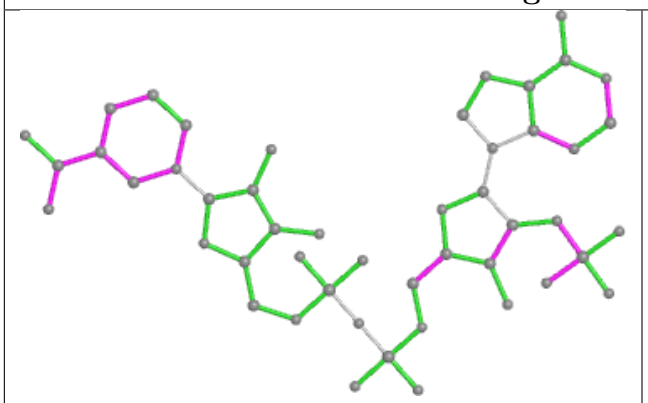


Torsions

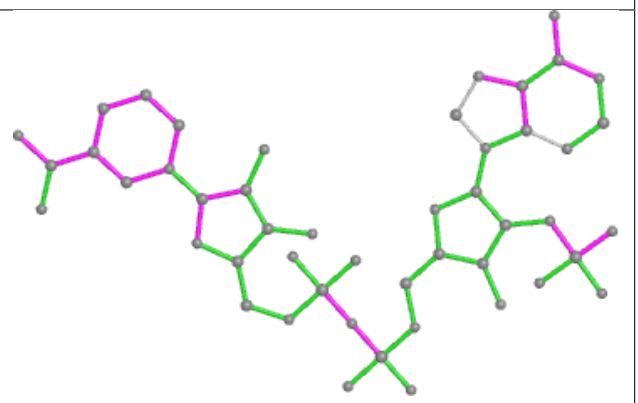


Rings

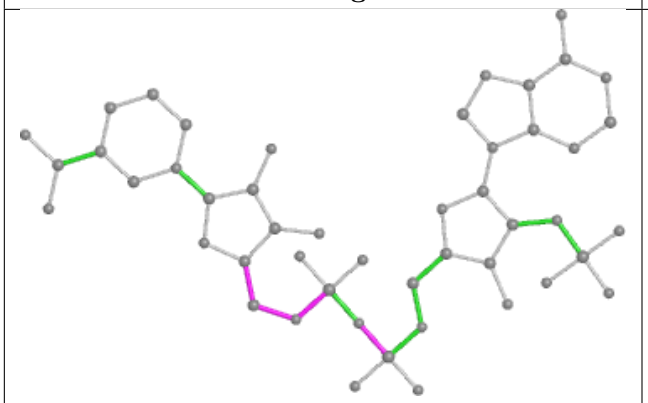
Ligand NAP B 750



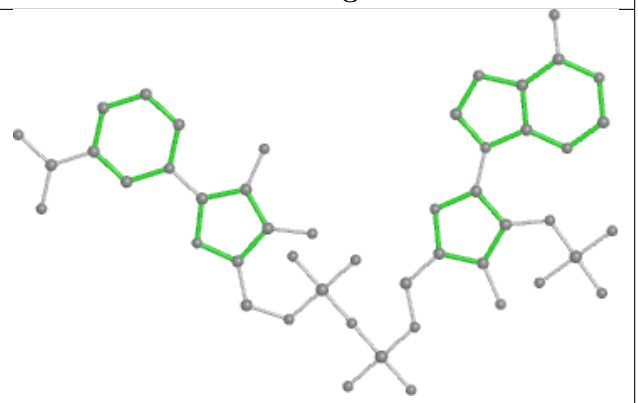
Bond lengths



Bond angles

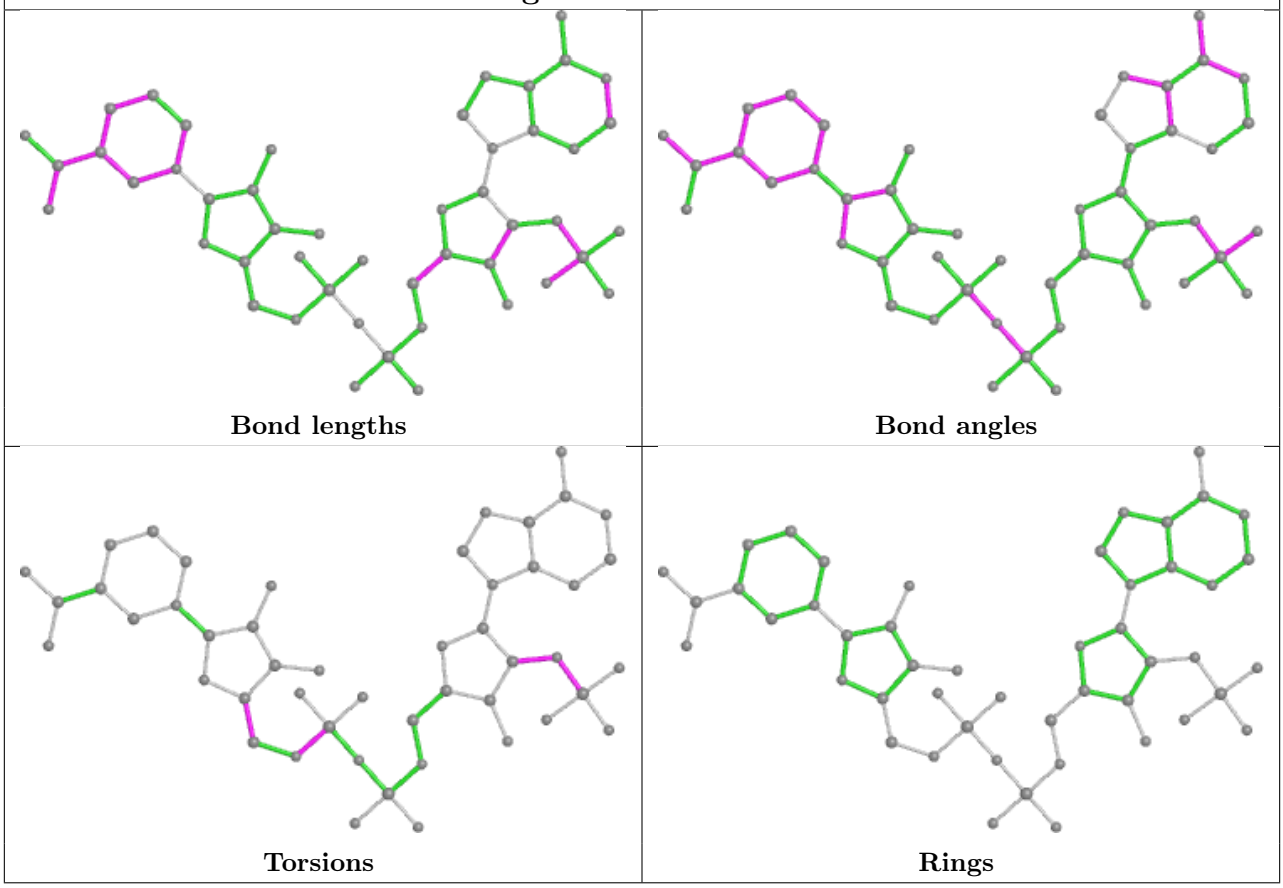


Torsions



Rings

Ligand NAP A 650



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	504/510 (98%)	0.04	12 (2%)	59	64	9, 18, 29, 47	0
1	B	502/510 (98%)	-0.03	15 (2%)	50	56	9, 17, 29, 47	0
1	C	502/510 (98%)	-0.01	12 (2%)	59	64	8, 17, 28, 48	0
1	D	502/510 (98%)	-0.01	9 (1%)	68	72	10, 18, 29, 45	0
All	All	2010/2040 (98%)	-0.00	48 (2%)	59	64	8, 17, 29, 48	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	507	ALA	10.0
1	C	508	ALA	8.3
1	A	507	ALA	7.2
1	B	123	ALA	5.7
1	B	125	LEU	4.6
1	D	123	ALA	4.6
1	A	508	ALA	4.4
1	B	507	ALA	4.0
1	A	123	ALA	3.9
1	D	125	LEU	3.8
1	C	342	ASP	3.8
1	A	121	THR	3.7
1	A	342	ASP	3.7
1	C	124	PRO	3.6
1	B	124	PRO	3.4
1	A	124	PRO	3.1
1	C	123	ALA	3.1
1	B	121	THR	3.1
1	A	125	LEU	3.1
1	D	121	THR	3.0
1	C	125	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	508	ALA	2.9
1	D	124	PRO	2.8
1	B	508	ALA	2.6
1	B	342	ASP	2.6
1	B	494	GLU	2.6
1	C	295	VAL	2.6
1	D	120	PRO	2.5
1	A	120	PRO	2.5
1	B	352	GLU	2.4
1	A	373	ALA	2.4
1	B	21	PRO	2.4
1	C	373	ALA	2.4
1	B	270	LYS	2.4
1	D	342	ASP	2.3
1	C	121	THR	2.3
1	B	269	ALA	2.2
1	C	120	PRO	2.2
1	B	120	PRO	2.2
1	B	304	GLN	2.2
1	A	17	GLY	2.2
1	C	506	LYS	2.2
1	A	5	THR	2.1
1	A	271	ALA	2.1
1	D	271	ALA	2.1
1	D	269	ALA	2.1
1	B	389	GLU	2.0
1	C	340	SER	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 monosaccharides 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,

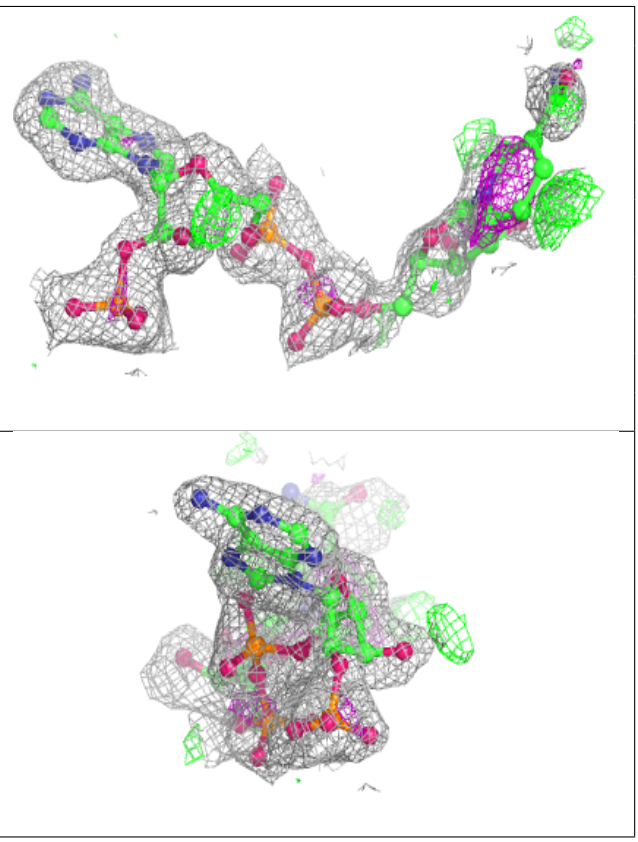
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	B	750	48/48	0.84	0.20	23,38,57,58	0
2	NAP	A	650	48/48	0.89	0.20	24,35,57,57	0
2	NAP	C	850	48/48	0.92	0.15	21,34,55,56	0
2	NAP	D	950	48/48	0.92	0.16	22,35,55,56	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.

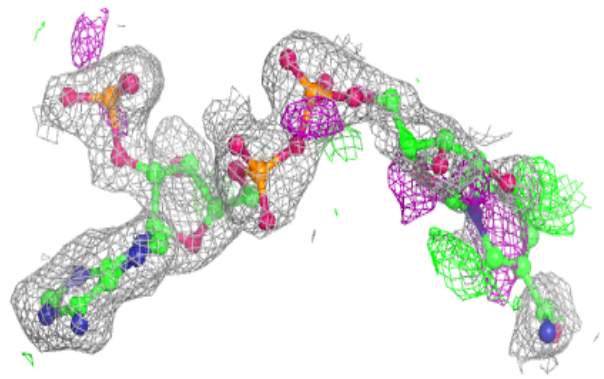
Electron density around NAP B 750:

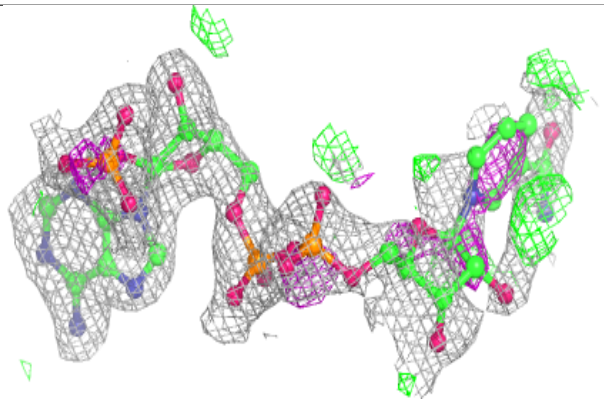
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

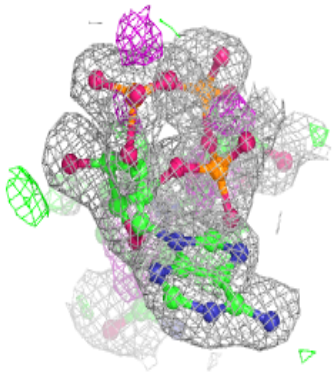


Electron density around NAP A 650:

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

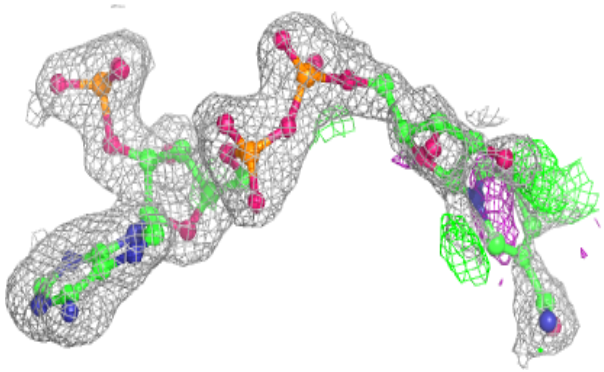


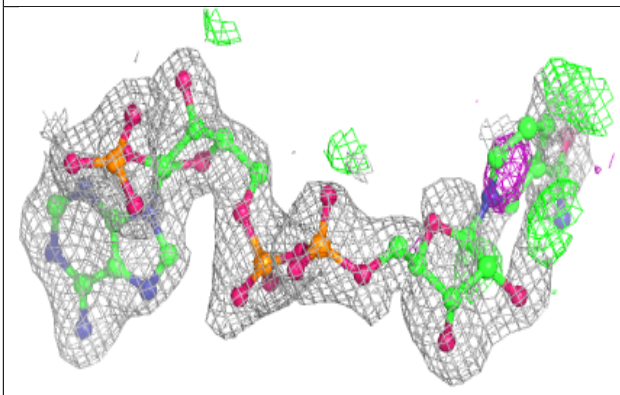


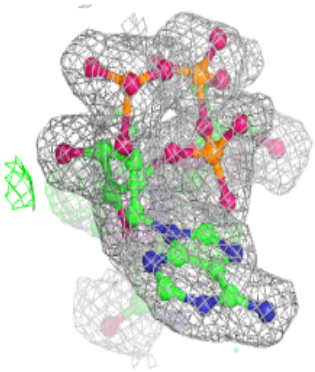


Electron density around NAP C 850:

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

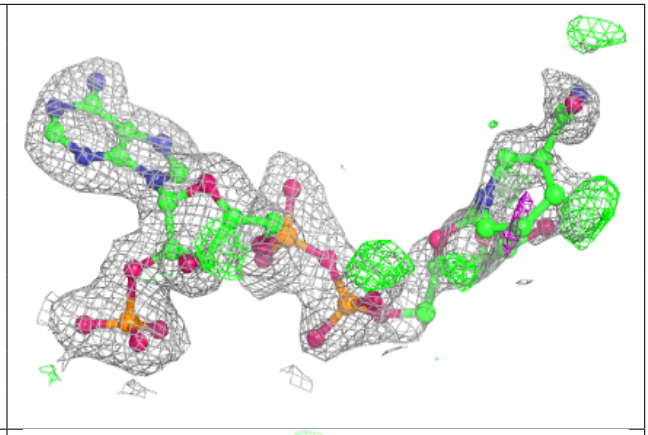


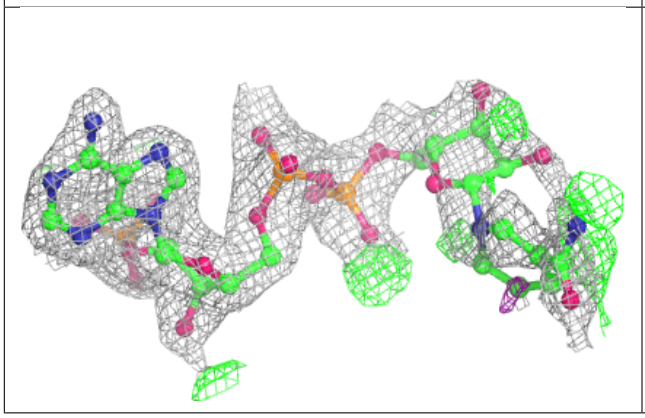


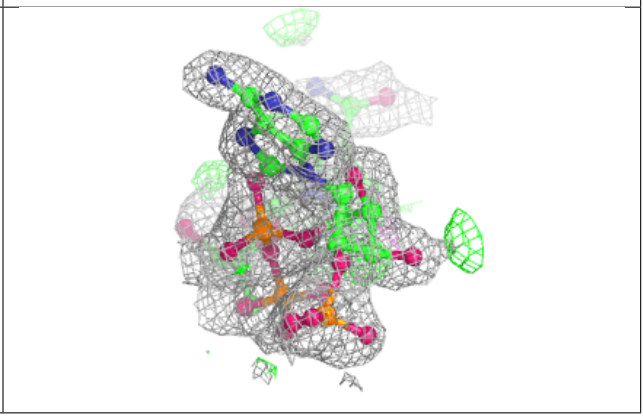


Electron density around NAP D 950:

$2mF_o$-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.