Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 06:32 pm GMT

PDB ID	:	4B7X
Title	:	Crystal structure of hypothetical protein PA1648 from Pseudomonas aeruginosa.
Authors	:	Alphey, M.S.; McMahon, S.A.; Duthie, F.; Naismith, J.H.
Deposited on	:	2012-08-24
Resolution	:	2.20 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:

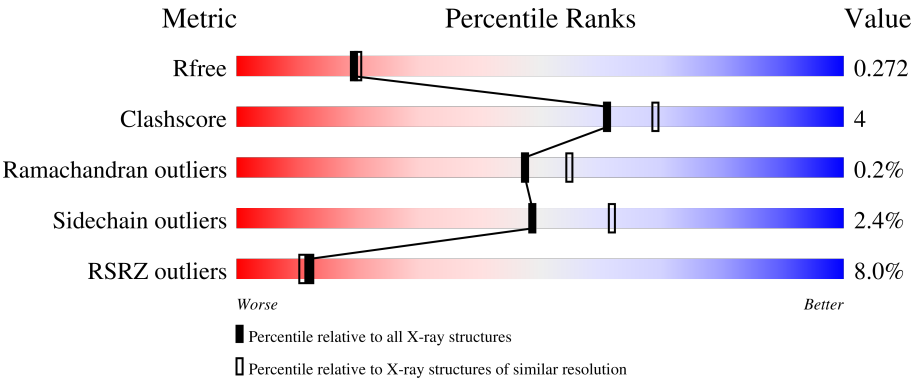
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	336	90% 7%
1	B	336	90% 9%
1	C	336	6% 85% 11%
1	D	336	7% 87% 10%
1	E	336	3% 91% 7%

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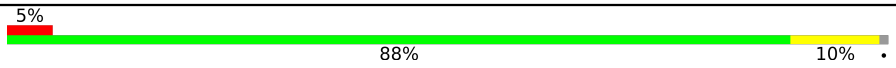
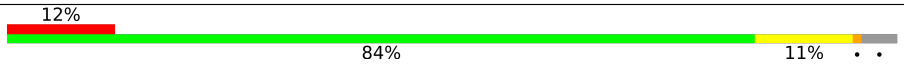
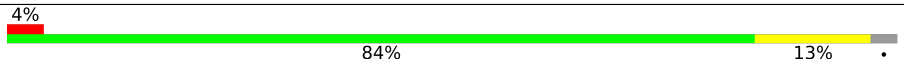
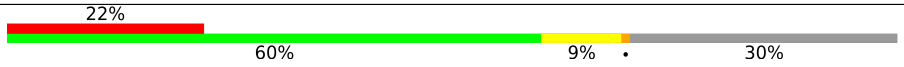
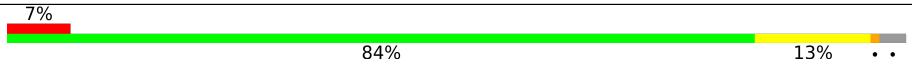
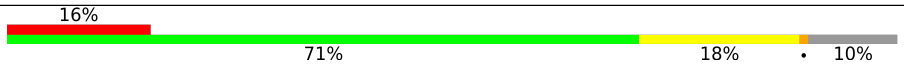
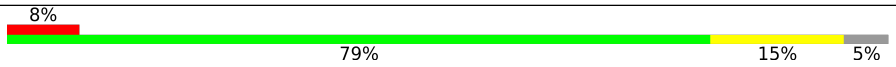
Mol	Chain	Length	Quality of chain
1	F	336	
1	G	336	
1	H	336	
1	I	336	
1	J	336	
1	K	336	
1	L	336	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30208 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 PROBABLE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2504	1597	431	463	13			
1	B	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	C	325	Total	C	N	O	S	0	0	0
			2473	1581	423	456	13			
1	D	327	Total	C	N	O	S	0	0	0
			2490	1590	428	459	13			
1	E	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	F	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	G	321	Total	C	N	O	S	0	0	0
			2446	1564	417	452	13			
1	H	327	Total	C	N	O	S	0	0	0
			2489	1591	426	459	13			
1	I	234	Total	C	N	O	S	0	0	0
			1768	1129	303	324	12			
1	J	327	Total	C	N	O	S	0	0	0
			2486	1586	428	459	13			
1	K	302	Total	C	N	O	S	0	0	0
			2316	1484	399	421	12			
1	L	320	Total	C	N	O	S	0	0	0
			2443	1563	417	450	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9I377
A	0	ALA	-	expression tag	UNP Q9I377
B	-1	GLY	-	expression tag	UNP Q9I377
B	0	ALA	-	expression tag	UNP Q9I377
C	-1	GLY	-	expression tag	UNP Q9I377

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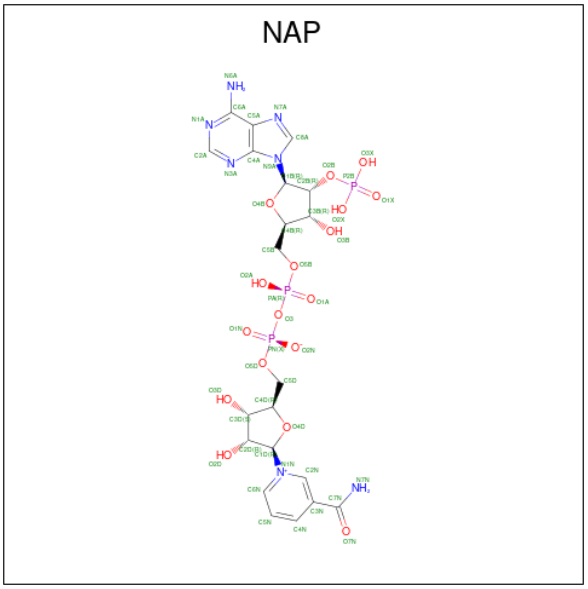
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP Q9I377
D	-1	GLY	-	expression tag	UNP Q9I377
D	0	ALA	-	expression tag	UNP Q9I377
E	-1	GLY	-	expression tag	UNP Q9I377
E	0	ALA	-	expression tag	UNP Q9I377
F	-1	GLY	-	expression tag	UNP Q9I377
F	0	ALA	-	expression tag	UNP Q9I377
G	-1	GLY	-	expression tag	UNP Q9I377
G	0	ALA	-	expression tag	UNP Q9I377
H	-1	GLY	-	expression tag	UNP Q9I377
H	0	ALA	-	expression tag	UNP Q9I377
I	-1	GLY	-	expression tag	UNP Q9I377
I	0	ALA	-	expression tag	UNP Q9I377
J	-1	GLY	-	expression tag	UNP Q9I377
J	0	ALA	-	expression tag	UNP Q9I377
K	-1	GLY	-	expression tag	UNP Q9I377
K	0	ALA	-	expression tag	UNP Q9I377
L	-1	GLY	-	expression tag	UNP Q9I377
L	0	ALA	-	expression tag	UNP Q9I377

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	68	Total	O	0	0
			68	68		
3	C	46	Total	O	0	0
			46	46		
3	D	60	Total	O	0	0
			60	60		
3	E	81	Total	O	0	0
			81	81		
3	F	67	Total	O	0	0
			67	67		
3	G	43	Total	O	0	0
			43	43		
3	H	41	Total	O	0	0
			41	41		

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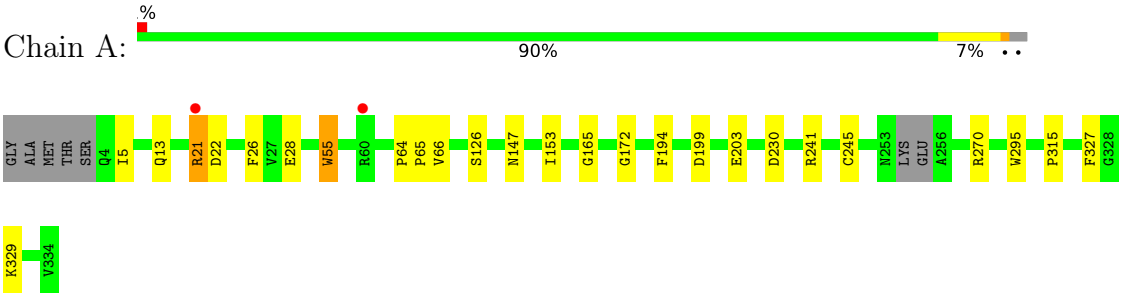
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	20	Total O 20 20	0	0
3	J	37	Total O 37 37	0	0
3	K	30	Total O 30 30	0	0
3	L	43	Total O 43 43	0	0

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.

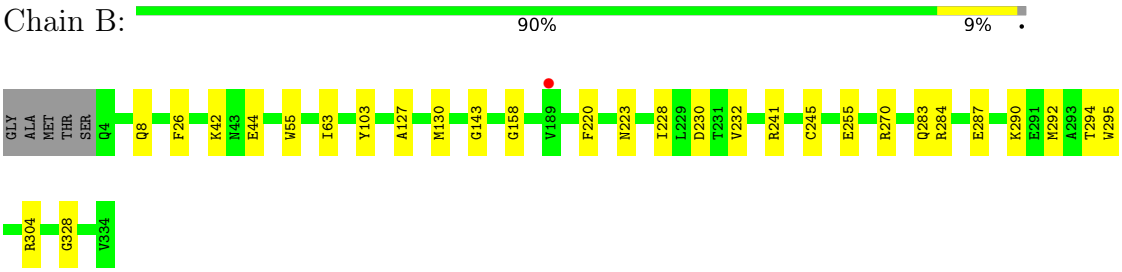
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain A:



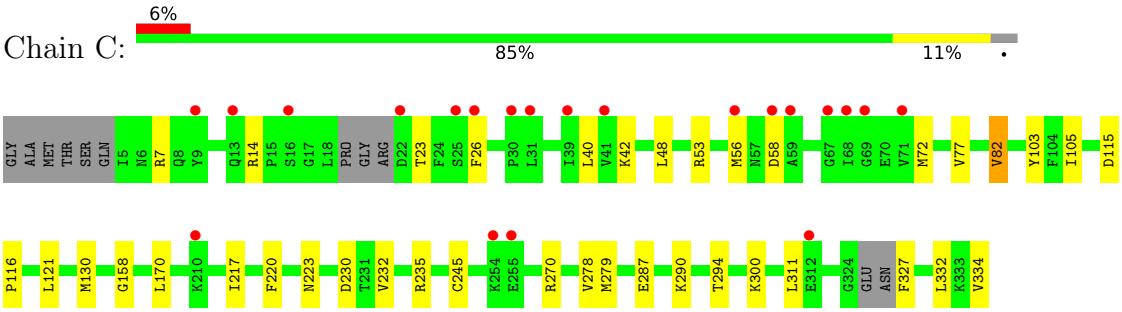
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain B:



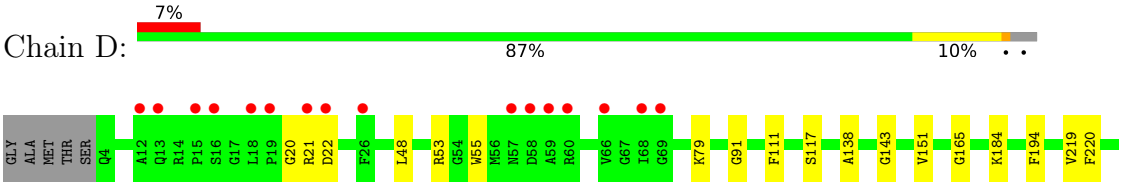
• Molecule 1: PROBABLE OXIDOREDUCTASE

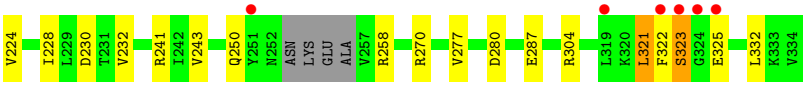
Chain C:



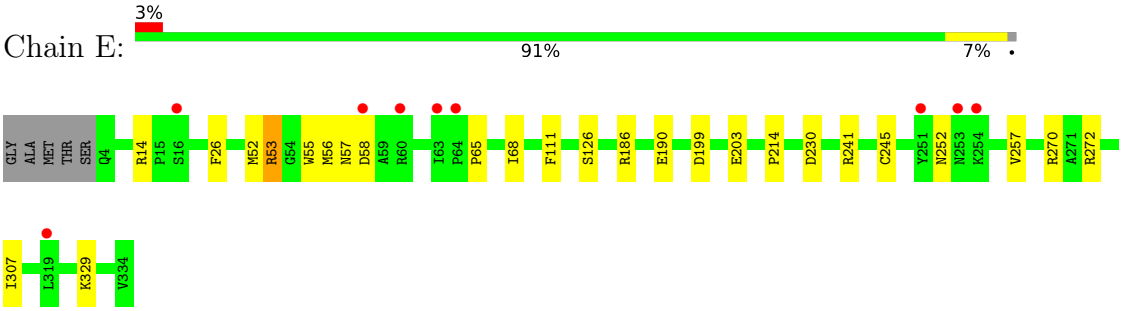
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain D:

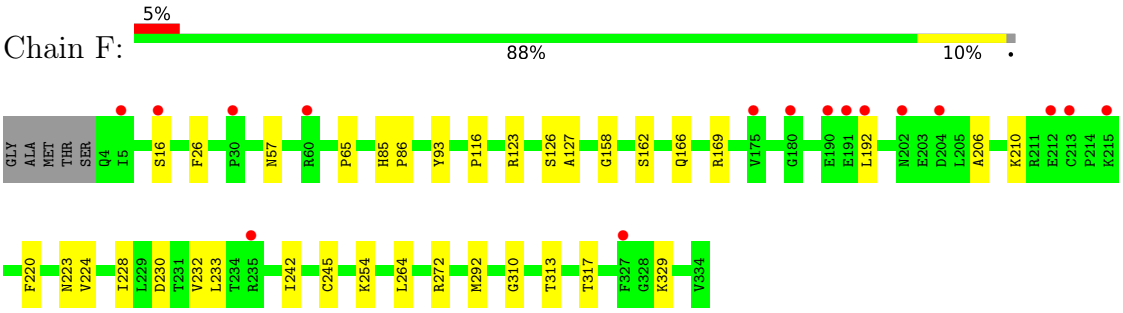




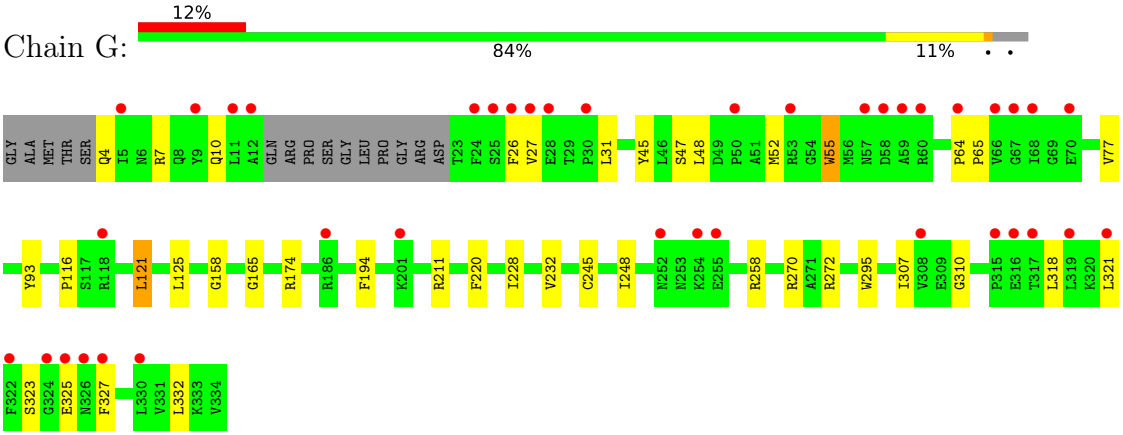
• Molecule 1: PROBABLE OXIDOREDUCTASE



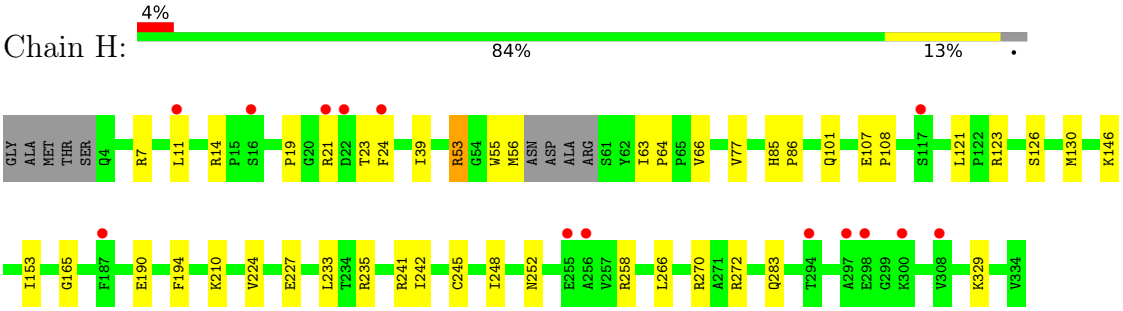
• Molecule 1: PROBABLE OXIDOREDUCTASE



• Molecule 1: PROBABLE OXIDOREDUCTASE

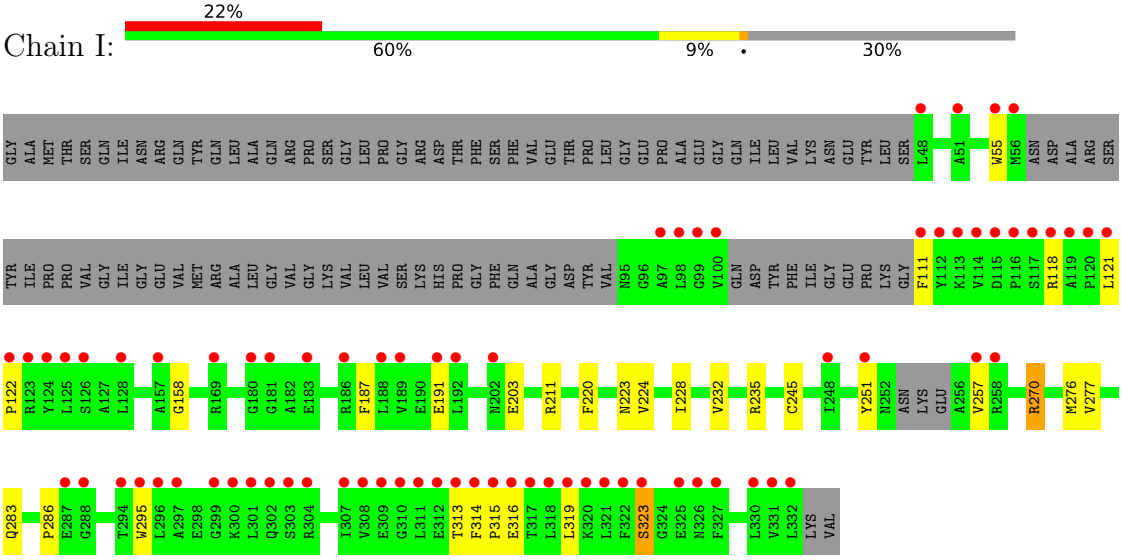


• Molecule 1: PROBABLE OXIDOREDUCTASE



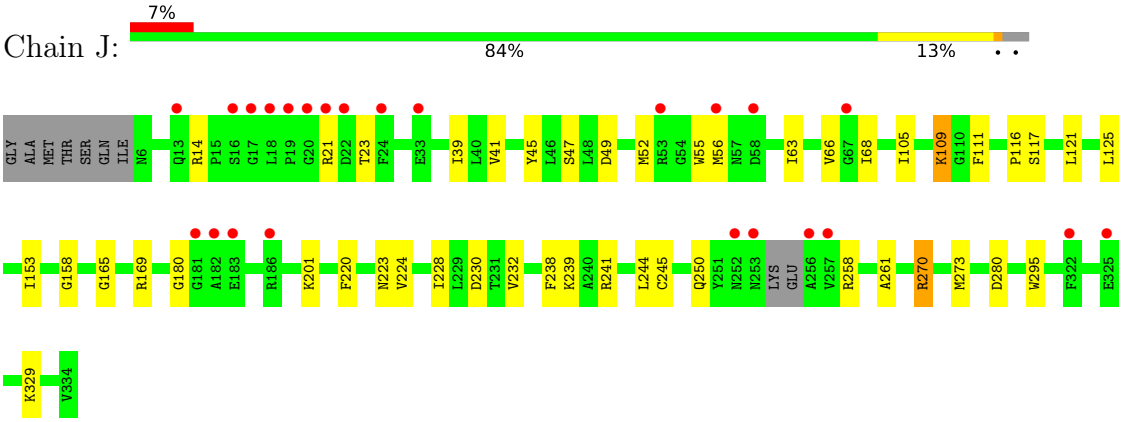
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain I:



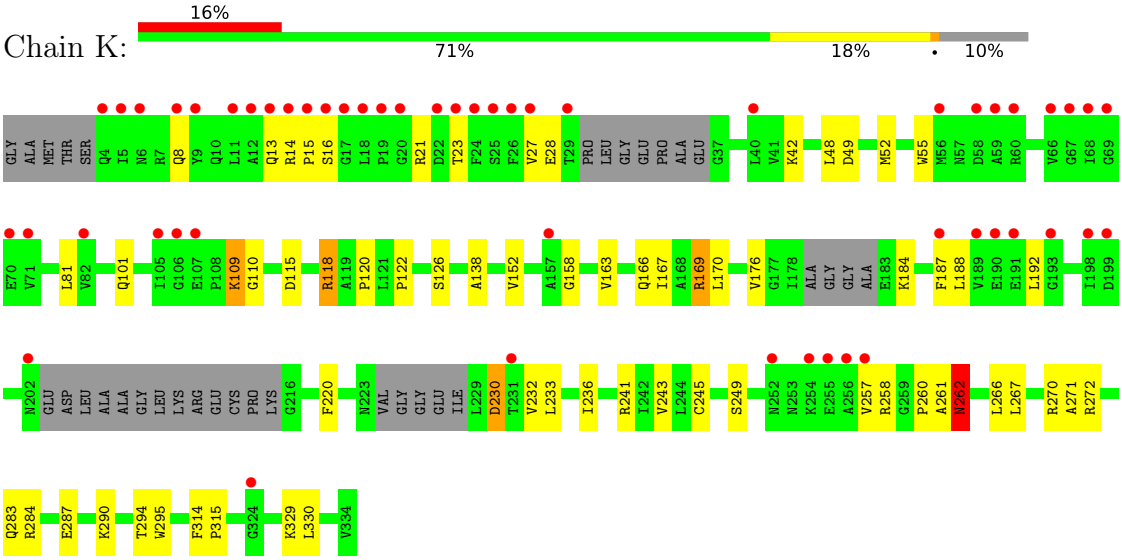
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain J:



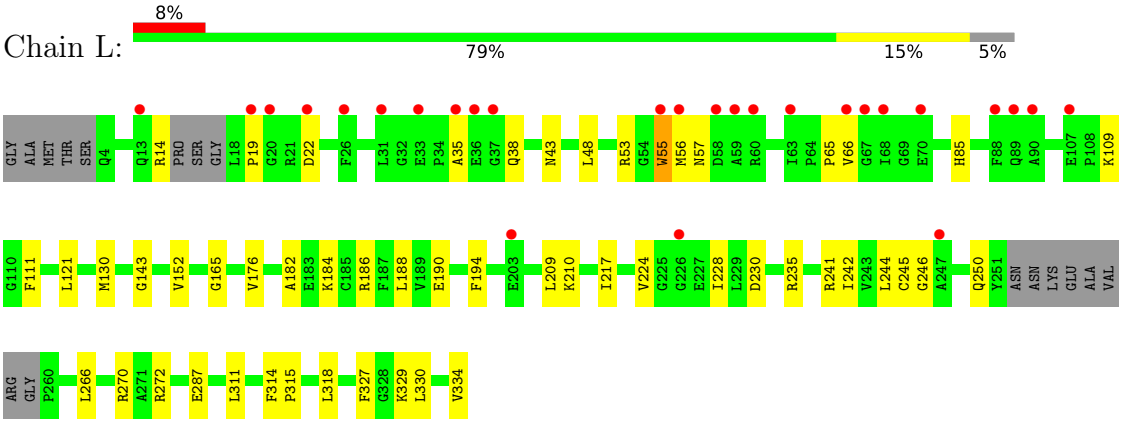
• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain K:



• Molecule 1: PROBABLE OXIDOREDUCTASE

Chain L:


8%
79%
15%
5%
GLY ALA MET THR SER Q4 Q13 R14 PRO SER GLY L18 P19 G20 R21 D22 F26 L31 G32 E33 P34 A35 E36 G37 Q38 N43 L48 R53 G54 W55 M56 N57 D58 A59 R60 I63 P64 P65 V66 G67 I68 G69 E70 H85 F88 Q89 A90 E107 P108 K109
G110 F111 L121 M130 G143 V152 G165 V176 A182 E183 K184 C185 R186 F187 L188 V189 E190 F194 E203 L209 K210 I217 V224 G225 G226 E227 I228 L229 D230 R235 R241 I242 V243 L244 C245 G246 A247 Q250 Y251 ASN ASN LYS GLU ALA VAL
ARG GLY P260 L266 R270 A271 R272 E287 L311 F314 P315 L318 F327 G328 K329 L330 V334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.26Å 175.97Å 182.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.42 – 2.20 55.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.42-2.20) 99.8 (55.83-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.276 0.234 , 0.272	Depositor DCC
R_{free} test set	13815 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30208	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	2/2551 (0.1%)	0.67	0/3443
1	B	0.50	1/2569 (0.0%)	0.63	0/3469
1	C	0.44	0/2518	0.59	0/3397
1	D	0.48	1/2537 (0.0%)	0.61	0/3425
1	E	0.53	1/2569 (0.0%)	0.67	0/3469
1	F	0.49	0/2569	0.60	0/3469
1	G	0.44	2/2491 (0.1%)	0.58	0/3362
1	H	0.42	1/2536 (0.0%)	0.56	0/3423
1	I	0.42	2/1795 (0.1%)	0.53	0/2416
1	J	0.43	1/2533 (0.0%)	0.58	0/3420
1	K	0.44	2/2357 (0.1%)	0.56	0/3177
1	L	0.44	1/2488 (0.0%)	0.58	0/3356
All	All	0.47	14/29513 (0.0%)	0.60	0/39826

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	TRP	CD2-CE2	5.67	1.48	1.41
1	K	295	TRP	CD2-CE2	5.32	1.47	1.41
1	E	55	TRP	CD2-CE2	5.20	1.47	1.41
1	B	295	TRP	CD2-CE2	5.18	1.47	1.41
1	A	55	TRP	CD2-CE2	5.18	1.47	1.41
1	D	55	TRP	CD2-CE2	5.17	1.47	1.41
1	G	295	TRP	CD2-CE2	5.16	1.47	1.41
1	H	55	TRP	CD2-CE2	5.16	1.47	1.41
1	I	55	TRP	CD2-CE2	5.13	1.47	1.41
1	I	295	TRP	CD2-CE2	5.10	1.47	1.41
1	K	55	TRP	CD2-CE2	5.08	1.47	1.41
1	J	295	TRP	CD2-CE2	5.04	1.47	1.41
1	L	55	TRP	CD2-CE2	5.02	1.47	1.41
1	G	55	TRP	CD2-CE2	5.01	1.47	1.41

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	2504	0	2524	16	0
1	B	2521	0	2544	14	0
1	C	2473	0	2499	24	0
1	D	2490	0	2513	22	0
1	E	2521	0	2544	18	0
1	F	2521	0	2544	25	0
1	G	2446	0	2469	24	0
1	H	2489	0	2515	29	0
1	I	1768	0	1794	18	0
1	J	2486	0	2505	35	0
1	K	2316	0	2334	33	0
1	L	2443	0	2467	28	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
2	E	48	0	25	2	0
2	F	48	0	25	3	0
2	G	48	0	25	4	0
2	H	48	0	25	2	0
2	I	48	0	25	4	0
2	J	48	0	25	3	0
2	K	48	0	25	2	0
2	L	48	0	25	2	0
3	A	118	0	0	0	0
3	B	68	0	0	0	0
3	C	46	0	0	1	0
3	D	60	0	0	0	0
3	E	81	0	0	0	0
3	F	67	0	0	0	0
3	G	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	41	0	0	0	0
3	I	20	0	0	0	0
3	J	37	0	0	1	0
3	K	30	0	0	0	0
3	L	43	0	0	0	0
All	All	30208	0	29552	264	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 4.

All (264) 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)
2:D:400:NAP:H4B	2:D:400:NAP:O2A	1.26	1.02
1:F:16:SER:O	1:F:254:LYS:HG3	1.65	0.96
1:C:48:LEU:HD11	1:C:332:LEU:HB2	1.51	0.91
2:D:400:NAP:O2A	2:D:400:NAP:C4B	2.19	0.84
1:F:206:ALA:O	1:F:210:LYS:HG3	1.80	0.81
1:I:319:LEU:O	1:I:323:SER:HB2	1.79	0.81
1:E:126:SER:HB3	1:E:329:LYS:HG2	1.69	0.72
1:L:224:VAL:HG11	1:L:228:ILE:HD12	1.71	0.70
1:L:182:ALA:O	1:L:186:ARG:HG2	1.93	0.69
1:I:283:GLN:NE2	1:L:111:PHE:O	2.27	0.67
1:F:57:ASN:O	1:F:65:PRO:HB3	1.96	0.66
1:D:53:ARG:HB2	1:D:322:PHE:CZ	2.30	0.66
1:I:224:VAL:HG11	1:I:228:ILE:HD12	1.78	0.66
1:F:16:SER:O	1:F:254:LYS:CG	2.41	0.65
1:J:244:LEU:HD21	1:J:273:MET:CE	2.28	0.64
1:H:227:GLU:HG2	1:H:258:ARG:HH21	1.62	0.64
1:J:245:CYS:O	2:J:400:NAP:H2N	1.98	0.62
1:H:24:PHE:CZ	1:H:56:MET:HE3	2.35	0.62
1:J:153:ILE:CD1	1:J:165:GLY:HA2	2.30	0.62
1:K:230:ASP:OD1	1:K:262:ASN:HB2	2.00	0.61
1:C:270:ARG:HD3	1:D:277:VAL:HB	1.82	0.61
1:A:153:ILE:HD11	1:A:165:GLY:HA2	1.82	0.60
1:A:126:SER:HB3	1:A:329:LYS:HG2	1.84	0.60
3:J:2014:HOH:O	1:L:287:GLU:HG3	2.01	0.59
1:K:27:VAL:HG12	1:K:28:GLU:H	1.68	0.59
1:J:111:PHE:O	1:K:283:GLN:NE2	2.36	0.59
1:K:284:ARG:O	1:K:287:GLU:HG2	2.03	0.59
1:H:24:PHE:CZ	1:H:56:MET:CE	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:LEU:HA	1:K:271:ALA:HB3	1.84	0.58
1:J:244:LEU:HD21	1:J:273:MET:HE2	1.85	0.58
1:H:210:LYS:HA	1:H:235:ARG:HH21	1.68	0.58
1:K:109:LYS:HG3	1:K:110:GLY:H	1.67	0.58
1:K:48:LEU:HD12	1:K:330:LEU:HG	1.86	0.58
1:D:250:GLN:HE21	1:D:258:ARG:H	1.51	0.57
1:E:272:ARG:CZ	1:F:272:ARG:HH21	2.16	0.57
1:H:165:GLY:HA3	1:H:194:PHE:CZ	2.39	0.57
1:K:314:PHE:HB3	1:K:315:PRO:HD3	1.85	0.57
1:F:313:THR:CG2	1:F:317:THR:OG1	2.53	0.57
1:H:153:ILE:CD1	1:H:165:GLY:HA2	2.35	0.57
1:J:47:SER:HB2	1:J:125:LEU:HD22	1.85	0.57
1:L:130:MET:SD	2:L:400:NAP:H5N	2.45	0.57
1:L:210:LYS:HA	1:L:235:ARG:HH21	1.69	0.57
1:A:21:ARG:HD2	1:A:21:ARG:O	2.04	0.57
1:J:14:ARG:NH1	1:J:66:VAL:O	2.37	0.57
1:L:329:LYS:HD2	1:L:330:LEU:N	2.20	0.57
1:G:45:TYR:OH	1:J:116:PRO:HG2	2.04	0.57
1:H:227:GLU:HG2	1:H:258:ARG:NH2	2.19	0.56
1:B:55:TRP:NE1	1:B:63:ILE:HD11	2.20	0.56
2:E:400:NAP:O2A	2:E:400:NAP:H4B	2.06	0.56
1:K:245:CYS:O	2:K:400:NAP:H2N	2.06	0.56
1:E:57:ASN:O	1:E:65:PRO:HB3	2.06	0.56
1:F:158:GLY:HA3	2:F:400:NAP:O2A	2.06	0.56
1:I:314:PHE:HB3	1:I:315:PRO:HD3	1.88	0.55
1:K:267:LEU:HD11	1:L:246:GLY:HA2	1.88	0.55
1:H:63:ILE:HG13	1:H:64:PRO:HD2	1.87	0.55
1:A:245:CYS:O	2:A:400:NAP:H2N	2.07	0.55
1:J:55:TRP:NE1	1:J:63:ILE:HD11	2.22	0.55
1:E:53:ARG:NH2	1:E:57:ASN:OD1	2.39	0.54
1:G:116:PRO:HG2	1:J:45:TYR:OH	2.06	0.54
1:H:126:SER:HB3	1:H:329:LYS:HG2	1.90	0.54
1:E:214:PRO:HB3	1:L:186:ARG:HH21	1.72	0.54
2:G:400:NAP:O2A	2:G:400:NAP:H4B	2.06	0.54
1:E:52:MET:O	1:E:56:MET:HG3	2.08	0.54
1:G:52:MET:HA	1:G:55:TRP:CE3	2.42	0.53
1:J:250:GLN:NE2	1:J:258:ARG:H	2.05	0.53
1:A:13:GLN:NE2	1:A:22:ASP:HB3	2.23	0.53
1:J:153:ILE:HD13	1:J:165:GLY:CA	2.39	0.53
1:H:39:ILE:HG12	1:H:108:PRO:HG3	1.90	0.53
1:C:245:CYS:O	2:C:400:NAP:H2N	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ILE:O	1:G:232:VAL:HG23	2.09	0.53
1:C:14:ARG:HD2	1:C:58:ASP:HB2	1.92	0.52
1:A:153:ILE:CD1	1:A:165:GLY:HA2	2.39	0.52
1:D:117:SER:CB	1:E:307:ILE:HD12	2.40	0.52
1:F:313:THR:HG22	1:F:317:THR:OG1	2.10	0.52
1:D:151:VAL:HG22	1:D:219:VAL:HB	1.93	0.51
1:I:121:LEU:HB3	1:I:122:PRO:HD3	1.92	0.51
1:B:223:ASN:HB3	2:B:400:NAP:H4D	1.93	0.51
1:K:158:GLY:HA3	2:K:400:NAP:O2A	2.11	0.51
1:F:233:LEU:HD21	1:F:242:ILE:CD1	2.41	0.50
1:H:233:LEU:HD21	1:H:242:ILE:HD13	1.92	0.50
1:L:143:GLY:O	1:L:241:ARG:HD2	2.10	0.50
1:G:47:SER:HB2	1:G:125:LEU:HD22	1.92	0.50
1:D:138:ALA:HB1	1:D:243:VAL:HG11	1.92	0.50
1:E:257:VAL:HG21	1:F:264:LEU:HD12	1.94	0.50
1:G:77:VAL:CG1	1:G:121:LEU:HD13	2.42	0.50
1:L:165:GLY:HA3	1:L:194:PHE:CZ	2.45	0.50
1:K:169:ARG:NH2	1:K:192:LEU:O	2.45	0.50
1:D:250:GLN:NE2	1:D:258:ARG:H	2.08	0.50
1:I:203:GLU:OE2	1:I:211:ARG:NH1	2.42	0.50
1:L:35:ALA:O	1:L:38:GLN:HB2	2.12	0.50
1:J:158:GLY:HA3	2:J:400:NAP:O2A	2.12	0.49
1:D:184:LYS:NZ	2:D:400:NAP:O2X	2.41	0.49
1:I:286:PRO:HG2	1:L:85:HIS:NE2	2.27	0.49
1:F:233:LEU:HD23	1:F:242:ILE:HD11	1.94	0.49
1:I:245:CYS:O	2:I:400:NAP:H2N	2.13	0.49
1:C:40:LEU:HD13	1:C:105:ILE:HG12	1.94	0.49
1:E:58:ASP:OD1	1:E:58:ASP:N	2.44	0.49
1:G:77:VAL:HG12	1:G:121:LEU:HD13	1.94	0.48
1:K:42:LYS:HB2	1:K:81:LEU:HD11	1.95	0.48
1:K:188:LEU:HD23	1:K:192:LEU:HD12	1.94	0.48
1:D:48:LEU:HD11	1:D:332:LEU:HB2	1.95	0.48
1:G:158:GLY:HA3	2:G:400:NAP:O2A	2.14	0.48
1:J:238:PHE:CE2	1:J:239:LYS:HD2	2.48	0.48
1:B:283:GLN:NE2	1:E:111:PHE:O	2.47	0.48
1:E:199:ASP:O	1:E:203:GLU:HG2	2.13	0.48
1:G:248:ILE:HD13	2:G:400:NAP:H52A	1.96	0.48
1:A:55:TRP:HB3	1:A:66:VAL:HG23	1.95	0.47
1:H:53:ARG:CD	1:H:252:ASN:OD1	2.63	0.47
1:I:276:MET:HA	1:J:270:ARG:HG3	1.96	0.47
1:J:39:ILE:HD12	1:J:41:VAL:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ARG:CD	1:D:280:ASP:OD2	2.63	0.47
1:H:77:VAL:HG11	1:H:121:LEU:HD22	1.96	0.47
1:I:187:PHE:O	1:I:191:GLU:HB2	2.14	0.47
1:D:321:LEU:O	1:D:322:PHE:HB2	2.14	0.47
1:F:233:LEU:HD21	1:F:242:ILE:HD12	1.97	0.47
1:F:310:GLY:O	1:F:313:THR:HB	2.14	0.47
1:H:233:LEU:CD2	1:H:242:ILE:CD1	2.93	0.47
1:L:242:ILE:HD12	1:L:266:LEU:HD21	1.95	0.47
1:E:14:ARG:HG2	1:E:68:ILE:HD11	1.97	0.47
1:A:199:ASP:O	1:A:203:GLU:HG2	2.16	0.46
1:D:224:VAL:HG11	1:D:228:ILE:HD12	1.96	0.46
1:J:153:ILE:HD13	1:J:165:GLY:HA2	1.96	0.46
1:K:260:PRO:O	1:K:262:ASN:N	2.48	0.46
1:E:186:ARG:NH2	1:G:211:ARG:O	2.48	0.46
1:A:13:GLN:HE21	1:A:22:ASP:HB3	1.80	0.46
1:F:223:ASN:HB3	2:F:400:NAP:H4D	1.97	0.46
1:G:64:PRO:HA	1:G:65:PRO:HD3	1.83	0.46
1:B:228:ILE:O	1:B:232:VAL:HG23	2.15	0.46
1:K:241:ARG:HD3	1:K:241:ARG:N	2.31	0.46
1:L:57:ASN:O	1:L:65:PRO:HB3	2.15	0.46
1:J:244:LEU:HD21	1:J:273:MET:HE1	1.98	0.46
1:B:245:CYS:O	2:B:400:NAP:H2N	2.16	0.46
1:C:42:LYS:HG2	1:C:103:TYR:CE2	2.51	0.46
1:C:48:LEU:CD1	1:C:332:LEU:HB2	2.36	0.46
1:I:220:PHE:CG	1:I:232:VAL:HG11	2.50	0.46
1:C:217:ILE:HD12	1:C:235:ARG:HB3	1.97	0.45
1:G:220:PHE:CG	1:G:232:VAL:HG11	2.50	0.45
1:E:245:CYS:O	2:E:400:NAP:H2N	2.16	0.45
1:E:190:GLU:OE1	1:G:174:ARG:NH1	2.49	0.45
1:G:310:GLY:O	1:G:332:LEU:HD11	2.17	0.45
1:J:49:ASP:OD1	1:J:329:LYS:NZ	2.49	0.45
1:J:223:ASN:HB3	2:J:400:NAP:H4D	1.99	0.45
1:K:120:PRO:HB2	1:K:122:PRO:HD2	1.98	0.45
1:F:224:VAL:HG11	1:F:228:ILE:HD12	1.98	0.45
1:G:307:ILE:HD13	1:J:117:SER:HB2	1.99	0.45
1:D:117:SER:HB2	1:E:307:ILE:HD12	1.99	0.45
1:G:272:ARG:HG3	1:H:272:ARG:HG3	1.99	0.45
1:C:158:GLY:HA3	2:C:400:NAP:O2A	2.17	0.45
1:L:184:LYS:O	1:L:188:LEU:HG	2.17	0.45
1:C:220:PHE:CG	1:C:232:VAL:HG11	2.52	0.44
1:B:127:ALA:O	1:B:292:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD23	1:C:82:VAL:HG23	1.99	0.44
1:D:165:GLY:HA3	1:D:194:PHE:CZ	2.52	0.44
1:G:4:GLN:HG2	1:G:31:LEU:HD22	1.99	0.44
1:L:14:ARG:HD2	1:L:56:MET:O	2.17	0.44
1:F:126:SER:HB3	1:F:329:LYS:HG2	1.98	0.44
1:G:7:ARG:HD2	1:G:26:PHE:HZ	1.83	0.44
1:G:318:LEU:O	1:G:321:LEU:HD12	2.17	0.44
1:H:245:CYS:O	2:H:400:NAP:H2N	2.17	0.44
1:D:220:PHE:CG	1:D:232:VAL:HG11	2.53	0.44
1:J:220:PHE:CG	1:J:232:VAL:HG11	2.52	0.44
1:A:147:ASN:OD1	1:A:172:GLY:HA3	2.18	0.44
1:C:7:ARG:HD2	1:C:26:PHE:HZ	1.83	0.44
1:D:79:LYS:HE2	1:D:91:GLY:HA2	2.00	0.44
1:H:7:ARG:O	1:H:101:GLN:HA	2.18	0.44
1:B:158:GLY:HA3	2:B:400:NAP:O2A	2.17	0.44
1:C:130:MET:SD	2:C:400:NAP:H5N	2.58	0.44
1:K:272:ARG:HD3	1:L:272:ARG:HD3	1.99	0.44
1:F:127:ALA:O	1:F:292:MET:HG2	2.18	0.44
1:I:277:VAL:HG13	1:J:270:ARG:HD2	2.00	0.44
1:J:270:ARG:HD3	1:J:270:ARG:N	2.33	0.44
1:A:5:ILE:CG2	1:A:28:GLU:HB3	2.48	0.43
1:B:220:PHE:CG	1:B:232:VAL:HG11	2.53	0.43
1:D:20:GLY:O	1:D:22:ASP:N	2.51	0.43
1:I:257:VAL:HG22	1:J:261:ALA:O	2.18	0.43
1:B:284:ARG:O	1:B:287:GLU:HG2	2.18	0.43
1:K:138:ALA:HB1	1:K:243:VAL:HG11	2.00	0.43
1:K:152:VAL:HA	1:K:176:VAL:O	2.18	0.43
1:L:314:PHE:N	1:L:315:PRO:HD2	2.33	0.43
1:K:233:LEU:O	1:K:236:ILE:HG12	2.19	0.43
1:A:165:GLY:HA3	1:A:194:PHE:CZ	2.53	0.43
1:D:117:SER:HB2	1:E:307:ILE:CD1	2.49	0.43
1:F:162:SER:HB2	1:F:192:LEU:HD21	2.00	0.43
1:F:233:LEU:CD2	1:F:242:ILE:CD1	2.96	0.43
1:J:14:ARG:HG2	1:J:68:ILE:HD11	2.01	0.43
1:K:115:ASP:HB3	1:K:118:ARG:HG3	2.00	0.43
1:C:115:ASP:HA	1:C:116:PRO:HD2	1.90	0.43
1:G:10:GLN:HE21	1:G:27:VAL:HG21	1.84	0.43
1:C:130:MET:HG2	1:C:278:VAL:HG11	2.00	0.43
1:D:111:PHE:O	1:H:283:GLN:NE2	2.48	0.43
1:H:19:PRO:HG3	1:H:53:ARG:HD2	2.00	0.43
1:H:130:MET:SD	2:H:400:NAP:H5N	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:VAL:O	1:K:167:ILE:HG13	2.19	0.43
1:K:220:PHE:CG	1:K:232:VAL:HG11	2.54	0.43
1:B:143:GLY:O	1:B:241:ARG:HD2	2.19	0.42
1:E:53:ARG:HD3	1:E:252:ASN:OD1	2.19	0.42
1:H:85:HIS:HA	1:H:86:PRO:HD3	1.91	0.42
1:G:93:TYR:CD1	1:G:116:PRO:HG3	2.54	0.42
1:J:14:ARG:HD2	1:J:56:MET:O	2.19	0.42
1:J:224:VAL:HG11	1:J:228:ILE:HD12	2.00	0.42
1:F:245:CYS:O	2:F:400:NAP:H2N	2.18	0.42
1:A:21:ARG:HD3	1:A:315:PRO:HG2	2.00	0.42
1:H:24:PHE:HZ	1:H:56:MET:CE	2.32	0.42
1:H:233:LEU:HD21	1:H:242:ILE:CD1	2.50	0.42
1:K:8:GLN:HG2	1:K:101:GLN:HB3	2.01	0.42
1:K:290:LYS:O	1:K:294:THR:HG23	2.19	0.42
1:L:43:ASN:O	1:L:334:VAL:HG23	2.19	0.42
1:G:165:GLY:HA3	1:G:194:PHE:CZ	2.54	0.42
1:I:158:GLY:HA3	2:I:400:NAP:O2A	2.20	0.42
1:C:311:LEU:HB2	1:C:334:VAL:HG13	2.01	0.42
1:L:245:CYS:O	2:L:400:NAP:H2N	2.20	0.42
1:B:130:MET:SD	2:B:400:NAP:H5N	2.60	0.42
1:J:250:GLN:HE22	1:J:258:ARG:H	1.67	0.42
1:K:257:VAL:HG12	1:K:258:ARG:N	2.35	0.42
1:L:48:LEU:HD23	1:L:318:LEU:HA	2.02	0.41
1:L:329:LYS:HD2	1:L:329:LYS:C	2.40	0.41
1:C:270:ARG:HD3	1:D:280:ASP:OD2	2.20	0.41
1:J:116:PRO:HB3	1:J:121:LEU:HD21	2.02	0.41
1:A:64:PRO:HA	1:A:65:PRO:HD3	1.94	0.41
1:G:245:CYS:O	2:G:400:NAP:H2N	2.19	0.41
1:I:223:ASN:HB3	2:I:400:NAP:H4D	2.03	0.41
1:H:14:ARG:NH1	1:H:66:VAL:O	2.53	0.41
1:H:224:VAL:HA	1:H:248:ILE:HG22	2.03	0.41
1:L:209:LEU:HD22	1:L:217:ILE:HD11	2.03	0.41
1:K:184:LYS:O	1:K:187:PHE:HB3	2.21	0.41
1:L:152:VAL:HA	1:L:176:VAL:O	2.20	0.41
1:B:42:LYS:HD2	1:B:103:TYR:CE1	2.56	0.41
1:F:93:TYR:CD1	1:F:116:PRO:HG3	2.55	0.41
1:H:242:ILE:HD12	1:H:266:LEU:HD21	2.03	0.41
1:L:55:TRP:HB3	1:L:66:VAL:HG23	2.02	0.41
1:K:13:GLN:HB3	1:K:23:THR:HA	2.02	0.41
1:A:153:ILE:CD1	1:A:165:GLY:CA	2.98	0.41
1:C:170:LEU:HD21	1:C:300:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:LEU:CD2	1:F:242:ILE:HD11	2.50	0.41
1:G:48:LEU:HD11	1:G:332:LEU:HB2	2.03	0.41
1:H:21:ARG:C	1:H:23:THR:H	2.24	0.41
1:J:55:TRP:HE1	1:J:63:ILE:HD11	1.85	0.41
1:J:109:LYS:O	1:J:109:LYS:HD3	2.21	0.41
1:K:14:ARG:HA	1:K:15:PRO:HD3	1.83	0.41
1:K:49:ASP:O	1:K:52:MET:HB2	2.21	0.41
1:K:126:SER:HB3	1:K:329:LYS:HG2	2.03	0.41
1:B:290:LYS:O	1:B:294:THR:HG23	2.21	0.41
1:F:85:HIS:HA	1:F:86:PRO:HD3	1.90	0.41
1:F:220:PHE:CG	1:F:232:VAL:HG11	2.56	0.41
1:I:251:TYR:HH	2:I:400:NAP:HO2N	1.69	0.41
1:J:180:GLY:HA3	1:J:201:LYS:HE3	2.03	0.41
1:A:241:ARG:HD3	1:A:241:ARG:N	2.35	0.40
1:B:304:ARG:HG2	1:B:328:GLY:HA3	2.03	0.40
1:C:77:VAL:HG11	1:C:121:LEU:HD22	2.03	0.40
1:C:223:ASN:HB3	2:C:400:NAP:H4D	2.03	0.40
1:F:166:GLN:HG2	1:F:169:ARG:HH21	1.86	0.40
1:K:166:GLN:O	1:K:170:LEU:HG	2.21	0.40
1:L:19:PRO:HG3	1:L:53:ARG:HG3	2.03	0.40
1:C:53:ARG:O	1:C:56:MET:HG2	2.22	0.40
1:C:290:LYS:O	1:C:294:THR:HG23	2.21	0.40
1:I:313:THR:HA	1:I:316:GLU:OE2	2.20	0.40
1:J:52:MET:HA	1:J:55:TRP:CE3	2.55	0.40
1:D:143:GLY:O	1:D:241:ARG:HD2	2.21	0.40
1:L:311:LEU:HB2	1:L:334:VAL:HG12	2.03	0.40
1:C:287:GLU:HG3	3:C:2040:HOH:O	2.20	0.40
1:H:53:ARG:HD3	1:H:252:ASN:OD1	2.21	0.40
1:I:270:ARG:HG2	1:J:280:ASP:OD2	2.21	0.40
1:D:323:SER:HB2	1:D:325:GLU:HG3	2.04	0.40
1:H:107:GLU:HA	1:H:108:PRO:HD3	1.93	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	325/336 (97%)	322 (99%)	3 (1%)	0	100	100
1	B	329/336 (98%)	324 (98%)	5 (2%)	0	100	100
1	C	319/336 (95%)	310 (97%)	9 (3%)	0	100	100
1	D	323/336 (96%)	316 (98%)	6 (2%)	1 (0%)	41	46
1	E	329/336 (98%)	323 (98%)	6 (2%)	0	100	100
1	F	329/336 (98%)	323 (98%)	6 (2%)	0	100	100
1	G	317/336 (94%)	307 (97%)	9 (3%)	1 (0%)	41	46
1	H	323/336 (96%)	313 (97%)	10 (3%)	0	100	100
1	I	226/336 (67%)	216 (96%)	10 (4%)	0	100	100
1	J	323/336 (96%)	314 (97%)	8 (2%)	1 (0%)	41	46
1	K	292/336 (87%)	277 (95%)	12 (4%)	3 (1%)	15	14
1	L	314/336 (94%)	308 (98%)	6 (2%)	0	100	100
All	All	3749/4032 (93%)	3653 (97%)	90 (2%)	6 (0%)	47	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	ARG
1	K	262	ASN
1	K	261	ALA
1	G	258	ARG
1	K	109	LYS
1	J	21	ARG

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	258/263 (98%)	253 (98%)	5 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	260/263 (99%)	254 (98%)	6 (2%)	50	63
1	C	255/263 (97%)	249 (98%)	6 (2%)	49	62
1	D	257/263 (98%)	251 (98%)	6 (2%)	50	63
1	E	260/263 (99%)	255 (98%)	5 (2%)	57	71
1	F	260/263 (99%)	257 (99%)	3 (1%)	71	83
1	G	252/263 (96%)	247 (98%)	5 (2%)	55	69
1	H	257/263 (98%)	250 (97%)	7 (3%)	44	57
1	I	180/263 (68%)	175 (97%)	5 (3%)	43	56
1	J	256/263 (97%)	249 (97%)	7 (3%)	44	57
1	K	239/263 (91%)	231 (97%)	8 (3%)	38	49
1	L	252/263 (96%)	243 (96%)	9 (4%)	35	45
All	All	2986/3156 (95%)	2914 (98%)	72 (2%)	49	62

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	26	PHE
1	A	230	ASP
1	A	270	ARG
1	A	327	PHE
1	B	8	GLN
1	B	26	PHE
1	B	44	GLU
1	B	230	ASP
1	B	255	GLU
1	B	270	ARG
1	C	23	THR
1	C	72	MET
1	C	82	VAL
1	C	230	ASP
1	C	279	MET
1	C	327	PHE
1	D	230	ASP
1	D	270	ARG
1	D	287	GLU
1	D	304	ARG
1	D	321	LEU

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Mol	Chain	Res	Type
1	D	323	SER
1	E	26	PHE
1	E	53	ARG
1	E	230	ASP
1	E	241	ARG
1	E	270	ARG
1	F	26	PHE
1	F	123	ARG
1	F	230	ASP
1	G	121	LEU
1	G	270	ARG
1	G	323	SER
1	G	325	GLU
1	G	327	PHE
1	H	11	LEU
1	H	53	ARG
1	H	123	ARG
1	H	146	LYS
1	H	190	GLU
1	H	241	ARG
1	H	270	ARG
1	I	111	PHE
1	I	118	ARG
1	I	235	ARG
1	I	270	ARG
1	I	323	SER
1	J	23	THR
1	J	105	ILE
1	J	109	LYS
1	J	169	ARG
1	J	230	ASP
1	J	241	ARG
1	J	270	ARG
1	K	16	SER
1	K	21	ARG
1	K	118	ARG
1	K	169	ARG
1	K	230	ASP
1	K	249	SER
1	K	262	ASN
1	K	270	ARG
1	L	22	ASP

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Mol	Chain	Res	Type
1	L	109	LYS
1	L	121	LEU
1	L	190	GLU
1	L	230	ASP
1	L	244	LEU
1	L	250	GLN
1	L	270	ARG
1	L	327	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	C	13	GLN
1	D	250	GLN
1	E	8	GLN
1	G	8	GLN
1	G	10	GLN
1	I	283	GLN
1	J	8	GLN
1	J	250	GLN
1	K	8	GLN
1	L	326	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	K	400	-	45,52,52	1.62	8 (17%)	56,80,80	1.29	7 (12%)
2	NAP	B	400	-	45,52,52	1.59	7 (15%)	56,80,80	1.26	6 (10%)
2	NAP	C	400	-	45,52,52	1.45	7 (15%)	56,80,80	1.28	6 (10%)
2	NAP	F	400	-	45,52,52	1.54	7 (15%)	56,80,80	1.25	5 (8%)
2	NAP	A	400	-	45,52,52	1.52	8 (17%)	56,80,80	1.21	7 (12%)
2	NAP	H	400	-	45,52,52	1.59	7 (15%)	56,80,80	1.17	2 (3%)
2	NAP	L	400	-	45,52,52	1.40	5 (11%)	56,80,80	1.35	7 (12%)
2	NAP	E	400	-	45,52,52	1.49	6 (13%)	56,80,80	1.35	8 (14%)
2	NAP	G	400	-	45,52,52	1.42	6 (13%)	56,80,80	1.20	4 (7%)
2	NAP	I	400	-	45,52,52	1.50	9 (20%)	56,80,80	1.20	5 (8%)
2	NAP	J	400	-	45,52,52	1.42	8 (17%)	56,80,80	1.27	5 (8%)
2	NAP	D	400	-	45,52,52	1.93	8 (17%)	56,80,80	1.44	7 (12%)

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	K	400	-	-	9/31/67/67	0/5/5/5
2	NAP	B	400	-	-	8/31/67/67	0/5/5/5
2	NAP	C	400	-	-	8/31/67/67	0/5/5/5
2	NAP	F	400	-	-	7/31/67/67	0/5/5/5
2	NAP	A	400	-	-	7/31/67/67	0/5/5/5
2	NAP	H	400	-	-	9/31/67/67	0/5/5/5
2	NAP	L	400	-	-	11/31/67/67	0/5/5/5
2	NAP	E	400	-	-	9/31/67/67	0/5/5/5
2	NAP	G	400	-	-	7/31/67/67	0/5/5/5
2	NAP	I	400	-	-	6/31/67/67	0/5/5/5
2	NAP	J	400	-	-	7/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	400	-	-	11/31/67/67	0/5/5/5

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAP	O4B-C1B	6.34	1.49	1.41
2	D	400	NAP	C2N-N1N	5.29	1.41	1.35
2	K	400	NAP	C2N-N1N	5.18	1.41	1.35
2	B	400	NAP	O4D-C1D	5.11	1.48	1.41
2	A	400	NAP	O4D-C1D	4.94	1.48	1.41
2	E	400	NAP	O4B-C1B	4.92	1.47	1.41
2	B	400	NAP	C2N-N1N	4.85	1.40	1.35
2	H	400	NAP	O4D-C1D	4.85	1.47	1.41
2	I	400	NAP	C2N-N1N	4.54	1.40	1.35
2	J	400	NAP	O4B-C1B	4.21	1.47	1.41
2	D	400	NAP	C5B-C4B	4.17	1.64	1.51
2	C	400	NAP	C2N-N1N	4.14	1.40	1.35
2	H	400	NAP	C2N-N1N	4.10	1.40	1.35
2	E	400	NAP	P2B-O1X	4.04	1.63	1.50
2	L	400	NAP	C2N-N1N	3.96	1.39	1.35
2	D	400	NAP	P2B-O1X	3.94	1.63	1.50
2	H	400	NAP	O4B-C1B	3.92	1.46	1.41
2	F	400	NAP	O4B-C1B	3.91	1.46	1.41
2	F	400	NAP	P2B-O1X	3.88	1.63	1.50
2	I	400	NAP	P2B-O1X	3.85	1.63	1.50
2	L	400	NAP	O4B-C1B	3.80	1.46	1.41
2	C	400	NAP	O4D-C1D	3.77	1.46	1.41
2	K	400	NAP	O4D-C1D	3.75	1.46	1.41
2	G	400	NAP	O4D-C1D	3.72	1.46	1.41
2	A	400	NAP	C2N-N1N	3.69	1.39	1.35
2	L	400	NAP	P2B-O1X	3.63	1.62	1.50
2	E	400	NAP	P2B-O2B	3.55	1.66	1.59
2	F	400	NAP	PA-O1A	3.55	1.63	1.50
2	F	400	NAP	O4D-C1D	3.54	1.46	1.41
2	D	400	NAP	O4D-C1D	3.46	1.45	1.41
2	J	400	NAP	C2N-N1N	3.44	1.39	1.35
2	G	400	NAP	P2B-O1X	3.41	1.61	1.50
2	B	400	NAP	O4B-C1B	3.32	1.45	1.41
2	F	400	NAP	C2N-N1N	3.31	1.39	1.35
2	H	400	NAP	P2B-O1X	3.29	1.61	1.50
2	G	400	NAP	PA-O1A	3.24	1.62	1.50
2	K	400	NAP	P2B-O1X	3.21	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	NAP	O4B-C1B	3.21	1.45	1.41
2	G	400	NAP	C2N-N1N	3.11	1.38	1.35
2	A	400	NAP	O4B-C1B	3.10	1.45	1.41
2	D	400	NAP	PA-O1A	3.10	1.61	1.50
2	K	400	NAP	PA-O1A	3.08	1.61	1.50
2	I	400	NAP	PA-O1A	3.05	1.61	1.50
2	A	400	NAP	P2B-O1X	3.00	1.60	1.50
2	J	400	NAP	P2B-O1X	2.97	1.60	1.50
2	C	400	NAP	P2B-O2X	2.93	1.66	1.54
2	K	400	NAP	O4B-C1B	2.91	1.45	1.41
2	C	400	NAP	P2B-O1X	2.86	1.59	1.50
2	E	400	NAP	O4D-C1D	2.86	1.45	1.41
2	J	400	NAP	O4D-C1D	2.85	1.45	1.41
2	H	400	NAP	PA-O1A	2.81	1.60	1.50
2	I	400	NAP	P2B-O2X	2.73	1.65	1.54
2	A	400	NAP	C2D-C1D	-2.73	1.49	1.53
2	G	400	NAP	C6N-N1N	2.72	1.42	1.35
2	K	400	NAP	P2B-O2B	2.71	1.64	1.59
2	B	400	NAP	P2B-O2B	2.70	1.64	1.59
2	I	400	NAP	C3N-C7N	2.66	1.54	1.50
2	I	400	NAP	O4B-C1B	2.64	1.44	1.41
2	I	400	NAP	O4D-C1D	2.63	1.44	1.41
2	L	400	NAP	PA-O1A	2.61	1.60	1.50
2	B	400	NAP	C6N-N1N	2.61	1.41	1.35
2	C	400	NAP	C6N-N1N	2.60	1.41	1.35
2	J	400	NAP	PA-O1A	2.56	1.60	1.50
2	D	400	NAP	C6N-N1N	2.55	1.41	1.35
2	C	400	NAP	PA-O1A	2.55	1.59	1.50
2	K	400	NAP	C6N-N1N	2.52	1.41	1.35
2	F	400	NAP	C6N-N1N	2.51	1.41	1.35
2	C	400	NAP	O4B-C1B	2.46	1.44	1.41
2	H	400	NAP	C3N-C7N	2.43	1.54	1.50
2	L	400	NAP	C6N-N1N	2.43	1.41	1.35
2	J	400	NAP	P2B-O2B	2.39	1.63	1.59
2	J	400	NAP	C2D-C1D	-2.34	1.50	1.53
2	J	400	NAP	C6N-N1N	2.31	1.41	1.35
2	H	400	NAP	C6N-N1N	2.31	1.41	1.35
2	K	400	NAP	C3N-C7N	2.31	1.54	1.50
2	F	400	NAP	C2D-C1D	-2.30	1.50	1.53
2	I	400	NAP	C6N-N1N	2.29	1.41	1.35
2	A	400	NAP	C6N-N1N	2.27	1.41	1.35
2	B	400	NAP	P2B-O1X	2.27	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAP	O5B-C5B	2.16	1.53	1.44
2	E	400	NAP	C6N-N1N	2.08	1.40	1.35
2	B	400	NAP	C3N-C7N	2.07	1.53	1.50
2	I	400	NAP	P2B-O2B	2.06	1.63	1.59
2	A	400	NAP	P2B-O3X	-2.06	1.46	1.54
2	E	400	NAP	P2B-O3X	-2.00	1.47	1.54
2	A	400	NAP	P2B-O2B	2.00	1.63	1.59

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	NAP	N3A-C2A-N1A	-5.10	120.70	128.68
2	C	400	NAP	N3A-C2A-N1A	-4.75	121.25	128.68
2	K	400	NAP	N3A-C2A-N1A	-4.73	121.29	128.68
2	I	400	NAP	N3A-C2A-N1A	-4.55	121.57	128.68
2	D	400	NAP	N3A-C2A-N1A	-4.53	121.59	128.68
2	J	400	NAP	N3A-C2A-N1A	-4.52	121.61	128.68
2	G	400	NAP	N3A-C2A-N1A	-4.43	121.76	128.68
2	H	400	NAP	N3A-C2A-N1A	-4.42	121.77	128.68
2	E	400	NAP	N3A-C2A-N1A	-4.42	121.77	128.68
2	A	400	NAP	N3A-C2A-N1A	-4.35	121.88	128.68
2	L	400	NAP	N3A-C2A-N1A	-4.33	121.91	128.68
2	F	400	NAP	N3A-C2A-N1A	-4.27	122.00	128.68
2	I	400	NAP	PN-O3-PA	-3.94	119.31	132.83
2	H	400	NAP	PN-O3-PA	-3.82	119.72	132.83
2	L	400	NAP	PN-O3-PA	-3.77	119.88	132.83
2	D	400	NAP	PN-O3-PA	-3.57	120.56	132.83
2	J	400	NAP	C3N-C7N-N7N	-3.57	113.46	117.75
2	L	400	NAP	C3N-C7N-N7N	-3.55	113.49	117.75
2	K	400	NAP	PN-O3-PA	-3.53	120.73	132.83
2	C	400	NAP	PN-O3-PA	-3.39	121.18	132.83
2	E	400	NAP	C3N-C7N-N7N	-3.38	113.70	117.75
2	J	400	NAP	PN-O3-PA	-3.37	121.28	132.83
2	F	400	NAP	PN-O3-PA	-3.34	121.38	132.83
2	K	400	NAP	C6N-N1N-C2N	-3.08	119.17	121.97
2	G	400	NAP	PN-O3-PA	-2.94	122.75	132.83
2	B	400	NAP	PN-O3-PA	-2.91	122.86	132.83
2	D	400	NAP	O5B-PA-O1A	2.80	120.00	109.07
2	D	400	NAP	C6N-N1N-C2N	-2.76	119.46	121.97
2	E	400	NAP	O3D-C3D-C4D	-2.73	103.14	111.05
2	D	400	NAP	O5B-C5B-C4B	2.67	118.19	108.99
2	C	400	NAP	C2N-C3N-C4N	2.65	121.27	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	400	NAP	C3N-C7N-N7N	-2.65	114.57	117.75
2	E	400	NAP	O3X-P2B-O2B	2.61	117.70	105.99
2	B	400	NAP	C1B-N9A-C4A	-2.57	122.12	126.64
2	A	400	NAP	C3N-C7N-N7N	-2.51	114.74	117.75
2	C	400	NAP	O4D-C1D-C2D	-2.49	103.29	106.93
2	B	400	NAP	O2X-P2B-O1X	-2.47	101.01	110.68
2	L	400	NAP	O4D-C1D-C2D	-2.44	103.36	106.93
2	I	400	NAP	O4B-C4B-C3B	-2.44	100.29	105.11
2	A	400	NAP	C4A-C5A-N7A	-2.42	106.87	109.40
2	E	400	NAP	C2N-C3N-C4N	2.37	120.95	118.26
2	J	400	NAP	O4D-C1D-C2D	-2.36	103.48	106.93
2	A	400	NAP	PN-O3-PA	-2.36	124.73	132.83
2	C	400	NAP	C6N-N1N-C2N	-2.35	119.83	121.97
2	K	400	NAP	O3X-P2B-O2B	2.32	116.39	105.99
2	F	400	NAP	C2N-C3N-C4N	2.31	120.88	118.26
2	B	400	NAP	C2A-N1A-C6A	2.30	122.69	118.75
2	G	400	NAP	C6N-N1N-C2N	-2.28	119.89	121.97
2	A	400	NAP	O4B-C4B-C3B	-2.25	100.67	105.11
2	L	400	NAP	C6N-N1N-C2N	-2.23	119.94	121.97
2	K	400	NAP	O7N-C7N-C3N	2.22	122.29	119.63
2	A	400	NAP	O4D-C1D-C2D	-2.20	103.71	106.93
2	E	400	NAP	C3N-C2N-N1N	-2.18	118.29	120.43
2	K	400	NAP	O4D-C1D-C2D	-2.17	103.76	106.93
2	F	400	NAP	C6N-N1N-C2N	-2.17	120.00	121.97
2	A	400	NAP	O3D-C3D-C4D	-2.14	104.87	111.05
2	F	400	NAP	C3N-C7N-N7N	-2.13	115.19	117.75
2	D	400	NAP	O2B-P2B-O1X	-2.12	101.22	109.39
2	G	400	NAP	C3N-C7N-N7N	-2.11	115.22	117.75
2	E	400	NAP	O4D-C1D-C2D	-2.10	103.85	106.93
2	D	400	NAP	O4D-C1D-C2D	-2.09	103.88	106.93
2	L	400	NAP	O2A-PA-O5B	2.08	117.41	107.75
2	C	400	NAP	C3N-C7N-N7N	-2.06	115.27	117.75
2	E	400	NAP	PN-O3-PA	-2.06	125.75	132.83
2	B	400	NAP	O3X-P2B-O2X	2.06	115.52	107.64
2	I	400	NAP	C6N-N1N-C2N	-2.06	120.10	121.97
2	I	400	NAP	C3N-C7N-N7N	-2.04	115.31	117.75
2	J	400	NAP	C2N-C3N-C4N	2.02	120.55	118.26
2	L	400	NAP	O7N-C7N-C3N	2.00	122.03	119.63

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NAP	O4D-C1D-N1N-C6N
2	B	400	NAP	O4D-C1D-N1N-C6N
2	C	400	NAP	O4D-C1D-N1N-C6N
2	D	400	NAP	C5B-O5B-PA-O1A
2	D	400	NAP	C5B-O5B-PA-O2A
2	D	400	NAP	C4B-C5B-O5B-PA
2	D	400	NAP	O4B-C4B-C5B-O5B
2	D	400	NAP	O4D-C1D-N1N-C6N
2	D	400	NAP	C2D-C1D-N1N-C2N
2	D	400	NAP	C2D-C1D-N1N-C6N
2	E	400	NAP	O4B-C4B-C5B-O5B
2	E	400	NAP	C2B-O2B-P2B-O2X
2	E	400	NAP	O4D-C1D-N1N-C6N
2	E	400	NAP	C2D-C1D-N1N-C2N
2	F	400	NAP	O4D-C1D-N1N-C6N
2	G	400	NAP	C4B-C5B-O5B-PA
2	G	400	NAP	O4B-C4B-C5B-O5B
2	G	400	NAP	O4D-C1D-N1N-C2N
2	G	400	NAP	O4D-C1D-N1N-C6N
2	G	400	NAP	C2D-C1D-N1N-C2N
2	G	400	NAP	C2D-C1D-N1N-C6N
2	H	400	NAP	O4D-C1D-N1N-C2N
2	H	400	NAP	O4D-C1D-N1N-C6N
2	J	400	NAP	O4B-C4B-C5B-O5B
2	J	400	NAP	O4D-C1D-N1N-C6N
2	K	400	NAP	O4B-C4B-C5B-O5B
2	K	400	NAP	O4D-C1D-N1N-C2N
2	K	400	NAP	O4D-C1D-N1N-C6N
2	K	400	NAP	C2D-C1D-N1N-C2N
2	L	400	NAP	C5B-O5B-PA-O1A
2	L	400	NAP	C5B-O5B-PA-O2A
2	L	400	NAP	C2B-O2B-P2B-O3X
2	L	400	NAP	C5D-O5D-PN-O2N
2	L	400	NAP	O4D-C1D-N1N-C6N
2	B	400	NAP	C3B-C4B-C5B-O5B
2	D	400	NAP	C3B-C4B-C5B-O5B
2	E	400	NAP	C3B-C4B-C5B-O5B
2	F	400	NAP	O4B-C4B-C5B-O5B
2	J	400	NAP	C3B-C4B-C5B-O5B
2	K	400	NAP	C3B-C4B-C5B-O5B
2	E	400	NAP	C4B-C5B-O5B-PA
2	B	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	400	NAP	C3B-C4B-C5B-O5B
2	G	400	NAP	C3B-C4B-C5B-O5B
2	H	400	NAP	C3B-C4B-C5B-O5B
2	J	400	NAP	C4B-C5B-O5B-PA
2	K	400	NAP	C4B-C5B-O5B-PA
2	C	400	NAP	O4B-C4B-C5B-O5B
2	H	400	NAP	O4B-C4B-C5B-O5B
2	B	400	NAP	C4B-C5B-O5B-PA
2	C	400	NAP	C4B-C5B-O5B-PA
2	F	400	NAP	C4B-C5B-O5B-PA
2	H	400	NAP	C4B-C5B-O5B-PA
2	L	400	NAP	C4B-C5B-O5B-PA
2	L	400	NAP	C2B-O2B-P2B-O1X
2	I	400	NAP	C4B-C5B-O5B-PA
2	C	400	NAP	C2B-O2B-P2B-O2X
2	D	400	NAP	C5B-O5B-PA-O3
2	K	400	NAP	C2B-O2B-P2B-O2X
2	L	400	NAP	C5D-O5D-PN-O3
2	H	400	NAP	PA-O3-PN-O2N
2	I	400	NAP	PA-O3-PN-O2N
2	K	400	NAP	PA-O3-PN-O2N
2	L	400	NAP	PN-O3-PA-O2A
2	A	400	NAP	C4B-C5B-O5B-PA
2	L	400	NAP	C5D-O5D-PN-O1N
2	A	400	NAP	PA-O3-PN-O2N
2	B	400	NAP	PA-O3-PN-O2N
2	C	400	NAP	PA-O3-PN-O2N
2	F	400	NAP	PA-O3-PN-O2N
2	J	400	NAP	PA-O3-PN-O2N
2	A	400	NAP	C3B-C4B-C5B-O5B
2	B	400	NAP	C2B-O2B-P2B-O1X
2	F	400	NAP	C2B-O2B-P2B-O1X
2	A	400	NAP	C2B-O2B-P2B-O3X
2	A	400	NAP	C2D-C1D-N1N-C2N
2	B	400	NAP	C2B-O2B-P2B-O3X
2	B	400	NAP	C2D-C1D-N1N-C2N
2	C	400	NAP	C2B-O2B-P2B-O3X
2	E	400	NAP	C2B-O2B-P2B-O3X
2	E	400	NAP	C2D-C1D-N1N-C6N
2	H	400	NAP	C5D-O5D-PN-O3
2	H	400	NAP	C2D-C1D-N1N-C2N
2	I	400	NAP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
2	J	400	NAP	C2B-O2B-P2B-O3X
2	J	400	NAP	C2D-C1D-N1N-C2N
2	K	400	NAP	C2B-O2B-P2B-O3X
2	L	400	NAP	C5B-O5B-PA-O3
2	A	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	PA-O3-PN-O1N
2	D	400	NAP	PA-O3-PN-O1N
2	D	400	NAP	PA-O3-PN-O2N
2	E	400	NAP	PA-O3-PN-O2N
2	F	400	NAP	PA-O3-PN-O1N
2	H	400	NAP	PA-O3-PN-O1N
2	I	400	NAP	PA-O3-PN-O1N
2	I	400	NAP	O4B-C4B-C5B-O5B
2	I	400	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

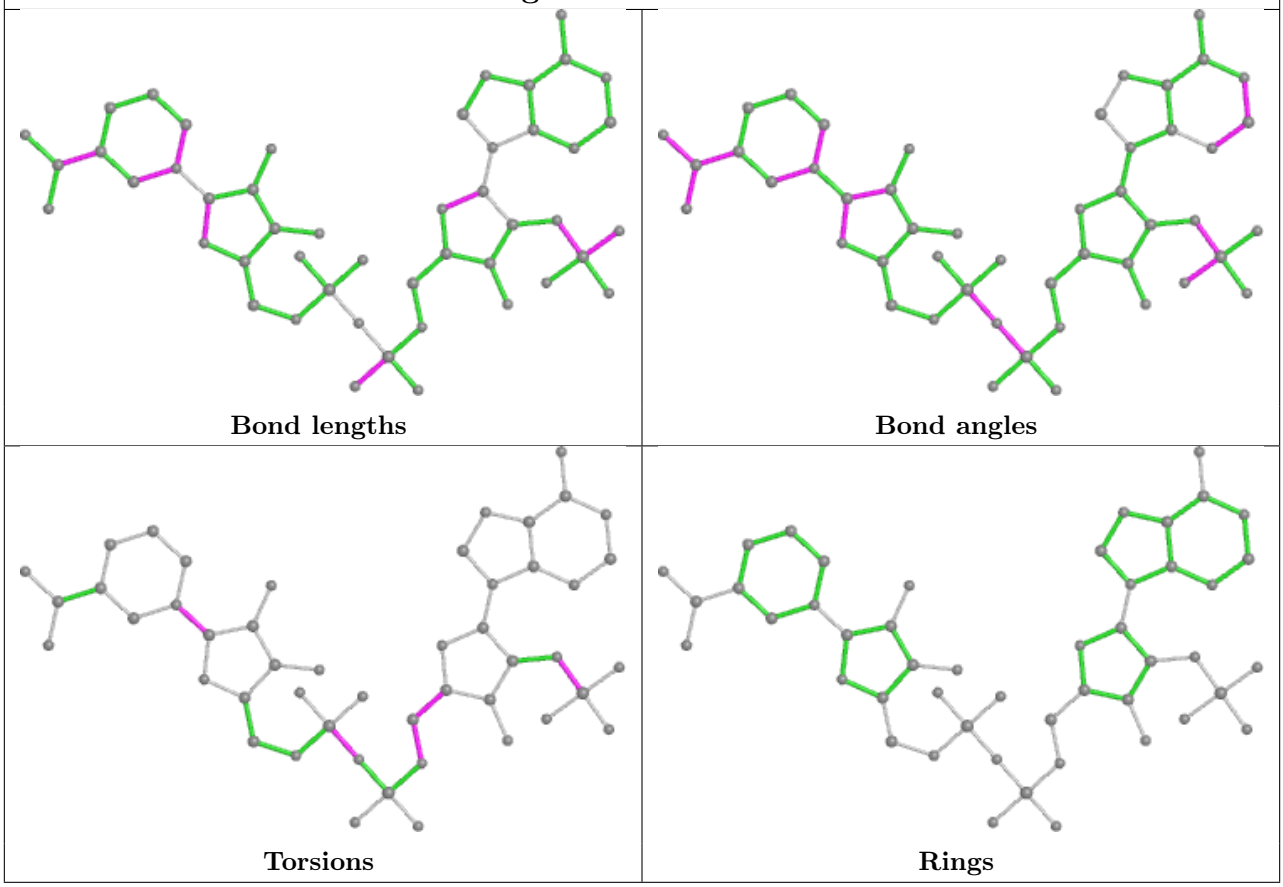
12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	400	NAP	2	0
2	B	400	NAP	4	0
2	C	400	NAP	4	0
2	F	400	NAP	3	0
2	A	400	NAP	1	0
2	H	400	NAP	2	0
2	L	400	NAP	2	0
2	E	400	NAP	2	0
2	G	400	NAP	4	0
2	I	400	NAP	4	0
2	J	400	NAP	3	0
2	D	400	NAP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 K 400



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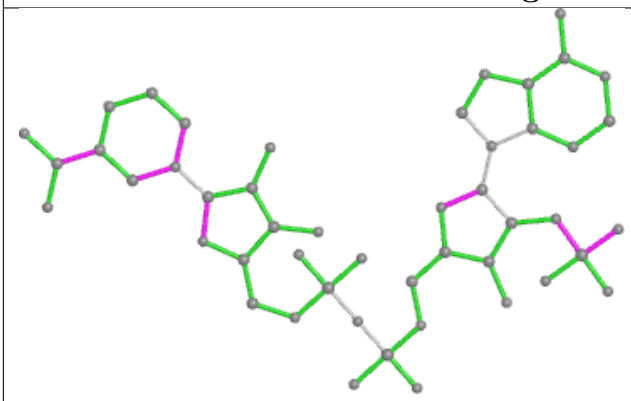
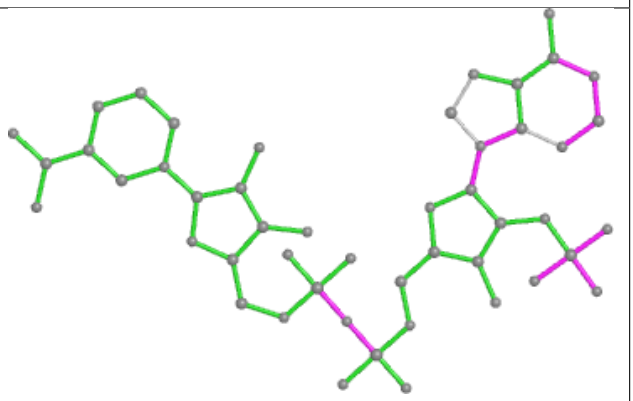
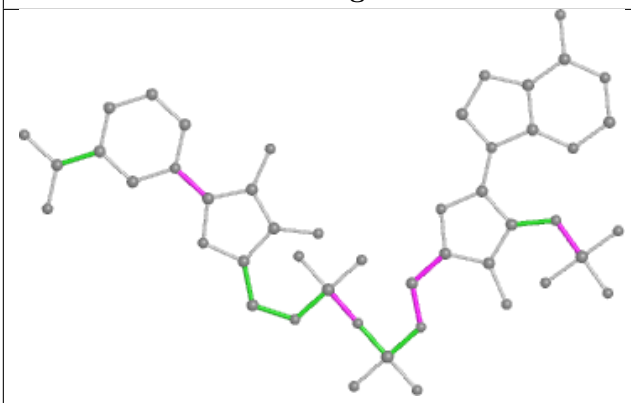


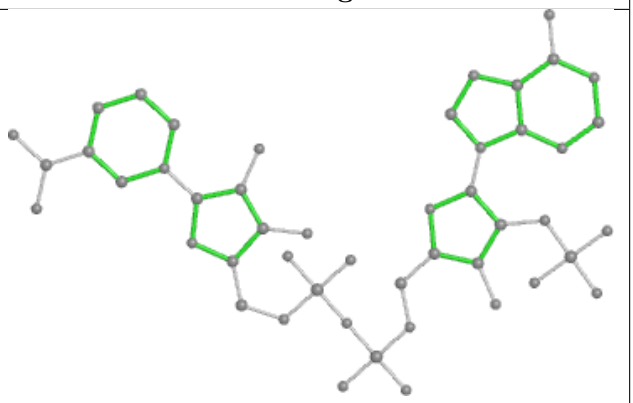
Bond lengths



Bond angles

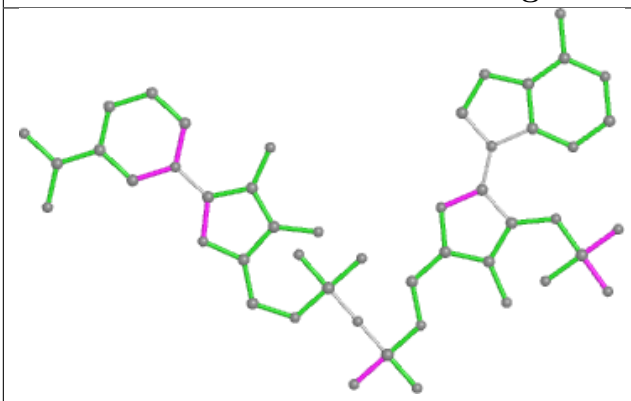


Torsions



Rings

Ligand NAP C 400



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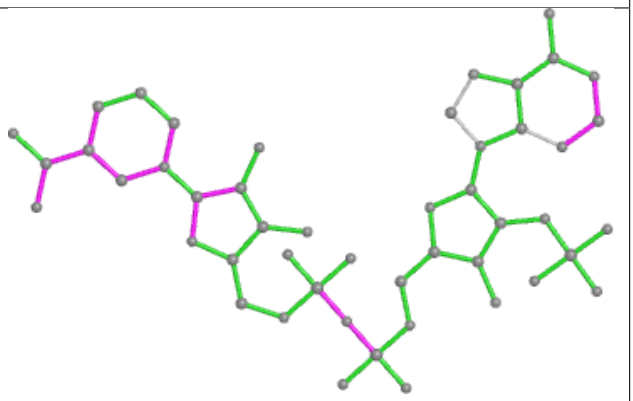

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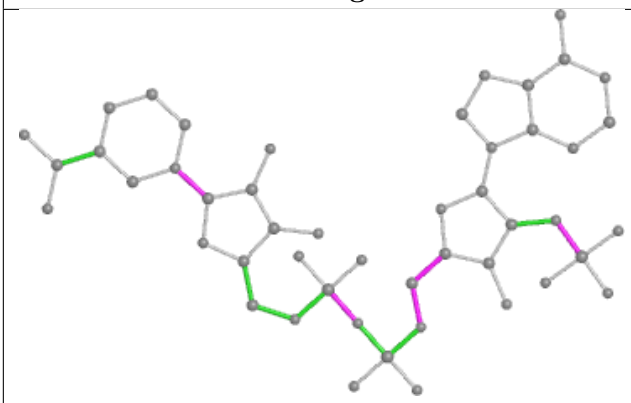

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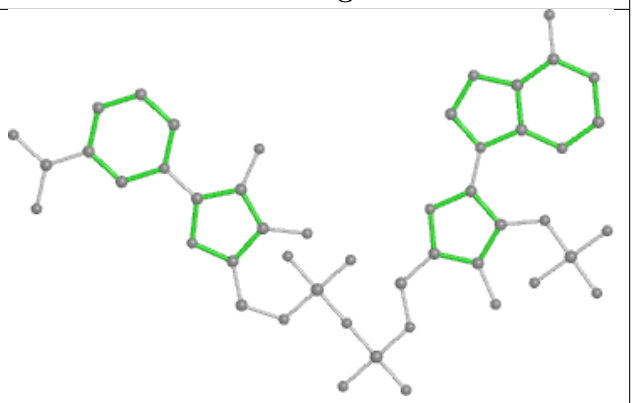

Rings

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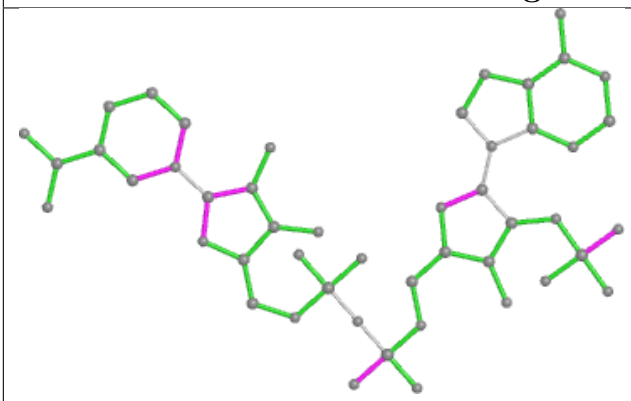

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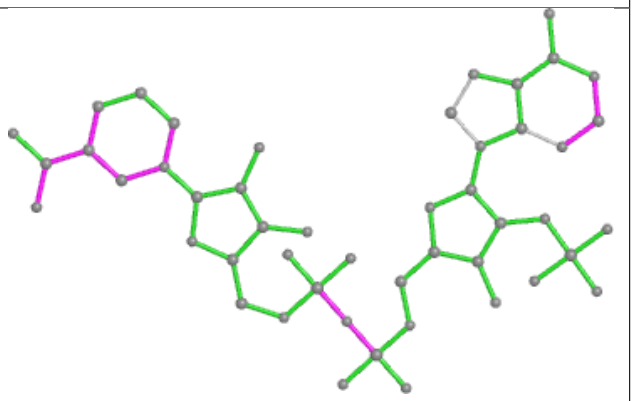

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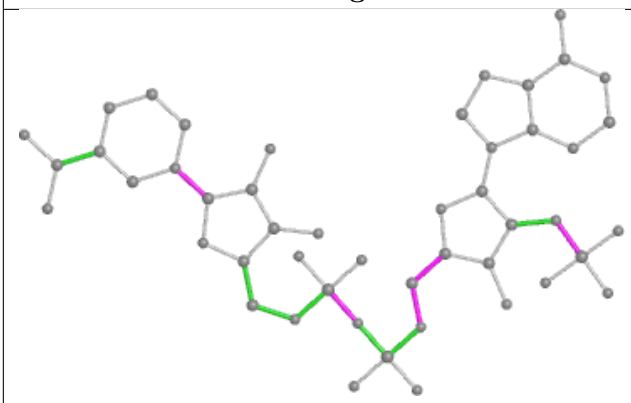

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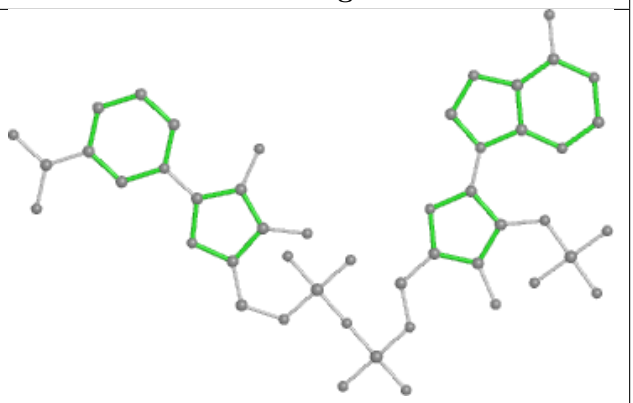
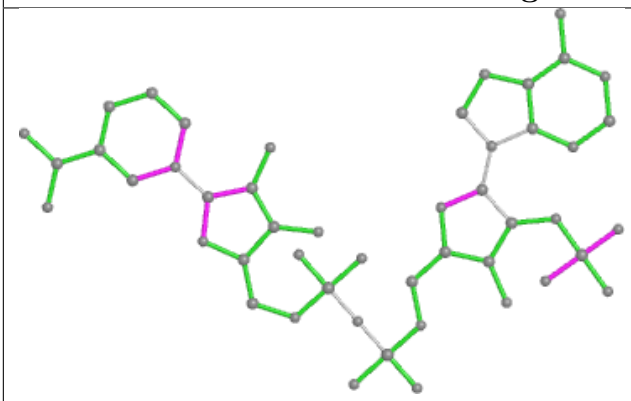


Rings

Ligand NAP A 400



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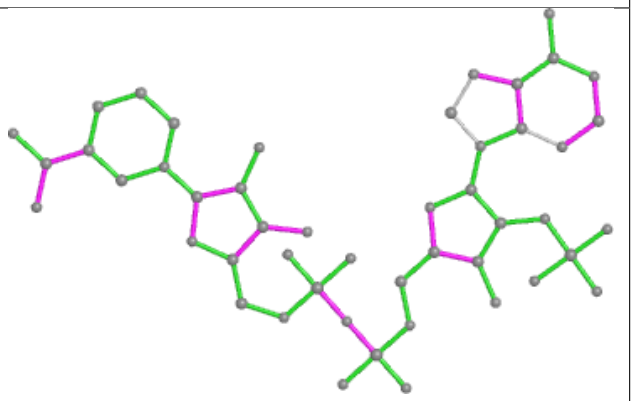
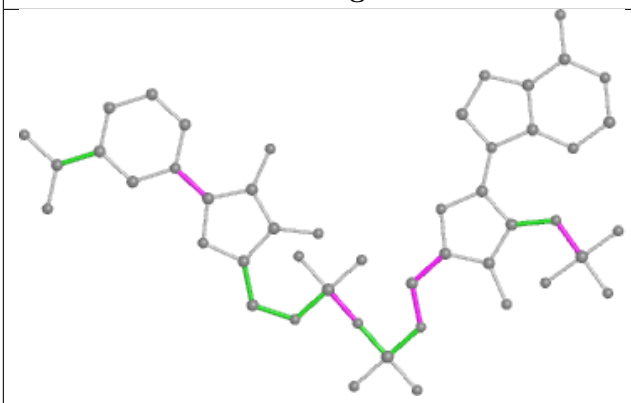


Bond angles



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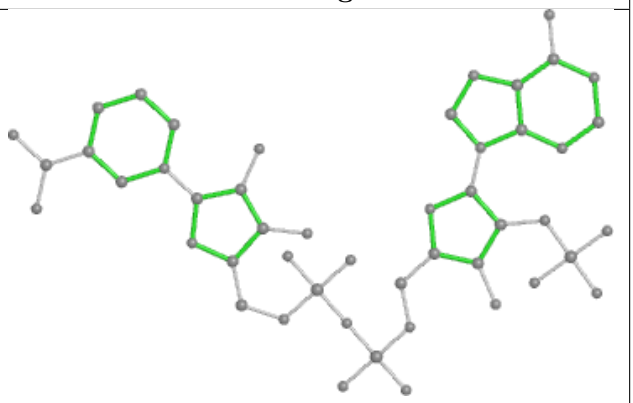

Rings

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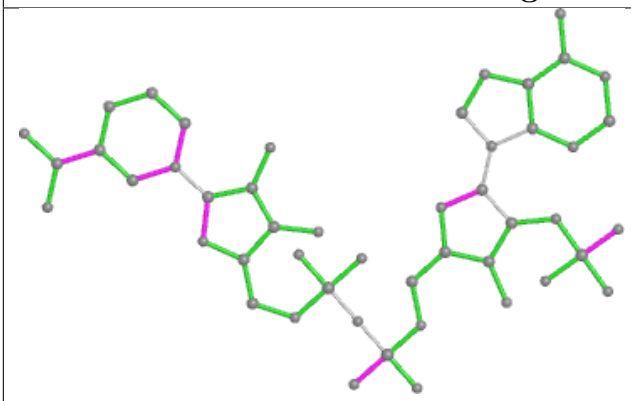

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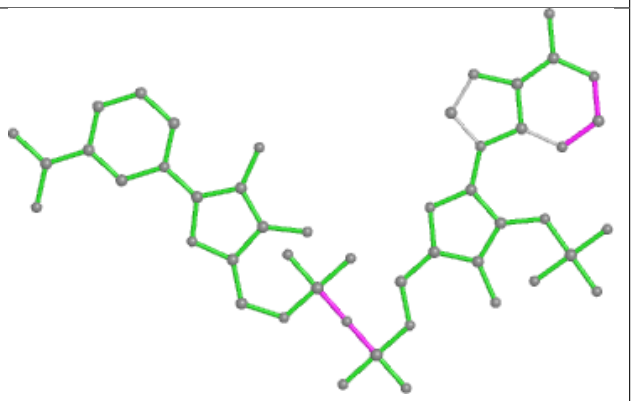

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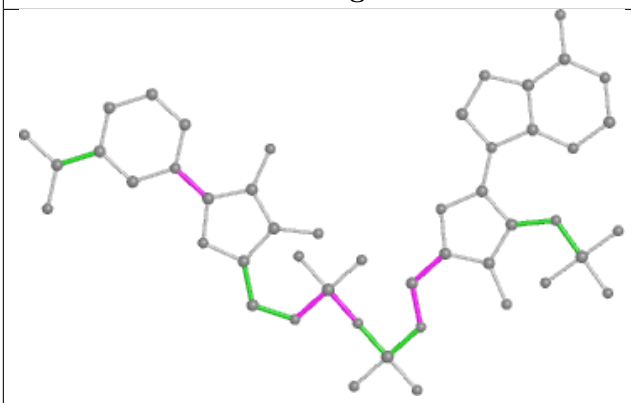

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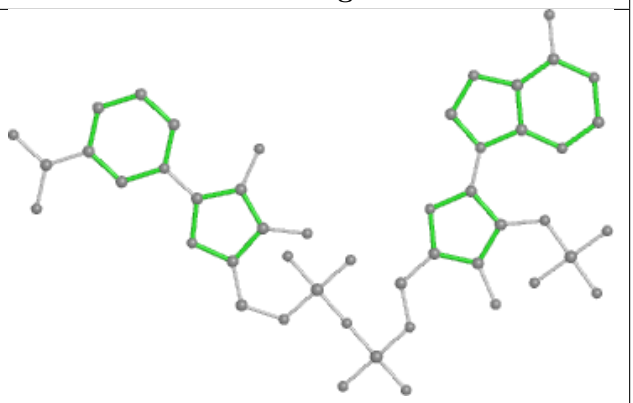
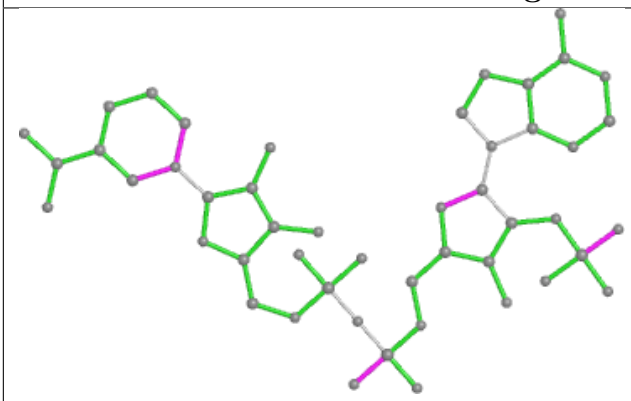


Rings

Ligand NAP L 400



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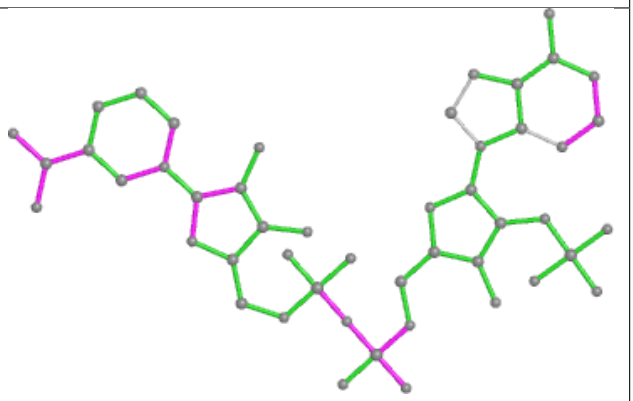

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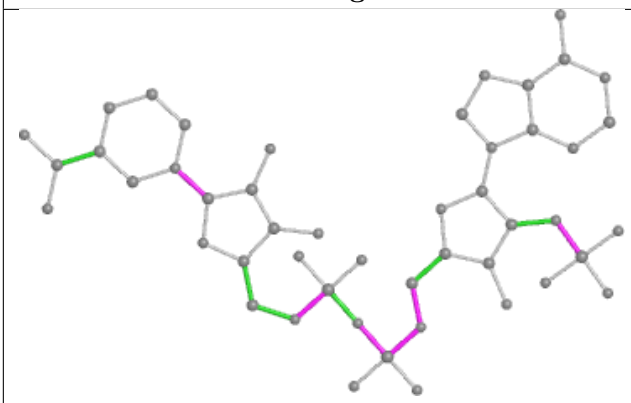

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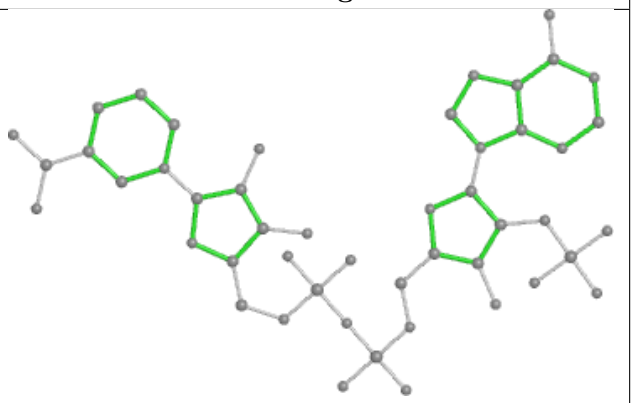
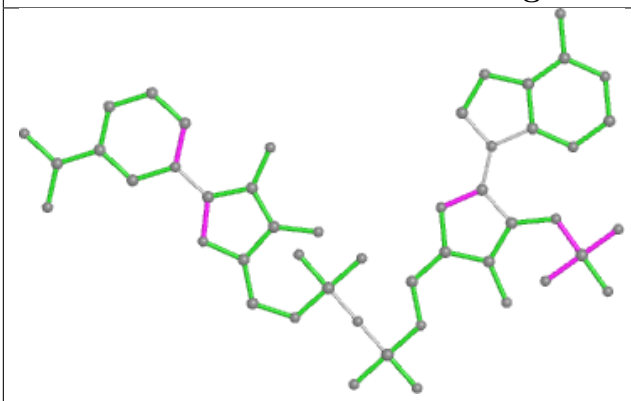
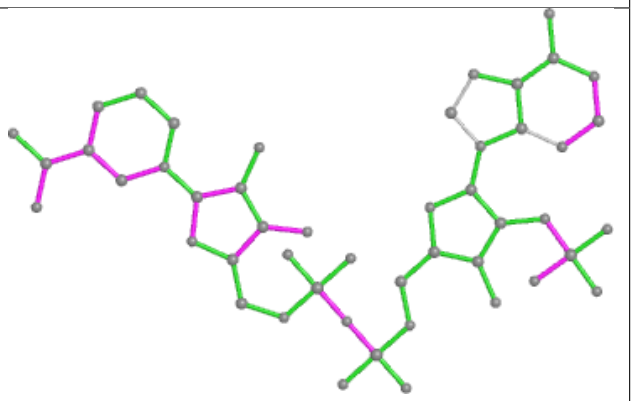


Rings

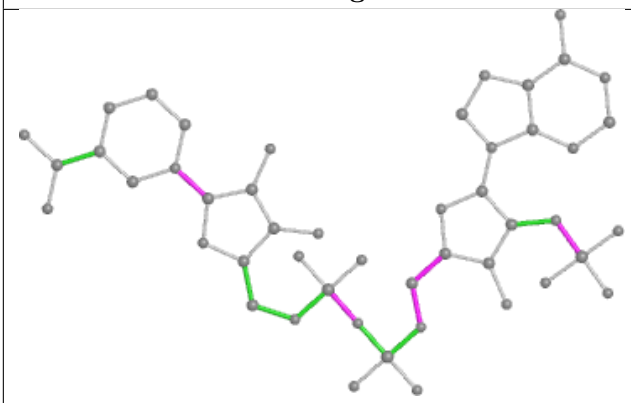
Ligand NAP E 400



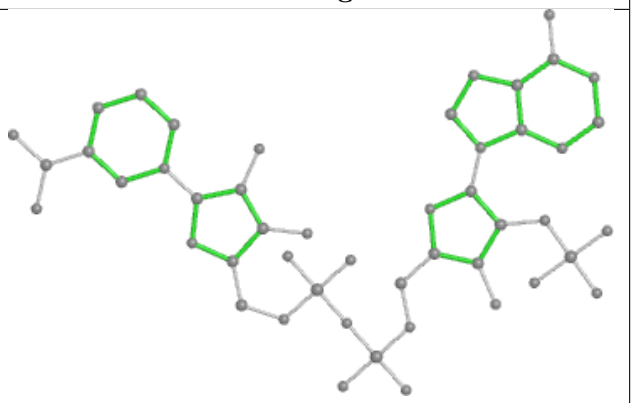
Bond lengths



Bond angles

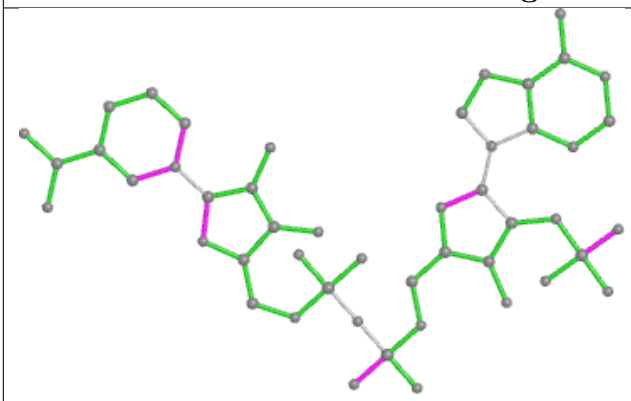


Torsions

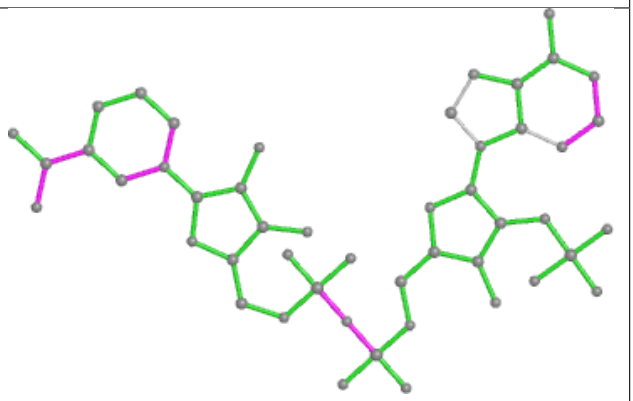


Rings

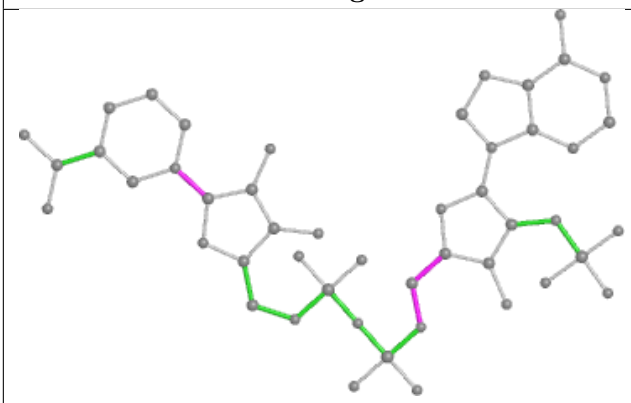
Ligand NAP G 400



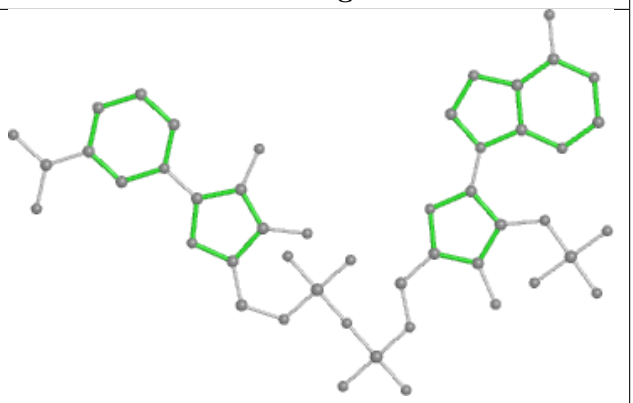
Bond lengths



Bond angles

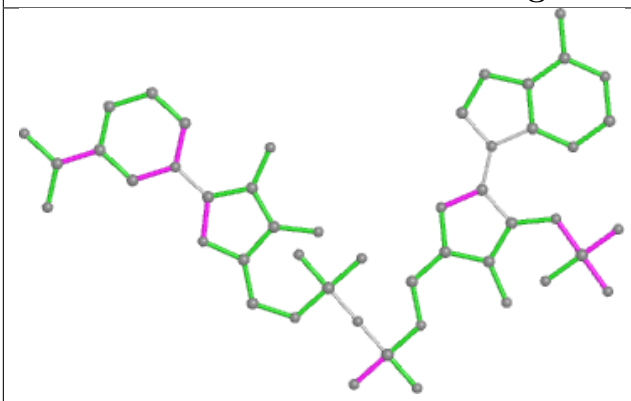


Torsions

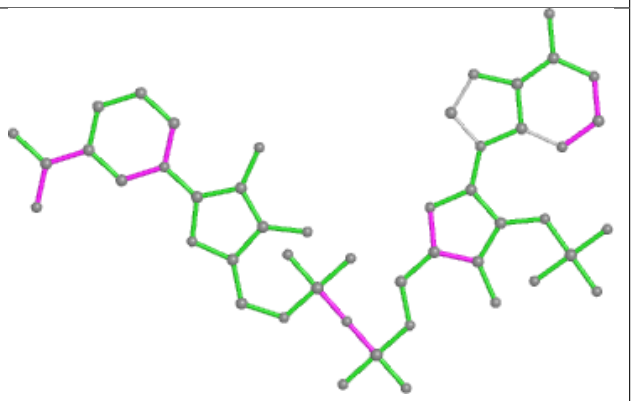


Rings

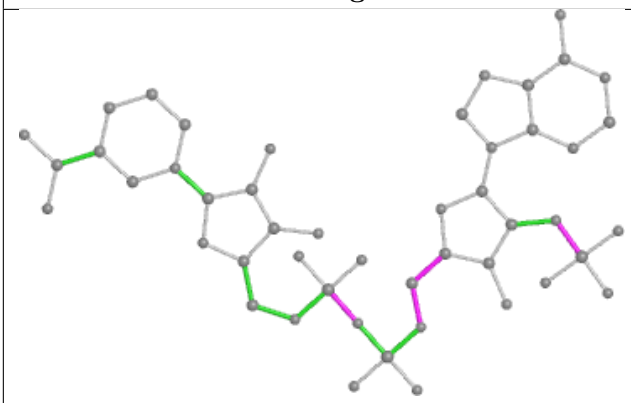
Ligand NAP I 400



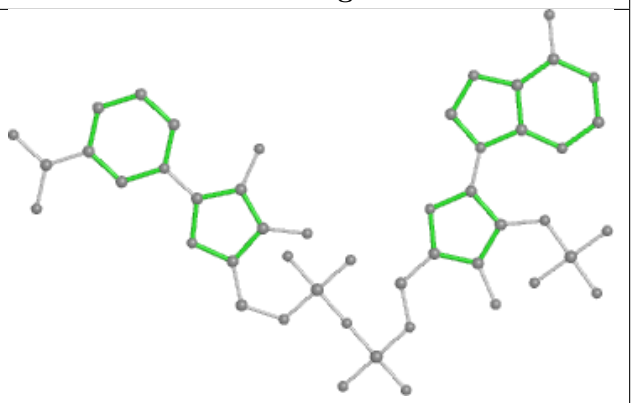
Bond lengths



Bond angles

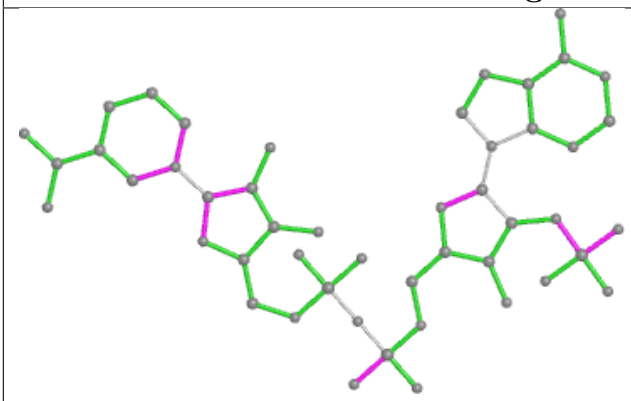


Torsions

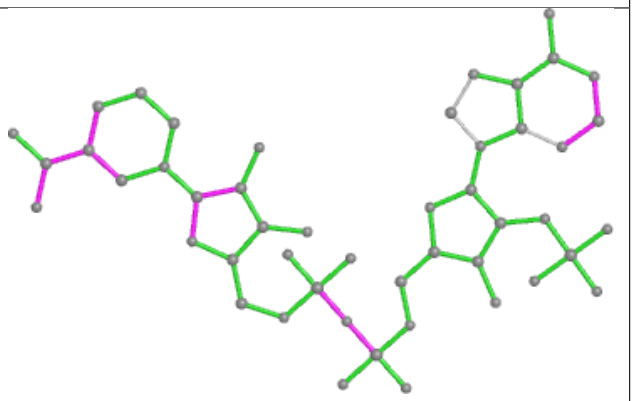


Rings

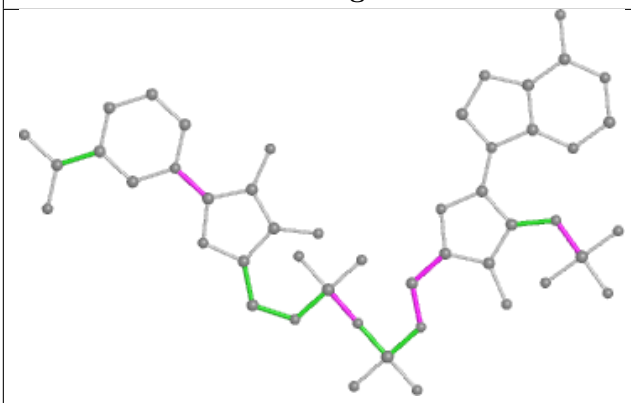
Ligand NAP J 400



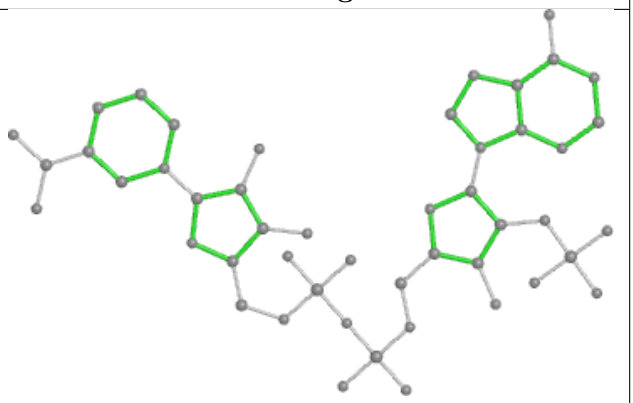
Bond lengths



Bond angles

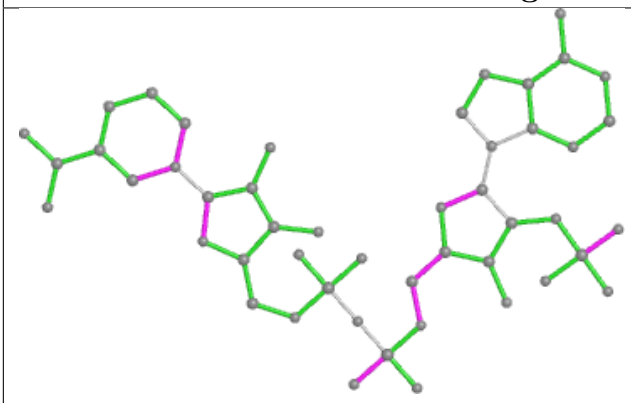


Torsions

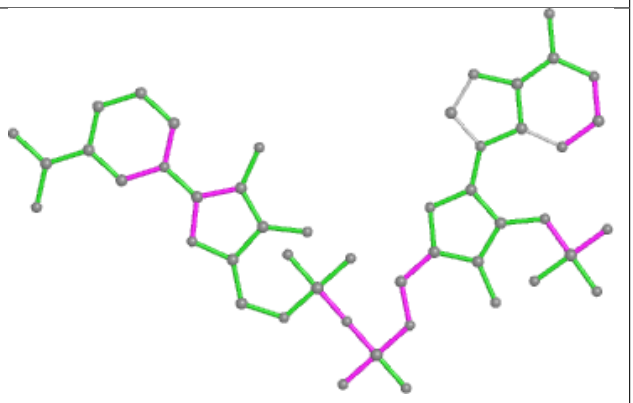


Rings

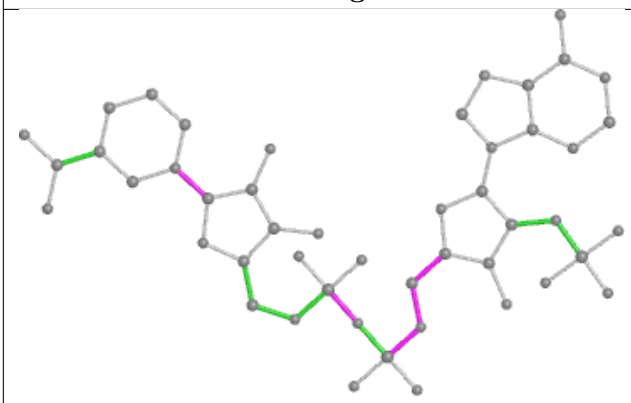
Ligand NAP D 400



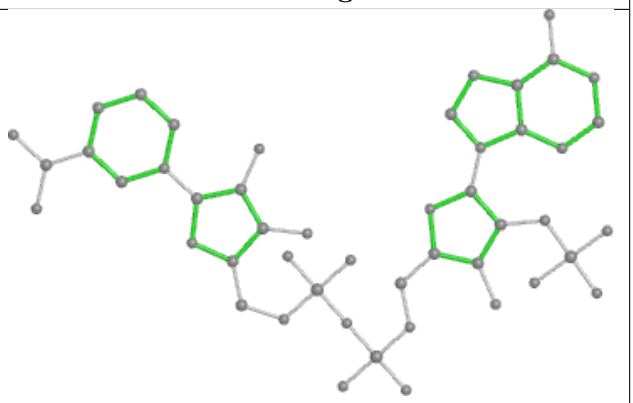
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	329/336 (97%)	-0.15	2 (0%) 89 88	14, 23, 42, 62	0
1	B	331/336 (98%)	-0.10	1 (0%) 94 93	20, 33, 51, 61	0
1	C	325/336 (96%)	0.47	21 (6%) 18 17	23, 45, 79, 98	0
1	D	327/336 (97%)	0.25	22 (6%) 17 16	20, 33, 83, 109	0
1	E	331/336 (98%)	-0.00	9 (2%) 54 52	14, 26, 55, 87	0
1	F	331/336 (98%)	0.06	16 (4%) 30 29	25, 37, 59, 77	0
1	G	321/336 (95%)	0.52	39 (12%) 4 3	23, 43, 96, 120	0
1	H	327/336 (97%)	0.34	14 (4%) 35 33	27, 49, 69, 92	0
1	I	234/336 (69%)	1.49	75 (32%) 0 0	31, 63, 122, 140	0
1	J	327/336 (97%)	0.36	24 (7%) 15 14	25, 47, 81, 109	0
1	K	302/336 (89%)	0.92	53 (17%) 1 1	27, 55, 91, 112	0
1	L	320/336 (95%)	0.54	27 (8%) 11 9	27, 47, 77, 105	0
All	All	3805/4032 (94%)	0.36	303 (7%) 12 11	14, 40, 84, 140	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	315	PRO	11.9
1	K	5	ILE	9.1
1	I	312	GLU	7.8
1	D	16	SER	7.5
1	J	21	ARG	7.3
1	G	321	LEU	7.3
1	I	318	LEU	7.1
1	J	182	ALA	7.1
1	I	307	ILE	6.9
1	K	256	ALA	6.8
1	I	117	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	I	319	LEU	6.5
1	I	327	PHE	6.5
1	I	310	GLY	6.4
1	G	24	PHE	6.3
1	I	114	VAL	6.2
1	I	116	PRO	6.1
1	I	308	VAL	6.0
1	G	57	ASN	5.9
1	K	22	ASP	5.9
1	K	67	GLY	5.7
1	G	26	PHE	5.7
1	I	118	ARG	5.7
1	I	313	THR	5.7
1	G	254	LYS	5.6
1	D	58	ASP	5.5
1	G	58	ASP	5.4
1	G	319	LEU	5.4
1	G	64	PRO	5.3
1	G	59	ALA	5.2
1	I	122	PRO	5.2
1	I	316	GLU	5.1
1	K	16	SER	5.1
1	G	12	ALA	5.1
1	G	322	PHE	5.1
1	D	319	LEU	5.0
1	I	111	PHE	5.0
1	I	331	VAL	5.0
1	I	317	THR	5.0
1	K	68	ILE	4.9
1	K	18	LEU	4.9
1	K	26	PHE	4.8
1	J	19	PRO	4.8
1	L	68	ILE	4.8
1	I	325	GLU	4.8
1	K	66	VAL	4.7
1	H	16	SER	4.7
1	C	58	ASP	4.7
1	C	67	GLY	4.7
1	J	181	GLY	4.6
1	K	11	LEU	4.6
1	K	105	ILE	4.6
1	I	330	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	16	SER	4.6
1	G	255	GLU	4.6
1	J	18	LEU	4.6
1	I	295	TRP	4.5
1	I	320	LYS	4.5
1	G	327	PHE	4.4
1	C	31	LEU	4.4
1	I	124	TYR	4.4
1	C	39	ILE	4.3
1	I	300	LYS	4.3
1	I	180	GLY	4.3
1	I	297	ALA	4.3
1	I	332	LEU	4.3
1	C	254	LYS	4.2
1	J	24	PHE	4.2
1	I	123	ARG	4.2
1	I	186	ARG	4.2
1	L	66	VAL	4.2
1	I	314	PHE	4.2
1	I	121	LEU	4.1
1	C	68	ILE	4.1
1	I	191	GLU	4.1
1	K	17	GLY	4.1
1	D	59	ALA	4.0
1	I	120	PRO	4.0
1	D	22	ASP	4.0
1	I	309	GLU	4.0
1	K	27	VAL	4.0
1	E	58	ASP	3.9
1	K	58	ASP	3.9
1	I	301	LEU	3.9
1	I	257	VAL	3.9
1	J	252	ASN	3.9
1	H	297	ALA	3.9
1	J	256	ALA	3.9
1	K	24	PHE	3.9
1	I	311	LEU	3.9
1	C	25	SER	3.9
1	L	37	GLY	3.8
1	G	60	ARG	3.8
1	K	13	GLN	3.8
1	I	113	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	66	VAL	3.7
1	E	16	SER	3.7
1	D	13	GLN	3.7
1	L	59	ALA	3.6
1	C	30	PRO	3.6
1	I	157	ALA	3.6
1	D	324	GLY	3.6
1	D	57	ASN	3.6
1	J	253	ASN	3.6
1	I	192	LEU	3.5
1	G	67	GLY	3.5
1	G	66	VAL	3.5
1	K	69	GLY	3.4
1	K	193	GLY	3.4
1	C	56	MET	3.4
1	G	11	LEU	3.4
1	L	33	GLU	3.4
1	I	202	ASN	3.4
1	F	180	GLY	3.4
1	L	22	ASP	3.4
1	K	324	GLY	3.3
1	L	67	GLY	3.3
1	I	304	ARG	3.3
1	G	316	GLU	3.3
1	I	55	TRP	3.3
1	I	119	ALA	3.3
1	C	71	VAL	3.3
1	K	19	PRO	3.2
1	C	9	TYR	3.2
1	C	16	SER	3.2
1	K	14	ARG	3.2
1	K	6	ASN	3.2
1	G	186	ARG	3.2
1	C	255	GLU	3.2
1	I	288	GLY	3.2
1	K	190	GLU	3.2
1	C	13	GLN	3.2
1	K	12	ALA	3.2
1	D	60	ARG	3.2
1	H	300	LYS	3.2
1	H	298	GLU	3.1
1	K	29	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	325	GLU	3.1
1	D	21	ARG	3.1
1	F	212	GLU	3.1
1	L	13	GLN	3.1
1	K	71	VAL	3.1
1	G	53	ARG	3.1
1	J	22	ASP	3.1
1	K	56	MET	3.1
1	K	20	GLY	3.1
1	I	98	LEU	3.0
1	I	188	LEU	3.0
1	D	15	PRO	3.0
1	H	256	ALA	3.0
1	K	231	THR	3.0
1	L	58	ASP	3.0
1	L	247	ALA	3.0
1	F	60	ARG	3.0
1	D	18	LEU	3.0
1	J	20	GLY	3.0
1	H	24	PHE	3.0
1	E	253	ASN	3.0
1	G	326	ASN	3.0
1	I	56	MET	2.9
1	I	321	LEU	2.9
1	K	202	ASN	2.9
1	C	41	VAL	2.9
1	J	58	ASP	2.9
1	E	254	LYS	2.9
1	F	202	ASN	2.9
1	I	99	GLY	2.9
1	I	287	GLU	2.9
1	C	26	PHE	2.9
1	I	294	THR	2.8
1	F	215	LYS	2.8
1	I	183	GLU	2.8
1	K	9	TYR	2.8
1	K	4	GLN	2.8
1	C	22	ASP	2.8
1	G	70	GLU	2.8
1	H	187	PHE	2.8
1	K	254	LYS	2.8
1	K	59	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	235	ARG	2.8
1	K	82	VAL	2.7
1	L	60	ARG	2.7
1	I	251	TYR	2.7
1	C	69	GLY	2.7
1	I	303	SER	2.7
1	L	36	GLU	2.7
1	E	60	ARG	2.7
1	I	302	GLN	2.7
1	I	299	GLY	2.7
1	L	63	ILE	2.7
1	I	115	ASP	2.7
1	I	326	ASN	2.7
1	C	210	LYS	2.6
1	F	190	GLU	2.6
1	K	198	ILE	2.6
1	K	23	THR	2.6
1	K	157	ALA	2.6
1	I	323	SER	2.6
1	I	48	LEU	2.6
1	K	187	PHE	2.6
1	H	294	THR	2.6
1	J	186	ARG	2.6
1	K	15	PRO	2.6
1	K	255	GLU	2.6
1	K	60	ARG	2.5
1	G	308	VAL	2.5
1	H	308	VAL	2.5
1	I	100	VAL	2.5
1	G	9	TYR	2.5
1	D	68	ILE	2.5
1	K	191	GLU	2.5
1	G	27	VAL	2.5
1	J	322	PHE	2.5
1	E	63	ILE	2.5
1	G	5	ILE	2.5
1	K	70	GLU	2.5
1	H	11	LEU	2.5
1	E	64	PRO	2.5
1	G	68	ILE	2.5
1	D	322	PHE	2.4
1	I	125	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	56	MET	2.4
1	L	89	GLN	2.4
1	F	30	PRO	2.4
1	I	169	ARG	2.4
1	E	319	LEU	2.4
1	G	325	GLU	2.4
1	L	107	GLU	2.4
1	G	252	ASN	2.3
1	H	21	ARG	2.3
1	G	50	PRO	2.3
1	G	330	LEU	2.3
1	L	35	ALA	2.3
1	J	17	GLY	2.3
1	D	19	PRO	2.3
1	D	12	ALA	2.3
1	I	112	TYR	2.3
1	F	191	GLU	2.3
1	G	25	SER	2.3
1	J	56	MET	2.3
1	J	183	GLU	2.3
1	J	67	GLY	2.3
1	I	322	PHE	2.3
1	L	19	PRO	2.3
1	F	5	ILE	2.3
1	G	317	THR	2.3
1	D	251	TYR	2.3
1	K	257	VAL	2.3
1	J	13	GLN	2.3
1	K	8	GLN	2.3
1	F	213	CYS	2.2
1	G	315	PRO	2.2
1	F	16	SER	2.2
1	H	117	SER	2.2
1	I	258	ARG	2.2
1	L	55	TRP	2.2
1	I	181	GLY	2.2
1	L	20	GLY	2.2
1	F	192	LEU	2.2
1	L	90	ALA	2.2
1	I	248	ILE	2.2
1	J	33	GLU	2.2
1	I	128	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	40	LEU	2.2
1	F	175	VAL	2.2
1	I	189	VAL	2.2
1	K	189	VAL	2.2
1	L	203	GLU	2.2
1	A	21	ARG	2.2
1	H	255	GLU	2.2
1	C	59	ALA	2.2
1	I	97	ALA	2.2
1	L	31	LEU	2.2
1	C	312	GLU	2.1
1	I	296	LEU	2.1
1	F	204	ASP	2.1
1	G	201	LYS	2.1
1	K	25	SER	2.1
1	J	53	ARG	2.1
1	F	327	PHE	2.1
1	I	51	ALA	2.1
1	J	325	GLU	2.1
1	K	107	GLU	2.1
1	K	199	ASP	2.1
1	K	252	ASN	2.1
1	D	323	SER	2.1
1	I	126	SER	2.1
1	L	226	GLY	2.1
1	G	30	PRO	2.1
1	G	324	GLY	2.0
1	G	28	GLU	2.0
1	L	70	GLU	2.0
1	B	189	VAL	2.0
1	K	106	GLY	2.0
1	H	22	ASP	2.0
1	J	257	VAL	2.0
1	D	26	PHE	2.0
1	L	26	PHE	2.0
1	L	88	PHE	2.0
1	E	251	TYR	2.0
1	D	69	GLY	2.0
1	A	60	ARG	2.0
1	G	118	ARG	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)

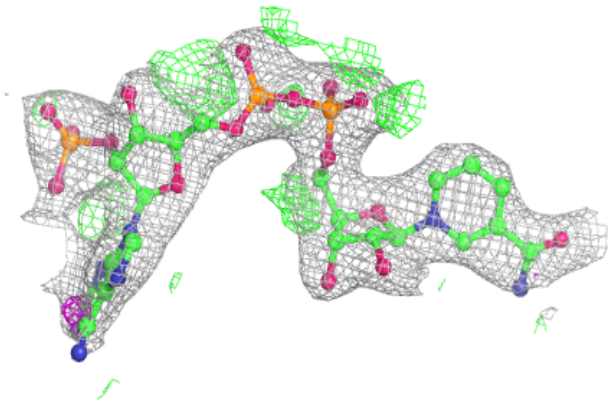
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

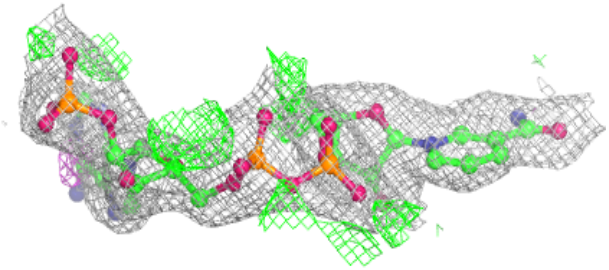
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	L	400	48/48	0.90	0.18	35,48,63,65	0
2	NAP	K	400	48/48	0.92	0.14	38,49,60,61	0
2	NAP	I	400	48/48	0.92	0.14	47,59,65,70	0
2	NAP	G	400	48/48	0.95	0.15	30,48,64,71	0
2	NAP	C	400	48/48	0.95	0.12	25,36,40,44	0
2	NAP	J	400	48/48	0.95	0.13	30,48,58,61	0
2	NAP	D	400	48/48	0.95	0.13	28,35,51,53	0
2	NAP	F	400	48/48	0.95	0.12	26,31,38,40	0
2	NAP	E	400	48/48	0.96	0.13	19,32,38,40	0
2	NAP	H	400	48/48	0.96	0.11	33,40,43,46	0
2	NAP	B	400	48/48	0.96	0.11	25,30,33,34	0
2	NAP	A	400	48/48	0.97	0.11	15,21,26,26	0

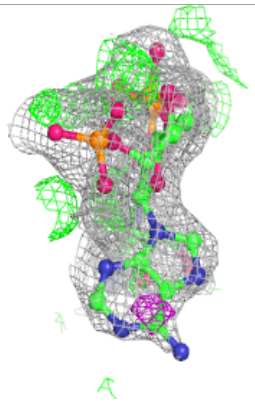
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP L 400:

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

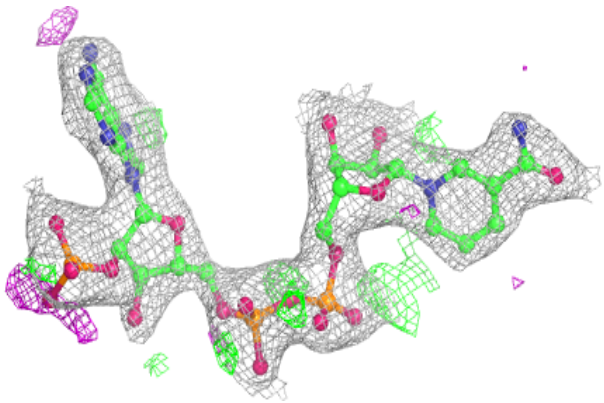


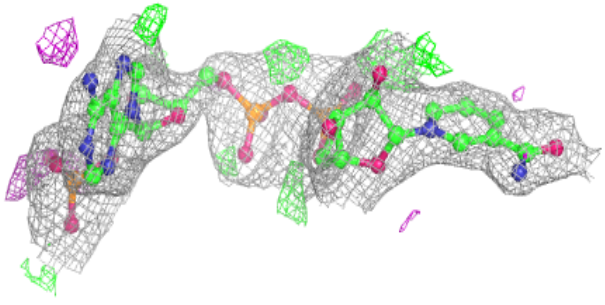


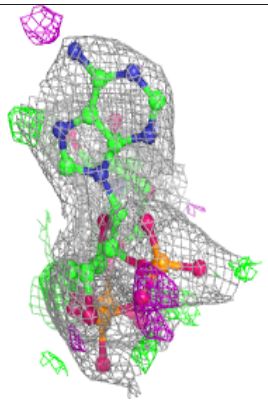


Electron density around NAP K 400:

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

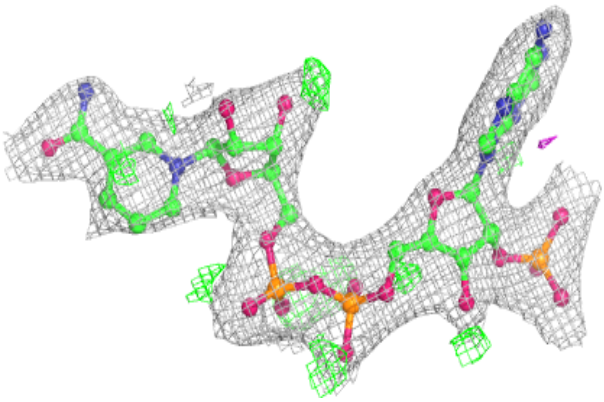


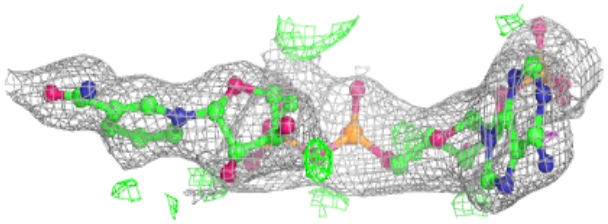


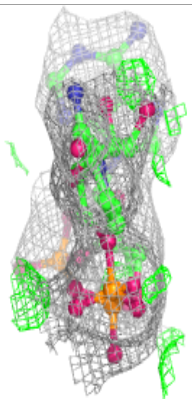


Electron density around NAP I 400:

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

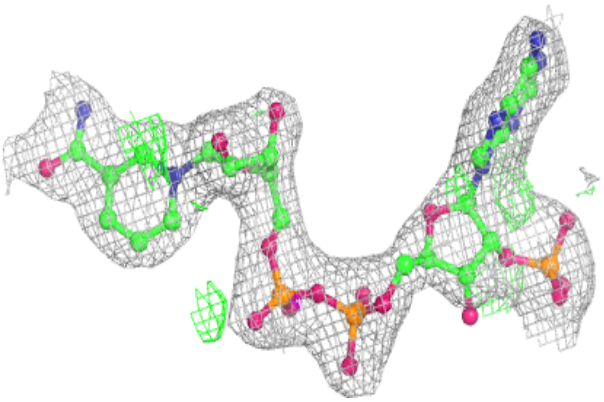


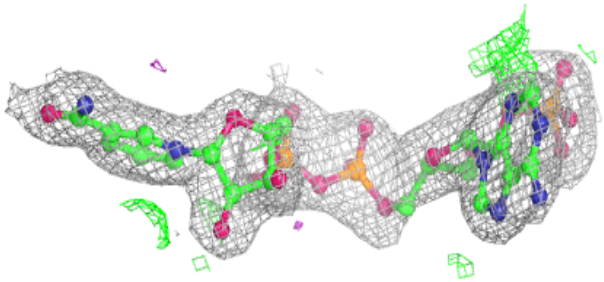


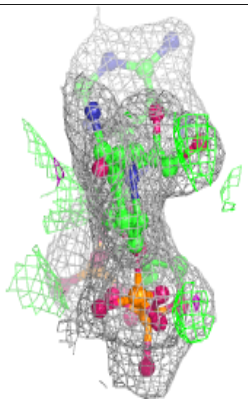


Electron density around NAP G 400:

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

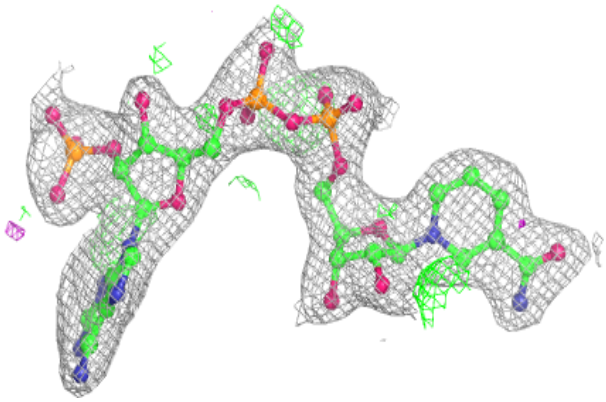


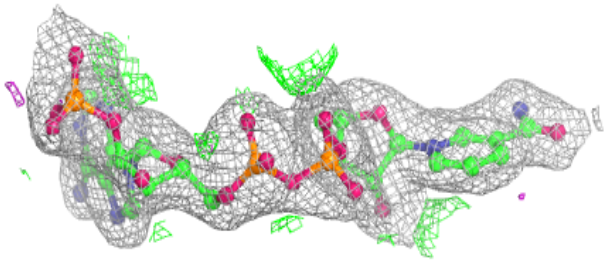


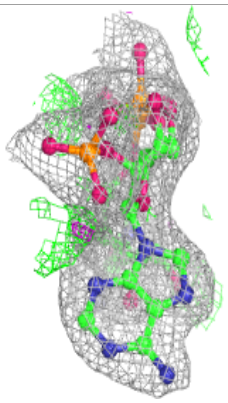


Electron density around NAP C 400:

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

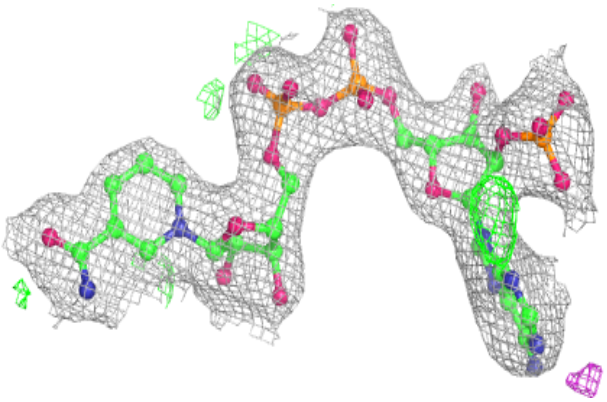


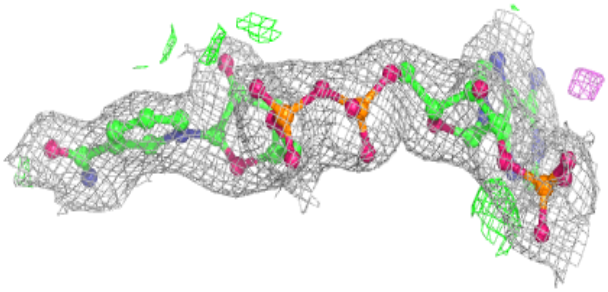


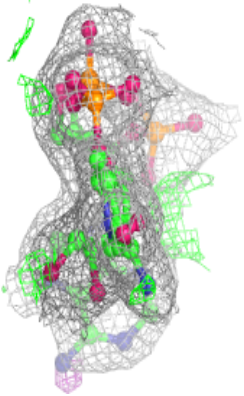


Electron density around NAP J 400:

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

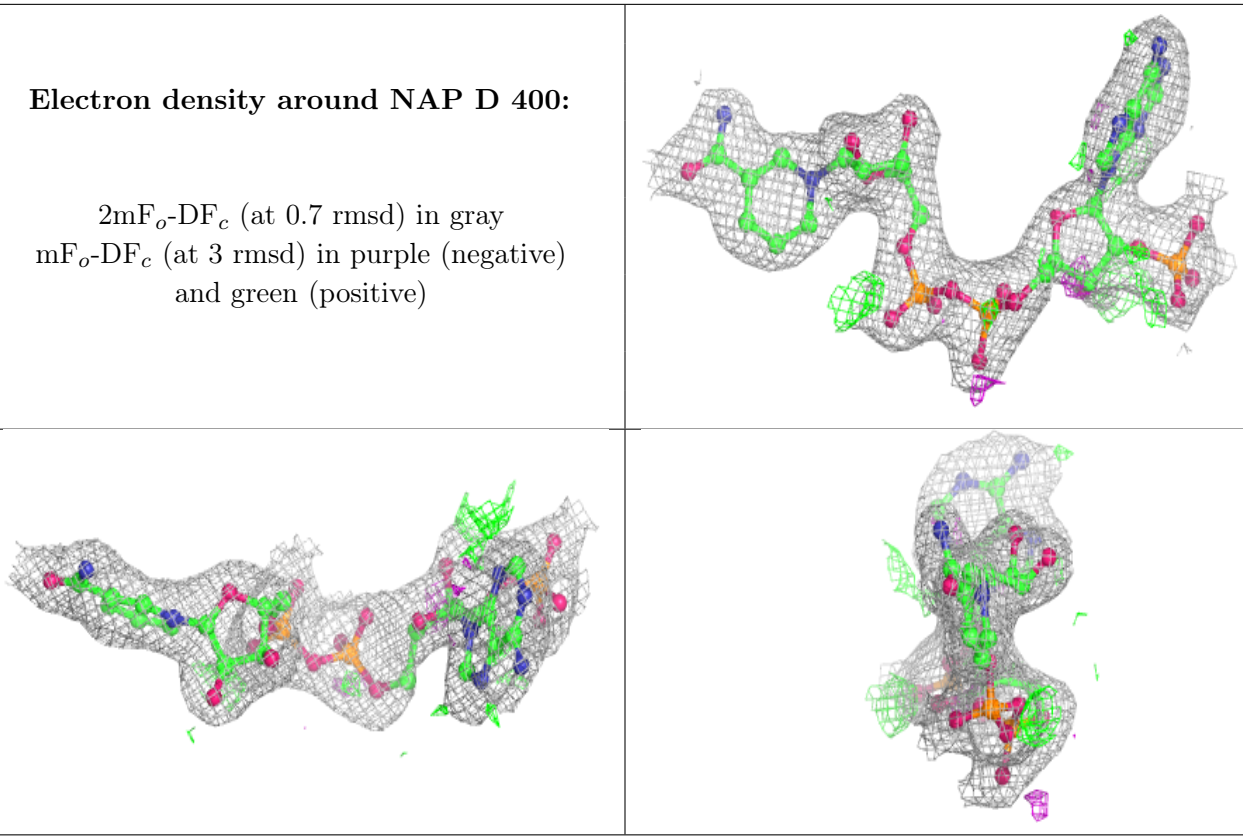






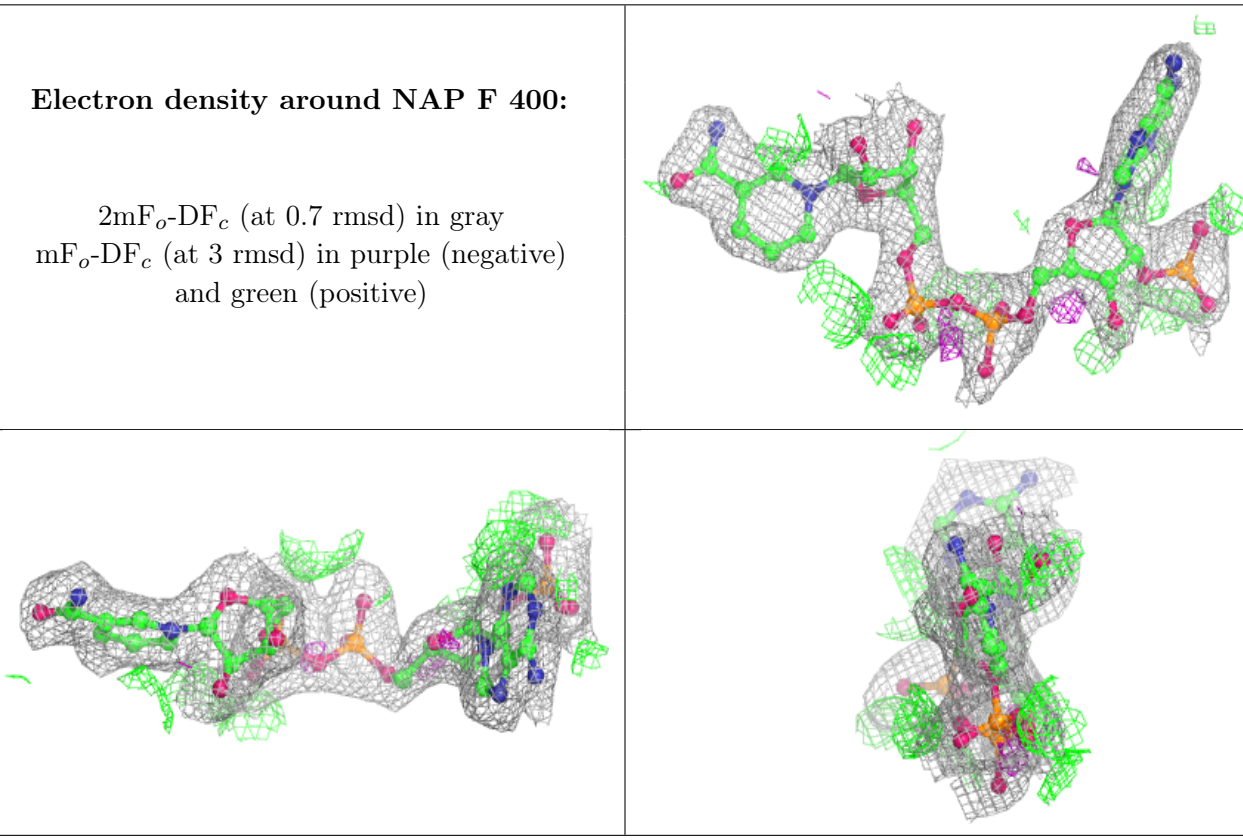
Electron density around NAP D 400:

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



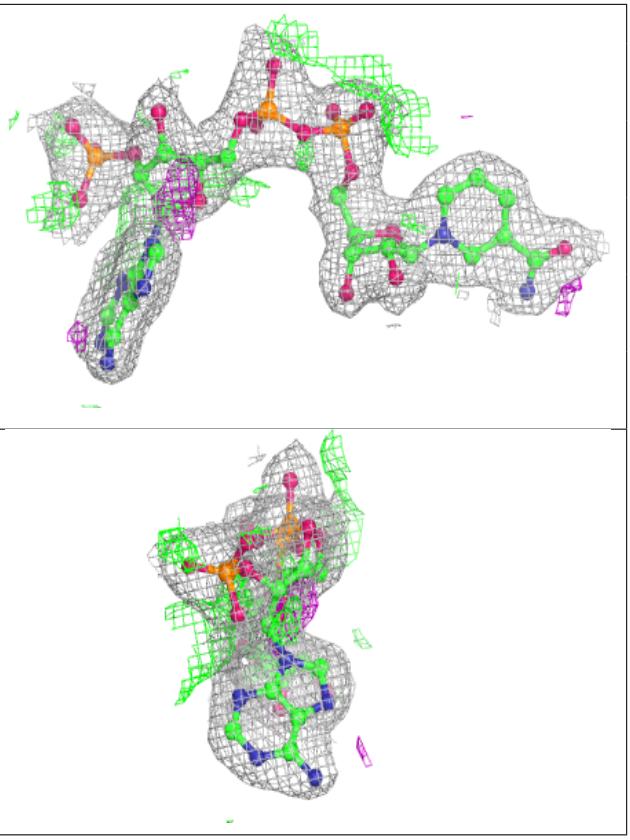
Electron density around NAP F 400:

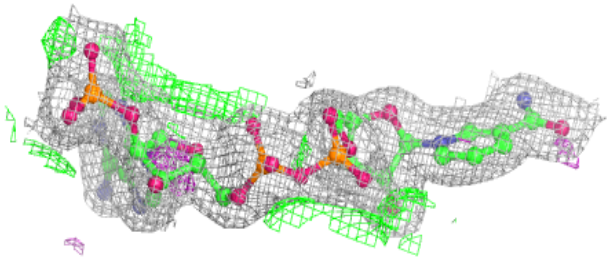
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP E 400:

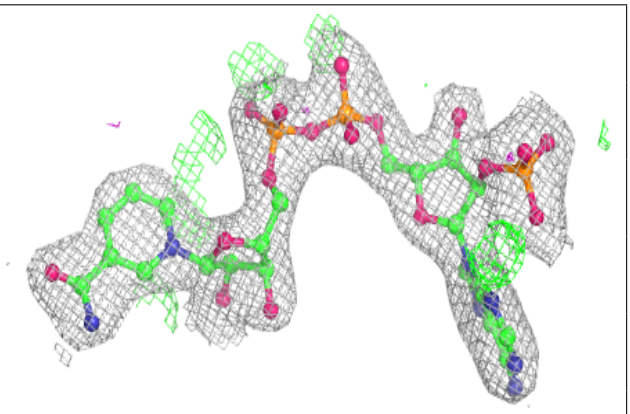
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

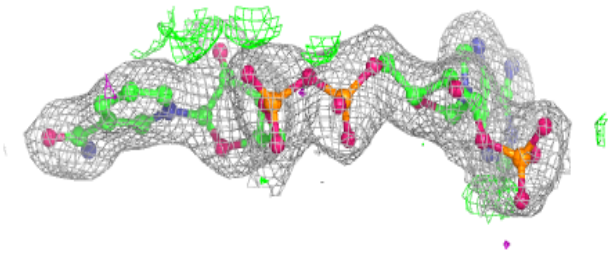


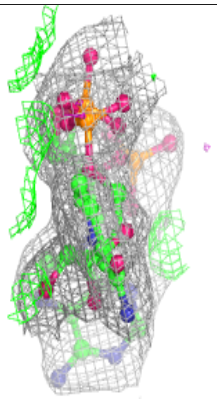


Electron density around NAP H 400:

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

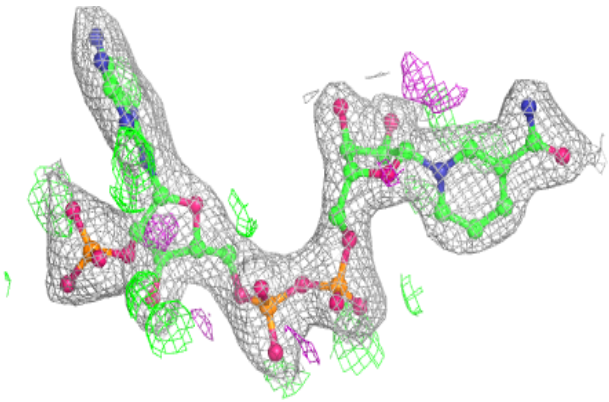


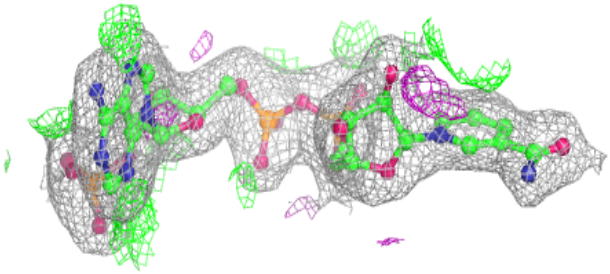


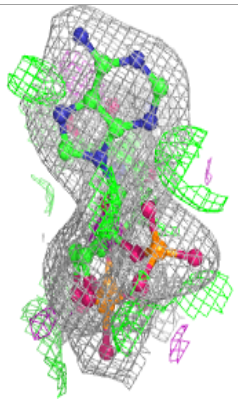


Electron density around NAP B 400:

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

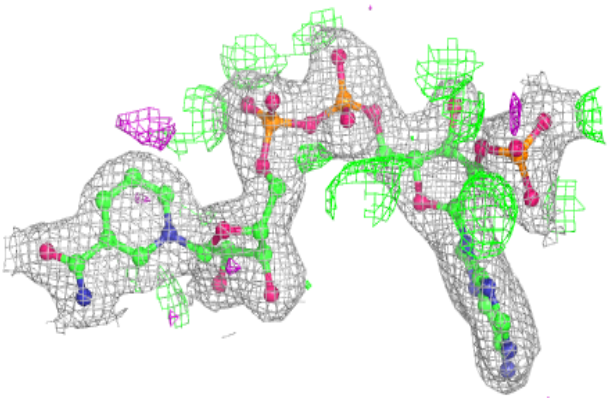


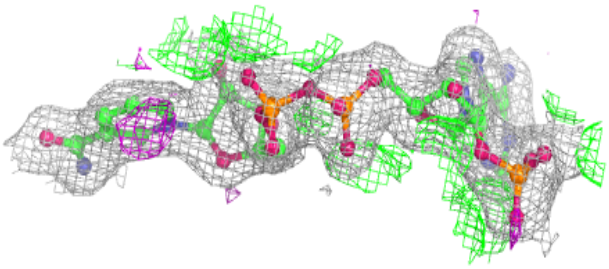


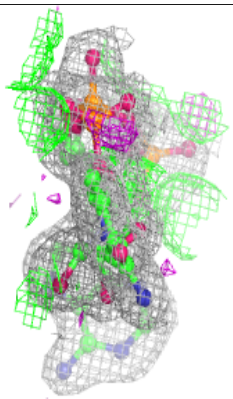


Electron density around NAP A 400:

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







6.5 Other polymers (i)

There are no such residues in this entry.