Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 04:31 AM EDT

PDB ID	:	4EJ0
Title	:	Crystal structure of ADP-L-glycero-D-manno-heptose-6-epimerase from Burkholderia thailandensis
Authors	:	Kim, M.S.; Shin, D.H.
Deposited on	:	2012-04-06
Resolution	:	2.61 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:

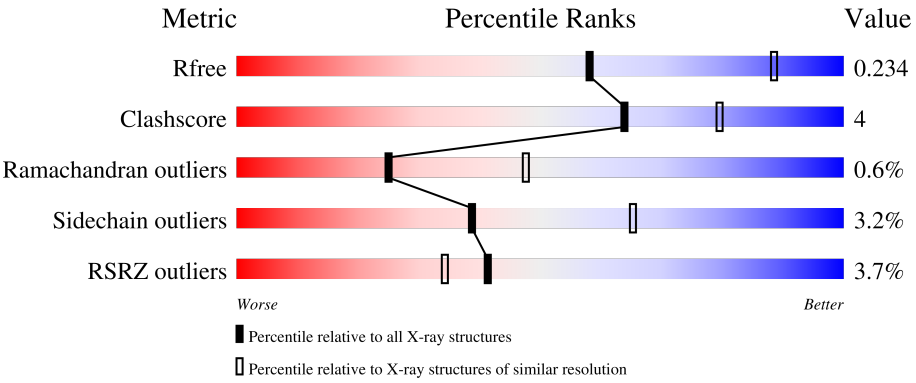
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.61 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	342	85% 11%
1	B	342	15% 75% 20%
1	C	342	3% 83% 13%
1	D	342	2% 86% 10%
1	E	342	87% 9%

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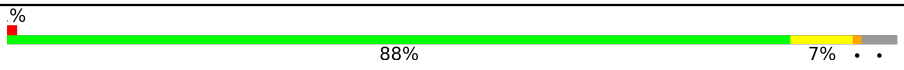
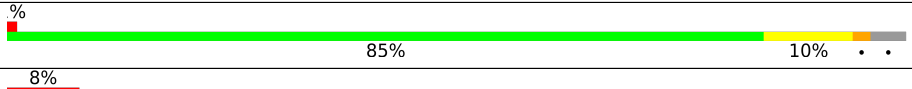
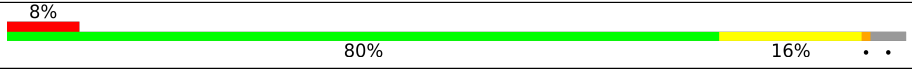
Mol	Chain	Length	Quality of chain
1	F	342	
1	G	342	
1	H	342	
1	I	342	
1	J	342	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27040 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 ADP-L-glycero-D-manno-heptose-6-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2611	1659	454	488	10			
1	B	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	C	330	Total	C	N	O	S	0	0	0
			2611	1659	454	488	10			
1	D	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	E	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	F	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	G	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	H	330	Total	C	N	O	S	0	0	0
			2611	1659	454	488	10			
1	I	330	Total	C	N	O	S	0	0	0
			2610	1659	454	487	10			
1	J	330	Total	C	N	O	S	0	0	0
			2611	1659	454	488	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q2SY18
A	-10	HIS	-	expression tag	UNP Q2SY18
A	-9	HIS	-	expression tag	UNP Q2SY18
A	-8	HIS	-	expression tag	UNP Q2SY18
A	-7	HIS	-	expression tag	UNP Q2SY18
A	-6	HIS	-	expression tag	UNP Q2SY18
A	-5	HIS	-	expression tag	UNP Q2SY18
A	-4	GLY	-	expression tag	UNP Q2SY18
A	-3	GLY	-	expression tag	UNP Q2SY18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q2SY18
A	-1	GLY	-	expression tag	UNP Q2SY18
A	0	GLY	-	expression tag	UNP Q2SY18
B	-11	MET	-	expression tag	UNP Q2SY18
B	-10	HIS	-	expression tag	UNP Q2SY18
B	-9	HIS	-	expression tag	UNP Q2SY18
B	-8	HIS	-	expression tag	UNP Q2SY18
B	-7	HIS	-	expression tag	UNP Q2SY18
B	-6	HIS	-	expression tag	UNP Q2SY18
B	-5	HIS	-	expression tag	UNP Q2SY18
B	-4	GLY	-	expression tag	UNP Q2SY18
B	-3	GLY	-	expression tag	UNP Q2SY18
B	-2	GLY	-	expression tag	UNP Q2SY18
B	-1	GLY	-	expression tag	UNP Q2SY18
B	0	GLY	-	expression tag	UNP Q2SY18
C	-11	MET	-	expression tag	UNP Q2SY18
C	-10	HIS	-	expression tag	UNP Q2SY18
C	-9	HIS	-	expression tag	UNP Q2SY18
C	-8	HIS	-	expression tag	UNP Q2SY18
C	-7	HIS	-	expression tag	UNP Q2SY18
C	-6	HIS	-	expression tag	UNP Q2SY18
C	-5	HIS	-	expression tag	UNP Q2SY18
C	-4	GLY	-	expression tag	UNP Q2SY18
C	-3	GLY	-	expression tag	UNP Q2SY18
C	-2	GLY	-	expression tag	UNP Q2SY18
C	-1	GLY	-	expression tag	UNP Q2SY18
C	0	GLY	-	expression tag	UNP Q2SY18
D	-11	MET	-	expression tag	UNP Q2SY18
D	-10	HIS	-	expression tag	UNP Q2SY18
D	-9	HIS	-	expression tag	UNP Q2SY18
D	-8	HIS	-	expression tag	UNP Q2SY18
D	-7	HIS	-	expression tag	UNP Q2SY18
D	-6	HIS	-	expression tag	UNP Q2SY18
D	-5	HIS	-	expression tag	UNP Q2SY18
D	-4	GLY	-	expression tag	UNP Q2SY18
D	-3	GLY	-	expression tag	UNP Q2SY18
D	-2	GLY	-	expression tag	UNP Q2SY18
D	-1	GLY	-	expression tag	UNP Q2SY18
D	0	GLY	-	expression tag	UNP Q2SY18
E	-11	MET	-	expression tag	UNP Q2SY18
E	-10	HIS	-	expression tag	UNP Q2SY18
E	-9	HIS	-	expression tag	UNP Q2SY18

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	HIS	-	expression tag	UNP Q2SY18
E	-7	HIS	-	expression tag	UNP Q2SY18
E	-6	HIS	-	expression tag	UNP Q2SY18
E	-5	HIS	-	expression tag	UNP Q2SY18
E	-4	GLY	-	expression tag	UNP Q2SY18
E	-3	GLY	-	expression tag	UNP Q2SY18
E	-2	GLY	-	expression tag	UNP Q2SY18
E	-1	GLY	-	expression tag	UNP Q2SY18
E	0	GLY	-	expression tag	UNP Q2SY18
F	-11	MET	-	expression tag	UNP Q2SY18
F	-10	HIS	-	expression tag	UNP Q2SY18
F	-9	HIS	-	expression tag	UNP Q2SY18
F	-8	HIS	-	expression tag	UNP Q2SY18
F	-7	HIS	-	expression tag	UNP Q2SY18
F	-6	HIS	-	expression tag	UNP Q2SY18
F	-5	HIS	-	expression tag	UNP Q2SY18
F	-4	GLY	-	expression tag	UNP Q2SY18
F	-3	GLY	-	expression tag	UNP Q2SY18
F	-2	GLY	-	expression tag	UNP Q2SY18
F	-1	GLY	-	expression tag	UNP Q2SY18
F	0	GLY	-	expression tag	UNP Q2SY18
G	-11	MET	-	expression tag	UNP Q2SY18
G	-10	HIS	-	expression tag	UNP Q2SY18
G	-9	HIS	-	expression tag	UNP Q2SY18
G	-8	HIS	-	expression tag	UNP Q2SY18
G	-7	HIS	-	expression tag	UNP Q2SY18
G	-6	HIS	-	expression tag	UNP Q2SY18
G	-5	HIS	-	expression tag	UNP Q2SY18
G	-4	GLY	-	expression tag	UNP Q2SY18
G	-3	GLY	-	expression tag	UNP Q2SY18
G	-2	GLY	-	expression tag	UNP Q2SY18
G	-1	GLY	-	expression tag	UNP Q2SY18
G	0	GLY	-	expression tag	UNP Q2SY18
H	-11	MET	-	expression tag	UNP Q2SY18
H	-10	HIS	-	expression tag	UNP Q2SY18
H	-9	HIS	-	expression tag	UNP Q2SY18
H	-8	HIS	-	expression tag	UNP Q2SY18
H	-7	HIS	-	expression tag	UNP Q2SY18
H	-6	HIS	-	expression tag	UNP Q2SY18
H	-5	HIS	-	expression tag	UNP Q2SY18
H	-4	GLY	-	expression tag	UNP Q2SY18
H	-3	GLY	-	expression tag	UNP Q2SY18

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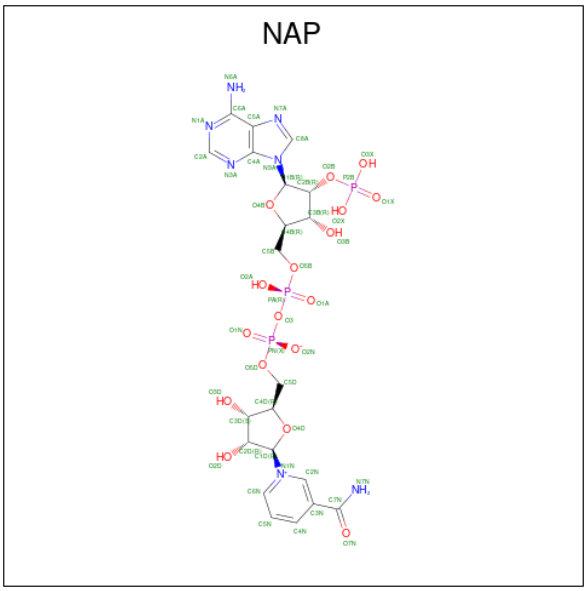
Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP Q2SY18
H	-1	GLY	-	expression tag	UNP Q2SY18
H	0	GLY	-	expression tag	UNP Q2SY18
I	-11	MET	-	expression tag	UNP Q2SY18
I	-10	HIS	-	expression tag	UNP Q2SY18
I	-9	HIS	-	expression tag	UNP Q2SY18
I	-8	HIS	-	expression tag	UNP Q2SY18
I	-7	HIS	-	expression tag	UNP Q2SY18
I	-6	HIS	-	expression tag	UNP Q2SY18
I	-5	HIS	-	expression tag	UNP Q2SY18
I	-4	GLY	-	expression tag	UNP Q2SY18
I	-3	GLY	-	expression tag	UNP Q2SY18
I	-2	GLY	-	expression tag	UNP Q2SY18
I	-1	GLY	-	expression tag	UNP Q2SY18
I	0	GLY	-	expression tag	UNP Q2SY18
J	-11	MET	-	expression tag	UNP Q2SY18
J	-10	HIS	-	expression tag	UNP Q2SY18
J	-9	HIS	-	expression tag	UNP Q2SY18
J	-8	HIS	-	expression tag	UNP Q2SY18
J	-7	HIS	-	expression tag	UNP Q2SY18
J	-6	HIS	-	expression tag	UNP Q2SY18
J	-5	HIS	-	expression tag	UNP Q2SY18
J	-4	GLY	-	expression tag	UNP Q2SY18
J	-3	GLY	-	expression tag	UNP Q2SY18
J	-2	GLY	-	expression tag	UNP Q2SY18
J	-1	GLY	-	expression tag	UNP Q2SY18
J	0	GLY	-	expression tag	UNP Q2SY18

- 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		
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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	18	Total	O	0	0
			18	18		

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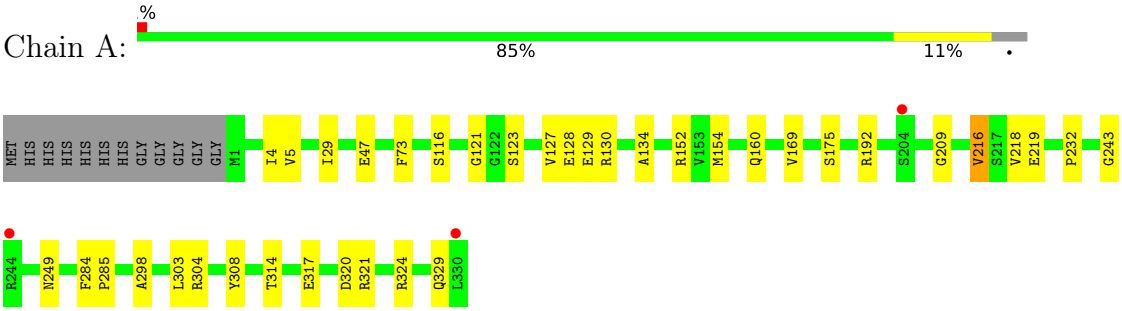
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	21	Total O 21 21	0	0
3	D	55	Total O 55 55	0	0
3	E	67	Total O 67 67	0	0
3	F	77	Total O 77 77	0	0
3	G	74	Total O 74 74	0	0
3	H	43	Total O 43 43	0	0
3	I	24	Total O 24 24	0	0
3	J	23	Total O 23 23	0	0

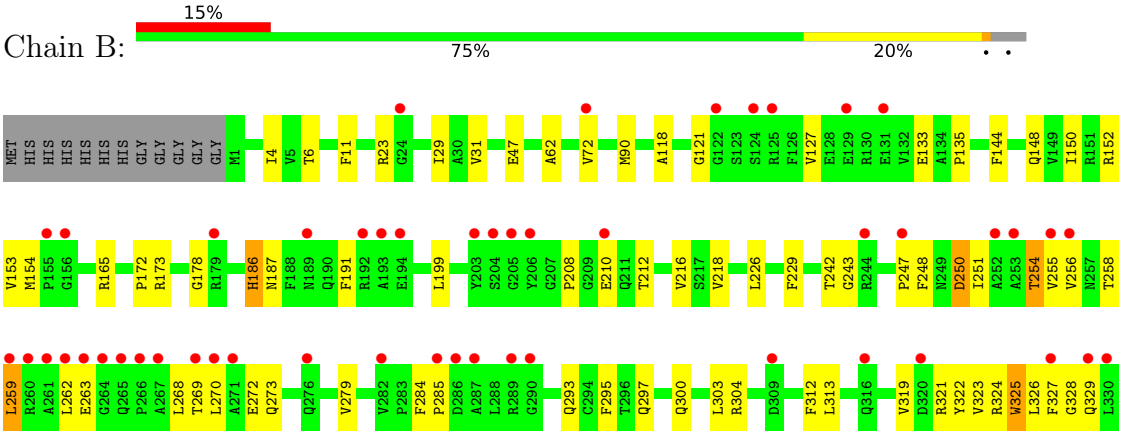
3 Residue-property plots (i)

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.

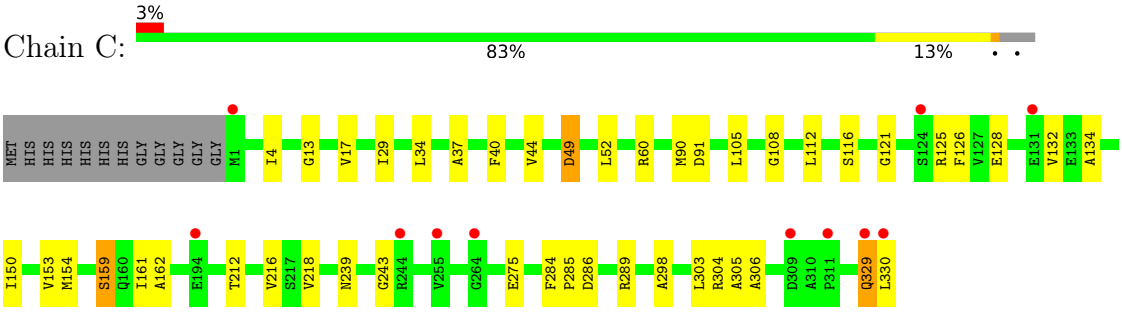
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase



• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

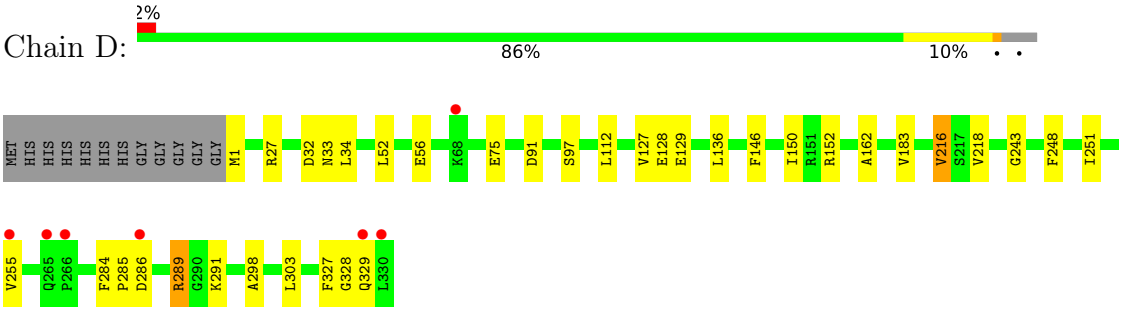


• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase



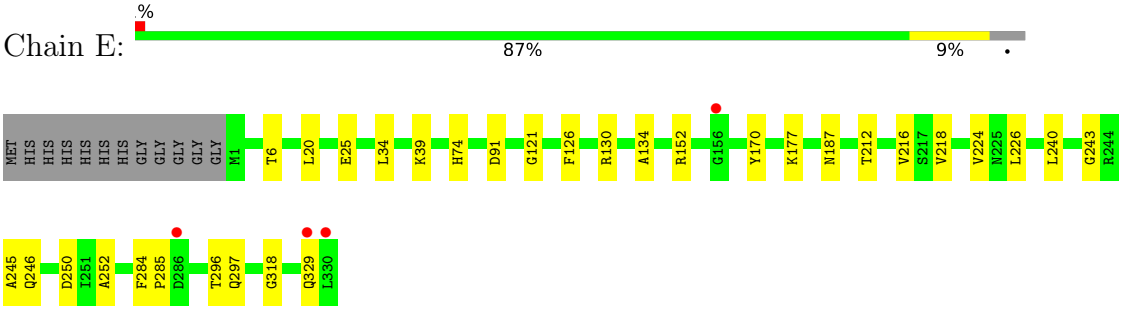
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

Chain D:



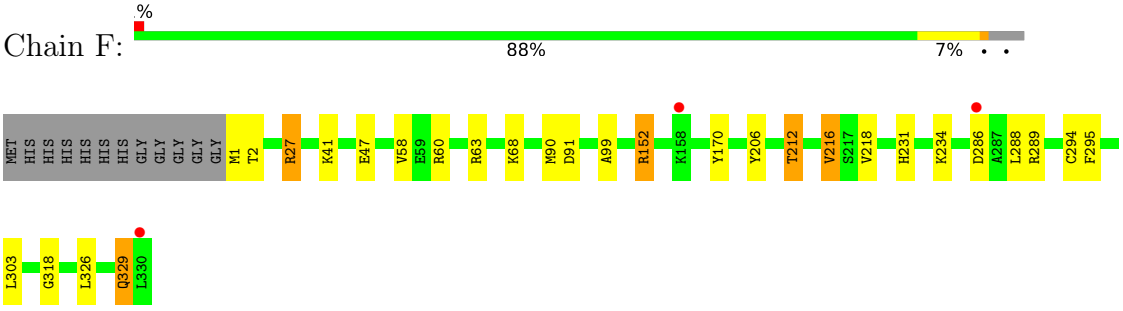
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

Chain E:



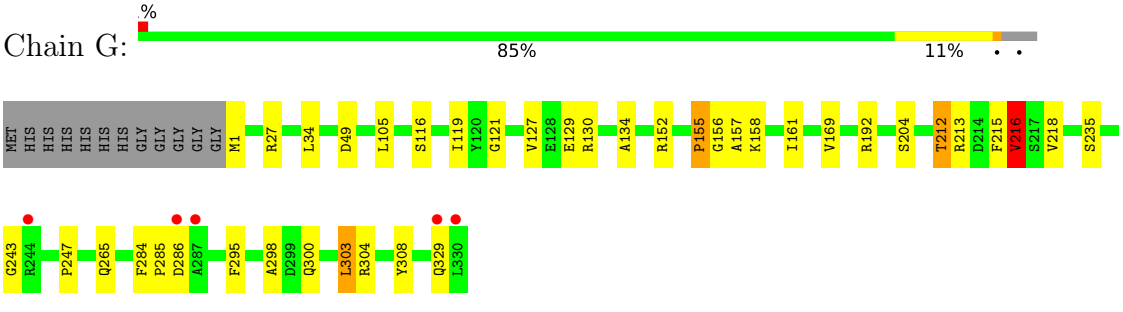
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

Chain F:



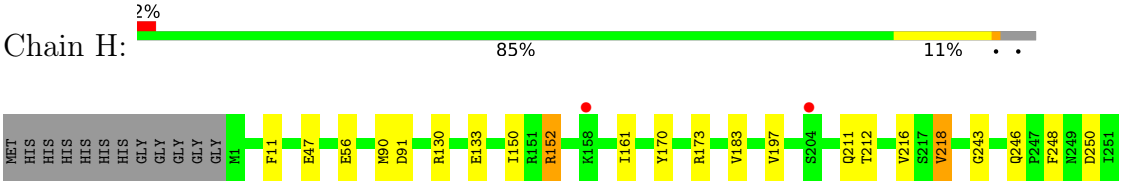
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

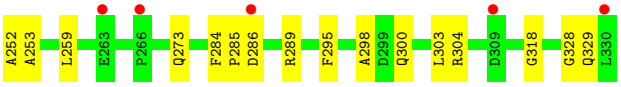
Chain G:



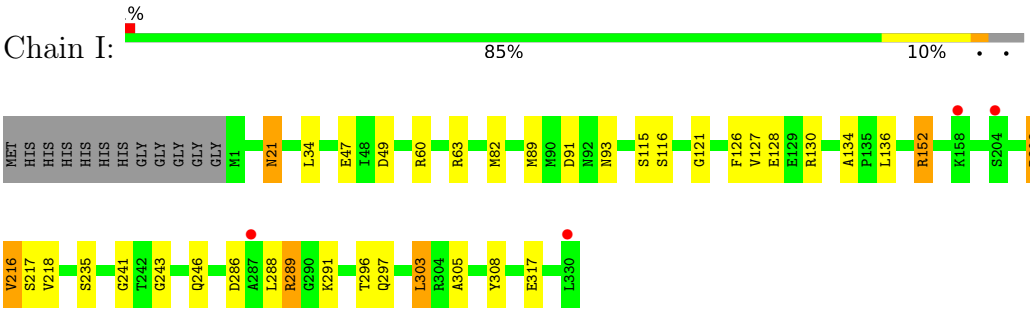
• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase

Chain H:

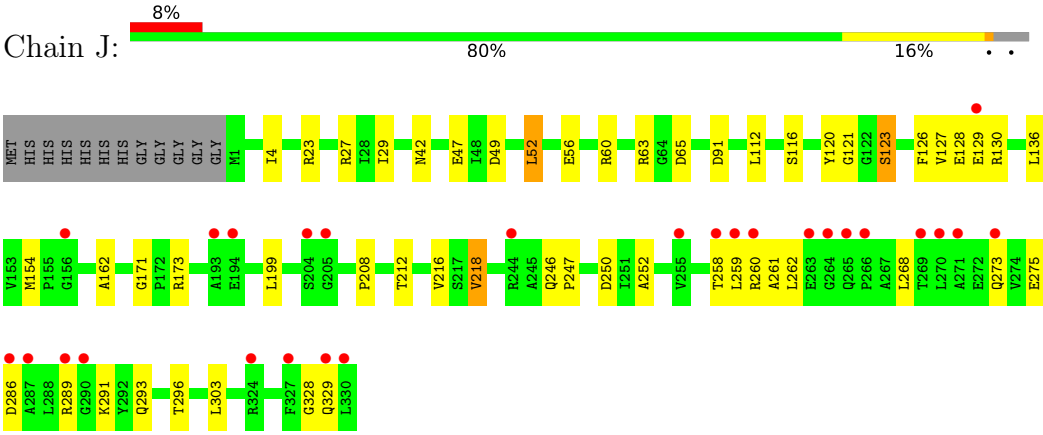




• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase



• Molecule 1: ADP-L-glycero-D-manno-heptose-6-epimerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	158.32Å 160.92Å 169.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.61 19.97 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.97-2.61) 99.8 (19.97-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.185 , 0.241 0.181 , 0.234	Depositor DCC
R_{free} test set	6600 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27040	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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	0.47	0/2668	0.56	0/3600
1	B	0.43	0/2667	0.54	0/3600
1	C	0.42	0/2668	0.56	0/3600
1	D	0.47	0/2667	0.57	1/3600 (0.0%)
1	E	0.48	0/2667	0.56	0/3600
1	F	0.49	0/2667	0.59	1/3600 (0.0%)
1	G	0.48	0/2667	0.60	1/3600 (0.0%)
1	H	0.46	0/2668	0.56	1/3600 (0.0%)
1	I	0.44	0/2667	0.55	0/3600
1	J	0.41	0/2668	0.54	0/3600
All	All	0.46	0/26674	0.56	4/36000 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	216	VAL	CB-CA-C	-5.61	100.74	111.40
1	H	218	VAL	CB-CA-C	-5.23	101.47	111.40
1	F	216	VAL	CB-CA-C	-5.06	101.79	111.40
1	D	216	VAL	CB-CA-C	-5.04	101.82	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2611	0	2528	16	0
1	B	2610	0	2528	53	0
1	C	2611	0	2528	23	0
1	D	2610	0	2528	18	0
1	E	2610	0	2528	15	0
1	F	2610	0	2528	17	0
1	G	2610	0	2528	22	0
1	H	2611	0	2528	19	0
1	I	2610	0	2528	19	0
1	J	2611	0	2528	31	0
2	A	48	0	24	1	0
2	B	48	0	24	0	0
2	C	48	0	24	1	0
2	D	48	0	24	0	0
2	E	48	0	24	0	0
2	F	48	0	24	0	0
2	G	48	0	24	0	0
2	H	48	0	24	0	0
2	I	48	0	24	0	0
2	J	48	0	24	1	0
3	A	54	0	0	0	0
3	B	18	0	0	7	0
3	C	21	0	0	0	0
3	D	55	0	0	2	0
3	E	67	0	0	0	0
3	F	77	0	0	3	0
3	G	74	0	0	1	0
3	H	43	0	0	0	0
3	I	24	0	0	0	0
3	J	23	0	0	2	0
All	All	27040	0	25520	216	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 (216) 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:150:ILE:O	3:B:514:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:N	3:F:532:HOH:O	2.19	0.74
1:B:212:THR:HA	1:B:247:PRO:HA	1.70	0.72
1:F:47:GLU:OE2	1:J:130:ARG:NE	2.19	0.71
1:J:52:LEU:HD21	1:J:60:ARG:HE	1.54	0.71
1:C:4:ILE:HG12	1:C:29:ILE:HB	1.74	0.70
1:H:286:ASP:HA	1:H:289:ARG:HG3	1.75	0.69
1:D:289:ARG:NH2	3:D:519:HOH:O	2.26	0.67
1:B:263:GLU:O	3:B:509:HOH:O	2.12	0.67
1:B:153:VAL:N	3:B:514:HOH:O	2.26	0.67
1:A:130:ARG:NE	1:B:47:GLU:OE2	2.28	0.67
1:J:260:ARG:NH2	3:J:522:HOH:O	2.28	0.65
1:B:263:GLU:OE2	3:B:517:HOH:O	2.14	0.65
1:J:127:VAL:O	1:J:129:GLU:N	2.28	0.65
1:D:1:MET:HG3	1:D:27:ARG:HD3	1.79	0.64
1:B:154:MET:N	3:B:514:HOH:O	2.17	0.63
1:B:268:LEU:HG	1:B:272:GLU:HB3	1.80	0.63
1:B:321:ARG:O	3:B:502:HOH:O	2.16	0.62
1:B:199:LEU:HD11	1:B:248:PHE:HB3	1.82	0.61
1:E:246:GLN:NE2	1:E:250:ASP:OD2	2.30	0.60
1:B:191:PHE:HE1	1:B:256:VAL:HG13	1.67	0.60
1:H:152:ARG:NH1	1:I:49:ASP:OD1	2.34	0.60
1:B:152:ARG:NH1	1:C:49:ASP:OD1	2.35	0.59
1:D:127:VAL:O	1:D:129:GLU:N	2.32	0.59
1:F:68:LYS:O	3:F:532:HOH:O	2.17	0.59
1:I:130:ARG:NE	1:J:47:GLU:OE2	2.30	0.59
1:H:197:VAL:HG21	1:H:252:ALA:HB1	1.85	0.58
1:A:116:SER:HB2	2:A:401:NAP:H6N	1.85	0.58
1:B:254:THR:O	1:B:258:THR:N	2.29	0.58
1:B:178:GLY:O	1:B:186:HIS:NE2	2.36	0.57
1:B:327:PHE:O	1:B:329:GLN:N	2.33	0.57
1:B:269:THR:H	1:B:272:GLU:HB2	1.70	0.56
1:B:135:PRO:HD2	1:C:44:VAL:HG13	1.88	0.56
1:C:90:MET:HG3	1:D:34:LEU:HD12	1.88	0.55
1:B:172:PRO:HB3	1:B:325:TRP:CH2	2.42	0.55
1:I:286:ASP:HA	1:I:289:ARG:HG3	1.89	0.54
1:G:155:PRO:O	1:G:157:ALA:N	2.35	0.54
1:I:21:ASN:OD1	1:I:47:GLU:N	2.35	0.53
1:J:171:GLY:HA3	1:J:218:VAL:HG22	1.91	0.53
1:B:250:ASP:OD1	1:B:250:ASP:N	2.42	0.53
1:J:4:ILE:HG12	1:J:29:ILE:HB	1.91	0.53
1:D:97:SER:HB3	1:D:146:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLN:HB3	1:B:279:VAL:HG23	1.89	0.53
1:B:172:PRO:HB3	1:B:325:TRP:CZ3	2.44	0.53
1:B:319:VAL:O	1:B:323:VAL:HG23	2.08	0.53
1:B:300:GLN:O	1:B:304:ARG:HG2	2.08	0.53
1:C:105:LEU:HD11	1:C:153:VAL:HG11	1.91	0.52
1:G:105:LEU:HD21	1:G:161:ILE:HD11	1.92	0.52
1:B:121:GLY:H	1:B:293:GLN:HE21	1.57	0.52
1:A:4:ILE:HG12	1:A:29:ILE:HB	1.91	0.51
1:A:47:GLU:OE2	1:E:130:ARG:NE	2.43	0.51
1:F:286:ASP:HA	1:F:289:ARG:HG3	1.93	0.51
1:B:242:THR:HG22	1:B:312:PHE:HB3	1.92	0.51
1:C:286:ASP:HA	1:C:289:ARG:HG3	1.93	0.51
1:J:246:GLN:NE2	1:J:250:ASP:OD2	2.38	0.51
1:B:210:GLU:O	1:B:247:PRO:HB3	2.10	0.50
1:I:213:ARG:HB2	1:I:215:PHE:CZ	2.46	0.50
1:G:204:SER:O	1:G:204:SER:OG	2.29	0.50
1:A:127:VAL:O	1:A:129:GLU:N	2.44	0.50
1:H:183:VAL:HG21	1:H:248:PHE:CE1	2.47	0.50
1:A:320:ASP:OD2	1:A:324:ARG:NH2	2.44	0.49
1:F:41:LYS:HE2	3:J:521:HOH:O	2.13	0.49
1:D:32:ASP:OD1	1:D:33:ASN:N	2.35	0.49
1:D:183:VAL:HG21	1:D:248:PHE:CE1	2.48	0.49
1:J:259:LEU:HA	1:J:262:LEU:HD12	1.93	0.49
1:F:2:THR:N	3:F:532:HOH:O	2.34	0.49
1:F:1:MET:HG3	1:F:27:ARG:HD2	1.95	0.48
1:H:246:GLN:NE2	1:H:250:ASP:OD2	2.44	0.48
1:B:4:ILE:HG12	1:B:29:ILE:HB	1.95	0.48
1:B:191:PHE:CE1	1:B:256:VAL:HG13	2.47	0.48
1:B:322:TYR:CE1	1:B:326:LEU:HD21	2.48	0.48
1:J:52:LEU:HD23	1:J:56:GLU:HG3	1.95	0.48
1:C:13:GLY:O	1:C:17:VAL:HG23	2.12	0.48
1:D:286:ASP:HA	1:D:289:ARG:HG3	1.96	0.48
1:G:300:GLN:O	1:G:304:ARG:HG2	2.14	0.48
1:F:170:TYR:OH	1:F:318:GLY:HA3	2.14	0.48
1:A:314:THR:OG1	1:A:317:GLU:HG3	2.14	0.48
1:H:243:GLY:HA2	1:H:298:ALA:O	2.13	0.48
1:C:37:ALA:O	1:C:40:PHE:HD2	1.98	0.47
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.73	0.47
1:I:152:ARG:NH1	1:J:49:ASP:OD1	2.44	0.47
1:C:125:ARG:HB2	1:C:132:VAL:HG11	1.97	0.47
1:G:213:ARG:HB2	1:G:215:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:GLY:HA2	1:G:298:ALA:O	2.14	0.47
1:E:243:GLY:O	1:E:297:GLN:NE2	2.38	0.46
1:C:128:GLU:OE1	1:C:128:GLU:N	2.42	0.46
1:A:121:GLY:HA3	1:A:134:ALA:O	2.15	0.46
1:C:121:GLY:HA3	1:C:134:ALA:O	2.16	0.46
1:J:199:LEU:HD11	1:J:252:ALA:HB2	1.97	0.46
1:B:4:ILE:HB	1:B:72:VAL:HG22	1.98	0.46
1:F:326:LEU:O	1:F:329:GLN:HG2	2.16	0.45
1:I:303:LEU:HD22	1:I:308:TYR:HB3	1.98	0.45
1:B:144:PHE:O	1:B:148:GLN:HG2	2.17	0.45
1:C:52:LEU:HD21	1:C:60:ARG:HE	1.80	0.45
1:H:170:TYR:OH	1:H:318:GLY:HA3	2.16	0.45
1:D:75:GLU:OE2	3:D:547:HOH:O	2.19	0.45
1:B:6:THR:HA	1:B:31:VAL:HB	1.98	0.45
1:B:243:GLY:O	1:B:297:GLN:NE2	2.41	0.45
1:B:251:ILE:O	1:B:255:VAL:HG23	2.15	0.45
1:B:256:VAL:HG11	1:B:273:GLN:HG2	1.98	0.45
1:D:284:PHE:HA	1:D:285:PRO:HD3	1.85	0.45
1:G:303:LEU:HD22	1:G:308:TYR:HB3	1.99	0.45
1:B:258:THR:O	1:B:262:LEU:HG	2.16	0.45
1:I:216:VAL:HG21	1:I:241:GLY:HA2	1.98	0.45
1:B:258:THR:HG23	1:B:324:ARG:NH2	2.31	0.45
1:G:192:ARG:HA	1:G:192:ARG:HD2	1.82	0.45
1:J:112:LEU:HA	1:J:162:ALA:O	2.17	0.45
1:C:275:GLU:HA	1:I:208:PRO:HD2	1.99	0.45
1:E:224:VAL:HB	1:E:240:LEU:HD11	1.99	0.45
1:J:63:ARG:NH2	1:J:65:ASP:OD2	2.32	0.45
1:B:208:PRO:HD3	1:J:275:GLU:HA	1.97	0.45
1:C:284:PHE:HA	1:C:285:PRO:HD3	1.84	0.45
1:F:90:MET:HG3	1:G:34:LEU:HD12	1.98	0.45
1:J:120:TYR:O	1:J:123:SER:HB2	2.16	0.45
1:A:169:VAL:HA	1:A:216:VAL:O	2.18	0.44
1:A:284:PHE:HA	1:A:285:PRO:HD3	1.81	0.44
1:G:158:LYS:HD3	1:G:158:LYS:HA	1.53	0.44
1:J:258:THR:O	1:J:262:LEU:HG	2.18	0.44
1:F:206:TYR:CE2	1:F:294:CYS:HB3	2.52	0.44
1:J:150:ILE:HG22	1:J:154:MET:HE2	2.00	0.44
1:J:212:THR:HG22	1:J:247:PRO:CA	2.47	0.44
1:B:212:THR:HG22	1:B:247:PRO:HB3	1.99	0.44
1:E:170:TYR:OH	1:E:318:GLY:HA3	2.17	0.44
1:C:108:GLY:HA2	1:C:159:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:PHE:CZ	1:E:296:THR:HA	2.53	0.44
1:G:116:SER:O	1:G:119:ILE:HB	2.18	0.44
1:I:60:ARG:HG2	1:I:63:ARG:NH2	2.33	0.44
1:H:286:ASP:OD1	1:H:289:ARG:NH1	2.51	0.44
1:J:42:ASN:O	1:J:173:ARG:NH1	2.51	0.44
1:J:136:LEU:HB3	1:J:291:LYS:HA	1.99	0.44
1:B:255:VAL:O	1:B:259:LEU:HB2	2.18	0.44
1:F:288:LEU:HD23	1:F:288:LEU:HA	1.90	0.43
1:H:211:GLN:H	1:H:211:GLN:CD	2.21	0.43
1:I:121:GLY:HA3	1:I:134:ALA:O	2.18	0.43
1:G:130:ARG:NE	1:H:47:GLU:OE2	2.52	0.43
1:B:284:PHE:HA	1:B:285:PRO:HD3	1.86	0.43
1:A:160:GLN:HB2	1:A:232:PRO:O	2.18	0.43
1:C:112:LEU:HA	1:C:162:ALA:O	2.17	0.43
1:D:251:ILE:O	1:D:255:VAL:HG23	2.18	0.43
1:I:126:PHE:CZ	1:I:296:THR:HA	2.54	0.43
1:D:327:PHE:O	1:D:329:GLN:N	2.52	0.43
1:E:284:PHE:HA	1:E:285:PRO:HD3	1.72	0.43
1:I:82:MET:SD	1:I:288:LEU:HD21	2.59	0.43
1:C:150:ILE:HG23	1:C:161:ILE:HG21	2.00	0.43
1:E:121:GLY:HA3	1:E:134:ALA:O	2.19	0.43
1:F:152:ARG:NH1	1:G:49:ASP:OD1	2.50	0.43
1:G:1:MET:HG3	1:G:27:ARG:HD3	2.00	0.43
1:H:300:GLN:O	1:H:304:ARG:HG2	2.19	0.43
1:C:126:PHE:O	1:C:239:ASN:ND2	2.51	0.42
1:D:52:LEU:HD23	1:D:56:GLU:HG3	2.01	0.42
1:H:253:ALA:HA	1:H:273:GLN:OE1	2.19	0.42
1:A:243:GLY:HA2	1:A:298:ALA:O	2.20	0.42
1:B:133:GLU:OE2	1:B:165:ARG:NH1	2.51	0.42
1:D:136:LEU:HB3	1:D:291:LYS:HA	2.02	0.42
1:E:187:ASN:ND2	1:E:252:ALA:HA	2.34	0.42
1:H:130:ARG:HA	1:H:133:GLU:OE1	2.19	0.42
1:B:212:THR:OG1	1:B:295:PHE:HD1	2.02	0.42
1:D:34:LEU:HD23	1:D:34:LEU:HA	1.87	0.42
1:I:152:ARG:NH2	1:J:47:GLU:OE1	2.52	0.42
1:A:219:GLU:OE1	1:A:321:ARG:NH2	2.52	0.42
1:B:226:LEU:O	1:B:229:PHE:HB3	2.19	0.42
1:J:212:THR:HA	1:J:247:PRO:HA	2.01	0.42
1:B:325:TRP:N	3:B:502:HOH:O	2.52	0.42
1:C:243:GLY:HA2	1:C:298:ALA:O	2.20	0.42
1:D:112:LEU:HA	1:D:162:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:GLY:HA3	1:G:134:ALA:O	2.18	0.42
1:J:116:SER:HB2	2:J:401:NAP:H6N	2.02	0.42
1:A:5:VAL:HG22	1:A:73:PHE:HB2	2.02	0.42
1:G:212:THR:HA	1:G:247:PRO:HA	2.02	0.42
1:I:136:LEU:HB3	1:I:291:LYS:HA	2.02	0.42
1:G:169:VAL:HA	1:G:216:VAL:O	2.19	0.42
1:J:268:LEU:HD12	1:J:273:GLN:HG2	2.02	0.42
1:H:212:THR:OG1	1:H:295:PHE:HD1	2.02	0.42
1:B:90:MET:HG3	1:C:34:LEU:HD12	2.02	0.42
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.87	0.42
1:E:245:ALA:HB2	1:E:297:GLN:HB2	2.02	0.42
1:J:60:ARG:HG2	1:J:60:ARG:HH11	1.85	0.42
1:J:260:ARG:C	1:J:262:LEU:H	2.23	0.41
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.91	0.41
1:F:58:VAL:HG11	1:F:99:ALA:HB1	2.01	0.41
1:G:212:THR:HG1	1:G:295:PHE:HD1	1.64	0.41
1:H:150:ILE:HG23	1:H:161:ILE:HG21	2.02	0.41
1:J:121:GLY:O	1:J:293:GLN:HG2	2.20	0.41
1:A:209:GLY:HA3	1:A:249:ASN:OD1	2.20	0.41
1:D:150:ILE:HD13	1:D:150:ILE:HA	1.95	0.41
1:G:127:VAL:O	1:G:129:GLU:N	2.48	0.41
1:B:187:ASN:HD22	1:B:187:ASN:HA	1.70	0.41
1:H:259:LEU:HD23	1:H:259:LEU:HA	1.85	0.41
1:F:212:THR:O	1:F:295:PHE:HA	2.21	0.41
1:H:284:PHE:HA	1:H:285:PRO:HD3	1.80	0.41
1:I:89:MET:O	1:I:93:ASN:HB2	2.20	0.41
1:J:126:PHE:CZ	1:J:296:THR:HA	2.55	0.41
1:E:34:LEU:CD2	1:E:39:LYS:HB2	2.50	0.41
1:J:284:PHE:HA	1:J:285:PRO:HD3	1.81	0.41
1:F:231:HIS:HB3	1:F:234:LYS:HD2	2.02	0.41
1:I:115:SER:OG	1:I:116:SER:N	2.52	0.41
1:A:304:ARG:HD3	1:A:308:TYR:O	2.21	0.41
1:B:259:LEU:HA	1:B:262:LEU:HD12	2.02	0.41
1:G:127:VAL:HG23	1:G:129:GLU:HG3	2.03	0.41
1:H:90:MET:HG3	1:I:34:LEU:HD12	2.01	0.41
1:C:304:ARG:C	1:C:306:ALA:H	2.25	0.41
1:D:243:GLY:HA2	1:D:298:ALA:O	2.21	0.41
1:G:284:PHE:HA	1:G:285:PRO:HD3	1.81	0.41
1:J:286:ASP:HA	1:J:289:ARG:HG3	2.02	0.41
1:B:11:PHE:HA	1:B:173:ARG:O	2.20	0.40
1:B:212:THR:HG22	1:B:247:PRO:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:THR:OG1	1:E:74:HIS:HA	2.21	0.40
1:E:20:LEU:HB3	1:E:25:GLU:HB2	2.02	0.40
1:E:177:LYS:HE2	1:E:177:LYS:HB3	1.70	0.40
1:B:118:ALA:HA	1:B:293:GLN:NE2	2.36	0.40
1:C:116:SER:HB2	2:C:401:NAP:H6N	2.04	0.40
1:H:11:PHE:HA	1:H:173:ARG:O	2.22	0.40
1:B:133:GLU:OE2	1:B:165:ARG:NH2	2.54	0.40
1:F:60:ARG:HG2	1:F:63:ARG:NH2	2.36	0.40
1:G:1:MET:N	3:G:506:HOH:O	2.53	0.40
1:I:243:GLY:O	1:I:297:GLN:NE2	2.50	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	328/342 (96%)	318 (97%)	9 (3%)	1 (0%)	41	64
1	B	328/342 (96%)	296 (90%)	30 (9%)	2 (1%)	25	47
1	C	328/342 (96%)	314 (96%)	12 (4%)	2 (1%)	25	47
1	D	328/342 (96%)	313 (95%)	13 (4%)	2 (1%)	25	47
1	E	328/342 (96%)	317 (97%)	11 (3%)	0	100	100
1	F	328/342 (96%)	313 (95%)	14 (4%)	1 (0%)	41	64
1	G	328/342 (96%)	313 (95%)	12 (4%)	3 (1%)	17	35
1	H	328/342 (96%)	316 (96%)	11 (3%)	1 (0%)	41	64
1	I	328/342 (96%)	312 (95%)	13 (4%)	3 (1%)	17	35
1	J	328/342 (96%)	306 (93%)	17 (5%)	5 (2%)	10	21
All	All	3280/3420 (96%)	3118 (95%)	142 (4%)	20 (1%)	25	47

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	329	GLN
1	J	128	GLU
1	B	328	GLY
1	C	305	ALA
1	D	328	GLY
1	G	155	PRO
1	G	156	GLY
1	J	329	GLN
1	A	128	GLU
1	D	128	GLU
1	I	305	ALA
1	C	329	GLN
1	G	329	GLN
1	I	128	GLU
1	J	328	GLY
1	B	62	ALA
1	J	208	PRO
1	J	261	ALA
1	H	328	GLY
1	I	208	PRO

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	266/273 (97%)	257 (97%)	9 (3%)	37	63
1	B	266/273 (97%)	255 (96%)	11 (4%)	30	56
1	C	266/273 (97%)	256 (96%)	10 (4%)	33	59
1	D	266/273 (97%)	260 (98%)	6 (2%)	50	75
1	E	266/273 (97%)	260 (98%)	6 (2%)	50	75
1	F	266/273 (97%)	259 (97%)	7 (3%)	46	72
1	G	266/273 (97%)	258 (97%)	8 (3%)	41	67
1	H	266/273 (97%)	259 (97%)	7 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	266/273 (97%)	254 (96%)	12 (4%)	27 52
1	J	266/273 (97%)	257 (97%)	9 (3%)	37 63
All	All	2660/2730 (97%)	2575 (97%)	85 (3%)	39 65

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	A	152	ARG
1	A	154	MET
1	A	175	SER
1	A	192	ARG
1	A	216	VAL
1	A	218	VAL
1	A	303	LEU
1	A	329	GLN
1	B	23	ARG
1	B	127	VAL
1	B	186	HIS
1	B	216	VAL
1	B	218	VAL
1	B	250	ASP
1	B	254	THR
1	B	259	LEU
1	B	270	LEU
1	B	303	LEU
1	B	325	TRP
1	C	49	ASP
1	C	91	ASP
1	C	154	MET
1	C	159	SER
1	C	212	THR
1	C	216	VAL
1	C	218	VAL
1	C	303	LEU
1	C	329	GLN
1	C	330	LEU
1	D	91	ASP
1	D	152	ARG
1	D	216	VAL
1	D	218	VAL

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Mol	Chain	Res	Type
1	D	289	ARG
1	D	303	LEU
1	E	91	ASP
1	E	152	ARG
1	E	212	THR
1	E	216	VAL
1	E	218	VAL
1	E	329	GLN
1	F	27	ARG
1	F	91	ASP
1	F	152	ARG
1	F	212	THR
1	F	216	VAL
1	F	218	VAL
1	F	303	LEU
1	G	152	ARG
1	G	212	THR
1	G	216	VAL
1	G	218	VAL
1	G	235	SER
1	G	265	GLN
1	G	286	ASP
1	G	303	LEU
1	H	56	GLU
1	H	91	ASP
1	H	152	ARG
1	H	216	VAL
1	H	218	VAL
1	H	303	LEU
1	H	329	GLN
1	I	21	ASN
1	I	91	ASP
1	I	127	VAL
1	I	152	ARG
1	I	216	VAL
1	I	217	SER
1	I	218	VAL
1	I	235	SER
1	I	246	GLN
1	I	289	ARG
1	I	303	LEU
1	I	317	GLU

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Mol	Chain	Res	Type
1	J	23	ARG
1	J	27	ARG
1	J	52	LEU
1	J	91	ASP
1	J	123	SER
1	J	152	ARG
1	J	216	VAL
1	J	218	VAL
1	J	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	ASN
1	B	293	GLN
1	H	316	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	F	401	-	45,52,52	1.97	11 (24%)	56,80,80	1.24	5 (8%)
2	NAP	I	401	-	45,52,52	2.04	11 (24%)	56,80,80	1.15	4 (7%)
2	NAP	E	401	-	45,52,52	1.98	12 (26%)	56,80,80	1.16	6 (10%)
2	NAP	J	401	-	45,52,52	2.00	11 (24%)	56,80,80	1.24	5 (8%)
2	NAP	C	401	-	45,52,52	2.05	11 (24%)	56,80,80	1.25	5 (8%)
2	NAP	H	401	-	45,52,52	2.01	11 (24%)	56,80,80	1.33	6 (10%)
2	NAP	D	401	-	45,52,52	2.09	12 (26%)	56,80,80	1.16	7 (12%)
2	NAP	B	401	-	45,52,52	1.98	11 (24%)	56,80,80	1.25	8 (14%)
2	NAP	A	401	-	45,52,52	1.89	11 (24%)	56,80,80	1.24	5 (8%)
2	NAP	G	401	-	45,52,52	2.01	11 (24%)	56,80,80	1.27	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	F	401	-	-	12/31/67/67	0/5/5/5
2	NAP	I	401	-	-	11/31/67/67	0/5/5/5
2	NAP	E	401	-	-	9/31/67/67	0/5/5/5
2	NAP	J	401	-	-	7/31/67/67	0/5/5/5
2	NAP	C	401	-	-	11/31/67/67	0/5/5/5
2	NAP	H	401	-	-	13/31/67/67	0/5/5/5
2	NAP	D	401	-	-	11/31/67/67	0/5/5/5
2	NAP	B	401	-	-	6/31/67/67	0/5/5/5
2	NAP	A	401	-	-	6/31/67/67	0/5/5/5
2	NAP	G	401	-	-	7/31/67/67	0/5/5/5

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	NAP	C7N-N7N	8.01	1.48	1.33
2	B	401	NAP	C7N-N7N	7.54	1.47	1.33
2	G	401	NAP	C7N-N7N	7.43	1.47	1.33
2	F	401	NAP	C7N-N7N	7.39	1.47	1.33
2	D	401	NAP	C7N-N7N	7.28	1.46	1.33
2	H	401	NAP	C7N-N7N	7.26	1.46	1.33
2	C	401	NAP	C7N-N7N	7.25	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C7N-N7N	7.08	1.46	1.33
2	J	401	NAP	C7N-N7N	7.01	1.46	1.33
2	E	401	NAP	C7N-N7N	6.96	1.46	1.33
2	J	401	NAP	C3B-C2B	-5.41	1.40	1.52
2	H	401	NAP	C3B-C2B	-5.19	1.41	1.52
2	I	401	NAP	C3B-C2B	-5.17	1.41	1.52
2	D	401	NAP	C3B-C2B	-5.15	1.41	1.52
2	C	401	NAP	C3B-C2B	-5.08	1.41	1.52
2	B	401	NAP	C3B-C2B	-5.01	1.41	1.52
2	E	401	NAP	C3B-C2B	-5.00	1.41	1.52
2	G	401	NAP	C3B-C2B	-4.95	1.41	1.52
2	A	401	NAP	C3B-C2B	-4.92	1.42	1.52
2	F	401	NAP	C3B-C2B	-4.51	1.42	1.52
2	C	401	NAP	C3N-C7N	4.19	1.56	1.50
2	I	401	NAP	C3N-C7N	3.93	1.56	1.50
2	D	401	NAP	O2D-C2D	-3.92	1.33	1.43
2	C	401	NAP	O2D-C2D	-3.89	1.33	1.43
2	J	401	NAP	O2D-C2D	-3.79	1.34	1.43
2	H	401	NAP	C3N-C7N	3.78	1.56	1.50
2	G	401	NAP	C3N-C7N	3.63	1.56	1.50
2	E	401	NAP	C3N-C7N	3.61	1.56	1.50
2	B	401	NAP	O2D-C2D	-3.58	1.34	1.43
2	E	401	NAP	O2D-C2D	-3.58	1.34	1.43
2	D	401	NAP	C2D-C1D	-3.55	1.48	1.53
2	D	401	NAP	C3N-C7N	3.54	1.55	1.50
2	F	401	NAP	O2D-C2D	-3.45	1.34	1.43
2	B	401	NAP	C2D-C1D	-3.38	1.48	1.53
2	H	401	NAP	O2D-C2D	-3.34	1.35	1.43
2	F	401	NAP	C2D-C1D	-3.34	1.48	1.53
2	I	401	NAP	O2D-C2D	-3.33	1.35	1.43
2	G	401	NAP	O2D-C2D	-3.13	1.35	1.43
2	B	401	NAP	C3N-C7N	3.11	1.55	1.50
2	J	401	NAP	C3N-C7N	3.11	1.55	1.50
2	A	401	NAP	O2D-C2D	-3.11	1.35	1.43
2	H	401	NAP	C6A-N6A	3.09	1.45	1.34
2	G	401	NAP	C2D-C1D	-3.03	1.49	1.53
2	C	401	NAP	C2D-C1D	-3.03	1.49	1.53
2	D	401	NAP	O4B-C4B	-3.02	1.38	1.45
2	E	401	NAP	O4B-C4B	-2.99	1.38	1.45
2	J	401	NAP	C2D-C1D	-2.96	1.49	1.53
2	H	401	NAP	C2D-C1D	-2.96	1.49	1.53
2	F	401	NAP	C3N-C7N	2.92	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O4B-C4B	-2.89	1.38	1.45
2	I	401	NAP	C2D-C1D	-2.87	1.49	1.53
2	A	401	NAP	C2D-C1D	-2.78	1.49	1.53
2	B	401	NAP	C6A-N6A	2.73	1.44	1.34
2	H	401	NAP	C5D-C4D	-2.73	1.43	1.51
2	C	401	NAP	C6A-N6A	2.70	1.43	1.34
2	B	401	NAP	O4B-C4B	-2.67	1.39	1.45
2	G	401	NAP	O4B-C4B	-2.64	1.39	1.45
2	D	401	NAP	C3B-C4B	-2.61	1.46	1.53
2	I	401	NAP	C5D-C4D	-2.59	1.43	1.51
2	J	401	NAP	C2D-C3D	-2.58	1.46	1.53
2	A	401	NAP	C6A-N6A	2.57	1.43	1.34
2	D	401	NAP	C2D-C3D	-2.57	1.46	1.53
2	D	401	NAP	C6A-N6A	2.57	1.43	1.34
2	A	401	NAP	C5D-C4D	-2.56	1.43	1.51
2	I	401	NAP	C6A-N6A	2.56	1.43	1.34
2	G	401	NAP	C6A-N6A	2.56	1.43	1.34
2	J	401	NAP	C6A-N6A	2.56	1.43	1.34
2	E	401	NAP	C2D-C1D	-2.55	1.49	1.53
2	F	401	NAP	C6A-N6A	2.55	1.43	1.34
2	E	401	NAP	C3B-C4B	-2.54	1.46	1.53
2	F	401	NAP	C3B-C4B	-2.54	1.46	1.53
2	E	401	NAP	C5D-C4D	-2.53	1.43	1.51
2	J	401	NAP	C3B-C4B	-2.50	1.46	1.53
2	C	401	NAP	C5D-C4D	-2.50	1.43	1.51
2	F	401	NAP	O5B-C5B	-2.49	1.35	1.44
2	A	401	NAP	C3N-C7N	2.47	1.54	1.50
2	B	401	NAP	C5D-C4D	-2.47	1.43	1.51
2	G	401	NAP	O5B-C5B	-2.47	1.35	1.44
2	C	401	NAP	C3B-C4B	-2.47	1.46	1.53
2	D	401	NAP	O3D-C3D	-2.44	1.37	1.43
2	F	401	NAP	C5D-C4D	-2.43	1.44	1.51
2	F	401	NAP	O4B-C4B	-2.42	1.39	1.45
2	E	401	NAP	C6A-N6A	2.39	1.42	1.34
2	D	401	NAP	O5B-C5B	-2.37	1.35	1.44
2	G	401	NAP	C5D-C4D	-2.36	1.44	1.51
2	E	401	NAP	C2D-C3D	-2.36	1.46	1.53
2	B	401	NAP	C3B-C4B	-2.35	1.47	1.53
2	D	401	NAP	C5D-C4D	-2.34	1.44	1.51
2	I	401	NAP	O4B-C4B	-2.33	1.39	1.45
2	C	401	NAP	O5B-C5B	-2.30	1.35	1.44
2	J	401	NAP	O4B-C4B	-2.29	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	O4B-C4B	-2.29	1.39	1.45
2	J	401	NAP	C5D-C4D	-2.29	1.44	1.51
2	B	401	NAP	C2D-C3D	-2.29	1.47	1.53
2	F	401	NAP	O5D-C5D	-2.28	1.36	1.44
2	C	401	NAP	C2D-C3D	-2.26	1.47	1.53
2	E	401	NAP	O5B-C5B	-2.20	1.36	1.44
2	A	401	NAP	C3B-C4B	-2.19	1.47	1.53
2	G	401	NAP	C3B-C4B	-2.19	1.47	1.53
2	J	401	NAP	O3D-C3D	-2.19	1.37	1.43
2	H	401	NAP	C3B-C4B	-2.19	1.47	1.53
2	G	401	NAP	C2D-C3D	-2.18	1.47	1.53
2	A	401	NAP	O5B-C5B	-2.16	1.36	1.44
2	I	401	NAP	O5B-C5B	-2.14	1.36	1.44
2	H	401	NAP	O3D-C3D	-2.13	1.37	1.43
2	H	401	NAP	O5B-C5B	-2.08	1.36	1.44
2	I	401	NAP	C3B-C4B	-2.07	1.47	1.53
2	A	401	NAP	C2D-C3D	-2.01	1.47	1.53
2	H	401	NAP	C2D-C3D	-2.01	1.47	1.53
2	B	401	NAP	O5B-C5B	-2.01	1.37	1.44
2	I	401	NAP	C2D-C3D	-2.01	1.47	1.53
2	E	401	NAP	O4B-C1B	-2.00	1.38	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	NAP	N3A-C2A-N1A	-4.67	121.38	128.68
2	B	401	NAP	N3A-C2A-N1A	-4.54	121.58	128.68
2	F	401	NAP	N3A-C2A-N1A	-4.54	121.59	128.68
2	A	401	NAP	N3A-C2A-N1A	-4.25	122.04	128.68
2	H	401	NAP	O7N-C7N-N7N	-4.18	116.63	122.58
2	E	401	NAP	N3A-C2A-N1A	-4.04	122.36	128.68
2	C	401	NAP	O7N-C7N-N7N	-3.92	117.01	122.58
2	G	401	NAP	N3A-C2A-N1A	-3.89	122.59	128.68
2	H	401	NAP	N3A-C2A-N1A	-3.85	122.66	128.68
2	C	401	NAP	N3A-C2A-N1A	-3.76	122.80	128.68
2	J	401	NAP	N3A-C2A-N1A	-3.75	122.82	128.68
2	A	401	NAP	C3N-C7N-N7N	3.71	122.20	117.75
2	H	401	NAP	C3N-C7N-N7N	3.68	122.17	117.75
2	D	401	NAP	N3A-C2A-N1A	-3.64	122.99	128.68
2	G	401	NAP	O7N-C7N-N7N	-3.49	117.62	122.58
2	C	401	NAP	C3N-C7N-N7N	3.42	121.86	117.75
2	G	401	NAP	C3N-C7N-N7N	3.28	121.69	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAP	C3N-C7N-N7N	3.25	121.66	117.75
2	E	401	NAP	O7N-C7N-N7N	-3.17	118.07	122.58
2	J	401	NAP	O4B-C1B-C2B	-2.93	101.50	106.59
2	J	401	NAP	C4A-C5A-N7A	-2.93	106.35	109.40
2	J	401	NAP	O7N-C7N-N7N	-2.84	118.54	122.58
2	D	401	NAP	PN-O3-PA	-2.81	123.19	132.83
2	D	401	NAP	O7N-C7N-N7N	-2.73	118.69	122.58
2	I	401	NAP	O7N-C7N-N7N	-2.71	118.72	122.58
2	D	401	NAP	O4D-C1D-C2D	-2.64	103.07	106.93
2	G	401	NAP	C4A-C5A-N7A	-2.61	106.68	109.40
2	F	401	NAP	C5N-C4N-C3N	-2.59	117.28	120.34
2	I	401	NAP	C4A-C5A-N7A	-2.55	106.74	109.40
2	E	401	NAP	O4B-C1B-C2B	-2.52	102.21	106.59
2	E	401	NAP	C4A-C5A-N7A	-2.49	106.81	109.40
2	C	401	NAP	PN-O3-PA	-2.45	124.44	132.83
2	B	401	NAP	O7N-C7N-N7N	-2.44	119.11	122.58
2	E	401	NAP	PN-O3-PA	-2.41	124.54	132.83
2	F	401	NAP	O4B-C1B-C2B	-2.35	102.52	106.59
2	B	401	NAP	C4A-C5A-N7A	-2.35	106.95	109.40
2	A	401	NAP	O7N-C7N-N7N	-2.29	119.32	122.58
2	F	401	NAP	C4A-C5A-N7A	-2.26	107.04	109.40
2	B	401	NAP	C1B-N9A-C4A	-2.22	122.74	126.64
2	H	401	NAP	PN-O3-PA	-2.21	125.23	132.83
2	D	401	NAP	C4A-C5A-N7A	-2.18	107.13	109.40
2	I	401	NAP	O4B-C1B-C2B	-2.18	102.81	106.59
2	H	401	NAP	C4A-C5A-N7A	-2.15	107.16	109.40
2	J	401	NAP	PN-O3-PA	-2.14	125.50	132.83
2	A	401	NAP	O4B-C1B-C2B	-2.13	102.89	106.59
2	H	401	NAP	O4B-C1B-C2B	-2.12	102.91	106.59
2	B	401	NAP	O4B-C1B-C2B	-2.10	102.94	106.59
2	B	401	NAP	PN-O3-PA	-2.10	125.62	132.83
2	A	401	NAP	C5N-C4N-C3N	-2.09	117.87	120.34
2	G	401	NAP	O4B-C1B-C2B	-2.08	102.98	106.59
2	D	401	NAP	C5N-C4N-C3N	-2.06	117.90	120.34
2	F	401	NAP	O7N-C7N-N7N	-2.06	119.65	122.58
2	C	401	NAP	C5N-C4N-C3N	-2.05	117.91	120.34
2	B	401	NAP	C5N-C4N-C3N	-2.05	117.92	120.34
2	D	401	NAP	C3N-C7N-N7N	2.04	120.20	117.75
2	E	401	NAP	O7N-C7N-C3N	2.00	122.03	119.63

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	C5D-O5D-PN-O2N
2	B	401	NAP	PN-O3-PA-O5B
2	B	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	C5D-O5D-PN-O2N
2	C	401	NAP	C5B-O5B-PA-O1A
2	C	401	NAP	PN-O3-PA-O5B
2	C	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	C5D-O5D-PN-O2N
2	D	401	NAP	PN-O3-PA-O5B
2	D	401	NAP	C5D-O5D-PN-O2N
2	F	401	NAP	PN-O3-PA-O5B
2	F	401	NAP	C5D-O5D-PN-O1N
2	F	401	NAP	C5D-O5D-PN-O2N
2	G	401	NAP	C5D-O5D-PN-O2N
2	H	401	NAP	PN-O3-PA-O5B
2	H	401	NAP	C5D-O5D-PN-O1N
2	H	401	NAP	C5D-O5D-PN-O2N
2	I	401	NAP	PN-O3-PA-O5B
2	I	401	NAP	C5D-O5D-PN-O1N
2	I	401	NAP	C5D-O5D-PN-O2N
2	J	401	NAP	C5D-O5D-PN-O1N
2	J	401	NAP	C5D-O5D-PN-O2N
2	C	401	NAP	C3B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	C3B-C4B-C5B-O5B
2	I	401	NAP	O4B-C4B-C5B-O5B
2	E	401	NAP	O4B-C4B-C5B-O5B
2	H	401	NAP	O4B-C4B-C5B-O5B
2	E	401	NAP	C3B-C4B-C5B-O5B
2	C	401	NAP	C4B-C5B-O5B-PA
2	C	401	NAP	C5B-O5B-PA-O3
2	D	401	NAP	C5B-O5B-PA-O3
2	D	401	NAP	C5D-O5D-PN-O3
2	E	401	NAP	C5D-O5D-PN-O3
2	F	401	NAP	C5B-O5B-PA-O3
2	F	401	NAP	C2B-O2B-P2B-O2X
2	F	401	NAP	C5D-O5D-PN-O3
2	G	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	O4B-C4B-C5B-O5B
2	F	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	PA-O3-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	B	401	NAP	PA-O3-PN-O2N
2	G	401	NAP	PA-O3-PN-O2N
2	C	401	NAP	C5B-O5B-PA-O2A
2	D	401	NAP	C5B-O5B-PA-O2A
2	D	401	NAP	C5D-O5D-PN-O1N
2	E	401	NAP	C5D-O5D-PN-O1N
2	G	401	NAP	C5D-O5D-PN-O1N
2	I	401	NAP	C5B-O5B-PA-O2A
2	I	401	NAP	C3B-C4B-C5B-O5B
2	D	401	NAP	C4B-C5B-O5B-PA
2	F	401	NAP	C4B-C5B-O5B-PA
2	J	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	PA-O3-PN-O2N
2	D	401	NAP	PA-O3-PN-O2N
2	E	401	NAP	PA-O3-PN-O2N
2	H	401	NAP	PA-O3-PN-O2N
2	I	401	NAP	PA-O3-PN-O2N
2	J	401	NAP	PA-O3-PN-O2N
2	H	401	NAP	C4B-C5B-O5B-PA
2	B	401	NAP	O4B-C4B-C5B-O5B
2	G	401	NAP	O4B-C4B-C5B-O5B
2	E	401	NAP	PA-O3-PN-O1N
2	F	401	NAP	PA-O3-PN-O1N
2	I	401	NAP	C4B-C5B-O5B-PA
2	G	401	NAP	C4B-C5B-O5B-PA
2	A	401	NAP	C3B-C4B-C5B-O5B
2	H	401	NAP	C3B-C4B-C5B-O5B
2	E	401	NAP	C2B-O2B-P2B-O1X
2	I	401	NAP	C2B-O2B-P2B-O1X
2	A	401	NAP	C5D-O5D-PN-O3
2	B	401	NAP	C5D-O5D-PN-O3
2	C	401	NAP	C5D-O5D-PN-O3
2	E	401	NAP	C2B-O2B-P2B-O3X
2	G	401	NAP	C2B-O2B-P2B-O2X
2	H	401	NAP	C5B-O5B-PA-O3
2	H	401	NAP	C2B-O2B-P2B-O2X
2	H	401	NAP	C2B-O2B-P2B-O3X
2	H	401	NAP	C5D-O5D-PN-O3
2	I	401	NAP	C5B-O5B-PA-O3
2	I	401	NAP	C5D-O5D-PN-O3
2	J	401	NAP	C2B-O2B-P2B-O2X
2	J	401	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	F	401	NAP	C3B-C4B-C5B-O5B
2	D	401	NAP	PA-O3-PN-O1N
2	F	401	NAP	PA-O3-PN-O2N
2	H	401	NAP	PA-O3-PN-O1N
2	E	401	NAP	C4B-C5B-O5B-PA
2	F	401	NAP	C5B-O5B-PA-O2A
2	H	401	NAP	C5B-O5B-PA-O2A
2	J	401	NAP	C4B-C5B-O5B-PA

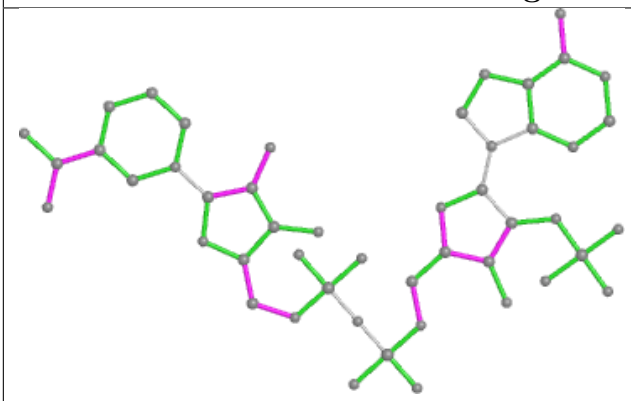
There are no ring outliers.

3 monomers are involved in 3 short contacts:

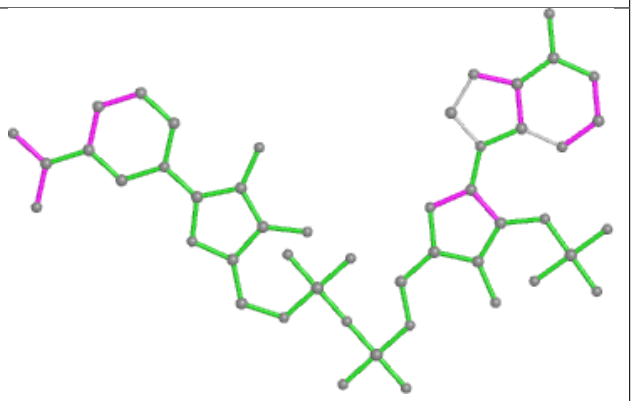
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	NAP	1	0
2	C	401	NAP	1	0
2	A	401	NAP	1	0

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.

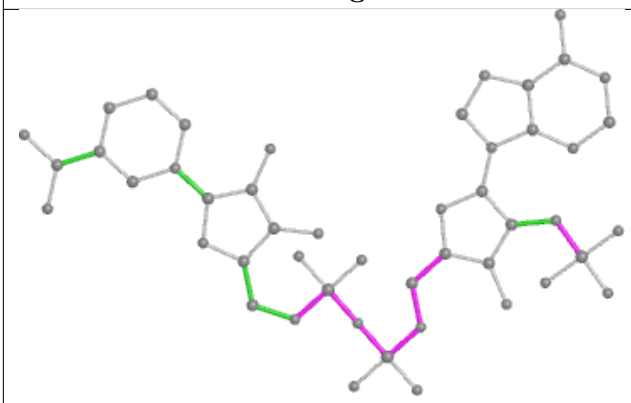
Ligand NAP F 401



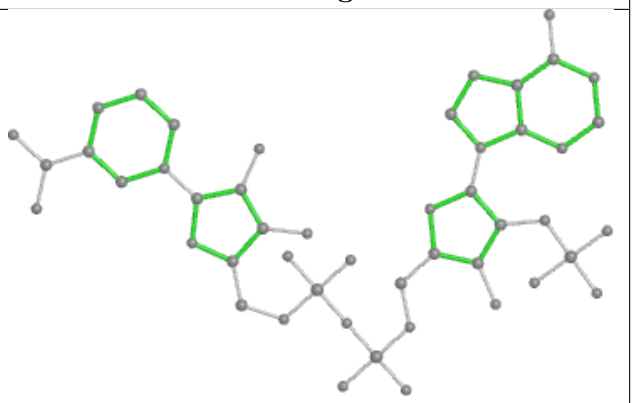
Bond lengths



Bond angles

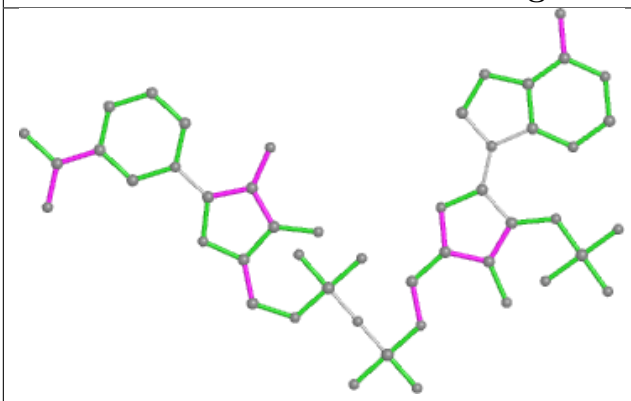


Torsions



Rings

Ligand NAP I 401



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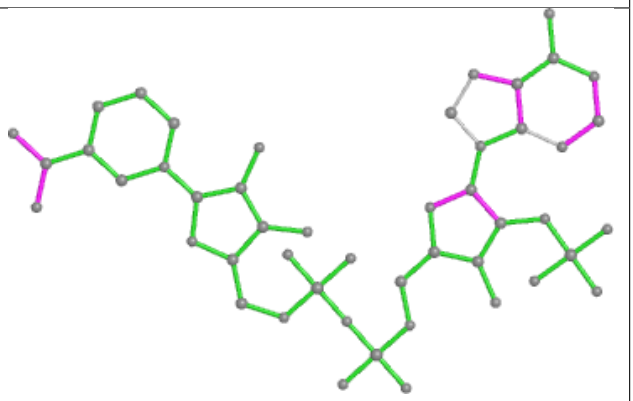

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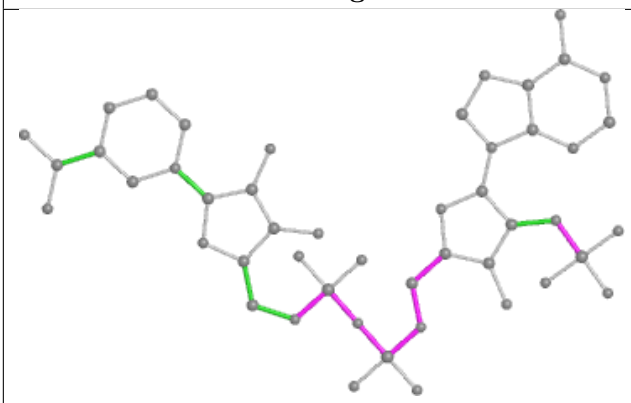

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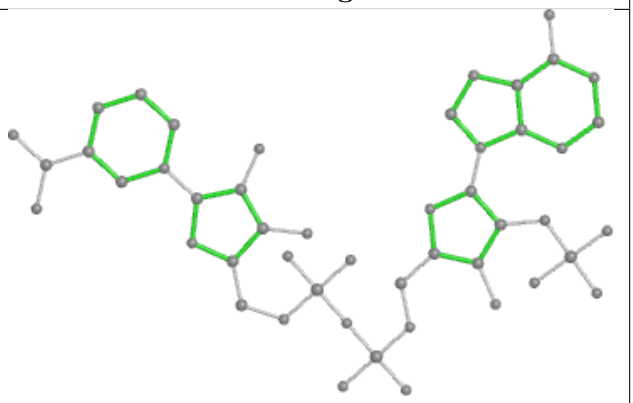

Rings

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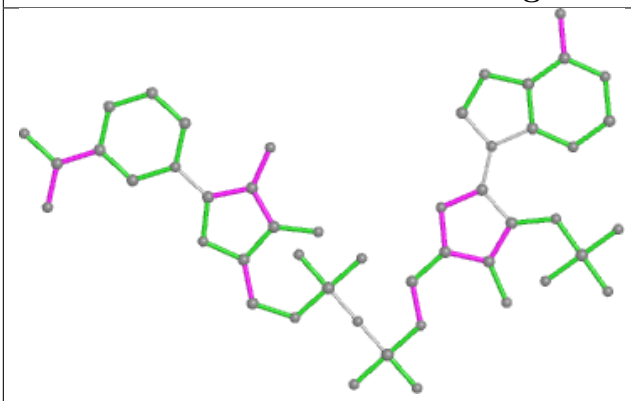

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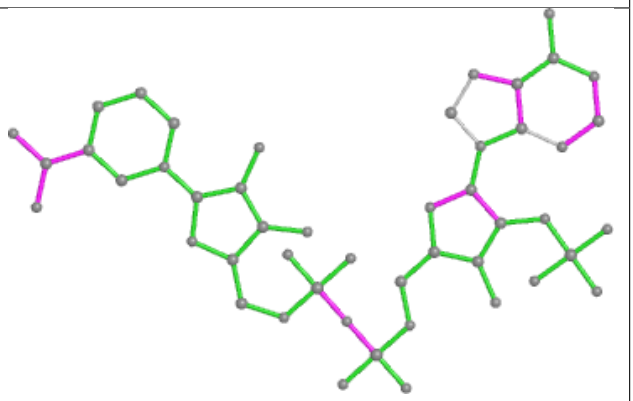
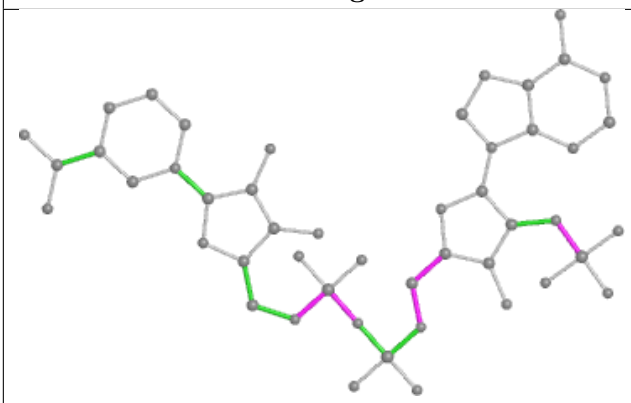


Bond angles



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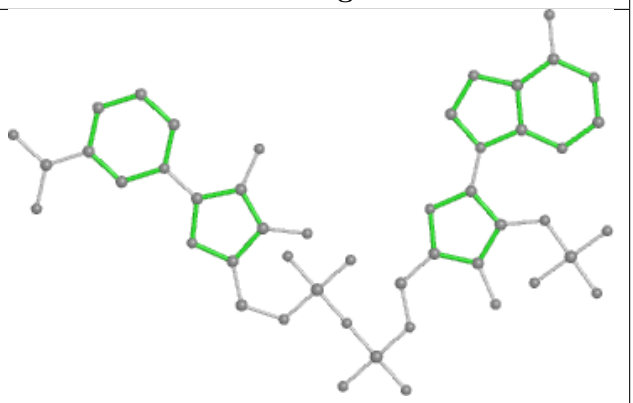
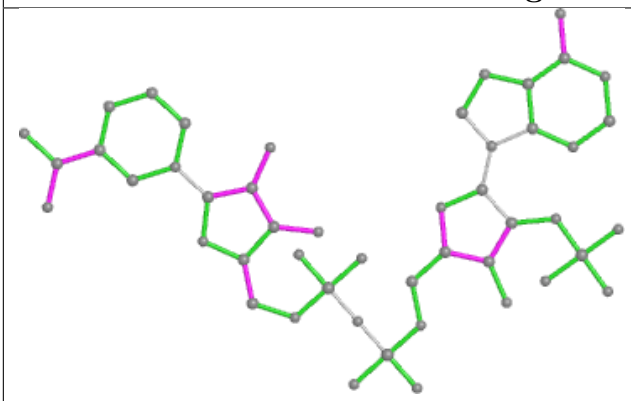


Rings

Ligand NAP J 401



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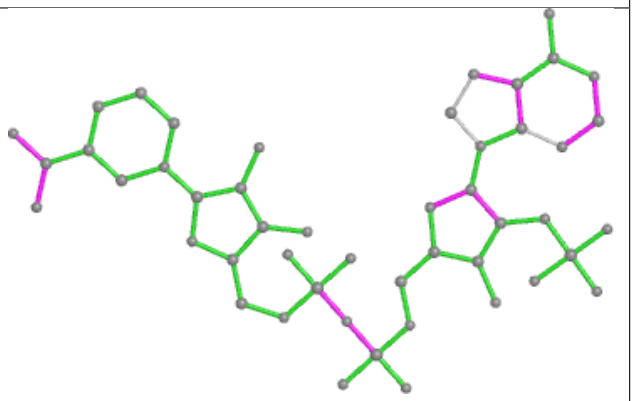
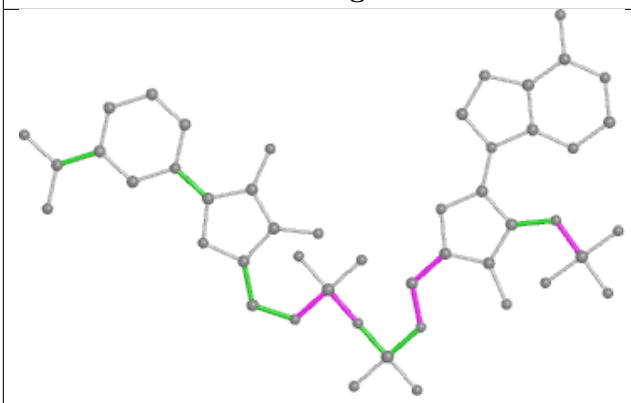


Bond angles



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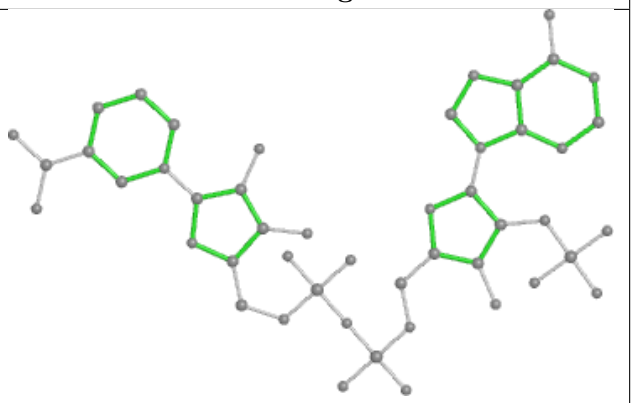
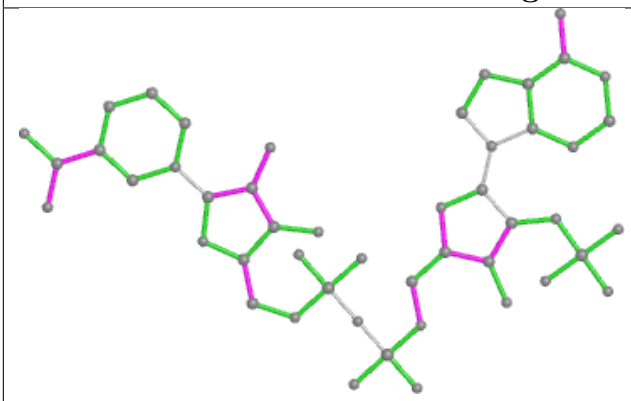


Rings

Ligand NAP C 401



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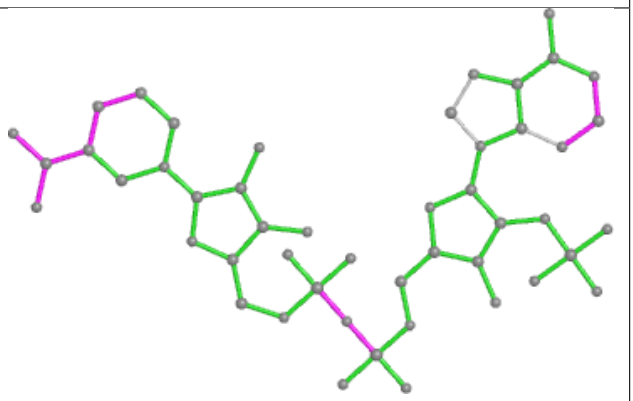

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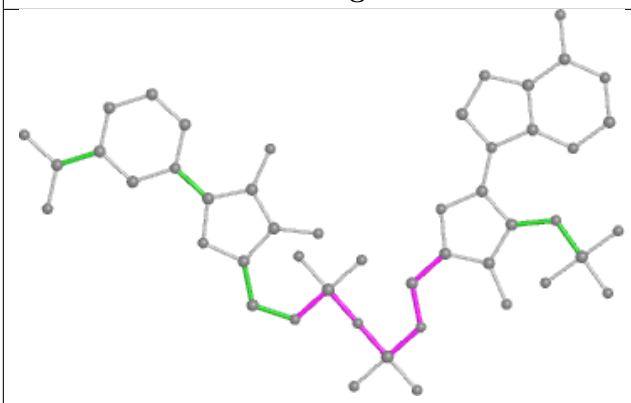

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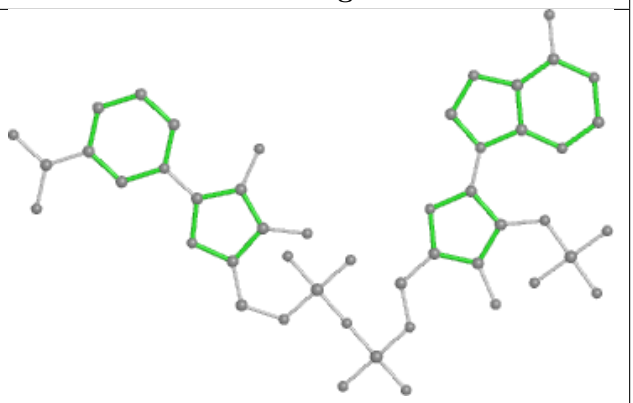

Rings

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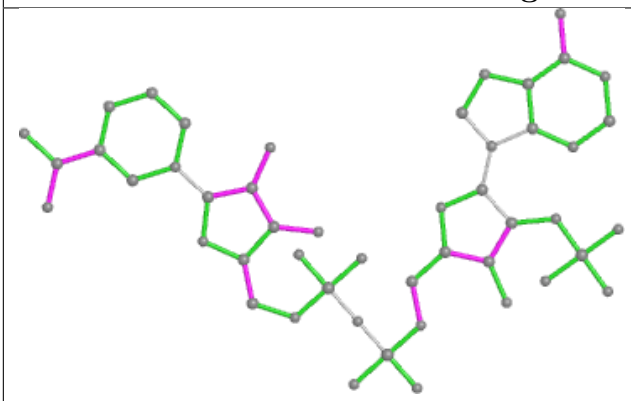

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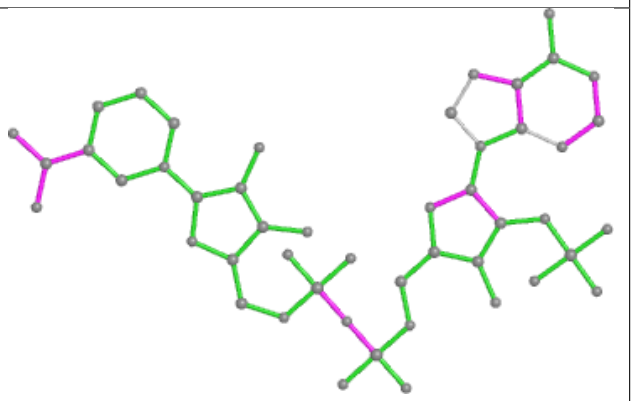
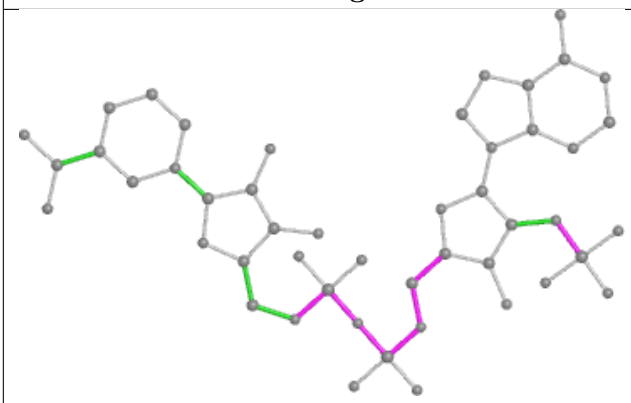


Bond angles



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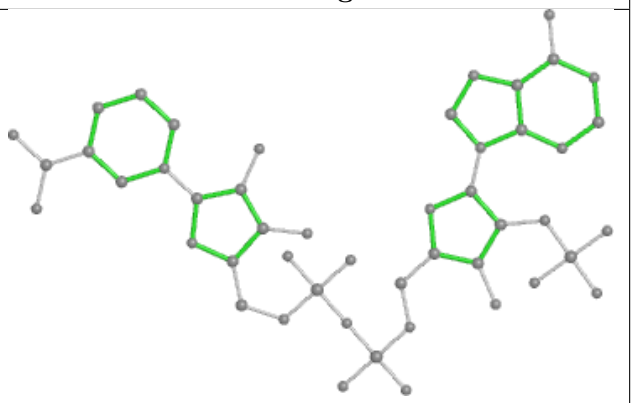
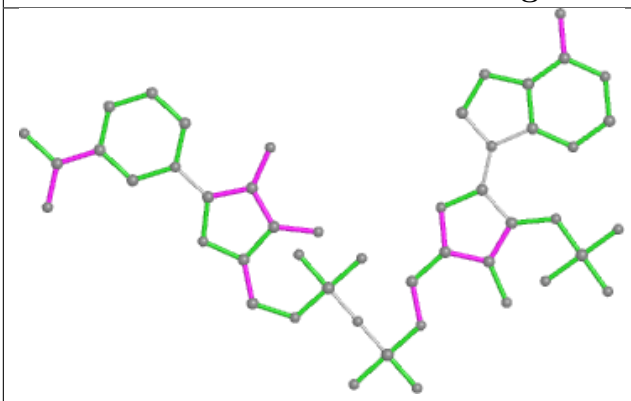


Rings

Ligand NAP D 401



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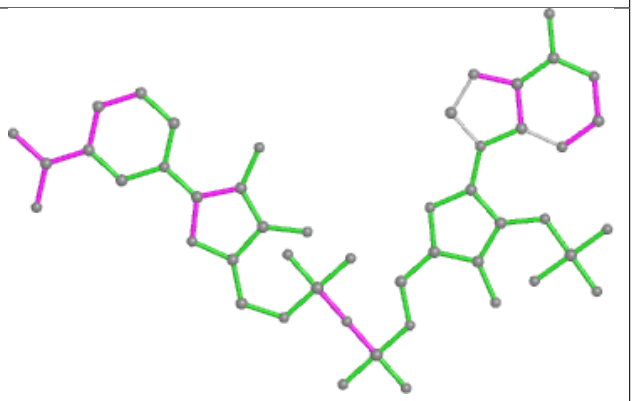
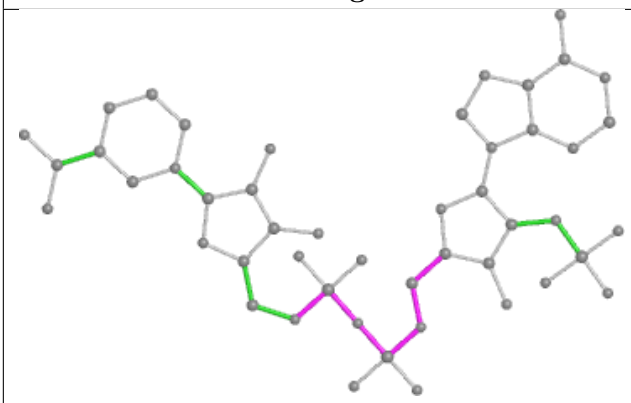


Bond angles



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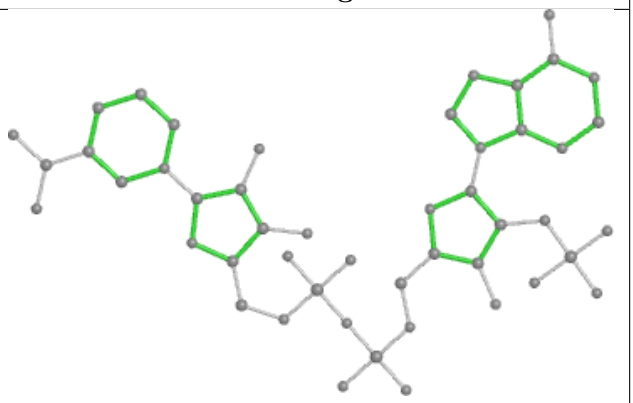
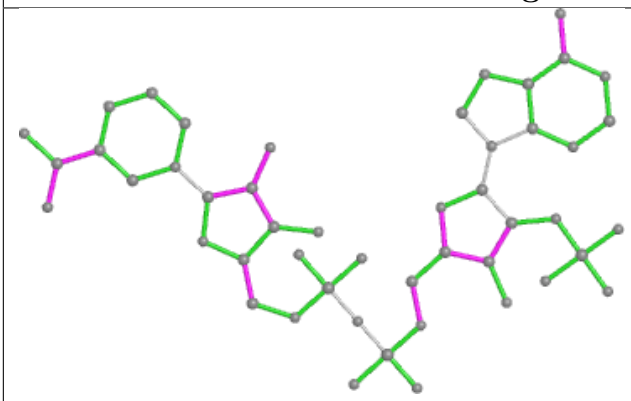


Rings

Ligand NAP B 401



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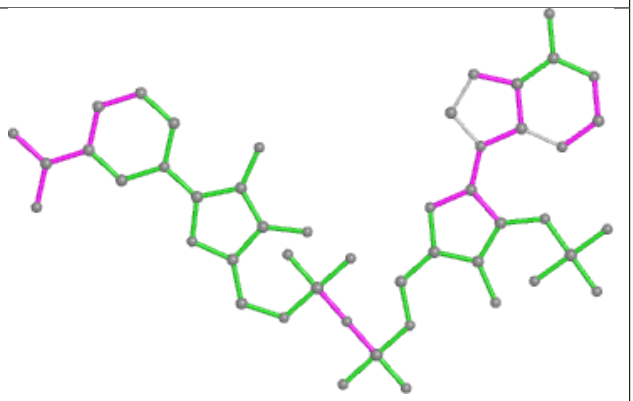
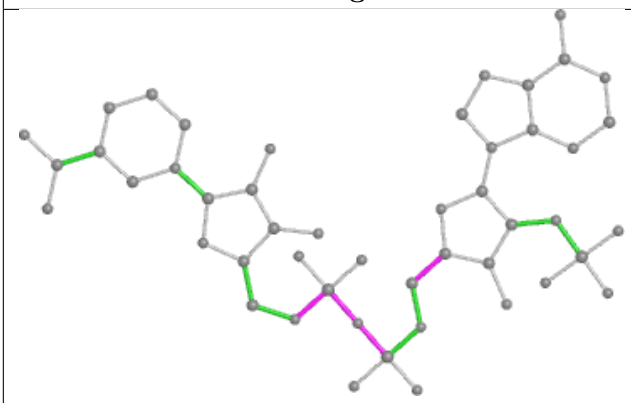
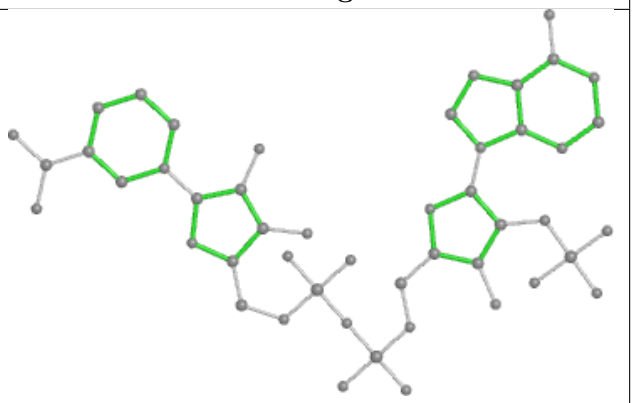


Bond angles

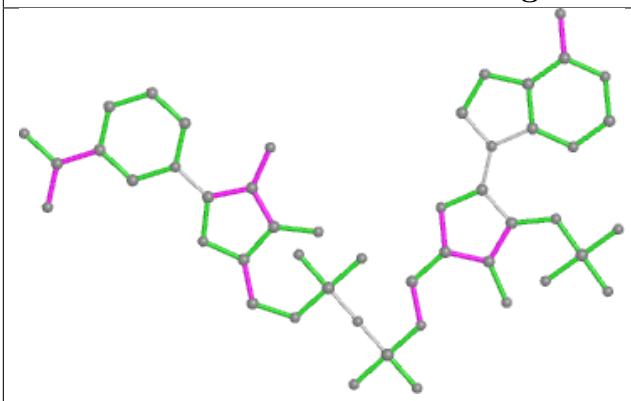


Torsions

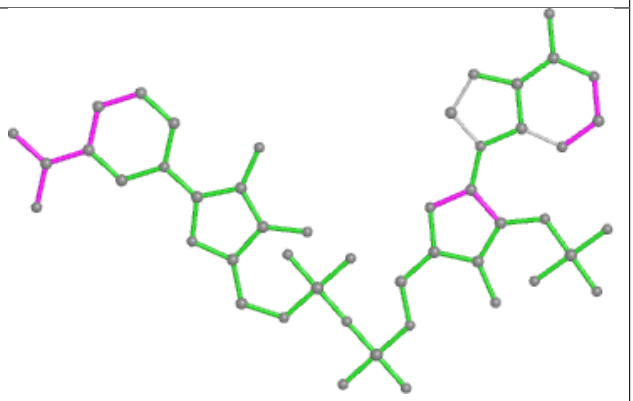


Rings

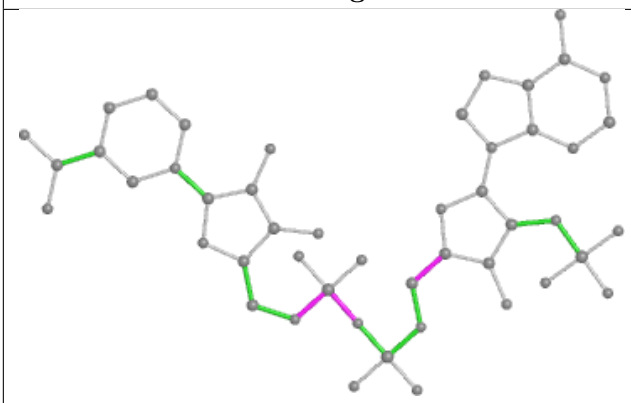
Ligand NAP A 401



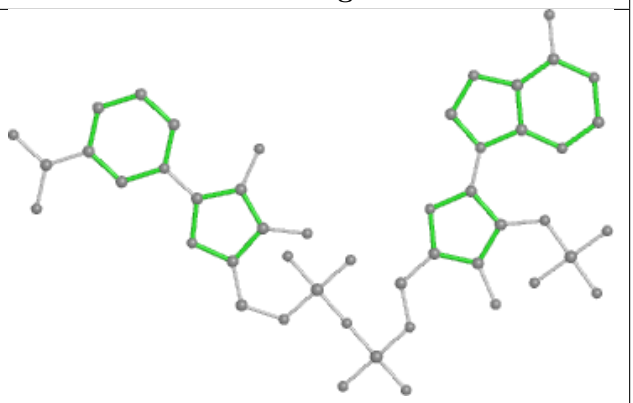
Bond lengths



Bond angles

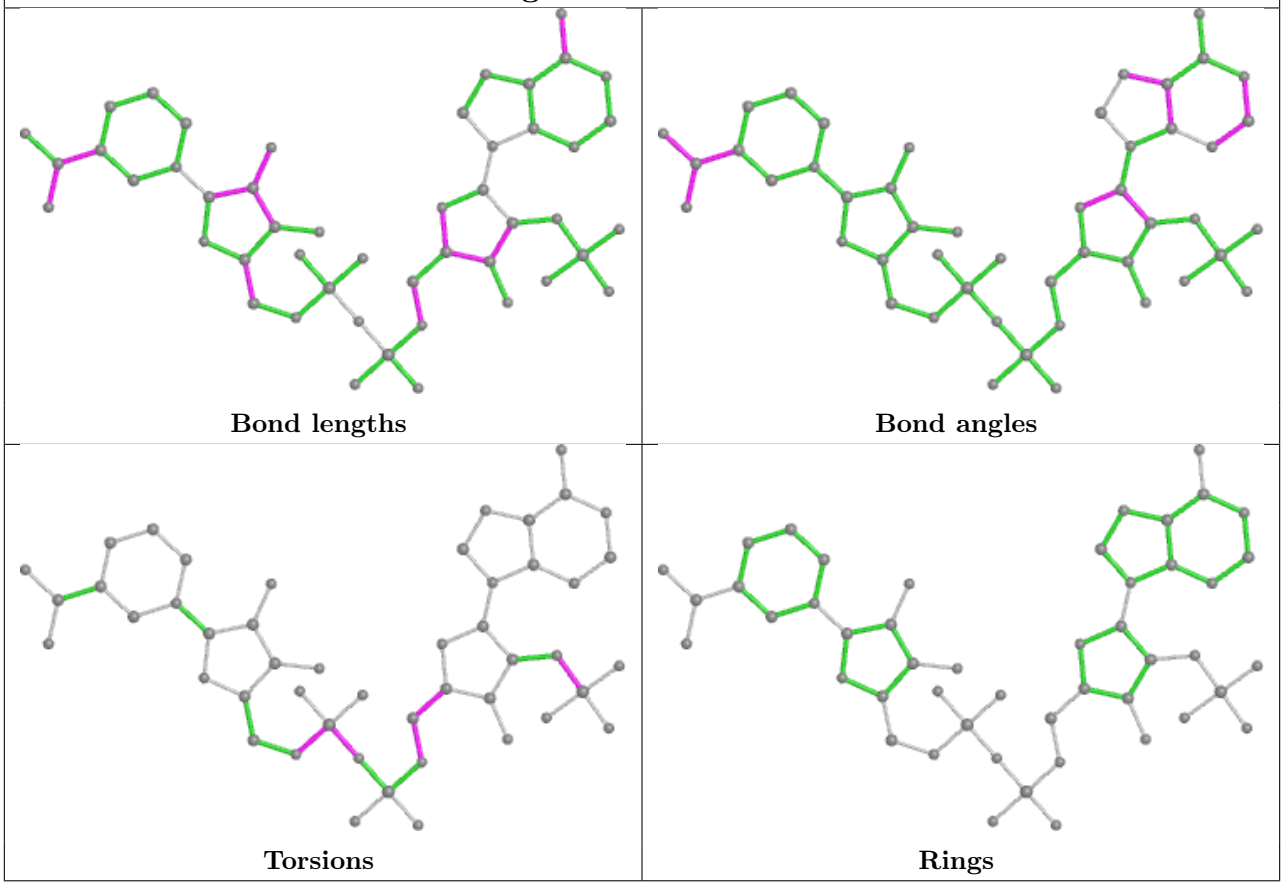


Torsions



Rings

Ligand NAP G 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/342 (96%)	-0.36	3 (0%) 84 82	31, 43, 65, 98	0
1	B	330/342 (96%)	0.59	50 (15%) 2 1	37, 68, 97, 116	0
1	C	330/342 (96%)	-0.10	11 (3%) 46 39	37, 56, 74, 126	0
1	D	330/342 (96%)	-0.31	7 (2%) 63 58	30, 44, 67, 108	0
1	E	330/342 (96%)	-0.35	4 (1%) 79 76	29, 43, 63, 106	0
1	F	330/342 (96%)	-0.42	3 (0%) 84 82	27, 38, 58, 105	0
1	G	330/342 (96%)	-0.40	5 (1%) 73 70	28, 40, 58, 109	0
1	H	330/342 (96%)	-0.31	7 (2%) 63 58	30, 45, 66, 114	0
1	I	330/342 (96%)	-0.25	4 (1%) 79 76	34, 51, 70, 109	0
1	J	330/342 (96%)	0.18	28 (8%) 10 7	33, 56, 96, 125	0
All	All	3300/3420 (96%)	-0.17	122 (3%) 41 34	27, 47, 85, 126	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	330	LEU	10.1
1	C	330	LEU	9.5
1	G	330	LEU	8.2
1	B	330	LEU	8.0
1	B	264	GLY	8.0
1	D	330	LEU	7.3
1	I	330	LEU	7.2
1	F	330	LEU	6.6
1	H	330	LEU	6.5
1	B	271	ALA	6.4
1	J	329	GLN	6.3
1	B	329	GLN	6.1
1	J	266	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	330	LEU	5.5
1	B	327	PHE	5.5
1	B	270	LEU	4.9
1	B	205	GLY	4.8
1	B	266	PRO	4.6
1	J	271	ALA	4.5
1	A	330	LEU	4.5
1	J	269	THR	4.4
1	B	290	GLY	4.4
1	B	193	ALA	4.3
1	B	316	GLN	4.2
1	J	204	SER	4.2
1	J	286	ASP	4.1
1	B	265	GLN	4.0
1	J	205	GLY	4.0
1	G	286	ASP	3.9
1	B	206	TYR	3.9
1	B	260	ARG	3.8
1	J	270	LEU	3.8
1	B	247	PRO	3.8
1	B	204	SER	3.8
1	J	263	GLU	3.7
1	J	327	PHE	3.7
1	I	287	ALA	3.6
1	B	267	ALA	3.6
1	D	329	GLN	3.6
1	B	286	ASP	3.5
1	J	289	ARG	3.5
1	J	264	GLY	3.5
1	B	262	LEU	3.5
1	B	252	ALA	3.4
1	J	324	ARG	3.4
1	B	287	ALA	3.3
1	B	285	PRO	3.3
1	G	329	GLN	3.3
1	B	255	VAL	3.3
1	B	124	SER	3.2
1	I	204	SER	3.2
1	B	309	ASP	3.2
1	B	256	VAL	3.2
1	E	329	GLN	3.2
1	B	253	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	189	ASN	3.1
1	B	155	PRO	3.1
1	J	194	GLU	3.1
1	B	263	GLU	3.1
1	B	261	ALA	3.0
1	B	156	GLY	3.0
1	J	273	GLN	3.0
1	C	329	GLN	2.9
1	F	286	ASP	2.8
1	C	124	SER	2.8
1	H	286	ASP	2.8
1	B	269	THR	2.8
1	D	286	ASP	2.7
1	C	309	ASP	2.6
1	B	276	GLN	2.6
1	C	1	MET	2.6
1	J	258	THR	2.6
1	J	265	GLN	2.5
1	B	210	GLU	2.5
1	B	320	ASP	2.5
1	B	129	GLU	2.5
1	J	156	GLY	2.5
1	E	156	GLY	2.4
1	J	129	GLU	2.4
1	B	289	ARG	2.4
1	B	192	ARG	2.4
1	H	204	SER	2.4
1	J	287	ALA	2.4
1	C	264	GLY	2.4
1	A	204	SER	2.4
1	J	255	VAL	2.4
1	J	283	PRO	2.3
1	D	255	VAL	2.3
1	B	131	GLU	2.3
1	B	122	GLY	2.3
1	C	311	PRO	2.3
1	B	194	GLU	2.3
1	B	259	LEU	2.2
1	F	158	LYS	2.2
1	C	244	ARG	2.2
1	B	282	VAL	2.2
1	D	265	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	309	ASP	2.2
1	H	266	PRO	2.2
1	H	158	LYS	2.2
1	J	244	ARG	2.2
1	B	24	GLY	2.2
1	J	193	ALA	2.2
1	I	158	LYS	2.1
1	C	194	GLU	2.1
1	E	286	ASP	2.1
1	G	244	ARG	2.1
1	B	203	TYR	2.1
1	J	259	LEU	2.1
1	A	244	ARG	2.1
1	D	266	PRO	2.1
1	B	179	ARG	2.1
1	B	244	ARG	2.1
1	J	260	ARG	2.1
1	B	125	ARG	2.1
1	H	263	GLU	2.1
1	J	290	GLY	2.1
1	C	255	VAL	2.0
1	C	131	GLU	2.0
1	G	287	ALA	2.0
1	B	72	VAL	2.0
1	D	68	LYS	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)

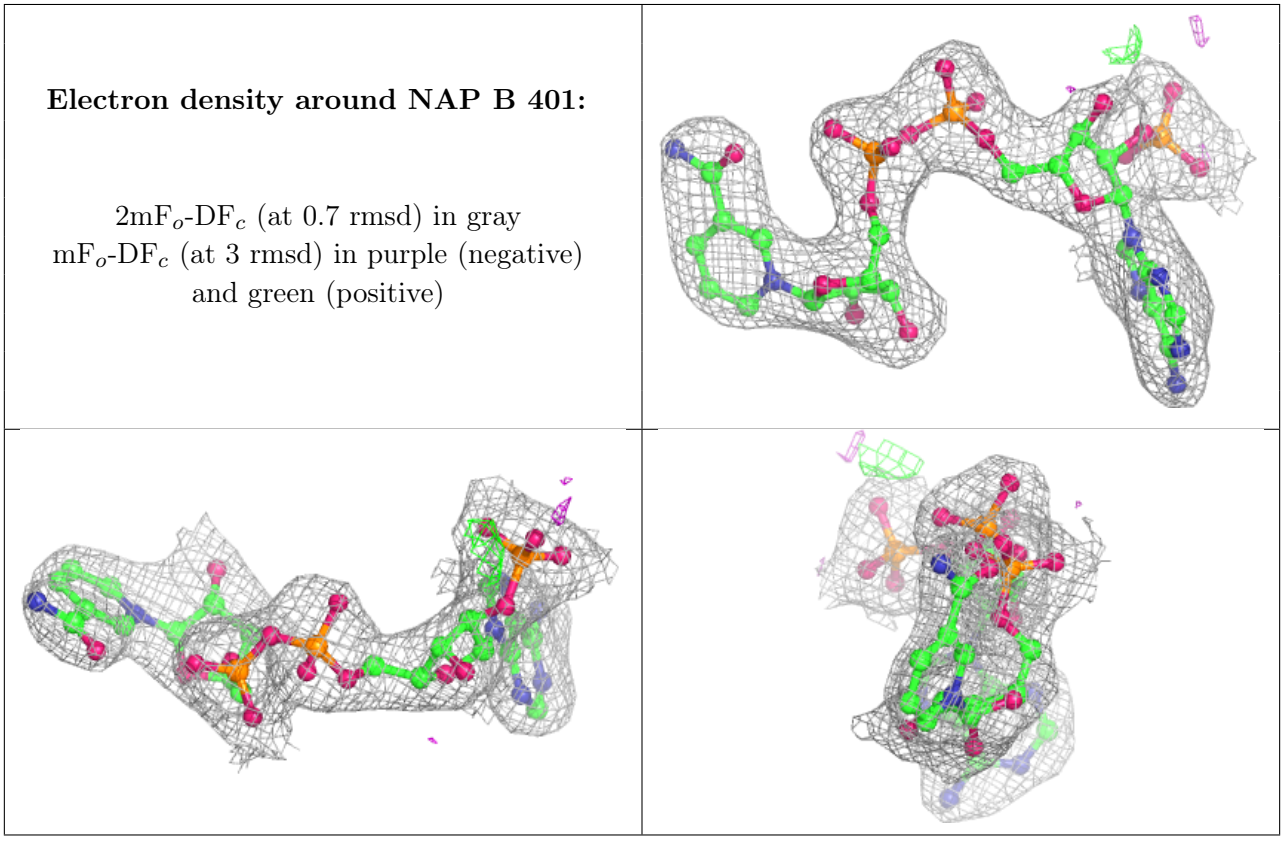
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B	401	48/48	0.97	0.11	34,46,54,57	0
2	NAP	C	401	48/48	0.98	0.10	35,40,46,48	0
2	NAP	D	401	48/48	0.98	0.12	29,35,40,43	0
2	NAP	E	401	48/48	0.98	0.10	24,30,35,37	0
2	NAP	G	401	48/48	0.98	0.12	25,31,34,39	0
2	NAP	I	401	48/48	0.98	0.10	32,38,44,49	0
2	NAP	A	401	48/48	0.99	0.10	27,34,38,40	0
2	NAP	H	401	48/48	0.99	0.10	27,33,39,42	0
2	NAP	F	401	48/48	0.99	0.10	24,31,34,34	0
2	NAP	J	401	48/48	0.99	0.10	31,39,46,48	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.

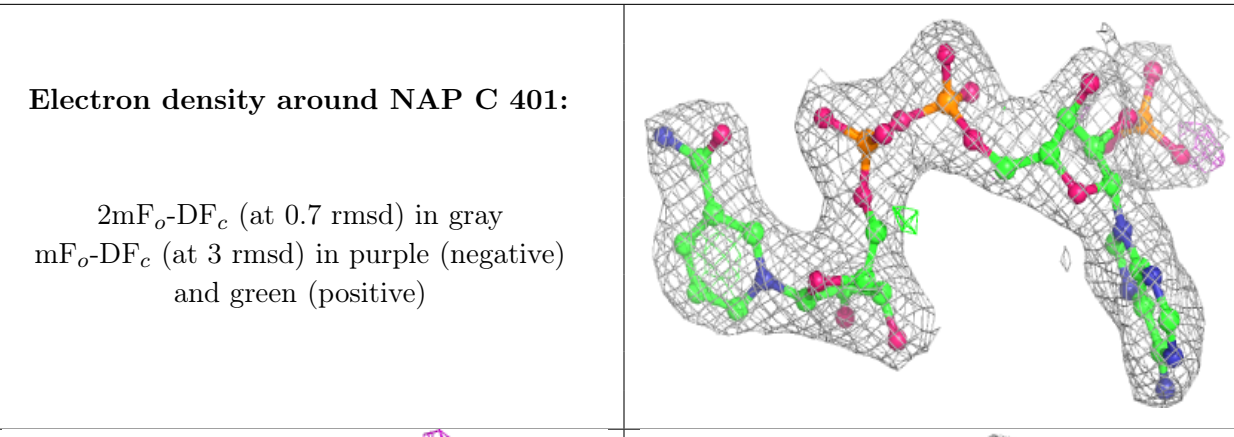
Electron density around NAP B 401:

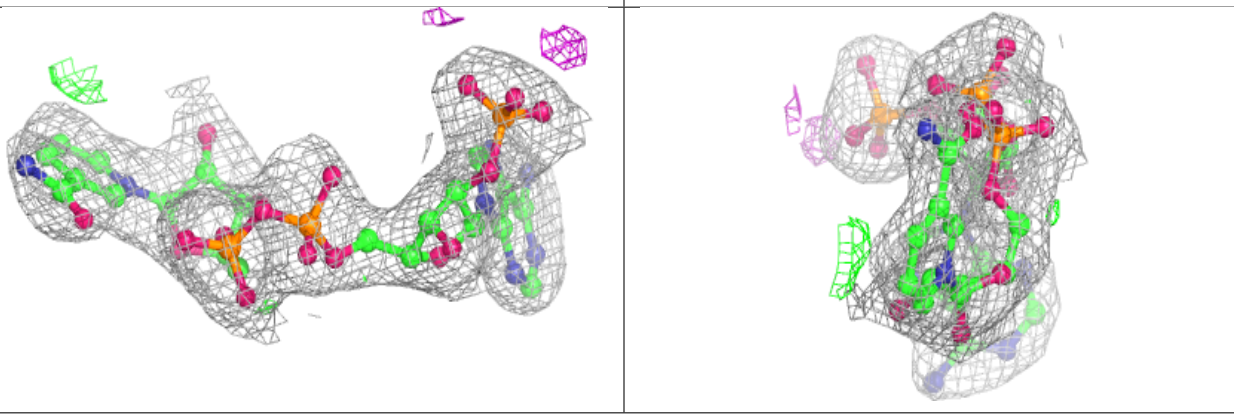
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP C 401:

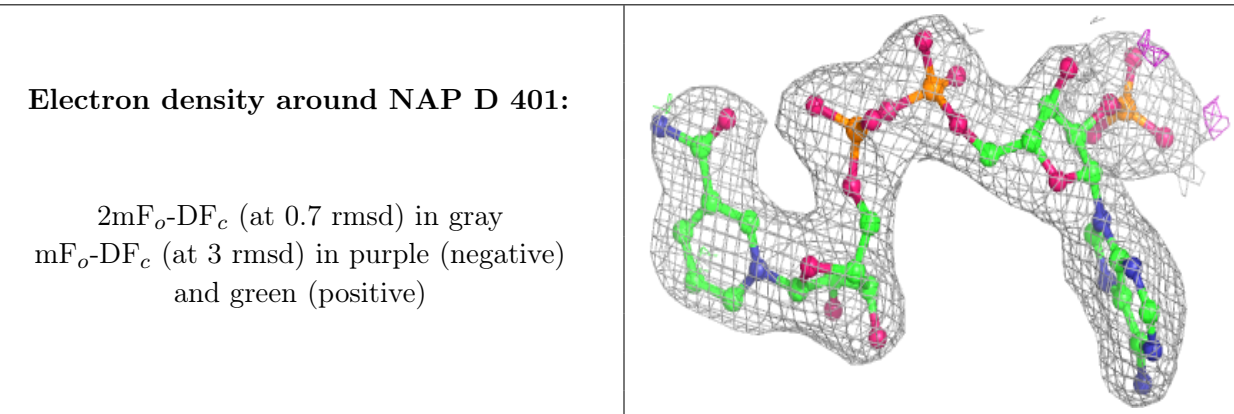
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

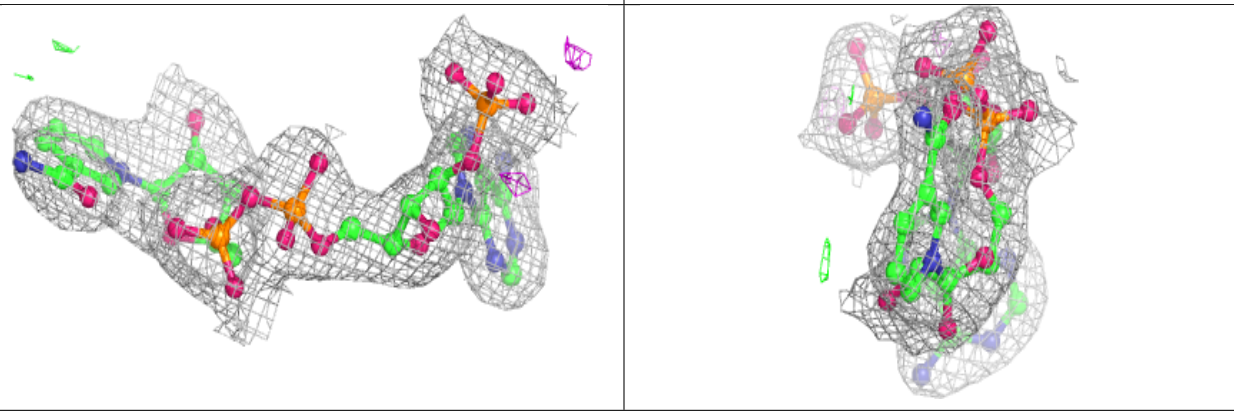




Electron density around NAP D 401:

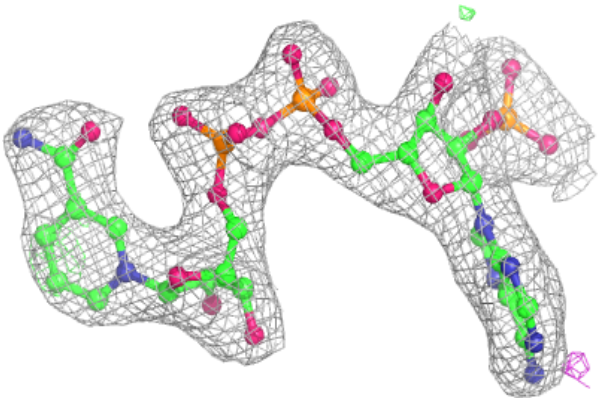
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

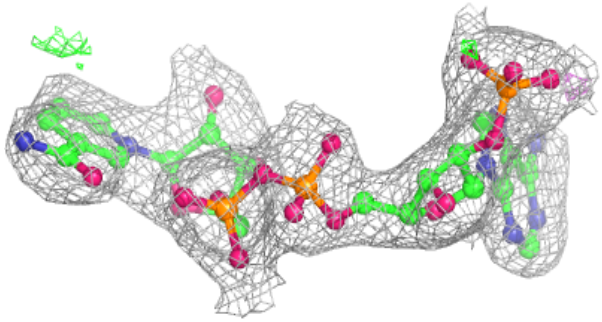


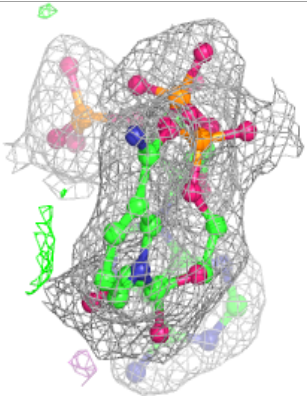


Electron density around NAP E 401:

$2mF_o$-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 401:

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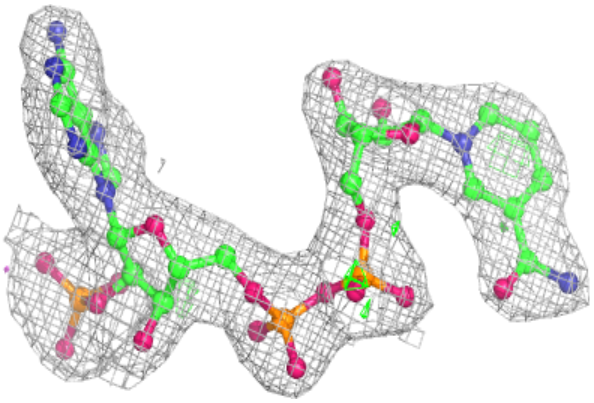
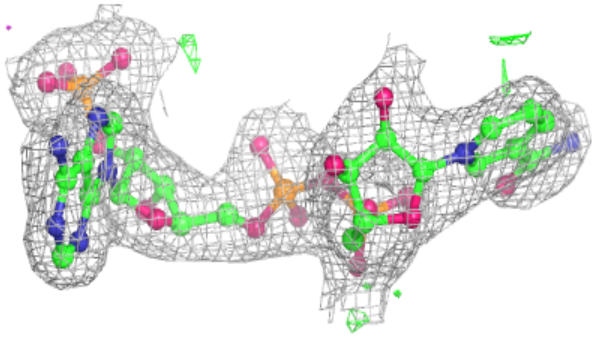
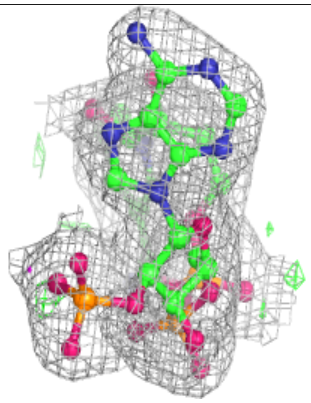
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around NAP I 401:

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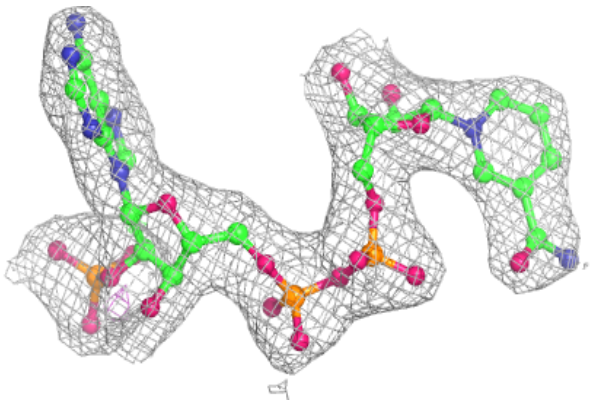
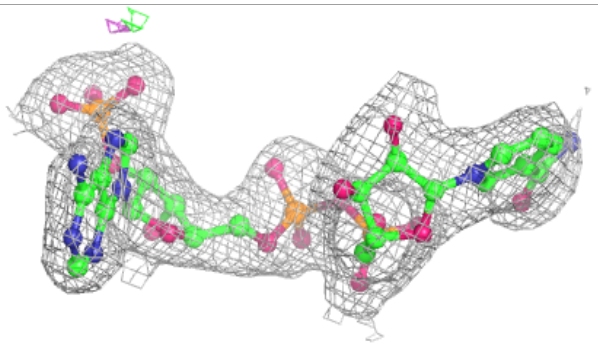
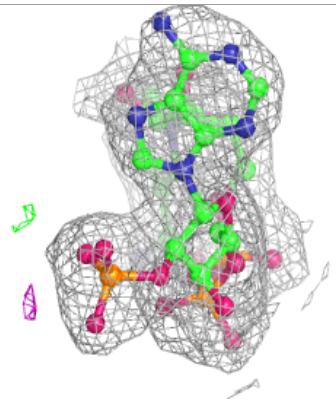
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around NAP A 401:

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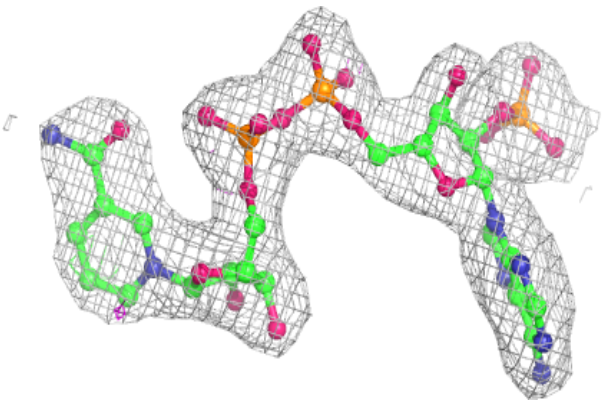
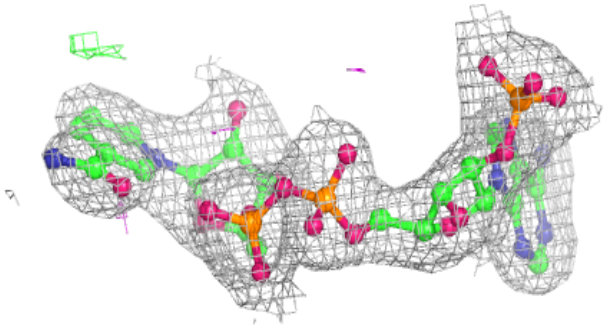
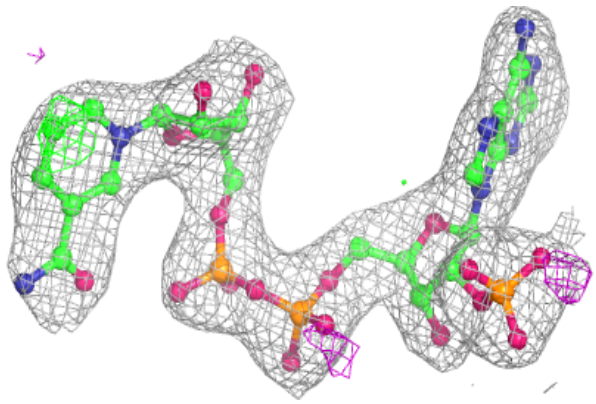
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

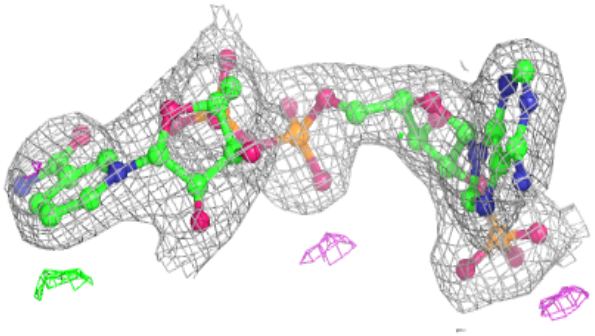


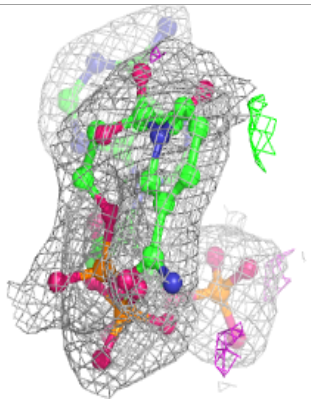


Electron density around NAP H 401:

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

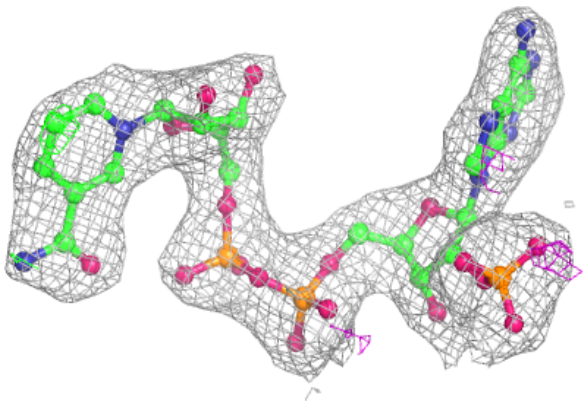


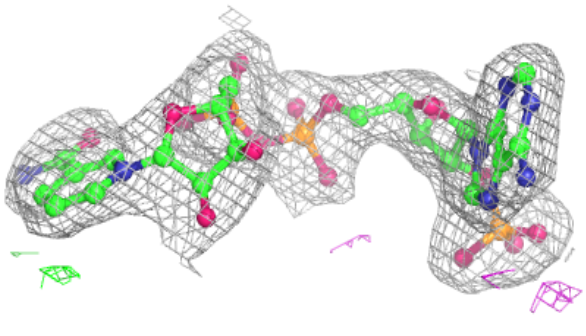


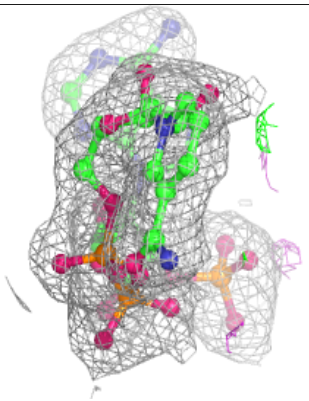


Electron density around NAP F 401:

$2mF_o$-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 401:

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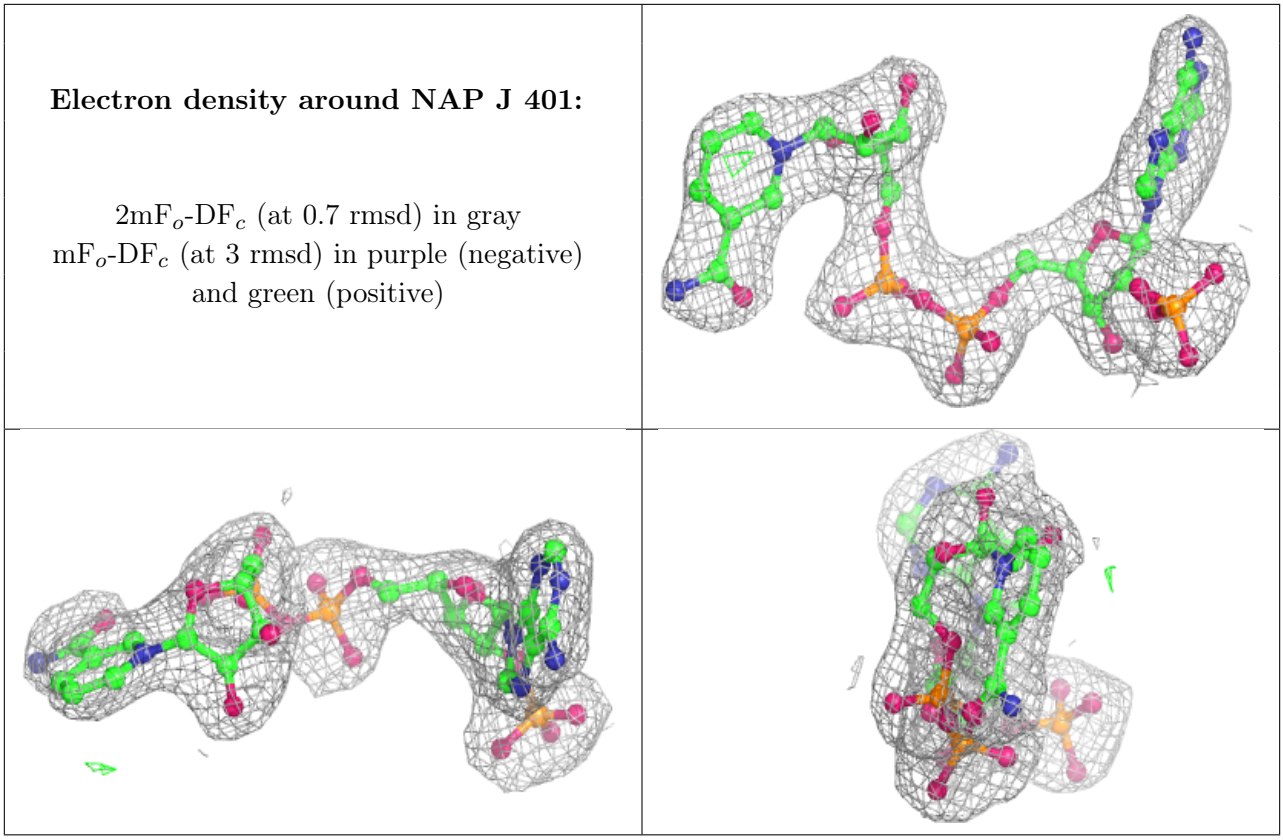
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.