Full wwPDB X-ray Structure Validation Report

Sep 5, 2023 – 06:28 AM EDT

PDB ID	:	3TOX
Title	:	Crystal structure of a short chain dehydrogenase in complex with NAD(P) from Sinorhizobium meliloti 1021
Authors	:	Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-09-06
Resolution	:	1.93 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 (1)) were used in the production of this report:

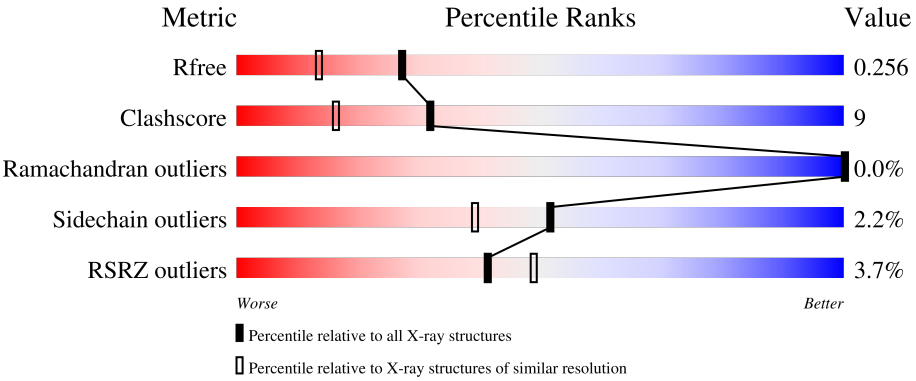
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	280	2% 79% 11% • 9%
1	B	280	5% 75% 12% • 11%
1	C	280	% 81% 9% • 9%
1	D	280	3% 80% 10% • 9%
1	E	280	6% 71% 18% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	280	
1	G	280	
1	I	280	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15313 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	B	248	Total	C	N	O	S	0	0	0
			1725	1080	306	338	1			
1	C	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	D	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	E	254	Total	C	N	O	S	0	0	0
			1764	1105	312	346	1			
1	F	254	Total	C	N	O	S	0	0	0
			1761	1102	312	346	1			
1	G	251	Total	C	N	O	S	0	0	0
			1745	1094	309	341	1			
1	I	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q92SS3
A	2	VAL	-	expression tag	UNP Q92SS3
A	259	ALA	-	expression tag	UNP Q92SS3
A	260	GLU	-	expression tag	UNP Q92SS3
A	261	ASN	-	expression tag	UNP Q92SS3
A	262	LEU	-	expression tag	UNP Q92SS3
A	263	TYR	-	expression tag	UNP Q92SS3
A	264	PHE	-	expression tag	UNP Q92SS3
A	265	GLN	-	expression tag	UNP Q92SS3
A	266	SER	-	expression tag	UNP Q92SS3
A	267	HIS	-	expression tag	UNP Q92SS3
A	268	HIS	-	expression tag	UNP Q92SS3
A	269	HIS	-	expression tag	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	HIS	-	expression tag	UNP Q92SS3
A	271	HIS	-	expression tag	UNP Q92SS3
A	272	HIS	-	expression tag	UNP Q92SS3
A	273	TRP	-	expression tag	UNP Q92SS3
A	274	SER	-	expression tag	UNP Q92SS3
A	275	HIS	-	expression tag	UNP Q92SS3
A	276	PRO	-	expression tag	UNP Q92SS3
A	277	GLN	-	expression tag	UNP Q92SS3
A	278	PHE	-	expression tag	UNP Q92SS3
A	279	GLU	-	expression tag	UNP Q92SS3
A	280	LYS	-	expression tag	UNP Q92SS3
B	1	MET	-	expression tag	UNP Q92SS3
B	2	VAL	-	expression tag	UNP Q92SS3
B	259	ALA	-	expression tag	UNP Q92SS3
B	260	GLU	-	expression tag	UNP Q92SS3
B	261	ASN	-	expression tag	UNP Q92SS3
B	262	LEU	-	expression tag	UNP Q92SS3
B	263	TYR	-	expression tag	UNP Q92SS3
B	264	PHE	-	expression tag	UNP Q92SS3
B	265	GLN	-	expression tag	UNP Q92SS3
B	266	SER	-	expression tag	UNP Q92SS3
B	267	HIS	-	expression tag	UNP Q92SS3
B	268	HIS	-	expression tag	UNP Q92SS3
B	269	HIS	-	expression tag	UNP Q92SS3
B	270	HIS	-	expression tag	UNP Q92SS3
B	271	HIS	-	expression tag	UNP Q92SS3
B	272	HIS	-	expression tag	UNP Q92SS3
B	273	TRP	-	expression tag	UNP Q92SS3
B	274	SER	-	expression tag	UNP Q92SS3
B	275	HIS	-	expression tag	UNP Q92SS3
B	276	PRO	-	expression tag	UNP Q92SS3
B	277	GLN	-	expression tag	UNP Q92SS3
B	278	PHE	-	expression tag	UNP Q92SS3
B	279	GLU	-	expression tag	UNP Q92SS3
B	280	LYS	-	expression tag	UNP Q92SS3
C	1	MET	-	expression tag	UNP Q92SS3
C	2	VAL	-	expression tag	UNP Q92SS3
C	259	ALA	-	expression tag	UNP Q92SS3
C	260	GLU	-	expression tag	UNP Q92SS3
C	261	ASN	-	expression tag	UNP Q92SS3
C	262	LEU	-	expression tag	UNP Q92SS3
C	263	TYR	-	expression tag	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	264	PHE	-	expression tag	UNP Q92SS3
C	265	GLN	-	expression tag	UNP Q92SS3
C	266	SER	-	expression tag	UNP Q92SS3
C	267	HIS	-	expression tag	UNP Q92SS3
C	268	HIS	-	expression tag	UNP Q92SS3
C	269	HIS	-	expression tag	UNP Q92SS3
C	270	HIS	-	expression tag	UNP Q92SS3
C	271	HIS	-	expression tag	UNP Q92SS3
C	272	HIS	-	expression tag	UNP Q92SS3
C	273	TRP	-	expression tag	UNP Q92SS3
C	274	SER	-	expression tag	UNP Q92SS3
C	275	HIS	-	expression tag	UNP Q92SS3
C	276	PRO	-	expression tag	UNP Q92SS3
C	277	GLN	-	expression tag	UNP Q92SS3
C	278	PHE	-	expression tag	UNP Q92SS3
C	279	GLU	-	expression tag	UNP Q92SS3
C	280	LYS	-	expression tag	UNP Q92SS3
D	1	MET	-	expression tag	UNP Q92SS3
D	2	VAL	-	expression tag	UNP Q92SS3
D	259	ALA	-	expression tag	UNP Q92SS3
D	260	GLU	-	expression tag	UNP Q92SS3
D	261	ASN	-	expression tag	UNP Q92SS3
D	262	LEU	-	expression tag	UNP Q92SS3
D	263	TYR	-	expression tag	UNP Q92SS3
D	264	PHE	-	expression tag	UNP Q92SS3
D	265	GLN	-	expression tag	UNP Q92SS3
D	266	SER	-	expression tag	UNP Q92SS3
D	267	HIS	-	expression tag	UNP Q92SS3
D	268	HIS	-	expression tag	UNP Q92SS3
D	269	HIS	-	expression tag	UNP Q92SS3
D	270	HIS	-	expression tag	UNP Q92SS3
D	271	HIS	-	expression tag	UNP Q92SS3
D	272	HIS	-	expression tag	UNP Q92SS3
D	273	TRP	-	expression tag	UNP Q92SS3
D	274	SER	-	expression tag	UNP Q92SS3
D	275	HIS	-	expression tag	UNP Q92SS3
D	276	PRO	-	expression tag	UNP Q92SS3
D	277	GLN	-	expression tag	UNP Q92SS3
D	278	PHE	-	expression tag	UNP Q92SS3
D	279	GLU	-	expression tag	UNP Q92SS3
D	280	LYS	-	expression tag	UNP Q92SS3
E	1	MET	-	expression tag	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	VAL	-	expression tag	UNP Q92SS3
E	259	ALA	-	expression tag	UNP Q92SS3
E	260	GLU	-	expression tag	UNP Q92SS3
E	261	ASN	-	expression tag	UNP Q92SS3
E	262	LEU	-	expression tag	UNP Q92SS3
E	263	TYR	-	expression tag	UNP Q92SS3
E	264	PHE	-	expression tag	UNP Q92SS3
E	265	GLN	-	expression tag	UNP Q92SS3
E	266	SER	-	expression tag	UNP Q92SS3
E	267	HIS	-	expression tag	UNP Q92SS3
E	268	HIS	-	expression tag	UNP Q92SS3
E	269	HIS	-	expression tag	UNP Q92SS3
E	270	HIS	-	expression tag	UNP Q92SS3
E	271	HIS	-	expression tag	UNP Q92SS3
E	272	HIS	-	expression tag	UNP Q92SS3
E	273	TRP	-	expression tag	UNP Q92SS3
E	274	SER	-	expression tag	UNP Q92SS3
E	275	HIS	-	expression tag	UNP Q92SS3
E	276	PRO	-	expression tag	UNP Q92SS3
E	277	GLN	-	expression tag	UNP Q92SS3
E	278	PHE	-	expression tag	UNP Q92SS3
E	279	GLU	-	expression tag	UNP Q92SS3
E	280	LYS	-	expression tag	UNP Q92SS3
F	1	MET	-	expression tag	UNP Q92SS3
F	2	VAL	-	expression tag	UNP Q92SS3
F	259	ALA	-	expression tag	UNP Q92SS3
F	260	GLU	-	expression tag	UNP Q92SS3
F	261	ASN	-	expression tag	UNP Q92SS3
F	262	LEU	-	expression tag	UNP Q92SS3
F	263	TYR	-	expression tag	UNP Q92SS3
F	264	PHE	-	expression tag	UNP Q92SS3
F	265	GLN	-	expression tag	UNP Q92SS3
F	266	SER	-	expression tag	UNP Q92SS3
F	267	HIS	-	expression tag	UNP Q92SS3
F	268	HIS	-	expression tag	UNP Q92SS3
F	269	HIS	-	expression tag	UNP Q92SS3
F	270	HIS	-	expression tag	UNP Q92SS3
F	271	HIS	-	expression tag	UNP Q92SS3
F	272	HIS	-	expression tag	UNP Q92SS3
F	273	TRP	-	expression tag	UNP Q92SS3
F	274	SER	-	expression tag	UNP Q92SS3
F	275	HIS	-	expression tag	UNP Q92SS3

Continued on next page...

Continued from previous page...

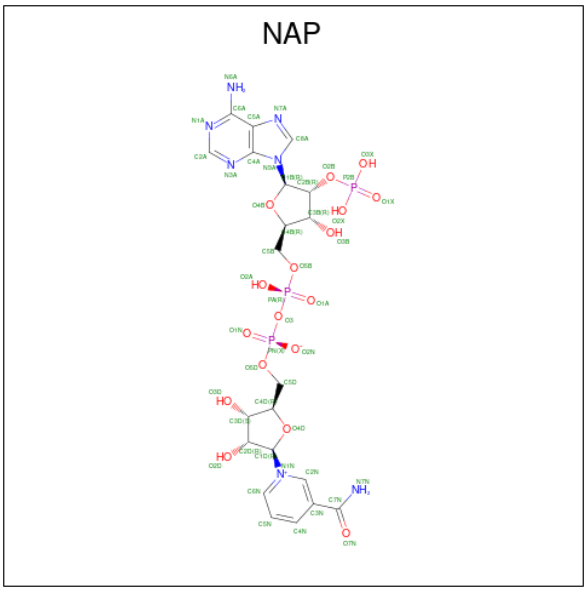
Chain	Residue	Modelled	Actual	Comment	Reference
F	276	PRO	-	expression tag	UNP Q92SS3
F	277	GLN	-	expression tag	UNP Q92SS3
F	278	PHE	-	expression tag	UNP Q92SS3
F	279	GLU	-	expression tag	UNP Q92SS3
F	280	LYS	-	expression tag	UNP Q92SS3
G	1	MET	-	expression tag	UNP Q92SS3
G	2	VAL	-	expression tag	UNP Q92SS3
G	259	ALA	-	expression tag	UNP Q92SS3
G	260	GLU	-	expression tag	UNP Q92SS3
G	261	ASN	-	expression tag	UNP Q92SS3
G	262	LEU	-	expression tag	UNP Q92SS3
G	263	TYR	-	expression tag	UNP Q92SS3
G	264	PHE	-	expression tag	UNP Q92SS3
G	265	GLN	-	expression tag	UNP Q92SS3
G	266	SER	-	expression tag	UNP Q92SS3
G	267	HIS	-	expression tag	UNP Q92SS3
G	268	HIS	-	expression tag	UNP Q92SS3
G	269	HIS	-	expression tag	UNP Q92SS3
G	270	HIS	-	expression tag	UNP Q92SS3
G	271	HIS	-	expression tag	UNP Q92SS3
G	272	HIS	-	expression tag	UNP Q92SS3
G	273	TRP	-	expression tag	UNP Q92SS3
G	274	SER	-	expression tag	UNP Q92SS3
G	275	HIS	-	expression tag	UNP Q92SS3
G	276	PRO	-	expression tag	UNP Q92SS3
G	277	GLN	-	expression tag	UNP Q92SS3
G	278	PHE	-	expression tag	UNP Q92SS3
G	279	GLU	-	expression tag	UNP Q92SS3
G	280	LYS	-	expression tag	UNP Q92SS3
I	1	MET	-	expression tag	UNP Q92SS3
I	2	VAL	-	expression tag	UNP Q92SS3
I	259	ALA	-	expression tag	UNP Q92SS3
I	260	GLU	-	expression tag	UNP Q92SS3
I	261	ASN	-	expression tag	UNP Q92SS3
I	262	LEU	-	expression tag	UNP Q92SS3
I	263	TYR	-	expression tag	UNP Q92SS3
I	264	PHE	-	expression tag	UNP Q92SS3
I	265	GLN	-	expression tag	UNP Q92SS3
I	266	SER	-	expression tag	UNP Q92SS3
I	267	HIS	-	expression tag	UNP Q92SS3
I	268	HIS	-	expression tag	UNP Q92SS3
I	269	HIS	-	expression tag	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	270	HIS	-	expression tag	UNP Q92SS3
I	271	HIS	-	expression tag	UNP Q92SS3
I	272	HIS	-	expression tag	UNP Q92SS3
I	273	TRP	-	expression tag	UNP Q92SS3
I	274	SER	-	expression tag	UNP Q92SS3
I	275	HIS	-	expression tag	UNP Q92SS3
I	276	PRO	-	expression tag	UNP Q92SS3
I	277	GLN	-	expression tag	UNP Q92SS3
I	278	PHE	-	expression tag	UNP Q92SS3
I	279	GLU	-	expression tag	UNP Q92SS3
I	280	LYS	-	expression tag	UNP Q92SS3

- 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		

Continued on next page...

Continued from previous page...

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

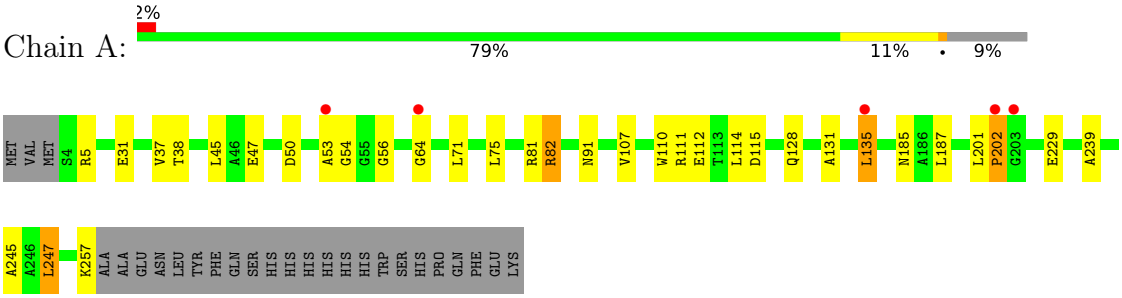
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	82	Total	O	0	0
			82	82		
3	C	130	Total	O	0	0
			130	130		
3	D	117	Total	O	0	0
			117	117		
3	E	96	Total	O	0	0
			96	96		
3	F	79	Total	O	0	0
			79	79		
3	G	92	Total	O	0	0
			92	92		
3	I	132	Total	O	0	0
			132	132		

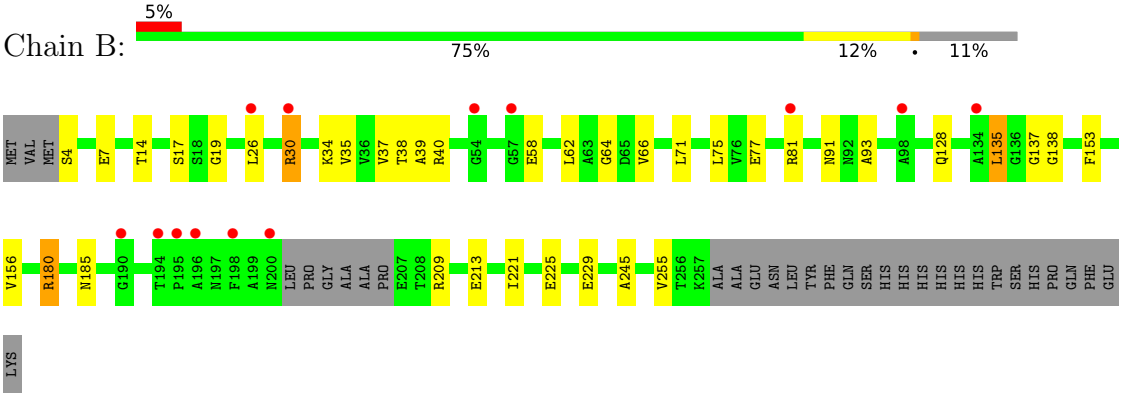
3 Residue-property plots (i)

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.

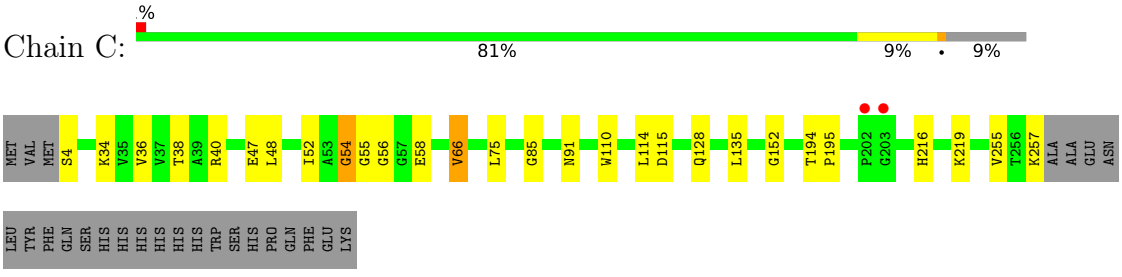
• Molecule 1: Short chain dehydrogenase



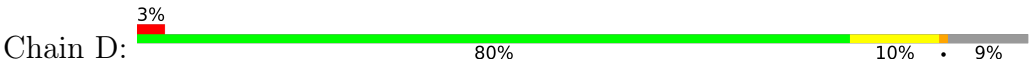
• Molecule 1: Short chain dehydrogenase

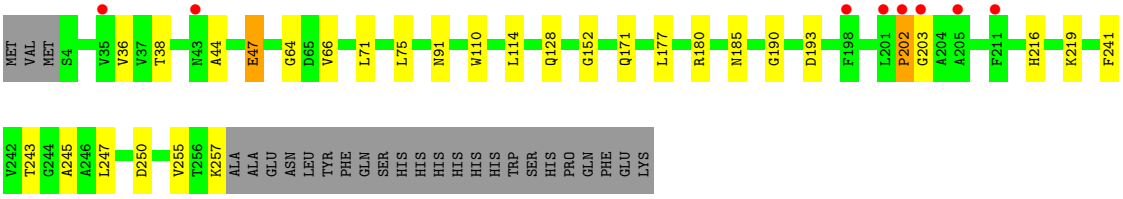


• Molecule 1: Short chain dehydrogenase



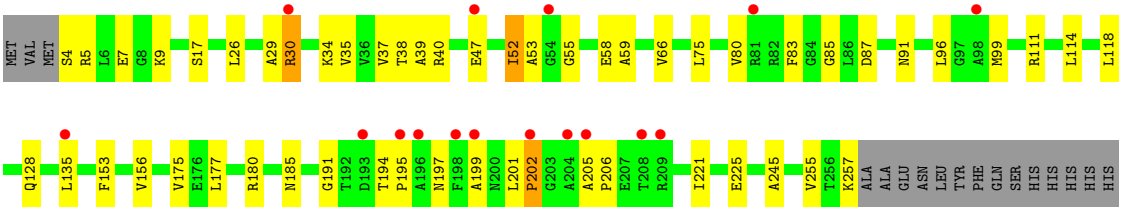
• Molecule 1: Short chain dehydrogenase





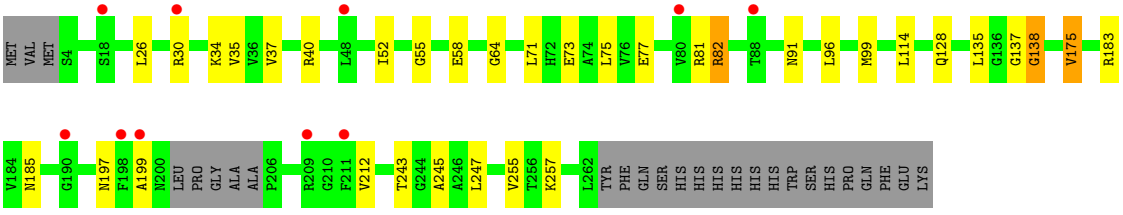
• Molecule 1: Short chain dehydrogenase

Chain E:



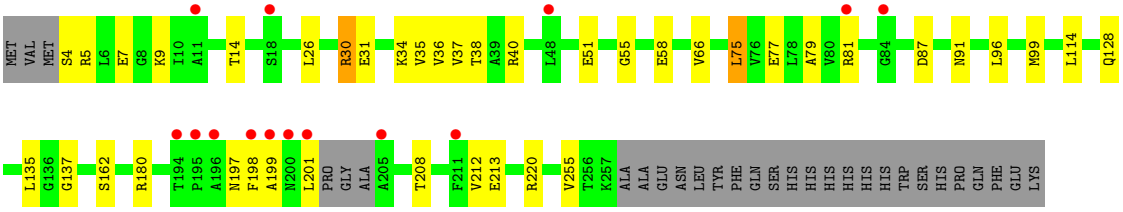
• Molecule 1: Short chain dehydrogenase

Chain F:



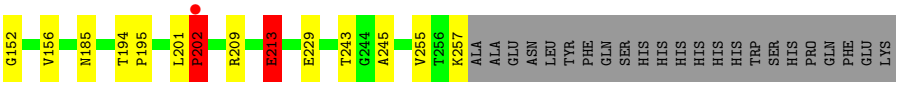
• Molecule 1: Short chain dehydrogenase

Chain G:



• Molecule 1: Short chain dehydrogenase

Chain I:


G152
V156
N185
T194
P195
L201
P202
R209
E213
E229
T243
G244
A245
V255
T256
K257
ALA
ALA
GLU
ASN
LEU
TYR
PHE
GLN
SER
HIS
HIS
HIS
HIS
HIS
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.97Å 122.94Å 139.82Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	43.47 – 1.93 43.47 – 1.93	Depositor EDS
% Data completeness (in resolution range)	87.4 (43.47-1.93) 87.4 (43.47-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.255 0.203 , 0.256	Depositor DCC
R_{free} test set	6812 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 27.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.417 for k,h,-l 0.387 for -k,-h,-l 0.399 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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	1.15	1/1795 (0.1%)	0.94	4/2437 (0.2%)
1	B	1.08	3/1745 (0.2%)	0.92	2/2366 (0.1%)
1	C	1.16	1/1795 (0.1%)	0.95	2/2437 (0.1%)
1	D	1.17	1/1795 (0.1%)	0.95	0/2437
1	E	1.03	2/1787 (0.1%)	0.92	3/2426 (0.1%)
1	F	1.06	2/1782 (0.1%)	0.91	1/2417 (0.0%)
1	G	1.05	0/1766	0.86	1/2396 (0.0%)
1	I	1.19	4/1795 (0.2%)	0.96	1/2437 (0.0%)
All	All	1.11	14/14260 (0.1%)	0.93	14/19353 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
1	I	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	VAL	CB-CG2	-5.89	1.40	1.52
1	I	213	GLU	CG-CD	-5.89	1.43	1.51
1	F	138	GLY	N-CA	-5.88	1.37	1.46
1	E	175	VAL	CB-CG1	5.83	1.65	1.52
1	F	175	VAL	CB-CG1	5.80	1.65	1.52
1	E	225	GLU	CB-CG	5.68	1.62	1.52
1	B	229	GLU	CB-CG	5.49	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	76	VAL	CB-CG2	5.48	1.64	1.52
1	A	239	ALA	CA-CB	5.42	1.63	1.52
1	I	255	VAL	CB-CG2	-5.34	1.41	1.52
1	B	137	GLY	C-O	-5.30	1.15	1.23
1	I	133	ALA	CA-CB	-5.11	1.41	1.52
1	D	241	PHE	CE2-CZ	5.08	1.47	1.37
1	B	225	GLU	CB-CG	5.01	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	GLY	N-CA-C	5.84	127.71	113.10
1	A	202	PRO	CA-C-N	5.74	127.67	116.20
1	C	55	GLY	N-CA-C	-5.74	98.76	113.10
1	I	30	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	115	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	202	PRO	N-CA-C	5.46	126.29	112.10
1	B	62	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	247	LEU	CB-CG-CD2	5.33	120.05	111.00
1	E	5	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	115	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	180	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	30	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	183	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	E	202	PRO	N-CA-C	5.07	125.29	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	GLY	Peptide
1	G	137	GLY	Peptide
1	I	202	PRO	Peptide

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	1771	0	1774	29	0
1	B	1725	0	1724	26	0
1	C	1771	0	1774	23	0
1	D	1771	0	1774	30	0
1	E	1764	0	1763	47	0
1	F	1761	0	1752	37	0
1	G	1745	0	1747	35	0
1	I	1771	0	1774	39	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	2	0
2	D	48	0	25	1	0
2	E	48	0	25	4	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	I	48	0	25	0	0
3	A	122	0	0	3	0
3	B	82	0	0	2	0
3	C	130	0	0	3	0
3	D	117	0	0	1	0
3	E	96	0	0	5	0
3	F	79	0	0	2	0
3	G	92	0	0	1	0
3	I	132	0	0	3	0
All	All	15313	0	14282	255	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 9.

All (255) 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:F:96:LEU:HB3	1:F:99:MET:HE3	1.31	1.10
1:G:96:LEU:HB3	1:G:99:MET:HE3	1.34	1.09
1:G:198:PHE:HA	1:G:201:LEU:HD13	1.30	1.06
1:I:135:LEU:N	1:I:135:LEU:CD1	2.18	1.05
1:G:198:PHE:HA	1:G:201:LEU:CD1	1.87	1.04
1:B:180:ARG:HG3	1:B:180:ARG:HH11	1.24	1.01
1:I:44:ALA:O	1:I:47:GLU:HG3	1.62	0.97
1:I:135:LEU:HD13	1:I:135:LEU:H	1.32	0.95
1:E:99:MET:HE2	1:E:156:VAL:HG12	1.47	0.94
1:I:135:LEU:N	1:I:135:LEU:HD13	1.84	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:MET:CE	1:E:156:VAL:HG12	2.07	0.84
1:I:135:LEU:N	1:I:135:LEU:HD12	1.94	0.82
1:I:99:MET:CE	1:I:156:VAL:HG12	2.11	0.81
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.43	0.81
1:I:99:MET:HE1	1:I:156:VAL:HG12	1.61	0.81
1:A:131:ALA:O	1:A:135:LEU:HD23	1.80	0.81
1:I:86:LEU:H	1:I:135:LEU:HD21	1.45	0.80
1:D:202:PRO:CG	1:D:202:PRO:O	2.30	0.80
1:D:202:PRO:O	1:D:202:PRO:CD	2.29	0.78
1:E:30:ARG:CZ	3:E:711:HOH:O	2.30	0.78
1:E:4:SER:HB2	1:E:7:GLU:HB2	1.66	0.77
1:G:30:ARG:HD3	1:G:30:ARG:N	1.96	0.77
1:A:91:ASN:HD21	1:A:128:GLN:HE22	1.34	0.76
1:E:40:ARG:HD3	3:E:794:HOH:O	1.85	0.76
1:E:91:ASN:HD21	1:E:128:GLN:HE22	1.36	0.74
1:G:91:ASN:HD21	1:G:128:GLN:HE22	1.36	0.73
1:G:198:PHE:CA	1:G:201:LEU:CD1	2.65	0.73
1:F:26:LEU:HD23	1:F:52:ILE:CD1	2.18	0.73
1:I:91:ASN:HD21	1:I:128:GLN:HE22	1.34	0.72
1:I:135:LEU:HD11	3:I:300:HOH:O	1.89	0.72
1:D:216:HIS:O	1:D:219:LYS:HE2	1.90	0.72
1:E:177:LEU:HD23	1:E:180:ARG:NH2	2.05	0.72
1:B:64:GLY:HA3	1:B:71:LEU:HD22	1.74	0.70
1:I:86:LEU:O	1:I:135:LEU:HD22	1.92	0.70
1:C:4:SER:N	3:C:743:HOH:O	2.25	0.70
1:D:202:PRO:O	1:D:202:PRO:HG2	1.90	0.70
1:F:30:ARG:NH2	1:F:55:GLY:HA3	2.06	0.70
1:B:180:ARG:HG3	1:B:180:ARG:NH1	1.99	0.70
1:A:38:THR:HG21	1:A:75:LEU:HD11	1.73	0.69
1:F:91:ASN:HD21	1:F:128:GLN:HE22	1.40	0.69
1:B:40:ARG:HB2	2:B:601:NAP:O2X	1.92	0.69
1:I:86:LEU:O	1:I:135:LEU:CD2	2.42	0.68
1:A:81:ARG:HD2	3:A:800:HOH:O	1.95	0.67
1:D:91:ASN:HD21	1:D:128:GLN:HE22	1.41	0.66
1:D:44:ALA:O	1:D:47:GLU:HG3	1.97	0.65
1:G:198:PHE:CA	1:G:201:LEU:HD13	2.17	0.65
1:D:38:THR:HG21	1:D:75:LEU:HD11	1.78	0.65
1:C:110:TRP:CZ2	1:C:114:LEU:HD11	2.31	0.65
1:E:177:LEU:HD23	1:E:180:ARG:HH21	1.61	0.65
1:D:152:GLY:N	1:E:255:VAL:HG13	2.12	0.65
1:B:91:ASN:HD21	1:B:128:GLN:HE22	1.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:HD21	1:C:128:GLN:HE22	1.44	0.64
1:B:30:ARG:HG2	1:B:30:ARG:NH1	2.10	0.64
1:I:49:THR:HG21	1:I:61:ALA:HB2	1.80	0.64
1:D:202:PRO:O	1:D:202:PRO:HD2	1.97	0.63
1:F:135:LEU:O	1:F:135:LEU:CD1	2.46	0.63
1:I:99:MET:HE1	1:I:156:VAL:CG1	2.28	0.63
1:F:35:VAL:HG12	1:F:37:VAL:HG13	1.81	0.63
1:E:177:LEU:CD2	1:E:180:ARG:HH21	2.11	0.63
1:E:34:LYS:HE3	1:E:58:GLU:OE2	1.99	0.62
1:C:110:TRP:NE1	1:C:114:LEU:HD12	2.15	0.62
1:G:197:ASN:O	1:G:201:LEU:HD12	1.99	0.62
1:E:205:ALA:HB1	1:E:206:PRO:HD2	1.81	0.62
1:F:34:LYS:HE3	1:F:58:GLU:OE2	2.00	0.62
1:A:82:ARG:NH2	3:A:336:HOH:O	2.31	0.62
1:A:135:LEU:N	1:A:135:LEU:CD2	2.63	0.61
1:G:199:ALA:HA	1:G:208:THR:HG21	1.83	0.61
1:I:54:GLY:H	1:I:56:GLY:H	1.48	0.60
1:A:201:LEU:HB3	1:A:202:PRO:HD2	1.84	0.60
1:A:81:ARG:NH2	1:D:193:ASP:OD1	2.34	0.60
1:B:77:GLU:O	1:B:81:ARG:HG3	2.01	0.59
1:B:135:LEU:HD23	1:B:135:LEU:N	2.16	0.59
1:A:81:ARG:HH22	1:D:193:ASP:CG	2.05	0.59
1:F:26:LEU:HD23	1:F:52:ILE:HD13	1.85	0.59
1:F:247:LEU:HD23	1:F:247:LEU:C	2.21	0.59
1:I:134:ALA:C	1:I:135:LEU:HD12	2.22	0.59
1:A:257:LYS:CD	3:B:742:HOH:O	2.50	0.59
1:A:110:TRP:NE1	1:A:114:LEU:HD12	2.18	0.58
1:E:96:LEU:HB3	1:E:99:MET:HE3	1.84	0.58
1:C:4:SER:N	3:C:304:HOH:O	2.35	0.58
1:E:38:THR:HG21	1:E:75:LEU:HD11	1.84	0.58
1:D:110:TRP:NE1	1:D:114:LEU:HD12	2.18	0.58
1:G:5:ARG:HD2	1:G:31:GLU:OE1	2.02	0.58
1:F:96:LEU:CB	1:F:99:MET:HE3	2.20	0.58
1:G:30:ARG:NH2	1:G:55:GLY:HA3	2.19	0.57
1:C:54:GLY:N	1:C:56:GLY:H	2.02	0.57
1:A:135:LEU:N	1:A:135:LEU:HD22	2.20	0.56
1:C:48:LEU:O	1:C:52:ILE:HG13	2.05	0.56
1:C:110:TRP:CE2	1:C:114:LEU:HD11	2.40	0.56
1:F:135:LEU:C	1:F:135:LEU:HD12	2.26	0.56
1:A:5:ARG:NH2	1:A:229:GLU:OE1	2.35	0.56
1:I:201:LEU:HB3	1:I:202:PRO:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:471:HOH:O	1:E:257:LYS:CD	2.53	0.55
1:B:26:LEU:O	1:B:30:ARG:HG2	2.06	0.55
1:F:40:ARG:HB2	2:F:601:NAP:O2X	2.06	0.55
1:A:5:ARG:HD3	1:A:31:GLU:OE1	2.07	0.55
1:A:50:ASP:O	1:A:53:ALA:O	2.25	0.54
1:I:99:MET:HE2	1:I:156:VAL:HG12	1.87	0.54
1:C:152:GLY:N	1:G:255:VAL:HG13	2.22	0.54
1:G:199:ALA:HA	1:G:208:THR:CG2	2.37	0.54
1:E:9:LYS:HA	1:E:87:ASP:OD2	2.08	0.54
1:E:30:ARG:NH2	1:E:55:GLY:HA3	2.22	0.54
1:C:34:LYS:HE3	1:C:58:GLU:OE2	2.09	0.53
1:G:34:LYS:HE3	1:G:58:GLU:OE2	2.09	0.53
1:G:255:VAL:CG1	1:G:255:VAL:O	2.56	0.53
1:C:110:TRP:NE1	1:C:114:LEU:CD1	2.72	0.52
1:G:5:ARG:HD2	1:G:31:GLU:CD	2.30	0.52
1:G:35:VAL:HG12	1:G:37:VAL:HG13	1.90	0.52
1:B:26:LEU:CD1	1:B:30:ARG:NH2	2.72	0.52
1:E:40:ARG:HB2	2:E:601:NAP:O2X	2.10	0.52
1:E:194:THR:HB	1:E:195:PRO:HD2	1.92	0.52
1:G:255:VAL:O	1:G:255:VAL:HG12	2.09	0.52
1:C:216:HIS:O	1:C:219:LYS:HE2	2.09	0.52
1:G:14:THR:HG22	1:G:38:THR:CG2	2.39	0.51
1:I:111:ARG:HD3	3:I:848:HOH:O	2.09	0.51
1:C:110:TRP:CE2	1:C:114:LEU:CD1	2.94	0.51
1:G:213:GLU:HG2	1:G:220:ARG:HA	1.92	0.51
1:B:185:ASN:HD22	1:B:245:ALA:H	1.59	0.51
1:C:34:LYS:HG2	3:C:578:HOH:O	2.11	0.51
1:F:77:GLU:O	1:F:81:ARG:HG2	2.11	0.51
1:G:36:VAL:HG21	1:G:79:ALA:HB2	1.93	0.50
1:I:38:THR:HG21	1:I:75:LEU:HD11	1.92	0.50
1:A:54:GLY:H	1:A:56:GLY:H	1.59	0.50
1:F:64:GLY:HA3	1:F:71:LEU:HD22	1.92	0.50
1:A:187:LEU:CD1	1:A:247:LEU:HD22	2.41	0.50
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.76	0.50
1:B:34:LYS:HE3	1:B:58:GLU:OE2	2.12	0.50
1:B:209:ARG:NH1	3:B:370:HOH:O	2.44	0.50
1:F:135:LEU:O	1:F:135:LEU:HD12	2.10	0.50
1:F:96:LEU:HB3	1:F:99:MET:CE	2.23	0.50
1:D:171:GLN:HB3	1:F:255:VAL:HG11	1.94	0.50
1:C:66:VAL:HB	2:C:601:NAP:C2A	2.43	0.49
1:F:30:ARG:NH2	1:F:55:GLY:CA	2.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:VAL:HG12	1:F:255:VAL:O	2.11	0.49
1:I:131:ALA:O	1:I:135:LEU:HD13	2.12	0.49
1:A:38:THR:HB	1:A:75:LEU:HD21	1.95	0.49
1:E:197:ASN:OD1	1:E:199:ALA:HB3	2.13	0.48
1:F:137:GLY:HA3	1:F:138:GLY:HA2	1.71	0.48
1:A:37:VAL:HG23	1:A:45:LEU:HD22	1.94	0.48
1:I:5:ARG:HD3	1:I:31:GLU:OE1	2.14	0.48
1:B:26:LEU:HD11	1:B:30:ARG:NH2	2.28	0.48
1:D:152:GLY:H	1:E:255:VAL:HG13	1.78	0.48
1:E:195:PRO:HD2	2:E:601:NAP:O2A	2.14	0.47
1:G:66:VAL:HB	2:G:601:NAP:C2A	2.44	0.47
1:G:4:SER:HB2	1:G:7:GLU:HB2	1.96	0.47
1:I:194:THR:HB	1:I:195:PRO:HD2	1.97	0.47
1:A:110:TRP:NE1	1:A:114:LEU:CD1	2.78	0.47
1:F:26:LEU:CD2	1:F:52:ILE:HD13	2.44	0.47
1:B:17:SER:HB3	1:B:39:ALA:CB	2.45	0.47
1:E:34:LYS:CE	1:E:58:GLU:OE2	2.63	0.47
1:E:111:ARG:NH2	3:E:785:HOH:O	2.33	0.47
2:E:601:NAP:O1N	2:E:601:NAP:H2N	2.14	0.47
1:G:9:LYS:HA	1:G:87:ASP:OD2	2.14	0.47
1:G:135:LEU:N	1:G:135:LEU:HD12	2.29	0.47
1:F:197:ASN:OD1	1:F:199:ALA:HB3	2.15	0.47
1:E:53:ALA:C	1:E:55:GLY:H	2.18	0.46
1:F:135:LEU:O	1:F:135:LEU:HD13	2.13	0.46
1:A:112:GLU:HG3	3:A:293:HOH:O	2.15	0.46
1:G:40:ARG:HB2	2:G:601:NAP:O2X	2.15	0.46
1:F:255:VAL:CG1	1:I:152:GLY:N	2.78	0.46
1:F:255:VAL:HG13	1:I:152:GLY:N	2.30	0.46
1:I:38:THR:HB	1:I:75:LEU:HD21	1.97	0.46
1:F:185:ASN:HD22	1:F:245:ALA:H	1.64	0.46
1:I:185:ASN:HD22	1:I:245:ALA:H	1.64	0.46
1:E:35:VAL:HG12	1:E:37:VAL:HG13	1.97	0.46
1:G:38:THR:HG21	1:G:75:LEU:HD11	1.98	0.46
1:I:64:GLY:C	1:I:71:LEU:HD22	2.36	0.46
1:A:64:GLY:HA3	1:A:71:LEU:HD13	1.98	0.46
1:D:185:ASN:HD22	1:D:245:ALA:H	1.65	0.45
1:C:36:VAL:HG12	1:C:75:LEU:HD22	1.98	0.45
1:D:257:LYS:CD	3:E:604:HOH:O	2.64	0.45
1:E:29:ALA:CB	1:E:52:ILE:HD13	2.46	0.45
1:C:257:LYS:CD	3:G:546:HOH:O	2.65	0.45
1:D:177:LEU:HD23	1:D:180:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:LEU:HD23	1:G:162:SER:CB	2.47	0.45
1:E:255:VAL:HG12	1:E:255:VAL:O	2.17	0.44
1:E:201:LEU:HB3	1:E:202:PRO:HD2	2.00	0.44
1:G:197:ASN:HD21	1:G:212:VAL:HG11	1.81	0.44
1:F:58:GLU:OE1	1:F:82:ARG:NH2	2.47	0.44
1:G:77:GLU:O	1:G:81:ARG:HG2	2.17	0.44
1:I:202:PRO:HG2	1:I:202:PRO:O	2.17	0.44
1:A:185:ASN:ND2	1:A:245:ALA:H	2.16	0.44
1:B:14:THR:HG22	1:B:38:THR:CG2	2.48	0.44
1:B:255:VAL:HG12	1:B:255:VAL:O	2.17	0.44
1:D:64:GLY:HA3	1:D:71:LEU:HD22	1.99	0.44
1:D:255:VAL:O	1:D:255:VAL:CG1	2.65	0.44
2:F:601:NAP:H2A	3:F:309:HOH:O	2.17	0.44
1:D:190:GLY:H	1:D:250:ASP:HA	1.83	0.44
1:A:185:ASN:HD22	1:A:245:ALA:H	1.64	0.44
1:I:45:LEU:O	1:I:49:THR:HG23	2.18	0.44
1:E:34:LYS:HD2	1:E:83:PHE:CE1	2.53	0.43
1:F:73:GLU:O	1:F:77:GLU:HG2	2.17	0.43
1:I:36:VAL:HG21	1:I:79:ALA:HB2	2.00	0.43
1:G:96:LEU:HD13	1:G:99:MET:HE3	2.00	0.43
1:D:36:VAL:HG12	1:D:75:LEU:HD22	2.01	0.43
1:B:35:VAL:HG12	1:B:37:VAL:HG13	2.00	0.43
1:E:66:VAL:HB	2:E:601:NAP:C2A	2.48	0.43
1:C:85:GLY:HA3	1:C:135:LEU:HD11	2.01	0.43
1:C:152:GLY:H	1:G:255:VAL:HG13	1.84	0.43
1:E:30:ARG:HG2	3:E:711:HOH:O	2.18	0.43
1:B:213:GLU:HG2	1:B:221:ILE:HG13	2.01	0.43
1:G:96:LEU:HB3	1:G:99:MET:CE	2.24	0.43
1:I:134:ALA:HB3	1:I:135:LEU:CD1	2.48	0.43
1:E:153:PHE:O	1:E:156:VAL:HG22	2.19	0.43
1:F:135:LEU:CD1	1:F:135:LEU:C	2.86	0.43
1:C:38:THR:HG21	1:C:75:LEU:HD11	2.00	0.43
1:E:185:ASN:HD22	1:E:245:ALA:H	1.66	0.43
3:F:322:HOH:O	1:I:257:LYS:CD	2.66	0.43
1:A:107:VAL:O	1:A:111:ARG:HG3	2.19	0.42
1:B:4:SER:HB2	1:B:7:GLU:HB2	2.01	0.42
1:E:255:VAL:O	1:E:255:VAL:CG1	2.67	0.42
1:F:30:ARG:HA	1:F:30:ARG:HD3	1.38	0.42
1:A:135:LEU:CD2	1:A:135:LEU:H	2.32	0.42
1:I:96:LEU:HD22	1:I:99:MET:HE3	2.01	0.42
1:C:194:THR:HB	1:C:195:PRO:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:VAL:HB	2:D:601:NAP:C2A	2.50	0.42
1:E:17:SER:HB3	1:E:39:ALA:CB	2.49	0.42
1:E:191:GLY:C	1:E:221:ILE:HG23	2.39	0.42
1:E:205:ALA:HB1	1:E:206:PRO:CD	2.49	0.42
1:D:38:THR:CG2	1:D:75:LEU:HD11	2.49	0.42
1:D:152:GLY:H	1:E:255:VAL:CG1	2.32	0.42
1:E:52:ILE:HG21	1:E:59:ALA:HB2	2.00	0.42
1:D:152:GLY:N	1:E:255:VAL:CG1	2.81	0.42
1:E:80:VAL:HG22	1:E:85:GLY:HA2	2.01	0.42
1:E:99:MET:HE1	1:E:156:VAL:HG12	1.96	0.42
1:B:185:ASN:ND2	1:B:245:ALA:H	2.18	0.42
1:D:247:LEU:HD23	1:D:247:LEU:C	2.40	0.42
1:F:257:LYS:CD	3:I:430:HOH:O	2.67	0.42
1:G:30:ARG:HD2	1:G:30:ARG:HA	1.67	0.42
1:I:131:ALA:O	1:I:135:LEU:CD1	2.67	0.42
1:F:185:ASN:HD21	1:F:243:THR:HA	1.85	0.41
1:B:153:PHE:O	1:B:156:VAL:HG22	2.20	0.41
1:E:29:ALA:HB3	1:E:52:ILE:HD13	2.02	0.41
1:E:38:THR:HB	1:E:75:LEU:HD21	2.01	0.41
1:I:209:ARG:O	1:I:213:GLU:HG2	2.20	0.41
1:A:64:GLY:C	1:A:71:LEU:HD22	2.40	0.41
1:B:135:LEU:N	1:B:135:LEU:CD2	2.83	0.41
1:E:118:LEU:HD23	1:F:114:LEU:HD11	2.01	0.41
1:F:30:ARG:CZ	1:F:55:GLY:HA3	2.50	0.41
1:F:197:ASN:HD21	1:F:212:VAL:HG11	1.86	0.41
1:A:187:LEU:HD12	1:A:247:LEU:HD22	2.01	0.41
1:F:247:LEU:C	1:F:247:LEU:CD2	2.88	0.41
1:I:185:ASN:HD21	1:I:243:THR:HA	1.86	0.41
1:D:202:PRO:HA	1:D:203:GLY:HA2	1.86	0.41
1:I:5:ARG:NH2	1:I:229:GLU:OE1	2.46	0.41
1:B:64:GLY:CA	1:B:71:LEU:HD22	2.47	0.41
1:C:54:GLY:CA	1:C:56:GLY:H	2.34	0.40
1:D:255:VAL:HG12	1:F:175:VAL:HG23	2.02	0.40
1:G:66:VAL:HG12	2:G:601:NAP:N1A	2.36	0.40
1:E:38:THR:CG2	1:E:75:LEU:HD11	2.51	0.40
1:I:185:ASN:ND2	1:I:245:ALA:H	2.19	0.40
1:B:66:VAL:HG11	1:B:93:ALA:HB1	2.03	0.40
1:C:40:ARG:HB2	2:C:601:NAP:O2X	2.22	0.40
1:D:185:ASN:HD21	1:D:243:THR:HA	1.87	0.40
1:D:110:TRP:CZ2	1:D:114:LEU:HD11	2.57	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	252/280 (90%)	246 (98%)	6 (2%)	0	100	100
1	B	244/280 (87%)	238 (98%)	5 (2%)	1 (0%)	34	24
1	C	252/280 (90%)	248 (98%)	4 (2%)	0	100	100
1	D	252/280 (90%)	245 (97%)	7 (3%)	0	100	100
1	E	252/280 (90%)	248 (98%)	4 (2%)	0	100	100
1	F	250/280 (89%)	245 (98%)	5 (2%)	0	100	100
1	G	247/280 (88%)	242 (98%)	5 (2%)	0	100	100
1	I	252/280 (90%)	246 (98%)	6 (2%)	0	100	100
All	All	2001/2240 (89%)	1958 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	GLY

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	163/188 (87%)	160 (98%)	3 (2%)	59	47
1	B	158/188 (84%)	154 (98%)	4 (2%)	47	35
1	C	163/188 (87%)	161 (99%)	2 (1%)	71	64
1	D	163/188 (87%)	161 (99%)	2 (1%)	71	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	162/188 (86%)	157 (97%)	5 (3%)	40 26
1	F	160/188 (85%)	158 (99%)	2 (1%)	69 62
1	G	160/188 (85%)	156 (98%)	4 (2%)	47 35
1	I	163/188 (87%)	157 (96%)	6 (4%)	34 19
All	All	1292/1504 (86%)	1264 (98%)	28 (2%)	52 39

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

Mol	Chain	Res	Type
1	A	47	GLU
1	A	82	ARG
1	A	135	LEU
1	B	30	ARG
1	B	75	LEU
1	B	135	LEU
1	B	180	ARG
1	C	47	GLU
1	C	66	VAL
1	D	47	GLU
1	D	202	PRO
1	E	26	LEU
1	E	47	GLU
1	E	52	ILE
1	E	114	LEU
1	E	135	LEU
1	F	75	LEU
1	F	82	ARG
1	G	26	LEU
1	G	30	ARG
1	G	51	GLU
1	G	75	LEU
1	I	47	GLU
1	I	52	ILE
1	I	112	GLU
1	I	135	LEU
1	I	202	PRO
1	I	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	185	ASN
1	B	91	ASN
1	B	185	ASN
1	C	91	ASN
1	C	185	ASN
1	D	91	ASN
1	D	185	ASN
1	E	91	ASN
1	E	185	ASN
1	F	91	ASN
1	F	185	ASN
1	G	91	ASN
1	G	185	ASN
1	I	43	ASN
1	I	91	ASN
1	I	185	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	G	601	-	45,52,52	2.93	10 (22%)	56,80,80	1.95	7 (12%)
2	NAP	I	601	-	45,52,52	3.04	14 (31%)	56,80,80	1.93	11 (19%)
2	NAP	D	601	-	45,52,52	2.64	11 (24%)	56,80,80	1.84	6 (10%)
2	NAP	C	601	-	45,52,52	2.96	10 (22%)	56,80,80	1.74	5 (8%)
2	NAP	F	601	-	45,52,52	2.85	10 (22%)	56,80,80	2.07	7 (12%)
2	NAP	A	601	-	45,52,52	2.78	13 (28%)	56,80,80	1.95	6 (10%)
2	NAP	E	601	-	45,52,52	2.97	10 (22%)	56,80,80	2.02	9 (16%)
2	NAP	B	601	-	45,52,52	2.89	12 (26%)	56,80,80	1.94	10 (17%)

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	G	601	-	-	6/31/67/67	0/5/5/5
2	NAP	I	601	-	-	6/31/67/67	0/5/5/5
2	NAP	D	601	-	-	8/31/67/67	0/5/5/5
2	NAP	C	601	-	-	4/31/67/67	0/5/5/5
2	NAP	F	601	-	-	7/31/67/67	0/5/5/5
2	NAP	A	601	-	-	4/31/67/67	0/5/5/5
2	NAP	E	601	-	-	5/31/67/67	0/5/5/5
2	NAP	B	601	-	-	6/31/67/67	0/5/5/5

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C2A-N3A	11.52	1.50	1.32
2	I	601	NAP	C2A-N3A	11.47	1.50	1.32
2	F	601	NAP	C2A-N3A	11.42	1.50	1.32
2	G	601	NAP	C2A-N3A	10.76	1.49	1.32
2	E	601	NAP	C2A-N3A	10.67	1.49	1.32
2	A	601	NAP	C2A-N3A	10.41	1.48	1.32
2	I	601	NAP	C2A-N1A	10.28	1.53	1.33
2	E	601	NAP	C2A-N1A	9.92	1.52	1.33
2	C	601	NAP	C2A-N3A	9.91	1.48	1.32
2	C	601	NAP	C2A-N1A	9.48	1.51	1.33
2	D	601	NAP	C2A-N1A	9.31	1.51	1.33
2	A	601	NAP	C2A-N1A	9.00	1.50	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C2A-N1A	8.92	1.50	1.33
2	F	601	NAP	C2A-N1A	8.91	1.50	1.33
2	E	601	NAP	C2N-N1N	8.89	1.45	1.35
2	D	601	NAP	C2A-N3A	8.86	1.46	1.32
2	G	601	NAP	C2A-N1A	8.86	1.50	1.33
2	G	601	NAP	C2N-N1N	8.51	1.45	1.35
2	I	601	NAP	C2N-N1N	7.36	1.43	1.35
2	D	601	NAP	C2N-N1N	7.35	1.43	1.35
2	C	601	NAP	C2N-N1N	6.81	1.43	1.35
2	A	601	NAP	C2N-N1N	6.56	1.43	1.35
2	B	601	NAP	C2N-N1N	6.52	1.42	1.35
2	C	601	NAP	O3B-C3B	6.30	1.57	1.43
2	F	601	NAP	C2N-N1N	6.18	1.42	1.35
2	G	601	NAP	O4B-C1B	5.33	1.48	1.41
2	F	601	NAP	C3N-C7N	-4.85	1.43	1.50
2	A	601	NAP	P2B-O2B	4.65	1.68	1.59
2	C	601	NAP	C3N-C7N	-4.64	1.43	1.50
2	C	601	NAP	P2B-O2B	4.47	1.67	1.59
2	A	601	NAP	C3N-C7N	-4.39	1.44	1.50
2	B	601	NAP	C3N-C7N	-4.22	1.44	1.50
2	G	601	NAP	C3N-C7N	-4.18	1.44	1.50
2	F	601	NAP	C6N-N1N	4.04	1.45	1.35
2	B	601	NAP	C6N-N1N	3.99	1.45	1.35
2	E	601	NAP	C6N-N1N	3.88	1.44	1.35
2	I	601	NAP	C6N-N1N	3.84	1.44	1.35
2	D	601	NAP	C3N-C7N	-3.77	1.44	1.50
2	D	601	NAP	O3B-C3B	3.67	1.51	1.43
2	E	601	NAP	O4D-C1D	3.57	1.46	1.41
2	E	601	NAP	P2B-O2B	3.55	1.66	1.59
2	B	601	NAP	P2B-O2B	3.47	1.65	1.59
2	I	601	NAP	C3N-C7N	-3.44	1.45	1.50
2	F	601	NAP	P2B-O2B	3.41	1.65	1.59
2	G	601	NAP	C6N-N1N	3.22	1.43	1.35
2	B	601	NAP	O4D-C1D	3.16	1.45	1.41
2	E	601	NAP	C3N-C7N	-3.16	1.45	1.50
2	C	601	NAP	O4D-C1D	3.05	1.45	1.41
2	I	601	NAP	O4B-C1B	3.00	1.45	1.41
2	B	601	NAP	O4B-C1B	2.91	1.45	1.41
2	I	601	NAP	P2B-O2B	2.88	1.64	1.59
2	A	601	NAP	C6N-N1N	2.75	1.42	1.35
2	I	601	NAP	O3B-C3B	2.73	1.49	1.43
2	D	601	NAP	O3D-C3D	2.70	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	O3D-C3D	2.64	1.49	1.43
2	I	601	NAP	C6N-C5N	2.64	1.44	1.38
2	A	601	NAP	C3D-C4D	2.57	1.59	1.53
2	E	601	NAP	PN-O5D	2.55	1.69	1.59
2	I	601	NAP	C2D-C3D	2.52	1.60	1.53
2	D	601	NAP	PN-O5D	2.52	1.69	1.59
2	I	601	NAP	PN-O5D	2.50	1.69	1.59
2	A	601	NAP	O3B-C3B	2.45	1.48	1.43
2	C	601	NAP	O4B-C1B	2.42	1.44	1.41
2	I	601	NAP	P2B-O2X	-2.40	1.45	1.54
2	E	601	NAP	C4N-C3N	2.38	1.43	1.39
2	A	601	NAP	PN-O5D	2.34	1.68	1.59
2	G	601	NAP	P2B-O2B	2.33	1.63	1.59
2	C	601	NAP	C2D-C1D	-2.30	1.50	1.53
2	D	601	NAP	C6N-N1N	2.27	1.40	1.35
2	G	601	NAP	O4B-C4B	-2.26	1.40	1.45
2	D	601	NAP	P2B-O2X	-2.24	1.46	1.54
2	B	601	NAP	PN-O5D	2.23	1.68	1.59
2	F	601	NAP	PN-O5D	2.22	1.68	1.59
2	G	601	NAP	PN-O5D	2.21	1.68	1.59
2	G	601	NAP	C4N-C3N	2.17	1.43	1.39
2	A	601	NAP	C6A-C5A	-2.17	1.35	1.43
2	B	601	NAP	PA-O5B	2.16	1.68	1.59
2	D	601	NAP	C6A-C5A	-2.15	1.35	1.43
2	A	601	NAP	O4B-C1B	2.13	1.44	1.41
2	F	601	NAP	P2B-O2X	-2.13	1.46	1.54
2	F	601	NAP	C5A-C4A	-2.11	1.35	1.40
2	D	601	NAP	PA-O2A	-2.11	1.45	1.55
2	E	601	NAP	PA-O5B	2.10	1.67	1.59
2	C	601	NAP	C6N-C5N	2.09	1.43	1.38
2	A	601	NAP	P2B-O2X	-2.09	1.46	1.54
2	B	601	NAP	C4N-C3N	2.09	1.42	1.39
2	I	601	NAP	C3B-C4B	-2.08	1.47	1.53
2	A	601	NAP	C6N-C5N	2.05	1.43	1.38
2	F	601	NAP	C4N-C3N	2.00	1.42	1.39
2	I	601	NAP	C5N-C4N	2.00	1.43	1.38

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	NAP	N3A-C2A-N1A	-10.97	111.54	128.68
2	A	601	NAP	N3A-C2A-N1A	-10.70	111.95	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	601	NAP	N3A-C2A-N1A	-10.54	112.20	128.68
2	D	601	NAP	N3A-C2A-N1A	-10.00	113.05	128.68
2	E	601	NAP	N3A-C2A-N1A	-9.89	113.22	128.68
2	G	601	NAP	N3A-C2A-N1A	-9.86	113.26	128.68
2	B	601	NAP	N3A-C2A-N1A	-9.73	113.47	128.68
2	C	601	NAP	N3A-C2A-N1A	-9.39	114.00	128.68
2	E	601	NAP	C1B-N9A-C4A	-5.53	116.92	126.64
2	B	601	NAP	C1B-N9A-C4A	-4.95	117.94	126.64
2	F	601	NAP	C1B-N9A-C4A	-4.40	118.92	126.64
2	G	601	NAP	O4D-C1D-C2D	-4.24	100.73	106.93
2	C	601	NAP	O4D-C1D-C2D	-4.18	100.81	106.93
2	F	601	NAP	O4D-C1D-C2D	-3.84	101.31	106.93
2	A	601	NAP	O4D-C1D-C2D	-3.84	101.32	106.93
2	D	601	NAP	C1B-N9A-C4A	-3.76	120.04	126.64
2	E	601	NAP	O4D-C1D-C2D	-3.69	101.53	106.93
2	F	601	NAP	O7N-C7N-C3N	3.47	123.78	119.63
2	B	601	NAP	O4D-C1D-C2D	-3.46	101.87	106.93
2	G	601	NAP	C5N-C4N-C3N	3.24	124.18	120.34
2	G	601	NAP	C4A-C5A-N7A	-3.20	106.06	109.40
2	E	601	NAP	C5N-C4N-C3N	3.18	124.11	120.34
2	I	601	NAP	O7N-C7N-N7N	-3.13	118.13	122.58
2	B	601	NAP	O7N-C7N-C3N	2.96	123.17	119.63
2	E	601	NAP	O7N-C7N-C3N	2.92	123.13	119.63
2	B	601	NAP	C6N-N1N-C2N	-2.92	119.31	121.97
2	C	601	NAP	C4A-C5A-N7A	-2.87	106.41	109.40
2	F	601	NAP	C3N-C7N-N7N	-2.83	114.36	117.75
2	D	601	NAP	O7N-C7N-C3N	2.77	122.94	119.63
2	D	601	NAP	O4D-C1D-C2D	-2.75	102.91	106.93
2	A	601	NAP	C5N-C4N-C3N	2.71	123.55	120.34
2	I	601	NAP	C3N-C7N-N7N	2.62	120.90	117.75
2	F	601	NAP	C4A-C5A-N7A	-2.62	106.67	109.40
2	C	601	NAP	C3D-C2D-C1D	-2.51	97.20	100.98
2	B	601	NAP	C5N-C4N-C3N	2.51	123.31	120.34
2	A	601	NAP	C1B-N9A-C4A	-2.44	122.36	126.64
2	B	601	NAP	C5A-C6A-N6A	-2.40	116.71	120.35
2	D	601	NAP	C6N-N1N-C2N	-2.37	119.81	121.97
2	E	601	NAP	O2X-P2B-O2B	-2.36	95.41	105.99
2	I	601	NAP	O4D-C1D-C2D	-2.32	103.54	106.93
2	E	601	NAP	C6N-N1N-C2N	-2.30	119.87	121.97
2	E	601	NAP	O3X-P2B-O2X	2.28	116.35	107.64
2	G	601	NAP	O7N-C7N-C3N	2.26	122.33	119.63
2	I	601	NAP	C4A-C5A-N7A	-2.24	107.07	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	601	NAP	C1B-N9A-C4A	-2.21	122.75	126.64
2	G	601	NAP	C1B-N9A-C4A	-2.20	122.77	126.64
2	I	601	NAP	O2X-P2B-O1X	2.19	119.25	110.68
2	B	601	NAP	O3B-C3B-C2B	-2.17	104.99	111.17
2	A	601	NAP	O3X-P2B-O2X	2.14	115.83	107.64
2	G	601	NAP	C5N-C6N-N1N	-2.14	117.33	120.40
2	I	601	NAP	O4B-C1B-C2B	-2.13	102.89	106.59
2	C	601	NAP	C1B-N9A-C4A	-2.13	122.91	126.64
2	I	601	NAP	C5N-C4N-C3N	2.10	122.83	120.34
2	E	601	NAP	C4A-C5A-N7A	-2.07	107.24	109.40
2	I	601	NAP	C3D-C2D-C1D	-2.07	97.87	100.98
2	F	601	NAP	PN-O3-PA	-2.05	125.81	132.83
2	D	601	NAP	C5B-C4B-C3B	-2.05	107.52	115.18
2	B	601	NAP	C3N-C2N-N1N	2.04	122.42	120.43
2	I	601	NAP	O2A-PA-O1A	2.03	122.25	112.24
2	B	601	NAP	O2N-PN-O1N	2.00	122.15	112.24
2	A	601	NAP	C3D-C2D-C1D	-2.00	97.97	100.98

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C5D-O5D-PN-O3
2	B	601	NAP	PN-O3-PA-O5B
2	C	601	NAP	C5D-O5D-PN-O3
2	D	601	NAP	C5B-O5B-PA-O1A
2	D	601	NAP	C5D-O5D-PN-O3
2	D	601	NAP	O4D-C1D-N1N-C2N
2	F	601	NAP	PN-O3-PA-O5B
2	F	601	NAP	C5D-O5D-PN-O3
2	G	601	NAP	PN-O3-PA-O5B
2	G	601	NAP	C5D-O5D-PN-O3
2	I	601	NAP	C5B-O5B-PA-O1A
2	I	601	NAP	C5D-O5D-PN-O3
2	A	601	NAP	PN-O3-PA-O5B
2	C	601	NAP	PN-O3-PA-O5B
2	D	601	NAP	PN-O3-PA-O5B
2	E	601	NAP	PN-O3-PA-O5B
2	I	601	NAP	PN-O3-PA-O5B
2	A	601	NAP	C5D-O5D-PN-O1N
2	B	601	NAP	C5D-O5D-PN-O1N
2	C	601	NAP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	601	NAP	C5D-O5D-PN-O1N
2	E	601	NAP	C5D-O5D-PN-O1N
2	F	601	NAP	C5D-O5D-PN-O1N
2	G	601	NAP	C5D-O5D-PN-O1N
2	I	601	NAP	C5D-O5D-PN-O1N
2	F	601	NAP	PA-O3-PN-O1N
2	D	601	NAP	O4B-C4B-C5B-O5B
2	E	601	NAP	O4B-C4B-C5B-O5B
2	C	601	NAP	O4B-C4B-C5B-O5B
2	B	601	NAP	C2B-O2B-P2B-O1X
2	B	601	NAP	C5D-O5D-PN-O3
2	D	601	NAP	C5B-O5B-PA-O3
2	D	601	NAP	C2B-O2B-P2B-O3X
2	E	601	NAP	C2B-O2B-P2B-O3X
2	E	601	NAP	C5D-O5D-PN-O3
2	F	601	NAP	C2B-O2B-P2B-O3X
2	G	601	NAP	C2B-O2B-P2B-O3X
2	I	601	NAP	C5B-O5B-PA-O3
2	B	601	NAP	O4B-C4B-C5B-O5B
2	F	601	NAP	O4B-C4B-C5B-O5B
2	G	601	NAP	O4B-C4B-C5B-O5B
2	B	601	NAP	PA-O3-PN-O2N
2	F	601	NAP	PA-O3-PN-O2N
2	G	601	NAP	PA-O3-PN-O2N
2	A	601	NAP	O4B-C4B-C5B-O5B
2	I	601	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

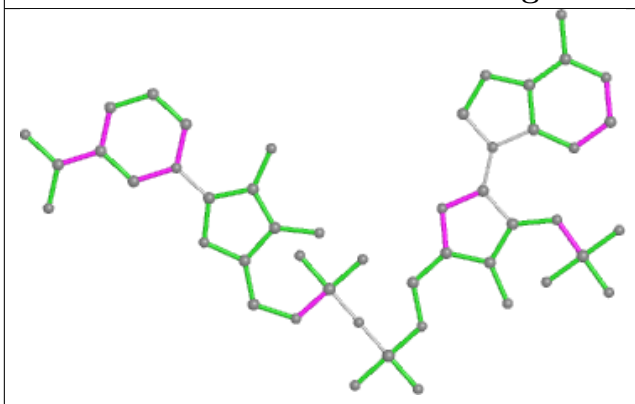
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	601	NAP	3	0
2	D	601	NAP	1	0
2	C	601	NAP	2	0
2	F	601	NAP	2	0
2	E	601	NAP	4	0
2	B	601	NAP	1	0

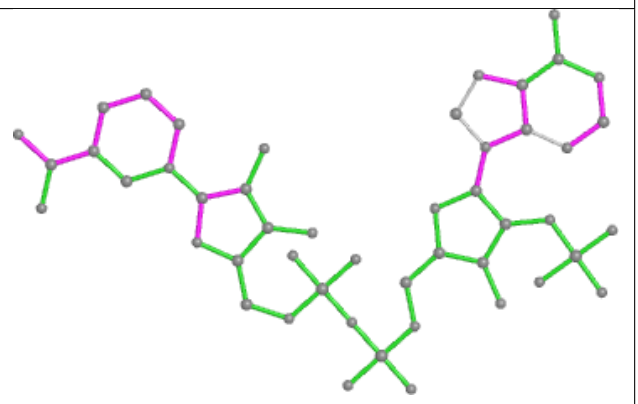
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

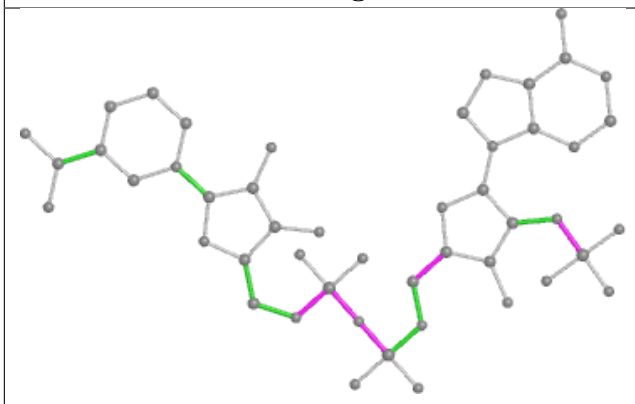
Ligand NAP G 601



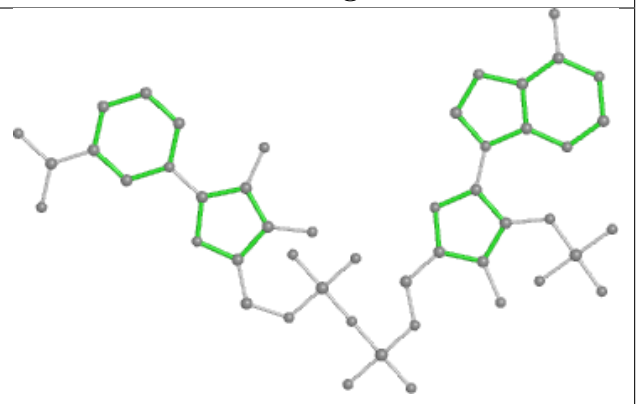
Bond lengths



Bond angles

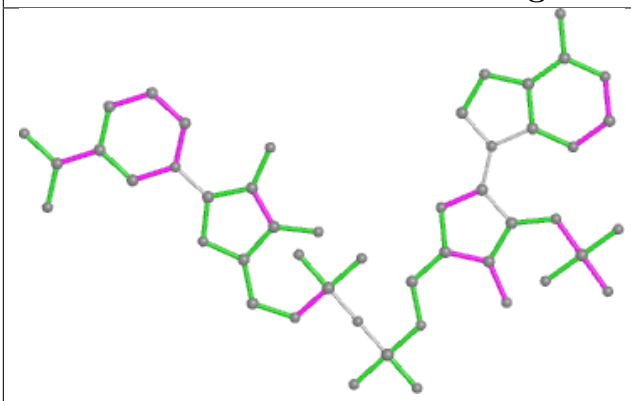


Torsions

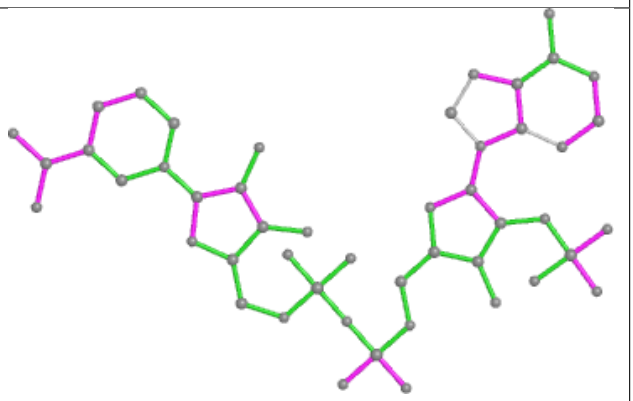


Rings

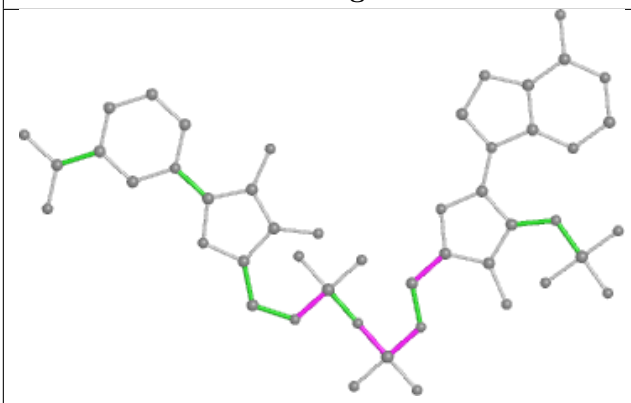
Ligand NAP I 601



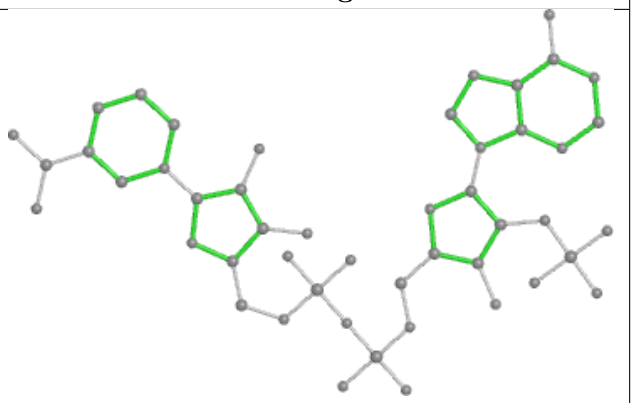
Bond lengths



Bond angles

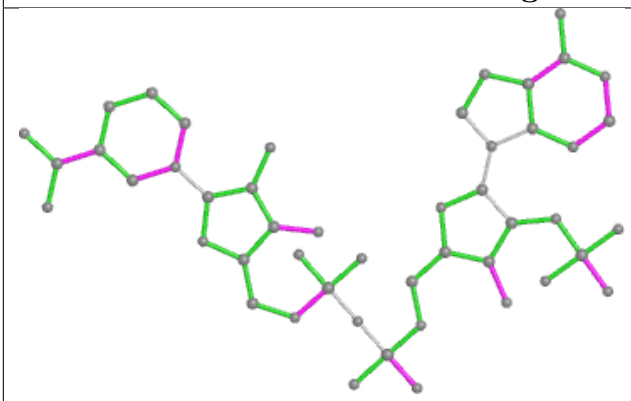


Torsions

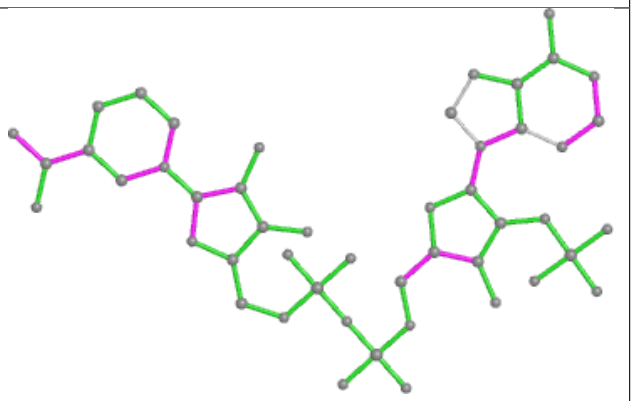


Rings

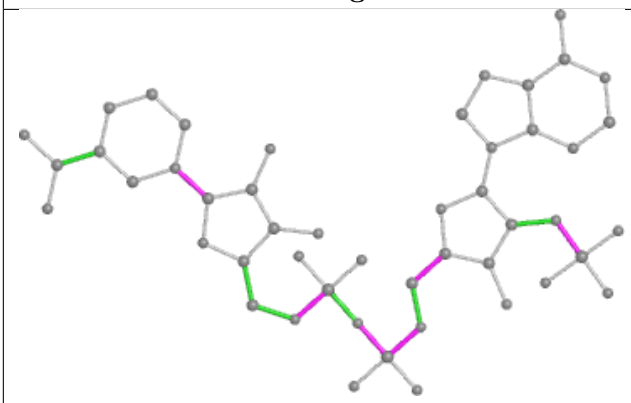
Ligand NAP D 601



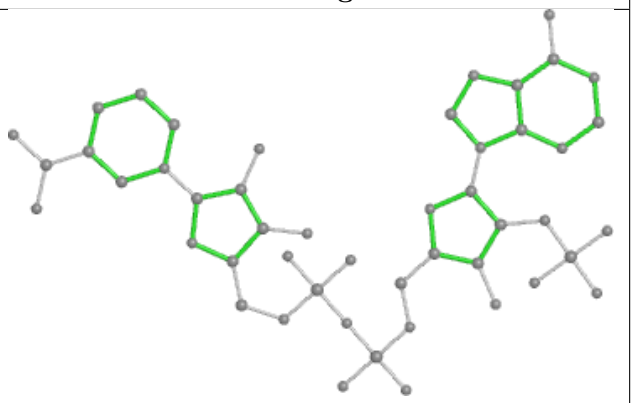
Bond lengths



Bond angles

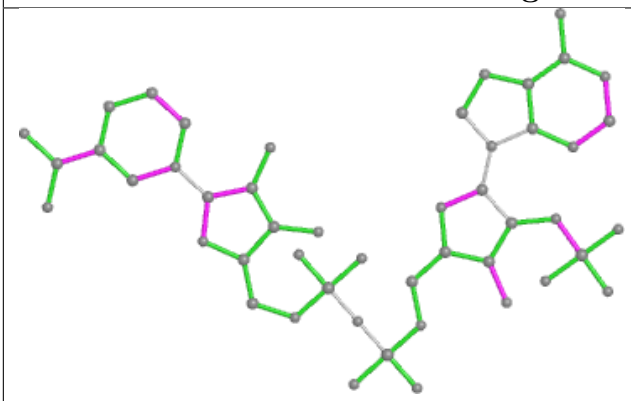


Torsions

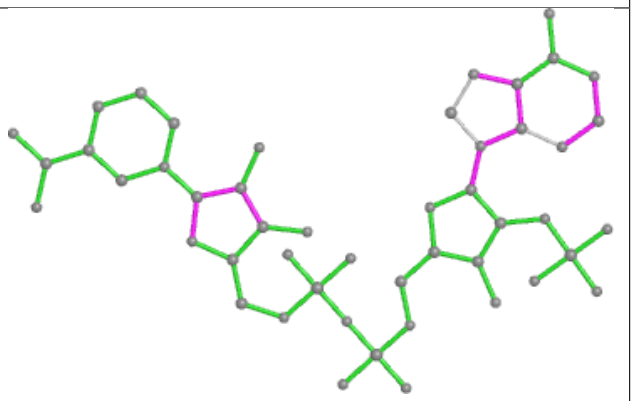


Rings

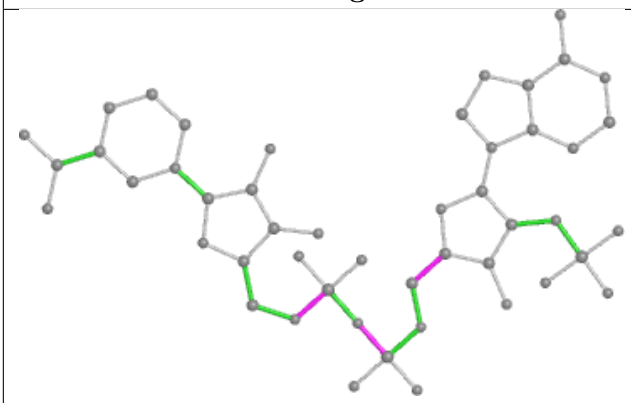
Ligand NAP C 601



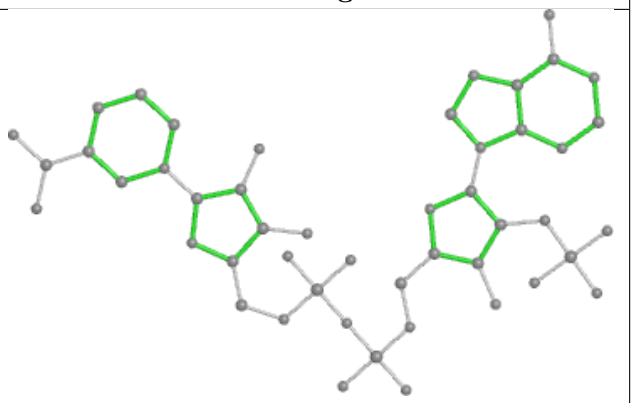
Bond lengths



Bond angles

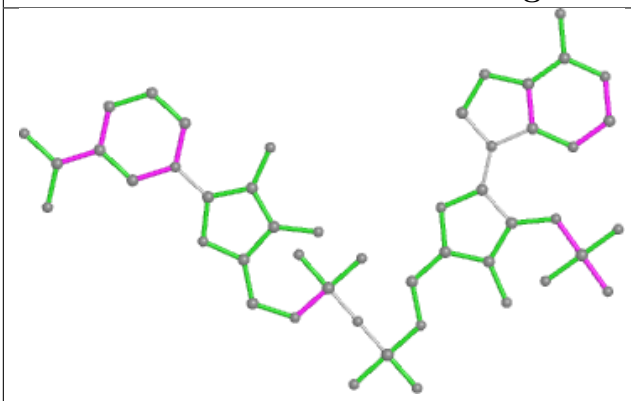


Torsions

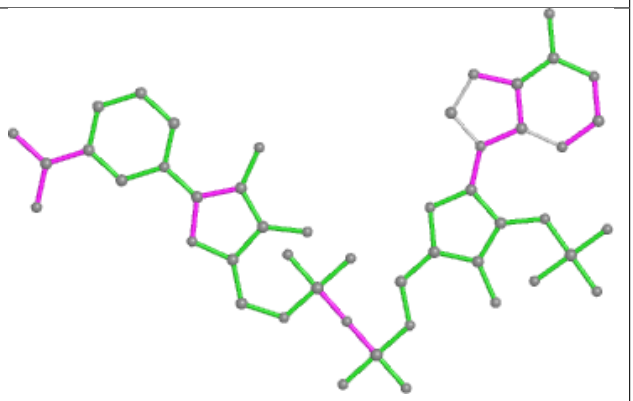


Rings

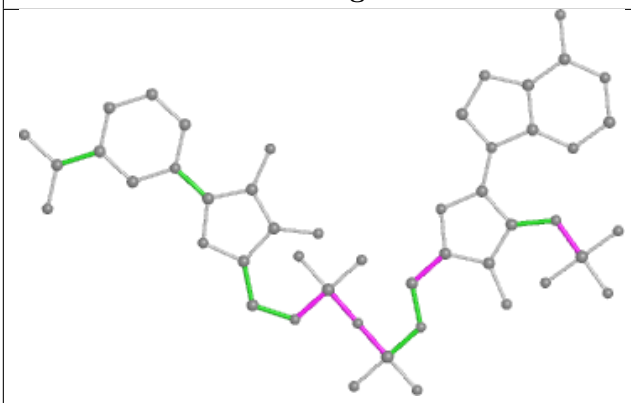
Ligand NAP F 601



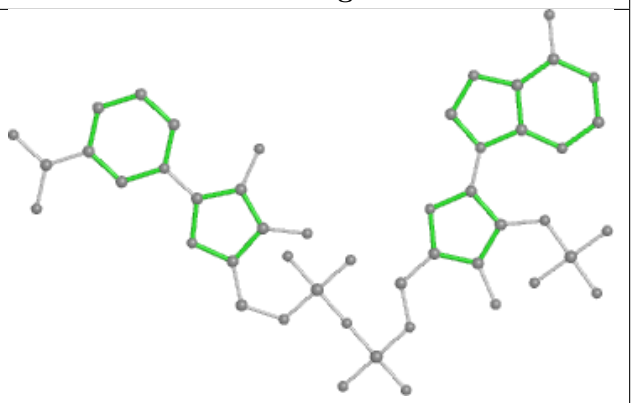
Bond lengths



Bond angles

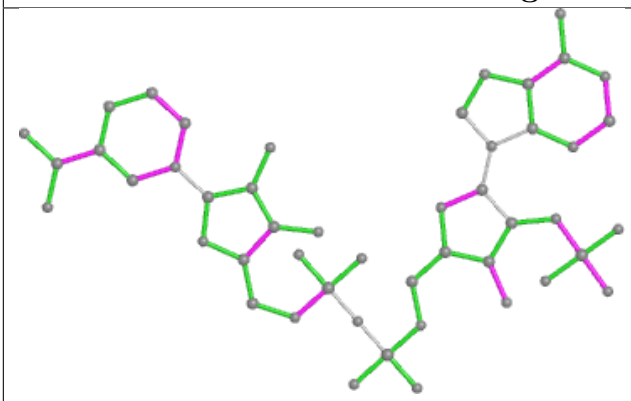


Torsions

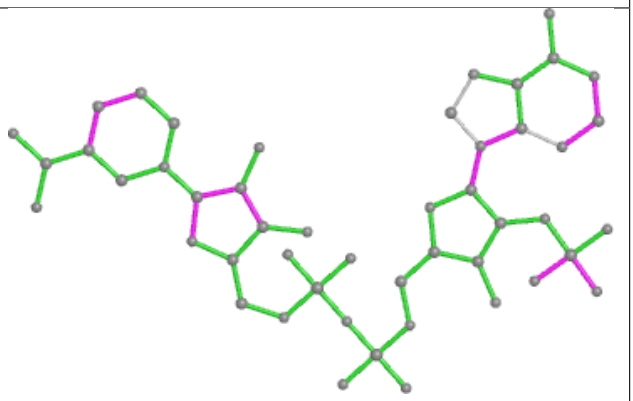


Rings

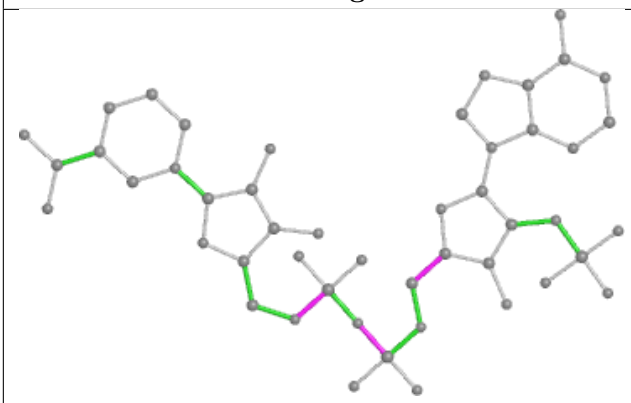
Ligand NAP A 601



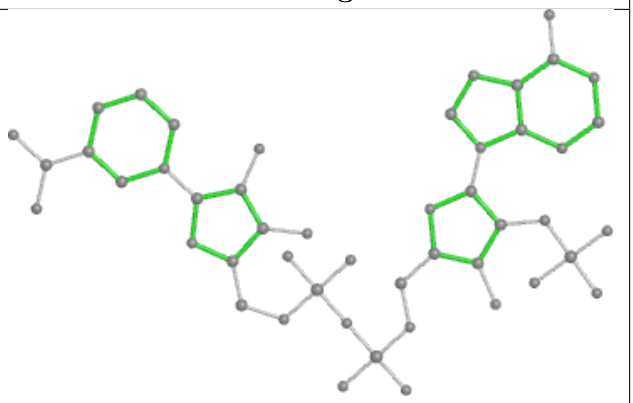
Bond lengths



Bond angles

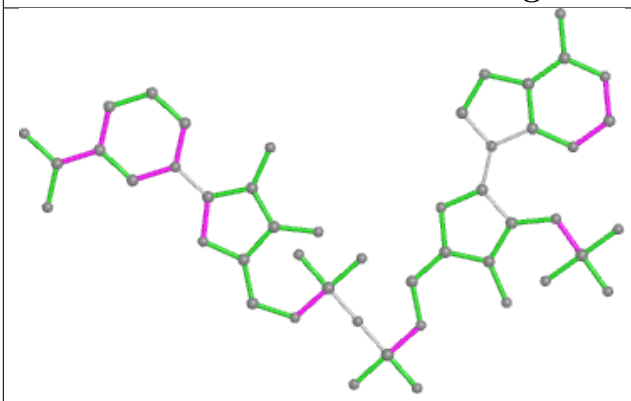


Torsions

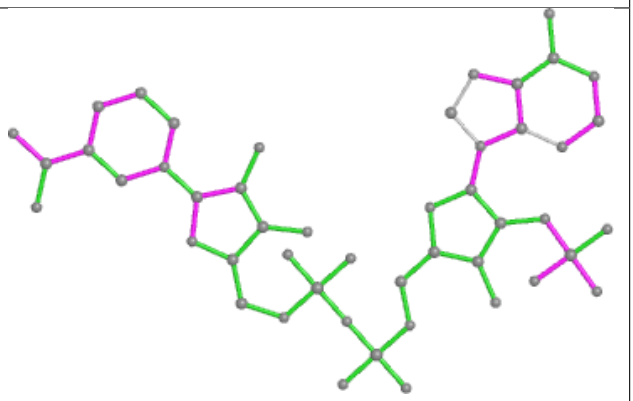


Rings

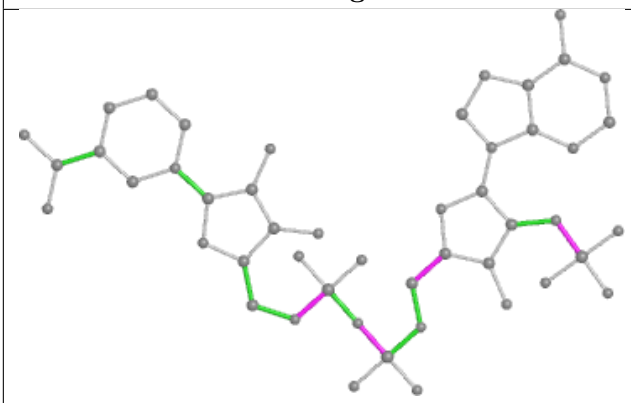
Ligand NAP E 601



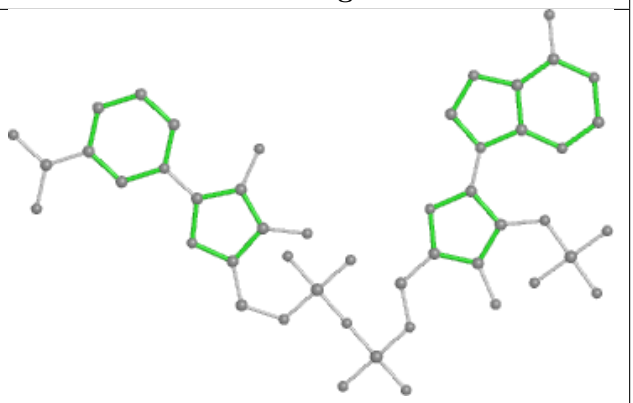
Bond lengths



Bond angles

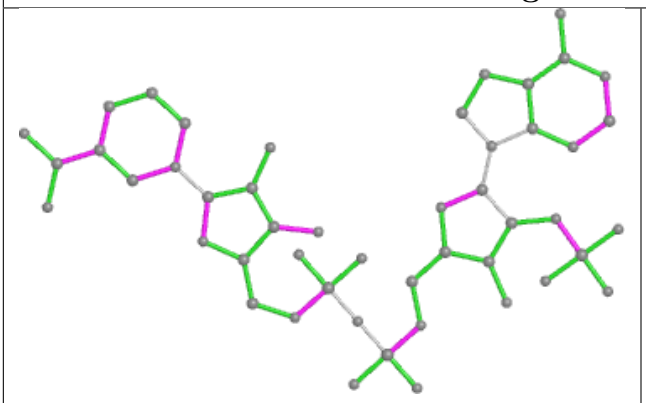


Torsions

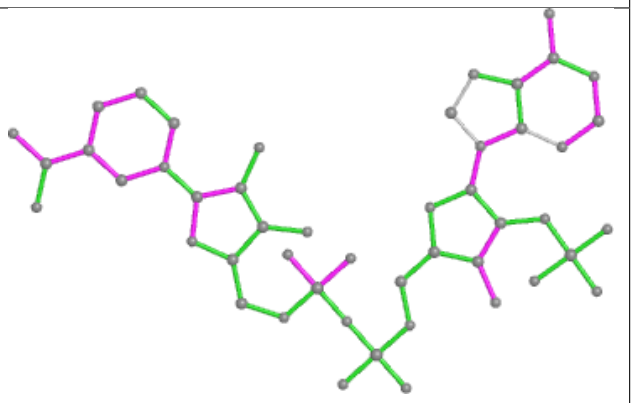


Rings

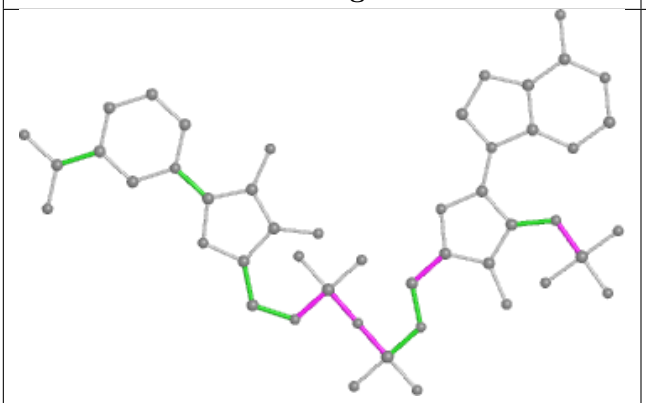
Ligand NAP B 601



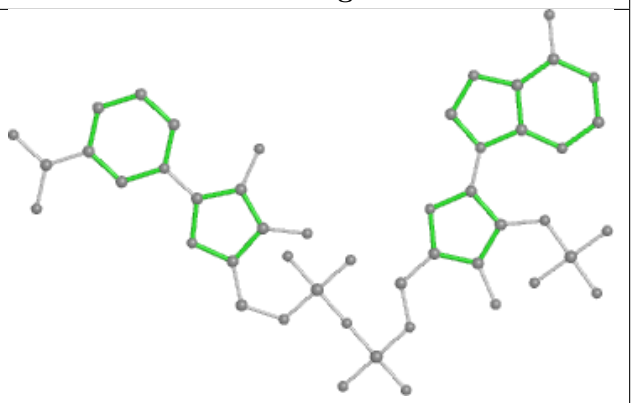
Bond lengths



Bond angles



Torsions



Rings

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	254/280 (90%)	0.33	5 (1%)	65	71	13, 21, 33, 41	0
1	B	248/280 (88%)	0.53	13 (5%)	27	34	15, 25, 43, 56	0
1	C	254/280 (90%)	0.35	2 (0%)	86	89	12, 20, 31, 40	0
1	D	254/280 (90%)	0.33	8 (3%)	49	56	12, 21, 33, 45	0
1	E	254/280 (90%)	0.60	16 (6%)	20	26	15, 25, 50, 70	0
1	F	254/280 (90%)	0.59	10 (3%)	39	47	15, 24, 43, 60	0
1	G	251/280 (89%)	0.58	14 (5%)	24	31	15, 24, 43, 63	0
1	I	254/280 (90%)	0.34	6 (2%)	59	66	12, 21, 33, 42	0
All	All	2023/2240 (90%)	0.46	74 (3%)	41	49	12, 23, 40, 70	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	PHE	6.9
1	E	202	PRO	6.2
1	E	205	ALA	5.3
1	G	194	THR	4.8
1	B	196	ALA	4.7
1	B	195	PRO	4.7
1	A	203	GLY	4.4
1	B	194	THR	4.4
1	B	57	GLY	4.3
1	E	204	ALA	4.3
1	E	208	THR	4.0
1	I	202	PRO	3.8
1	G	18	SER	3.8
1	G	48	LEU	3.8
1	F	80	VAL	3.7
1	G	205	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	196	ALA	3.7
1	E	193	ASP	3.6
1	G	201	LEU	3.6
1	B	54	GLY	3.5
1	G	195	PRO	3.5
1	F	211	PHE	3.4
1	I	53	ALA	3.3
1	E	198	PHE	3.3
1	E	54	GLY	3.3
1	B	200	ASN	3.3
1	D	202	PRO	3.3
1	F	198	PHE	3.2
1	E	196	ALA	3.2
1	D	198	PHE	3.2
1	D	203	GLY	3.2
1	E	135	LEU	3.1
1	E	30	ARG	3.1
1	B	190	GLY	3.0
1	F	30	ARG	2.9
1	D	211	PHE	2.9
1	F	190	GLY	2.9
1	E	81	ARG	2.9
1	C	202	PRO	2.9
1	G	211	PHE	2.8
1	D	201	LEU	2.8
1	B	98	ALA	2.8
1	F	199	ALA	2.8
1	G	199	ALA	2.8
1	B	30	ARG	2.8
1	D	43	ASN	2.8
1	A	64	GLY	2.7
1	A	202	PRO	2.6
1	E	98	ALA	2.5
1	I	79	ALA	2.5
1	B	26	LEU	2.5
1	F	88	THR	2.5
1	C	203	GLY	2.4
1	E	209	ARG	2.4
1	A	135	LEU	2.4
1	B	134	ALA	2.4
1	E	199	ALA	2.3
1	G	200	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	205	ALA	2.3
1	I	81	ARG	2.3
1	I	28	PHE	2.2
1	E	47	GLU	2.2
1	F	18	SER	2.2
1	B	81	ARG	2.2
1	A	53	ALA	2.2
1	B	198	PHE	2.1
1	G	84	GLY	2.1
1	E	195	PRO	2.1
1	D	35	VAL	2.1
1	F	209	ARG	2.1
1	F	48	LEU	2.1
1	G	81	ARG	2.0
1	G	11	ALA	2.0
1	I	135	LEU	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	E	601	48/48	0.81	0.25	30,37,49,52	0
2	NAP	G	601	48/48	0.82	0.26	28,39,45,46	0
2	NAP	F	601	48/48	0.83	0.23	29,41,46,51	0
2	NAP	B	601	48/48	0.86	0.22	30,39,47,48	0
2	NAP	I	601	48/48	0.92	0.12	16,24,30,33	0
2	NAP	A	601	48/48	0.94	0.12	19,25,32,35	0
2	NAP	C	601	48/48	0.94	0.12	18,23,31,34	0

Continued on next page...

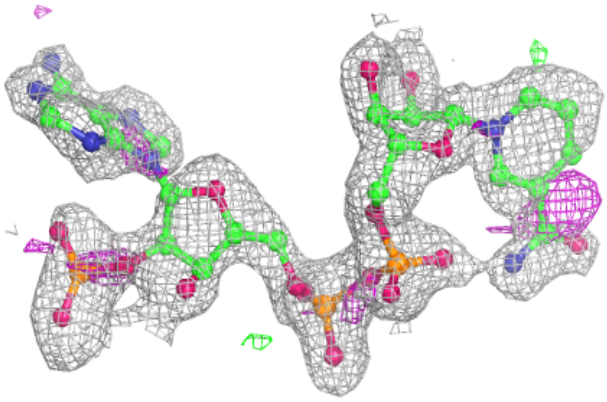
Continued from previous page...

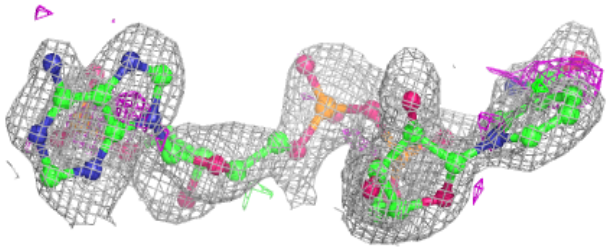
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	D	601	48/48	0.95	0.11	15,23,30,35	0

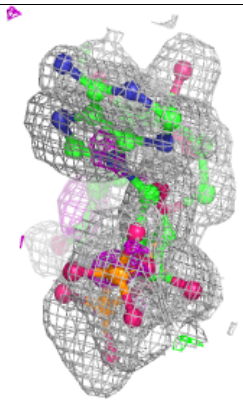
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP E 601:

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

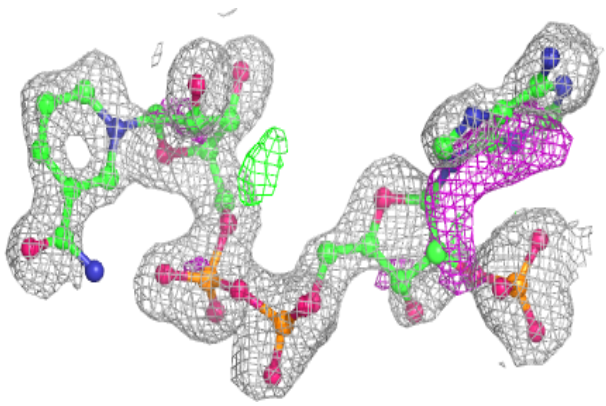


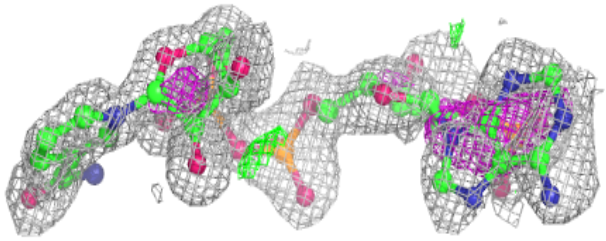


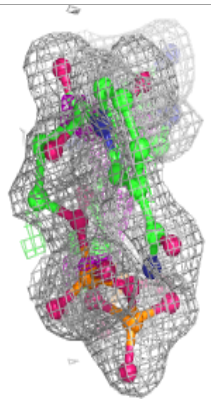


Electron density around NAP G 601:

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

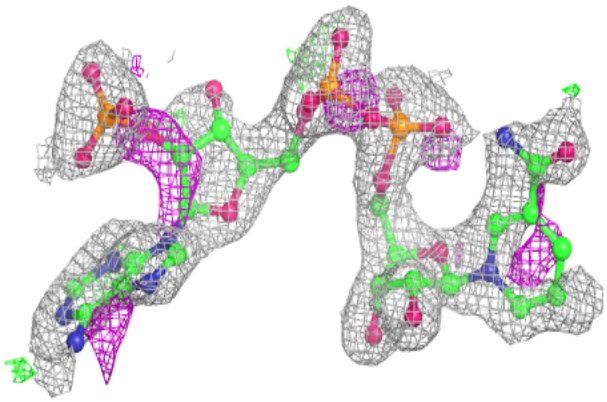


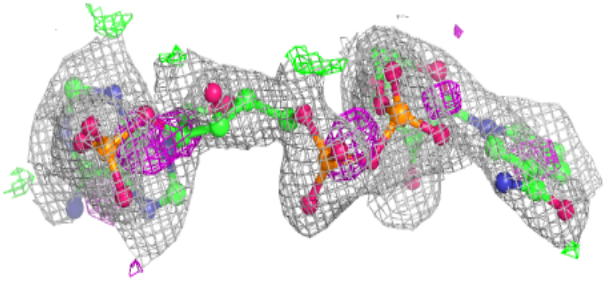


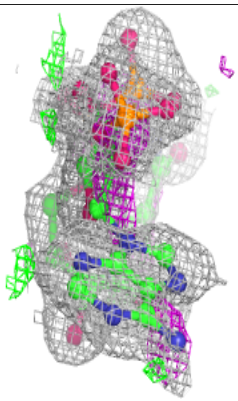


Electron density around NAP F 601:

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

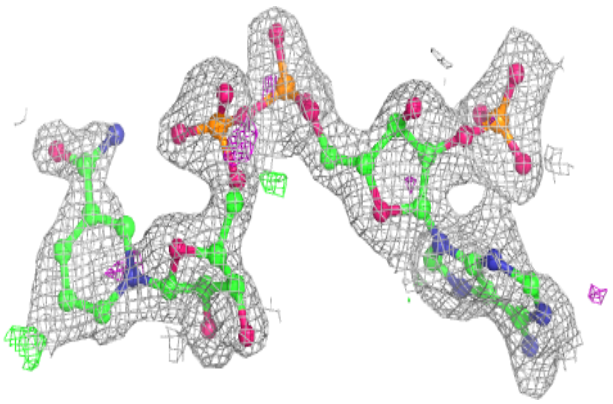


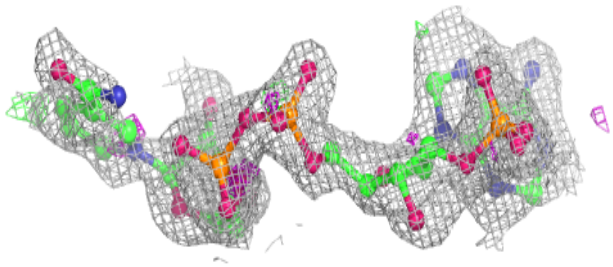


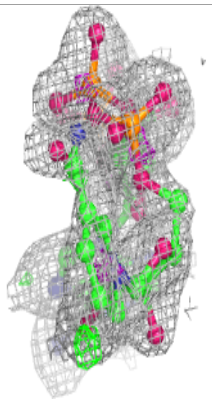


Electron density around NAP B 601:

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

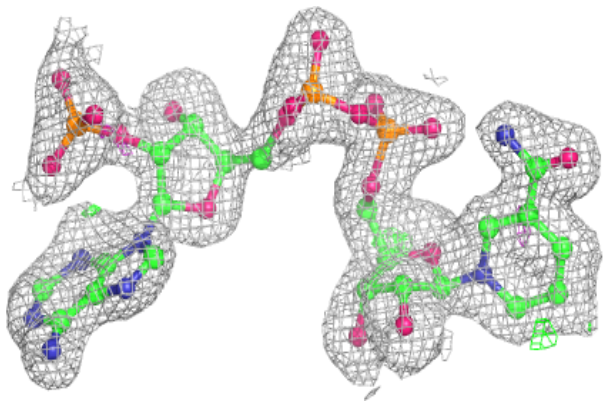


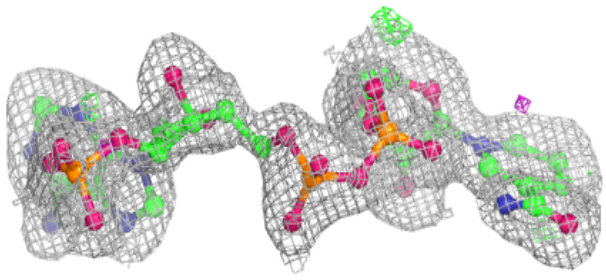


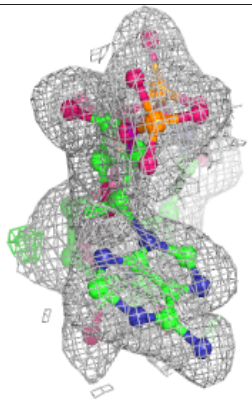


Electron density around NAP I 601:

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

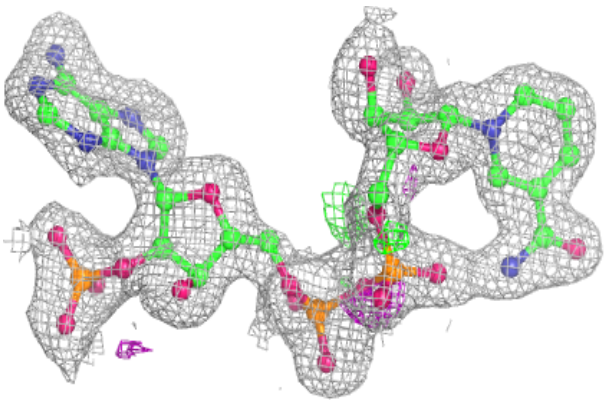


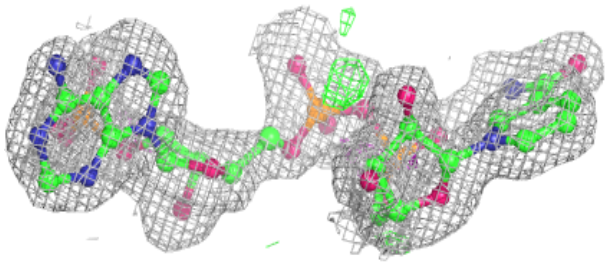


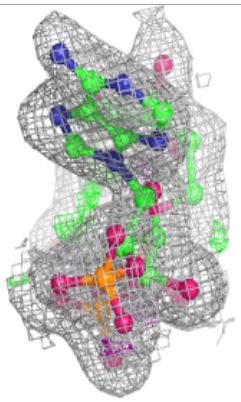


Electron density around NAP A 601:

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

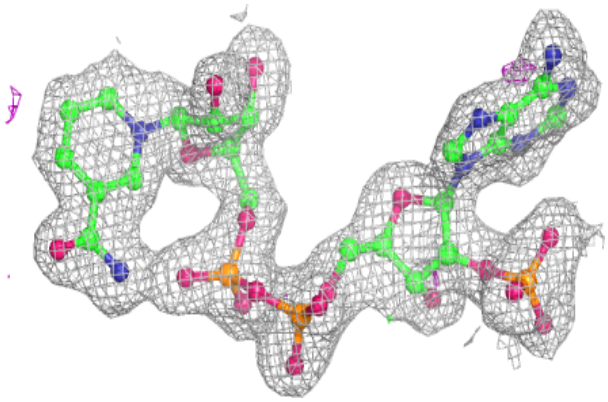


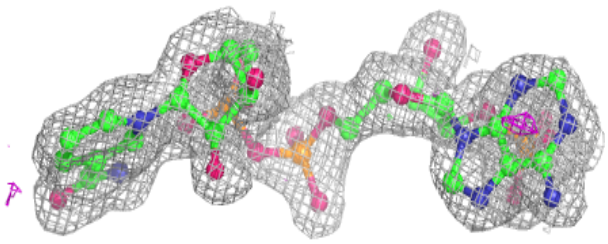


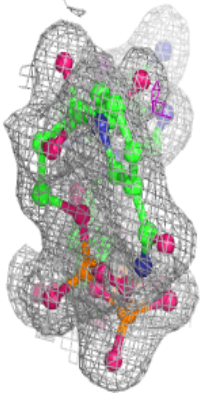


Electron density around NAP C 601:

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

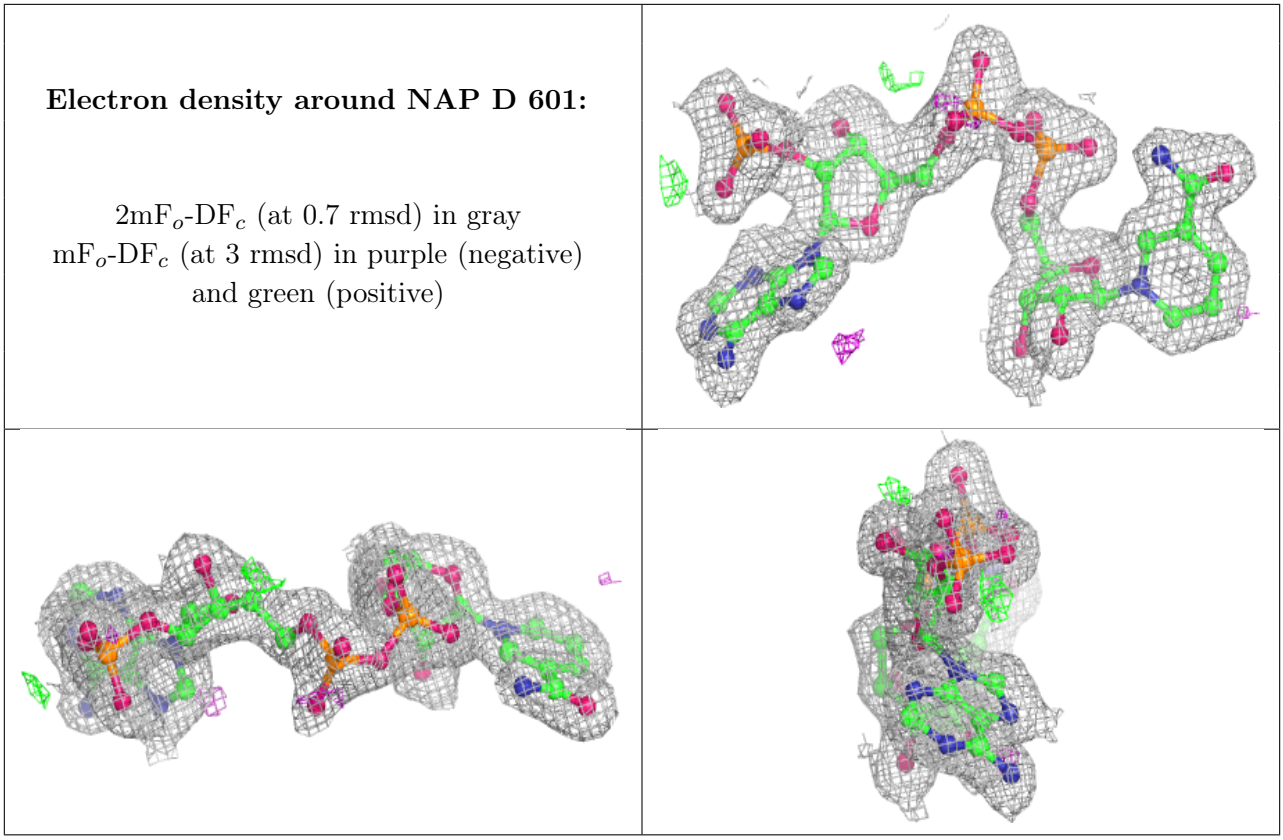






Electron density around NAP D 601:

$2mF_o$-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.