wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2024 – 02:43 AM EST

PDB ID	:	4L04
Title	:	Crystal Structure Analysis of human IDH1 mutants in complex with NADP+ and Ca2+/alpha-Ketoglutarate
Authors	:	Concha, N.O.; Smallwood, A.M.
Deposited on	:	2013-05-30
Resolution	:	2.87 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

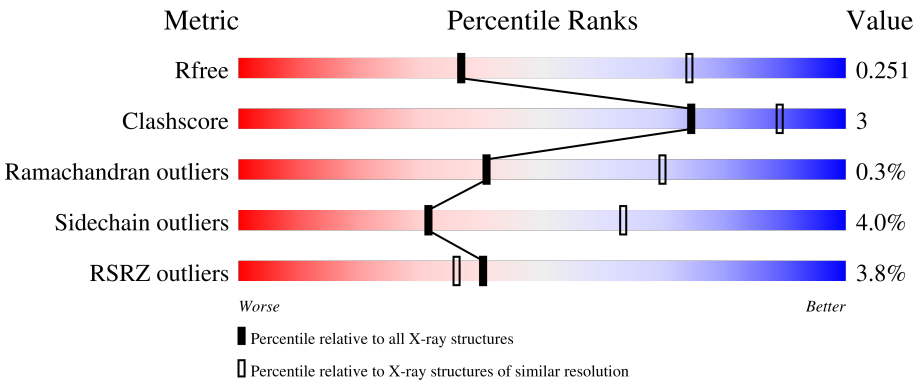
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	425	2% 87% 9% • •
1	B	425	% 85% 12% •
1	C	425	4% 84% 12% •
1	D	425	5% 84% 13% •
1	E	425	5% 84% 13% •

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Mol	Chain	Length	Quality of chain
1	F	425	6% 88% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19647 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	411	3221	2048	546	609	18	0	0	0
1	B	412	3258	2071	553	616	18	0	2	0
1	C	412	3206	2030	547	611	18	0	0	0
1	D	412	3129	1982	535	596	16	0	1	0
1	E	412	3226	2047	547	614	18	0	1	0
1	F	412	3184	2025	543	598	18	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	GLY	conflict	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	97	ASN	GLY	conflict	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874
B	425	HIS	-	expression tag	UNP O75874
C	97	ASN	GLY	conflict	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874
D	97	ASN	GLY	conflict	UNP O75874
D	415	SER	-	expression tag	UNP O75874
D	416	LEU	-	expression tag	UNP O75874
D	417	GLU	-	expression tag	UNP O75874
D	418	HIS	-	expression tag	UNP O75874
D	419	HIS	-	expression tag	UNP O75874
D	420	HIS	-	expression tag	UNP O75874
D	421	HIS	-	expression tag	UNP O75874
D	422	HIS	-	expression tag	UNP O75874
D	423	HIS	-	expression tag	UNP O75874
D	424	HIS	-	expression tag	UNP O75874
D	425	HIS	-	expression tag	UNP O75874
E	97	ASN	GLY	conflict	UNP O75874
E	415	SER	-	expression tag	UNP O75874
E	416	LEU	-	expression tag	UNP O75874
E	417	GLU	-	expression tag	UNP O75874
E	418	HIS	-	expression tag	UNP O75874
E	419	HIS	-	expression tag	UNP O75874
E	420	HIS	-	expression tag	UNP O75874
E	421	HIS	-	expression tag	UNP O75874
E	422	HIS	-	expression tag	UNP O75874
E	423	HIS	-	expression tag	UNP O75874
E	424	HIS	-	expression tag	UNP O75874

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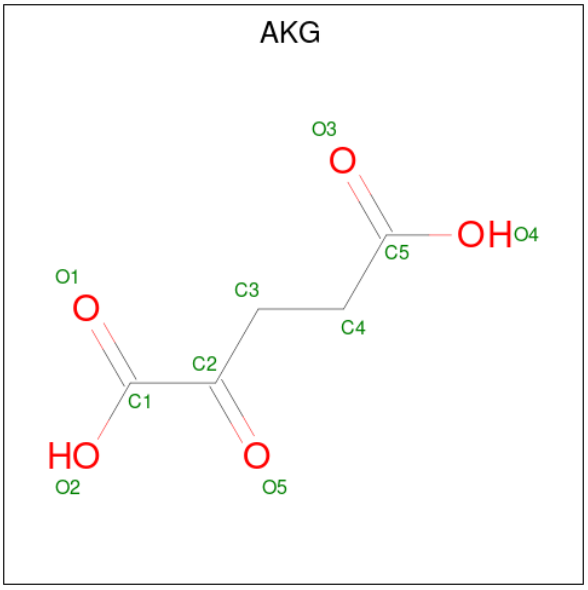
Chain	Residue	Modelled	Actual	Comment	Reference
E	425	HIS	-	expression tag	UNP O75874
F	97	ASN	GLY	conflict	UNP O75874
F	415	SER	-	expression tag	UNP O75874
F	416	LEU	-	expression tag	UNP O75874
F	417	GLU	-	expression tag	UNP O75874
F	418	HIS	-	expression tag	UNP O75874
F	419	HIS	-	expression tag	UNP O75874
F	420	HIS	-	expression tag	UNP O75874
F	421	HIS	-	expression tag	UNP O75874
F	422	HIS	-	expression tag	UNP O75874
F	423	HIS	-	expression tag	UNP O75874
F	424	HIS	-	expression tag	UNP O75874
F	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			10	5	5			
2	B	1	Total	C	O		0	0
			10	5	5			
2	C	1	Total	C	O		0	0
			10	5	5			
2	D	1	Total	C	O		0	0
			10	5	5			
2	E	1	Total	C	O		0	0
			10	5	5			

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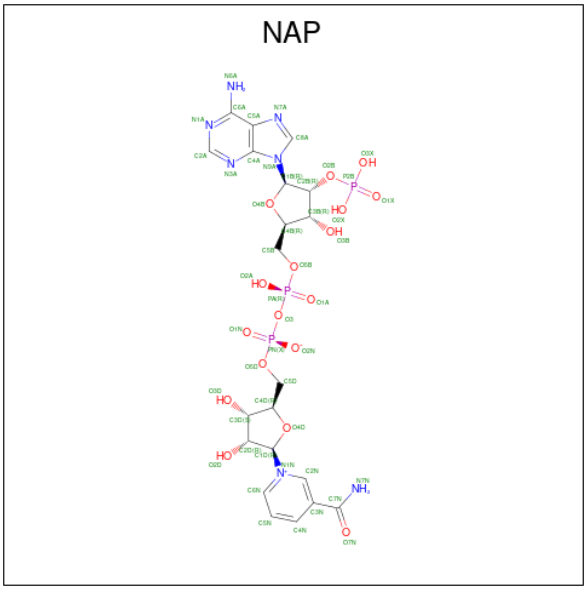
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	F	1	10	5	5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0
			Total	Ca		
3	C	1	1	1	0	0
			Total	Ca		
3	D	1	1	1	0	0
			Total	Ca		
3	E	1	1	1	0	0
			Total	Ca		
3	F	1	1	1	0	0

- Molecule 4 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
			Total	C	N	O	P		
4	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
4	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
4	C	1	48	21	7	17	3	0	0

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

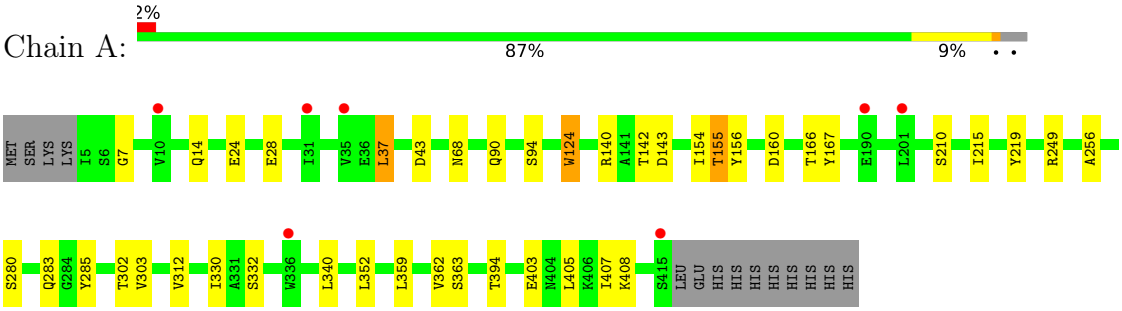
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	18	18	18	0	0
			Total	O		
5	B	13	13	13	0	0
			Total	O		
5	C	16	16	16	0	0
			Total	O		
5	D	8	8	8	0	0
			Total	O		
5	E	7	7	7	0	0
			Total	O		
5	F	7	7	7	0	0

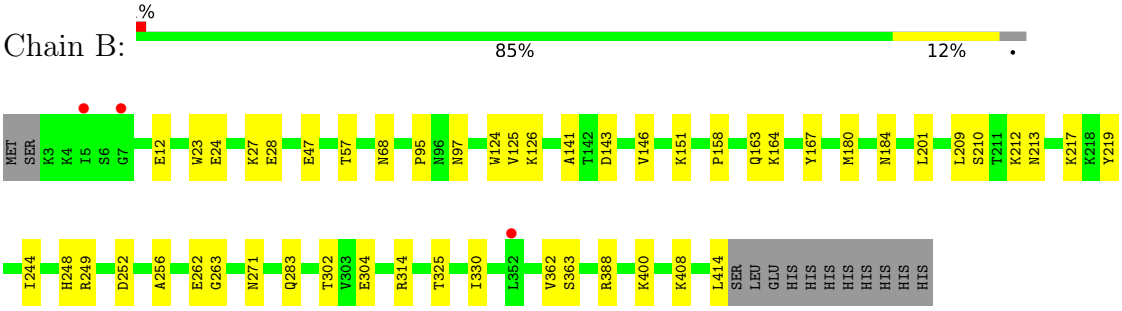
3 Residue-property plots (i)

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.

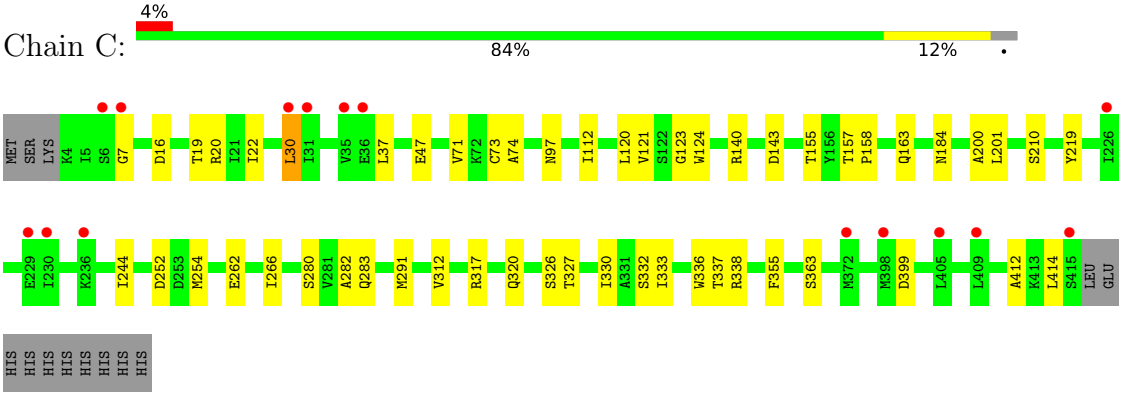
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



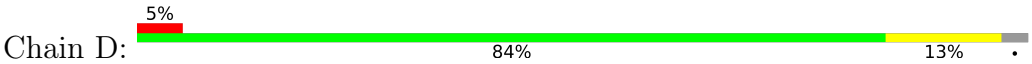
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

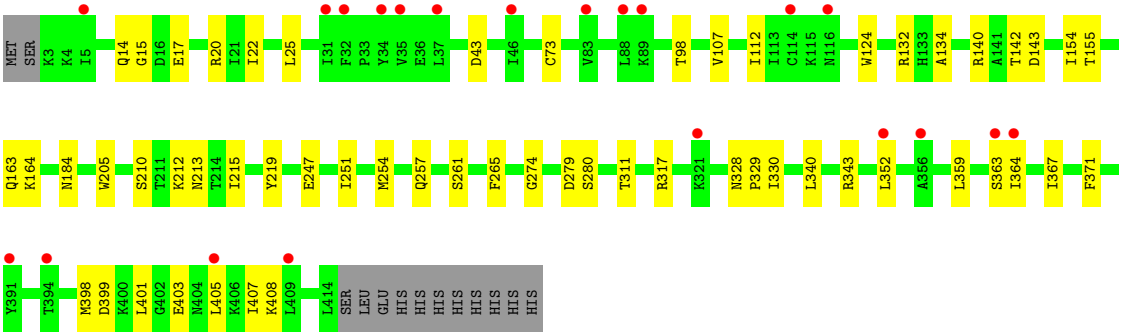


• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



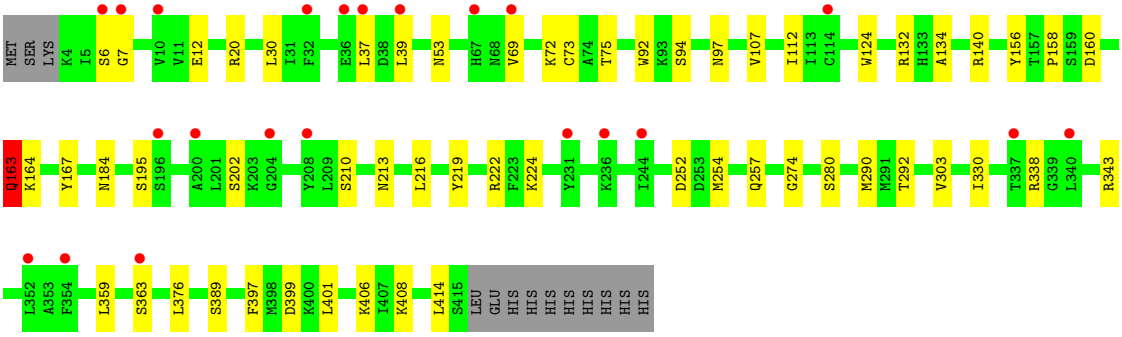
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic





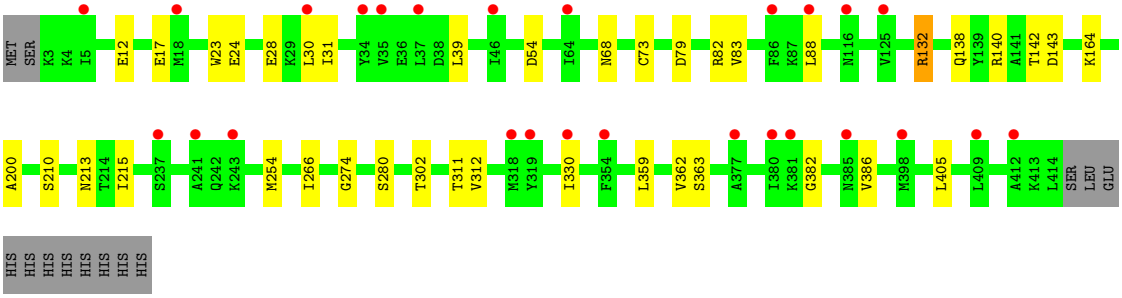
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain E:



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.41Å 116.62Å 275.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.87 49.24 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.24-2.87) 98.0 (49.24-2.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.86Å)	Xtriage
Refinement program	PHENIX, BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.259 0.195 , 0.251	Depositor DCC
R_{free} test set	3578 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19647	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6255e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, AKG, CA

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	0/3289	0.68	0/4446
1	B	0.47	0/3332	0.68	0/4499
1	C	0.47	0/3272	0.68	0/4422
1	D	0.45	0/3197	0.68	0/4336
1	E	0.47	0/3296	0.68	1/4456 (0.0%)
1	F	0.46	0/3255	0.69	0/4406
All	All	0.46	0/19641	0.68	1/26565 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	163	GLN	C-N-CA	5.21	134.72	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3221	0	3144	20	0
1	B	3258	0	3208	23	0
1	C	3206	0	3111	24	0
1	D	3129	0	2959	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3226	0	3147	25	0
1	F	3184	0	3075	19	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	0	0
4	C	48	0	25	1	0
4	D	48	0	25	0	0
4	E	48	0	25	1	0
4	F	48	0	25	0	0
5	A	18	0	0	0	0
5	B	13	0	0	0	0
5	C	16	0	0	0	0
5	D	8	0	0	0	0
5	E	7	0	0	0	0
5	F	7	0	0	0	0
All	All	19647	0	18818	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 121 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:E:163:GLN:NE2	1:E:164:LYS:H	1.59	0.99
1:C:19:THR:HG21	1:C:74:ALA:HB3	1.64	0.79
1:E:163:GLN:HA	1:E:163:GLN:OE1	1.90	0.69
1:D:205:TRP:HB3	1:D:265:PHE:HA	1.75	0.68
1:A:142:THR:HG21	1:B:167:TYR:HB3	1.80	0.64

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	409/425 (96%)	389 (95%)	19 (5%)	1 (0%)	47	76
1	B	412/425 (97%)	391 (95%)	19 (5%)	2 (0%)	29	59
1	C	410/425 (96%)	384 (94%)	26 (6%)	0	100	100
1	D	411/425 (97%)	386 (94%)	23 (6%)	2 (0%)	29	59
1	E	411/425 (97%)	389 (95%)	21 (5%)	1 (0%)	47	76
1	F	411/425 (97%)	387 (94%)	22 (5%)	2 (0%)	29	59
All	All	2464/2550 (97%)	2326 (94%)	130 (5%)	8 (0%)	41	70

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	TRP
1	D	163	GLN
1	E	124	TRP
1	F	164	LYS
1	A	124	TRP

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	337/362 (93%)	326 (97%)	11 (3%)	38	70
1	B	345/362 (95%)	332 (96%)	13 (4%)	33	65
1	C	333/362 (92%)	320 (96%)	13 (4%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	312/362 (86%)	297 (95%)	15 (5%)	25	56
1	E	339/362 (94%)	318 (94%)	21 (6%)	18	45
1	F	326/362 (90%)	318 (98%)	8 (2%)	47	77
All	All	1992/2172 (92%)	1911 (96%)	81 (4%)	31	62

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	163	GLN
1	E	408	LYS
1	E	195	SER
1	E	280	SER
1	F	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	309	HIS
1	F	68	ASN
1	F	404	ASN
1	F	96	ASN
1	C	96	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAP	C	503	-	45,52,52	1.82	3 (6%)	56,80,80	1.10	1 (1%)
2	AKG	B	501	3	9,9,9	2.04	1 (11%)	11,11,11	1.56	2 (18%)
4	NAP	E	503	-	45,52,52	1.73	3 (6%)	56,80,80	1.22	4 (7%)
2	AKG	E	501	3	9,9,9	2.24	1 (11%)	11,11,11	1.42	1 (9%)
4	NAP	F	503	-	45,52,52	1.76	4 (8%)	56,80,80	1.20	4 (7%)
2	AKG	A	501	3	9,9,9	2.15	1 (11%)	11,11,11	1.51	1 (9%)
2	AKG	F	501	3	9,9,9	1.93	1 (11%)	11,11,11	1.64	3 (27%)
2	AKG	D	501	3	9,9,9	2.05	1 (11%)	11,11,11	1.15	1 (9%)
4	NAP	A	504	-	45,52,52	1.77	4 (8%)	56,80,80	1.09	2 (3%)
4	NAP	B	502	-	45,52,52	1.65	4 (8%)	56,80,80	1.30	2 (3%)
4	NAP	D	503	-	45,52,52	1.79	4 (8%)	56,80,80	1.11	2 (3%)
2	AKG	C	501	3	9,9,9	1.97	1 (11%)	11,11,11	1.35	1 (9%)

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
4	NAP	C	503	-	-	10/31/67/67	0/5/5/5
2	AKG	B	501	3	-	1/9/9/9	-
4	NAP	E	503	-	-	10/31/67/67	0/5/5/5
2	AKG	E	501	3	-	6/9/9/9	-
4	NAP	F	503	-	-	11/31/67/67	0/5/5/5
2	AKG	A	501	3	-	6/9/9/9	-
2	AKG	F	501	3	-	6/9/9/9	-
2	AKG	D	501	3	-	5/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	A	504	-	-	12/31/67/67	0/5/5/5
4	NAP	B	502	-	-	9/31/67/67	0/5/5/5
4	NAP	D	503	-	-	4/31/67/67	0/5/5/5
2	AKG	C	501	3	-	4/9/9/9	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	NAP	O7N-C7N	9.41	1.42	1.24
4	D	503	NAP	O7N-C7N	9.15	1.41	1.24
4	F	503	NAP	O7N-C7N	8.98	1.41	1.24
4	E	503	NAP	O7N-C7N	8.93	1.41	1.24
4	A	504	NAP	O7N-C7N	8.83	1.41	1.24

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	NAP	N3A-C2A-N1A	-6.48	118.55	128.68
4	E	503	NAP	N3A-C2A-N1A	-5.85	119.54	128.68
4	F	503	NAP	N3A-C2A-N1A	-5.83	119.57	128.68
4	D	503	NAP	N3A-C2A-N1A	-5.67	119.82	128.68
4	A	504	NAP	N3A-C2A-N1A	-5.17	120.60	128.68

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AKG	O1-C1-C2-O5
2	A	501	AKG	O1-C1-C2-C3
2	A	501	AKG	O2-C1-C2-C3
2	C	501	AKG	C2-C3-C4-C5
2	D	501	AKG	O2-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	NAP	1	0
4	E	503	NAP	1	0
2	A	501	AKG	1	0

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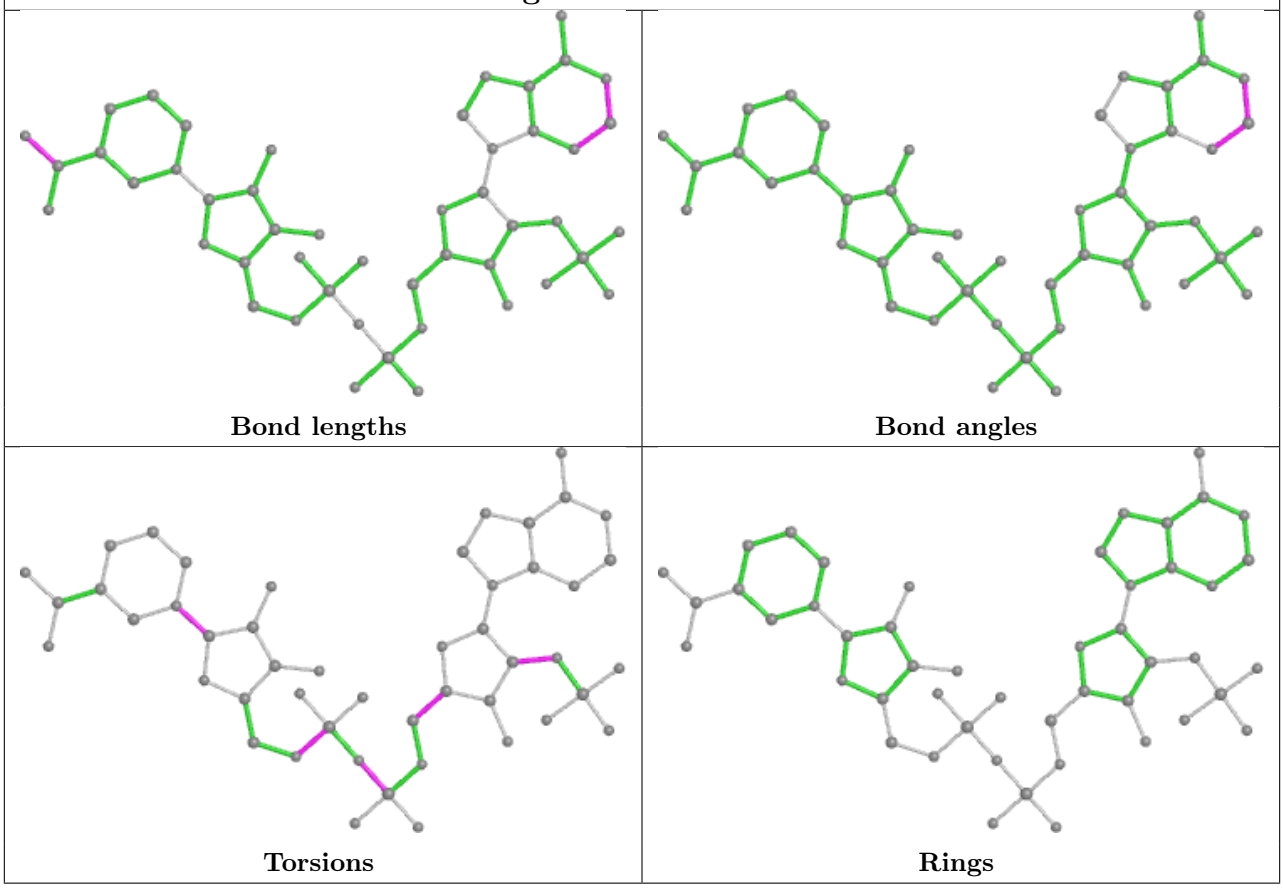
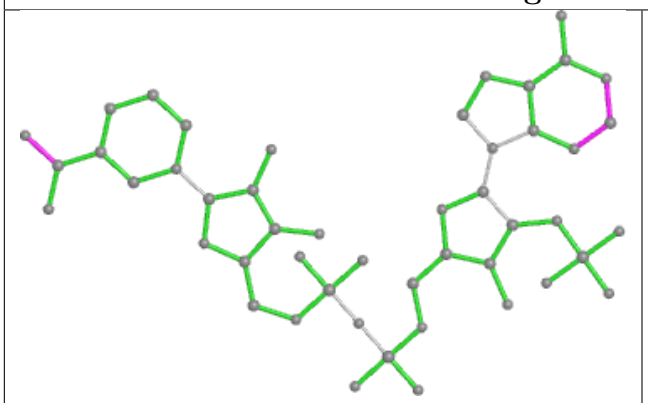
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	NAP	1	0

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.

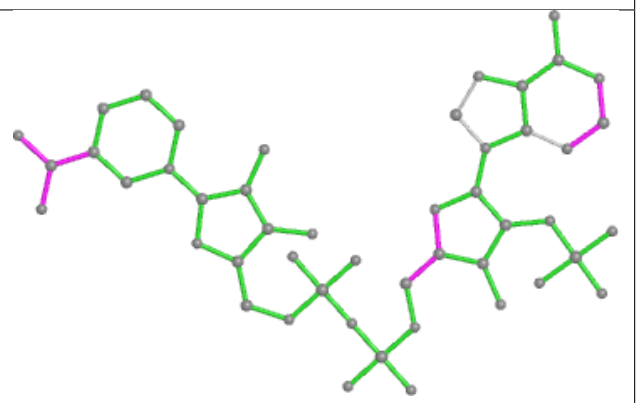
Ligand NAP C 503



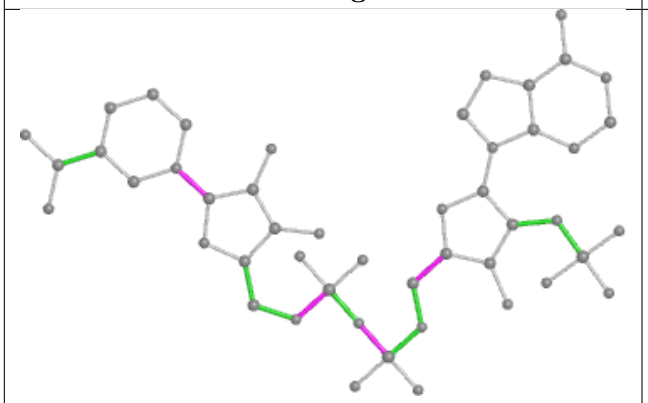
Ligand NAP E 503



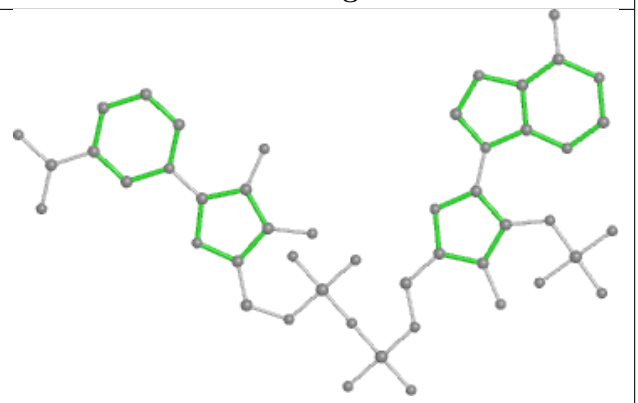
Bond lengths



Bond angles

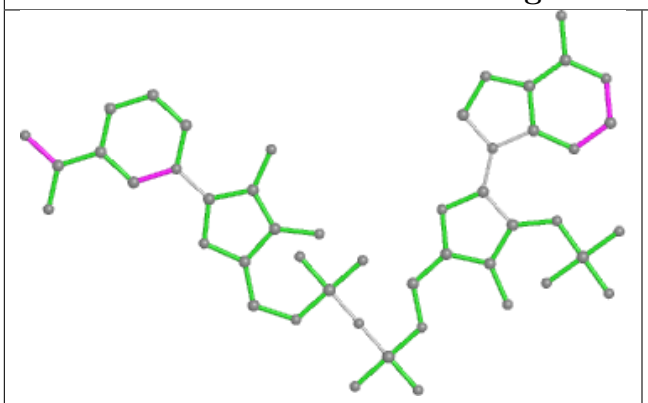


Torsions

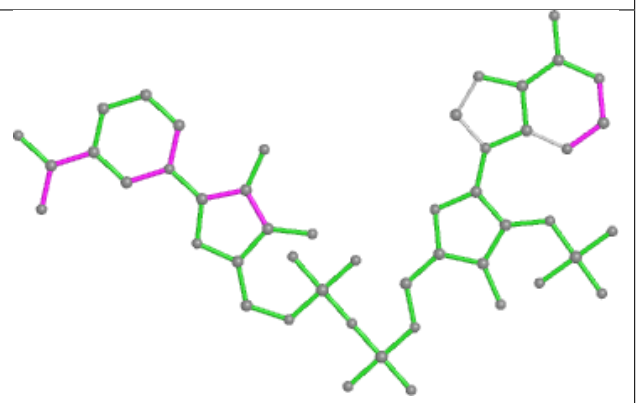


Rings

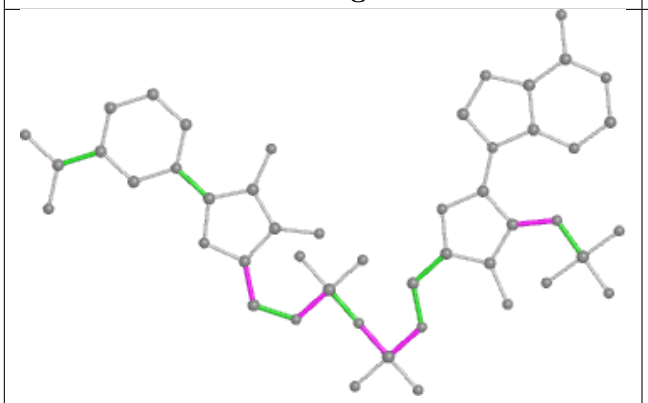
Ligand NAP F 503



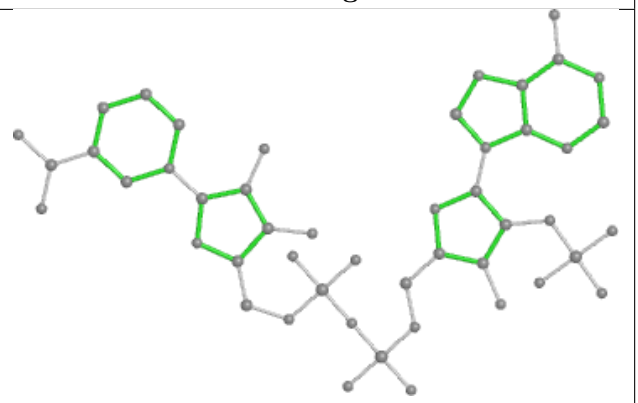
Bond lengths



Bond angles

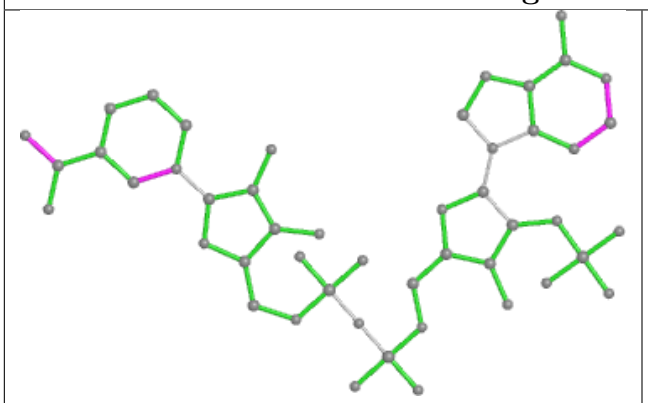


Torsions

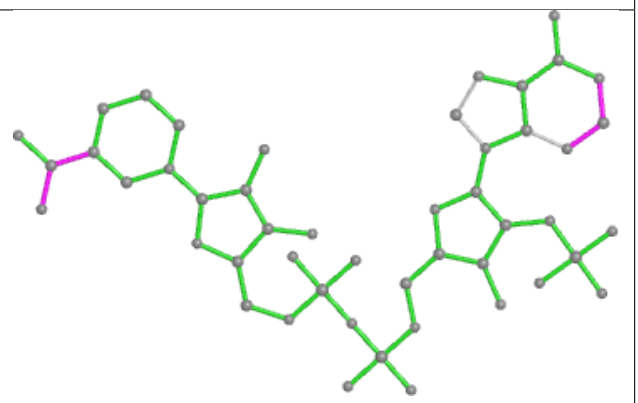


Rings

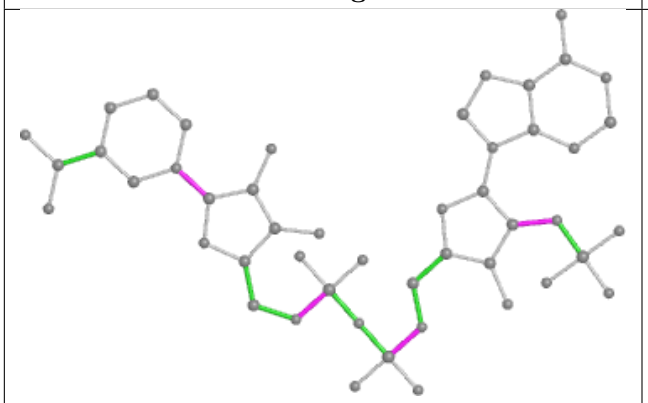
Ligand NAP A 504



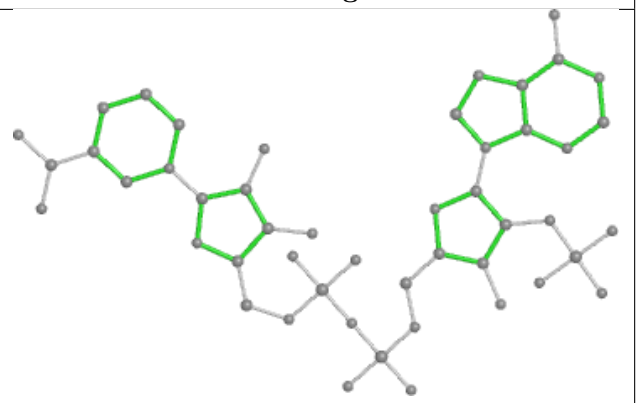
Bond lengths



Bond angles

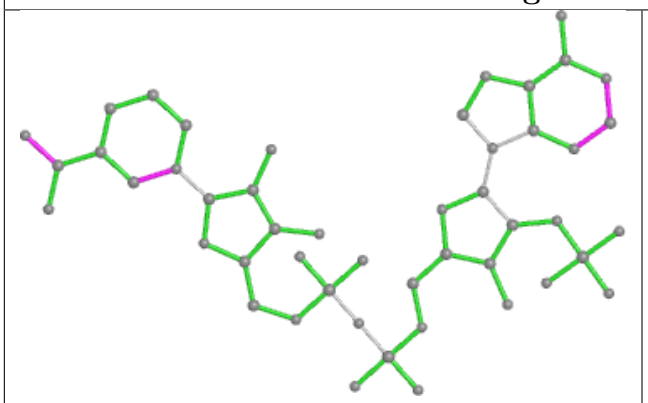


Torsions

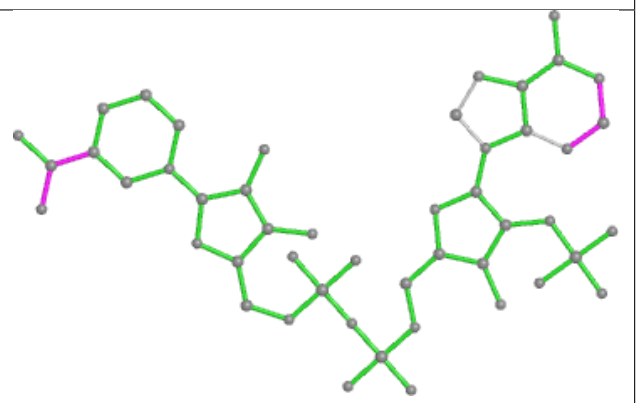


Rings

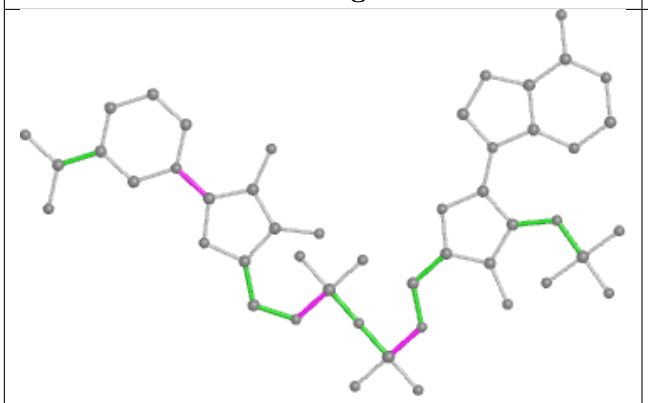
Ligand NAP B 502



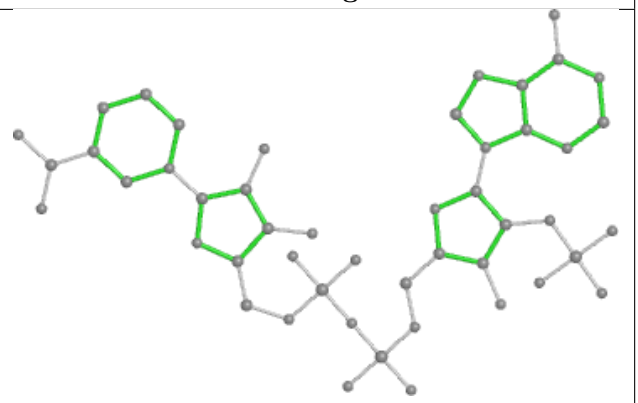
Bond lengths



Bond angles

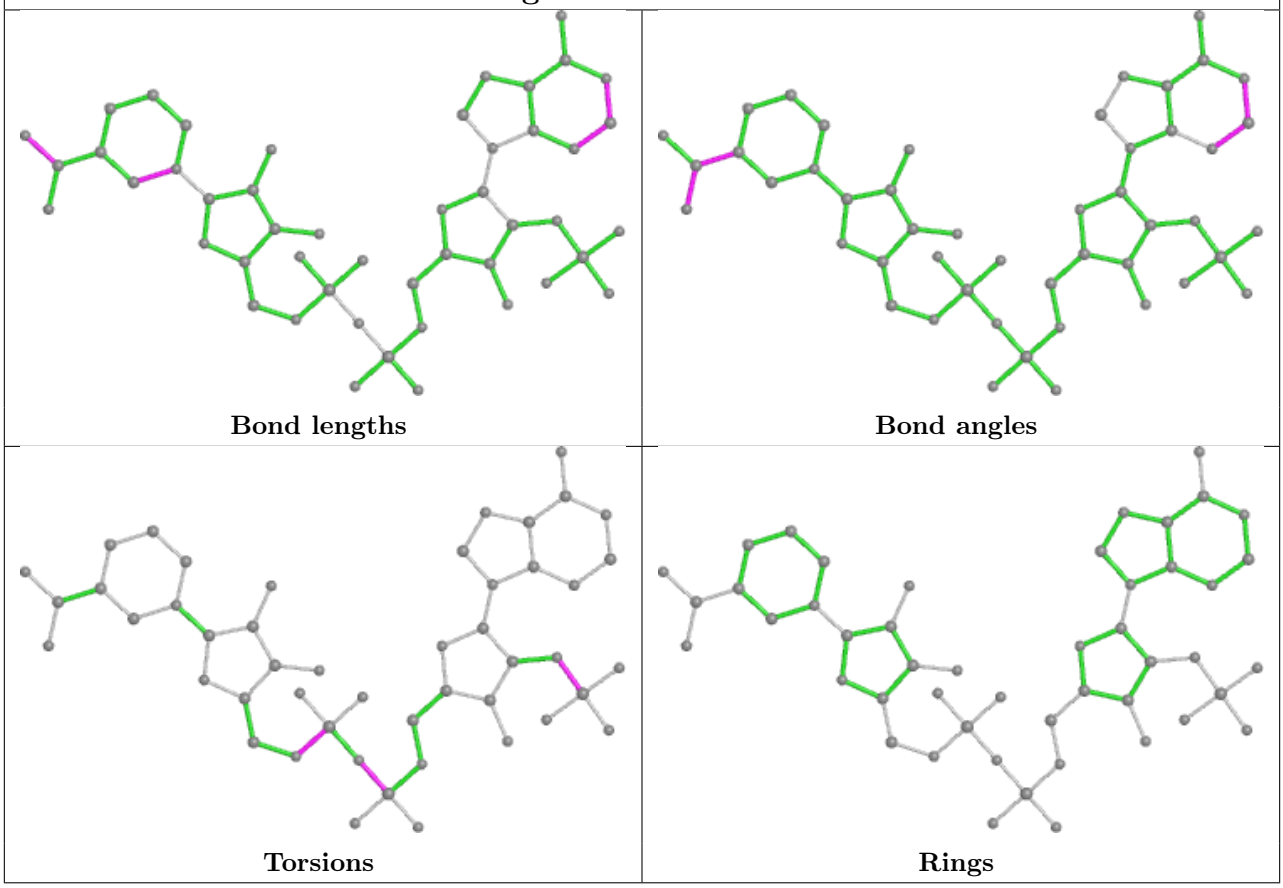


Torsions



Rings

Ligand NAP D 503



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/425 (96%)	-0.11	7 (1%)	70	70	39, 69, 98, 124	0
1	B	412/425 (96%)	-0.34	3 (0%)	87	87	38, 55, 79, 94	0
1	C	412/425 (96%)	0.01	15 (3%)	42	38	40, 69, 96, 130	0
1	D	412/425 (96%)	0.12	21 (5%)	28	24	40, 83, 116, 147	0
1	E	412/425 (96%)	0.09	22 (5%)	26	22	40, 71, 101, 121	0
1	F	412/425 (96%)	0.20	26 (6%)	20	16	42, 81, 112, 151	0
All	All	2471/2550 (96%)	-0.01	94 (3%)	40	36	38, 70, 105, 151	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	SER	9.0
1	D	35	VAL	6.6
1	F	35	VAL	6.0
1	D	363	SER	5.5
1	E	7	GLY	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

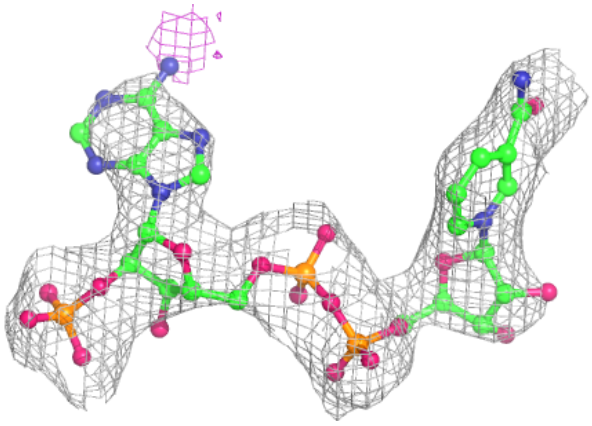
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

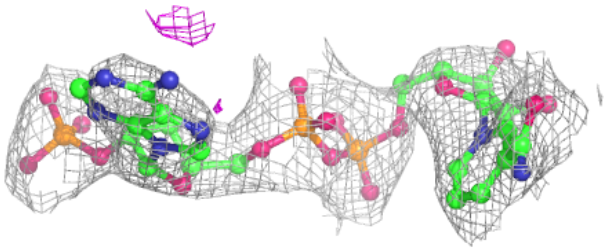
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAP	D	503	48/48	0.87	0.21	98,109,113,114	0
2	AKG	C	501	10/10	0.88	0.30	79,85,88,88	0
2	AKG	F	501	10/10	0.89	0.29	86,90,99,99	0
2	AKG	E	501	10/10	0.90	0.35	91,96,98,98	0
4	NAP	F	503	48/48	0.91	0.20	84,99,103,105	0
2	AKG	D	501	10/10	0.92	0.24	100,101,102,102	0
4	NAP	E	503	48/48	0.94	0.20	54,68,77,79	0
2	AKG	A	501	10/10	0.94	0.21	74,77,79,79	0
2	AKG	B	501	10/10	0.95	0.15	41,55,58,58	0
3	CA	F	502	1/1	0.96	0.20	74,74,74,74	0
4	NAP	A	504	48/48	0.96	0.16	43,59,68,71	0
4	NAP	C	503	48/48	0.96	0.18	50,61,74,75	0
3	CA	A	502	1/1	0.97	0.25	70,70,70,70	0
3	CA	E	502	1/1	0.98	0.23	72,72,72,72	0
3	CA	C	502	1/1	0.98	0.24	62,62,62,62	0
3	CA	D	502	1/1	0.98	0.24	70,70,70,70	0
4	NAP	B	502	48/48	0.98	0.17	44,51,59,62	0
3	CA	A	503	1/1	0.99	0.17	53,53,53,53	0

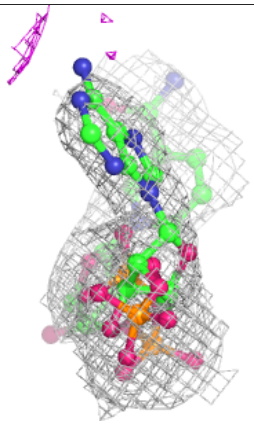
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 503:

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

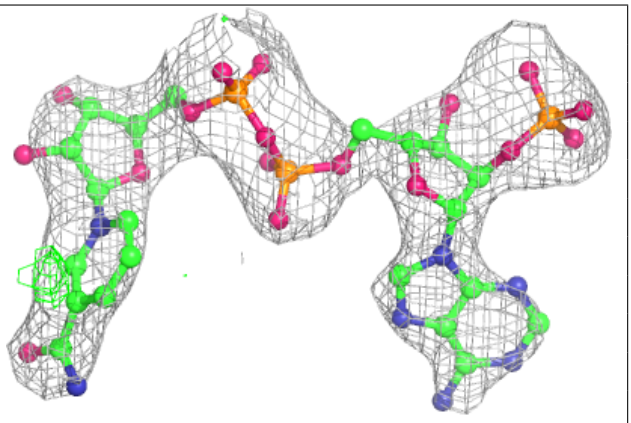


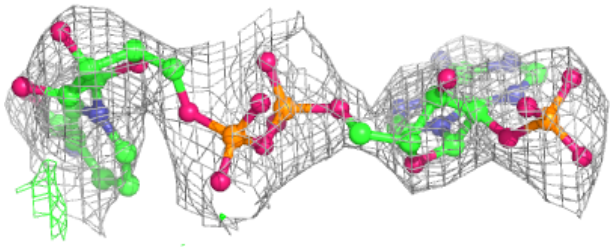


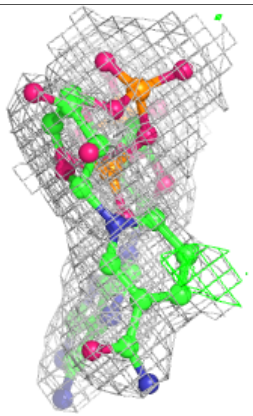


Electron density around NAP F 503:

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

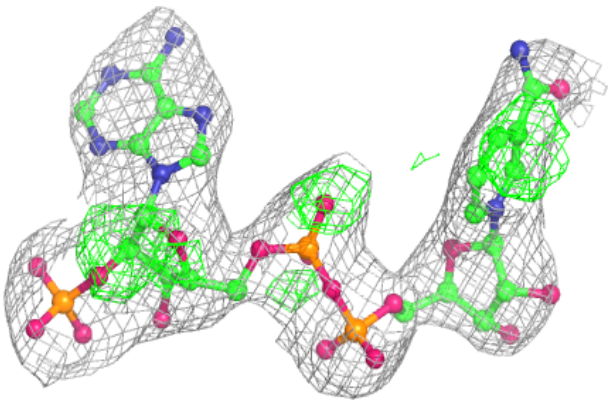


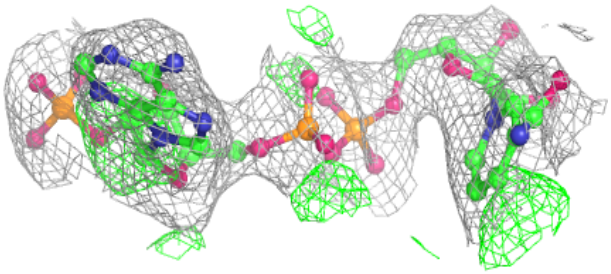


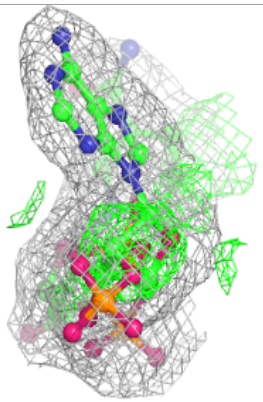


Electron density around NAP E 503:

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

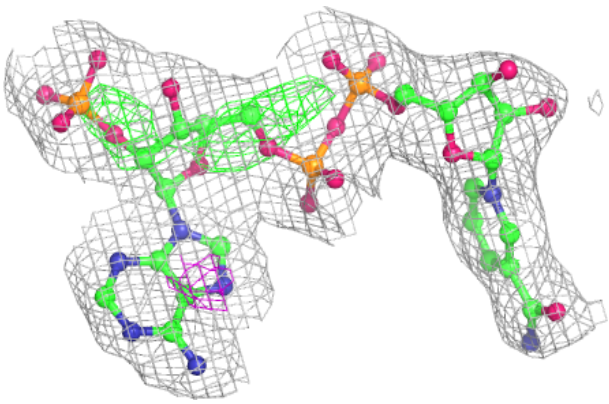


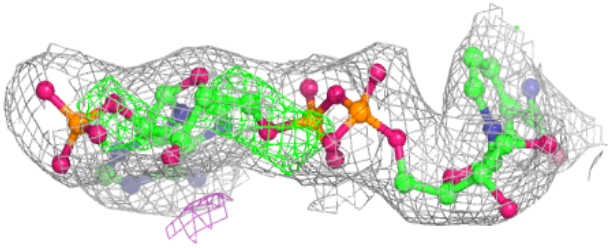


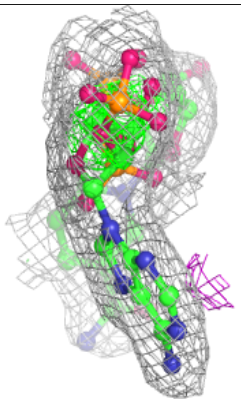


Electron density around NAP A 504:

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

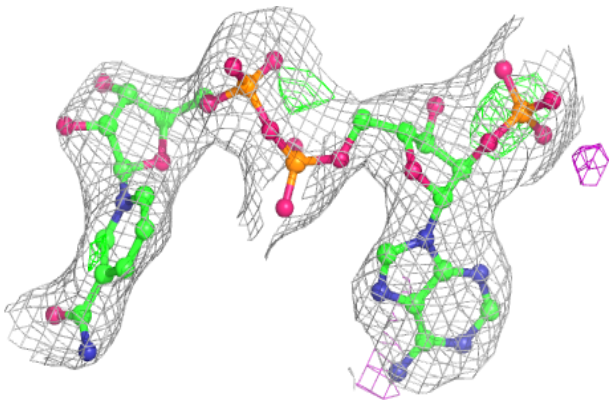


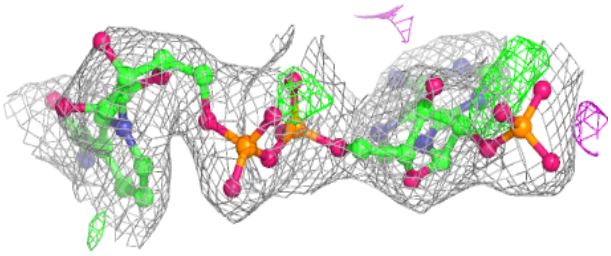


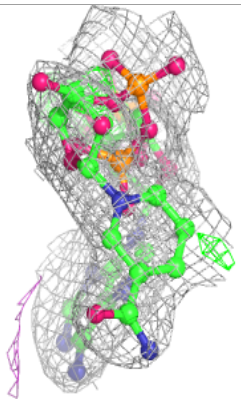


Electron density around NAP C 503:

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

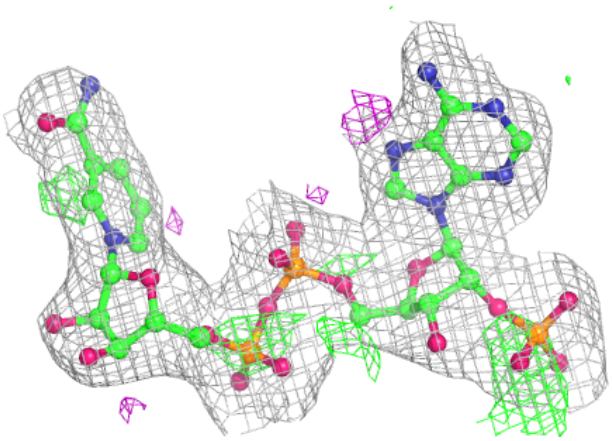


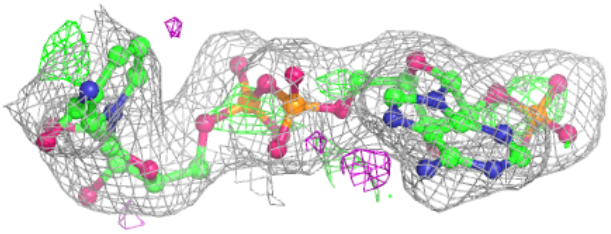


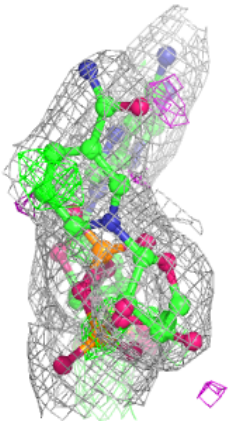


Electron density around NAP B 502:

$2mF_o$-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.