wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 11:13 PM EDT

PDB ID	:	2D2I
Title	:	Crystal Structure of NADP-Dependent Glyceraldehyde-3-Phosphate Dehydrogenase from Synechococcus Sp. complexed with Nadp+
Authors	:	Kitatani, T.; Nakamura, Y.; Wada, K.; Kinoshita, T.; Tamoi, M.; Shigeoka, S.; Tada, T.
Deposited on	:	2005-09-09
Resolution	:	2.50 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:

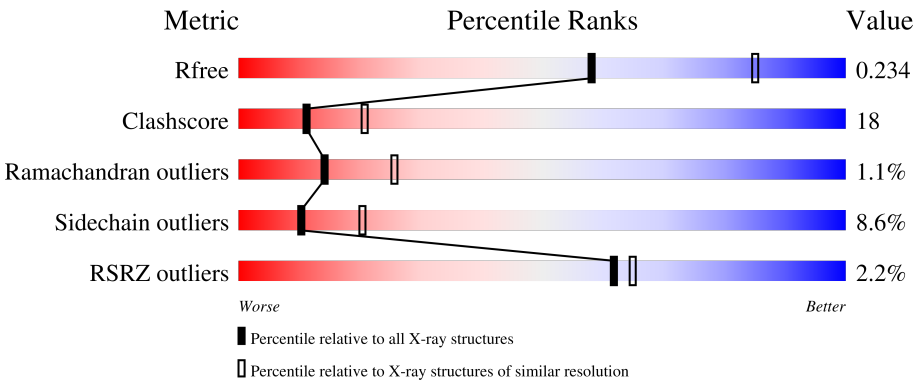
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	380	% 61% 24% • • 11%
1	B	380	% 63% 21% 5% • 11%
1	O	380	% 62% 23% • 11%
1	P	380	3% 58% 28% • • 11%

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Mol	Chain	Length	Quality of chain
1	Q	380	4% 59% 27% • 11%
1	R	380	2% 61% 24% • 11%

2 Entry composition (i)

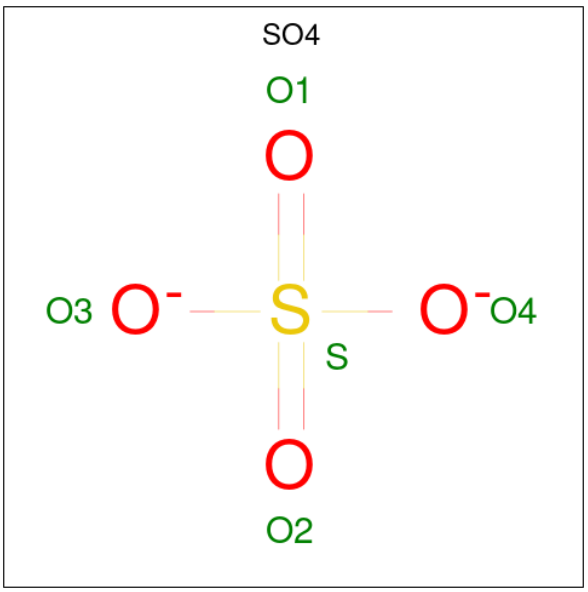
There are 4 unique types of molecules in this entry. The entry contains 16415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glyceraldehyde 3-phosphate dehydrogenase.

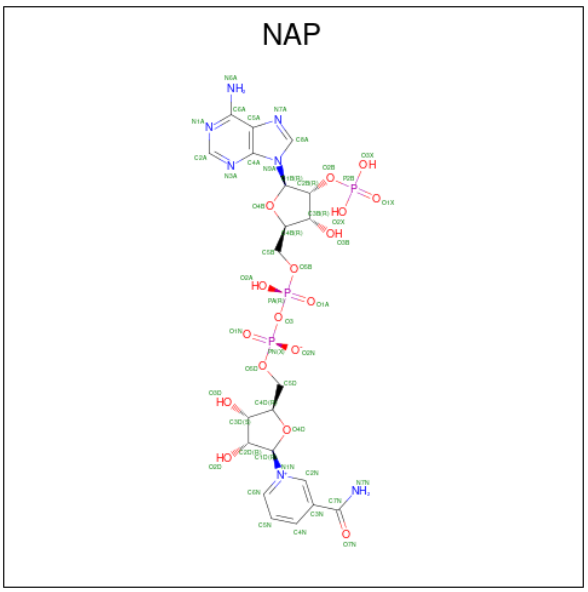
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2588	1625	454	500	9	0	0	0
1	B	338	2588	1625	454	500	9	0	0	0
1	O	338	2588	1625	454	500	9	0	0	0
1	P	338	2588	1625	454	500	9	0	0	0
1	Q	338	2588	1625	454	500	9	0	0	0
1	R	338	2588	1625	454	500	9	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	O	1	5	4	1	0	0
			Total	O	S		
2	O	1	5	4	1	0	0
			Total	O	S		
2	P	1	5	4	1	0	0
			Total	O	S		
2	P	1	5	4	1	0	0
			Total	O	S		
2	Q	1	5	4	1	0	0
			Total	O	S		
2	Q	1	5	4	1	0	0
			Total	O	S		
2	R	1	5	4	1	0	0
			Total	O	S		
2	R	1	5	4	1	0	0

- Molecule 3 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		
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0
3	O	1	48	21	7	17	3	0	0
3	P	1	48	21	7	17	3	0	0
3	Q	1	48	21	7	17	3	0	0
3	R	1	48	21	7	17	3	0	0

- Molecule 4 is water.

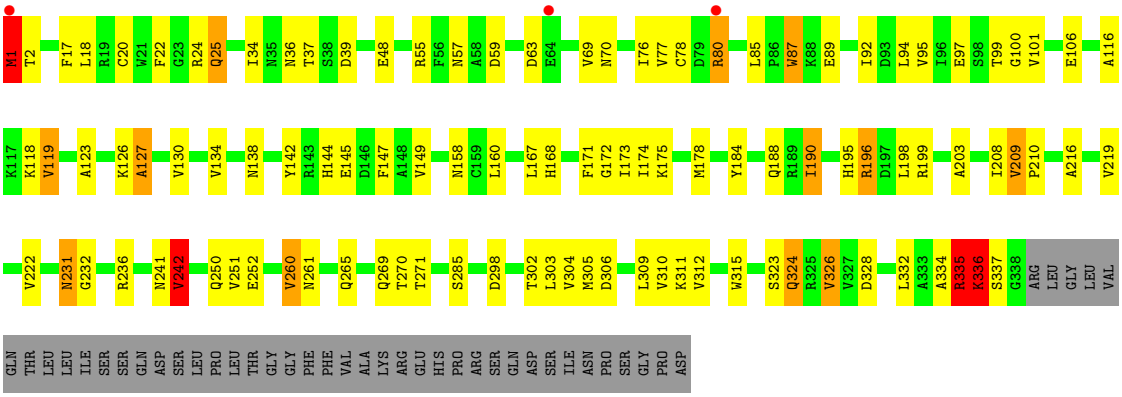
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	107	107	107	0	0
4	B	142	142	142	0	0
4	O	86	86	86	0	0
4	P	82	82	82	0	0
4	Q	47	47	47	0	0
4	R	75	75	75	0	0

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.

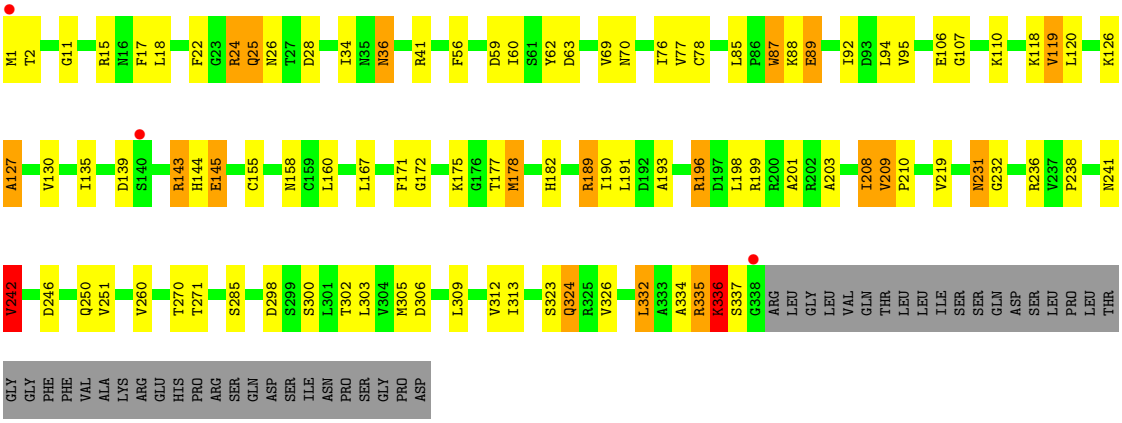
• Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

Chain A:



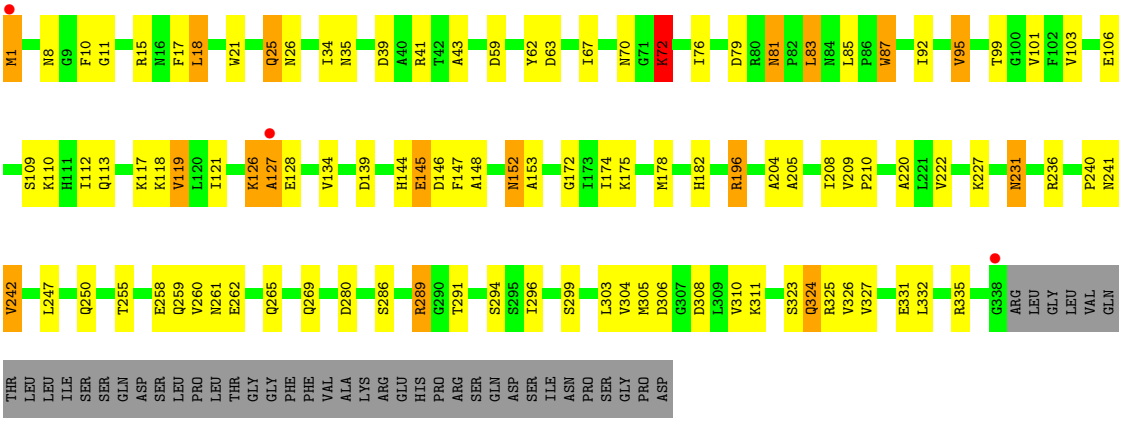
• Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

Chain B:



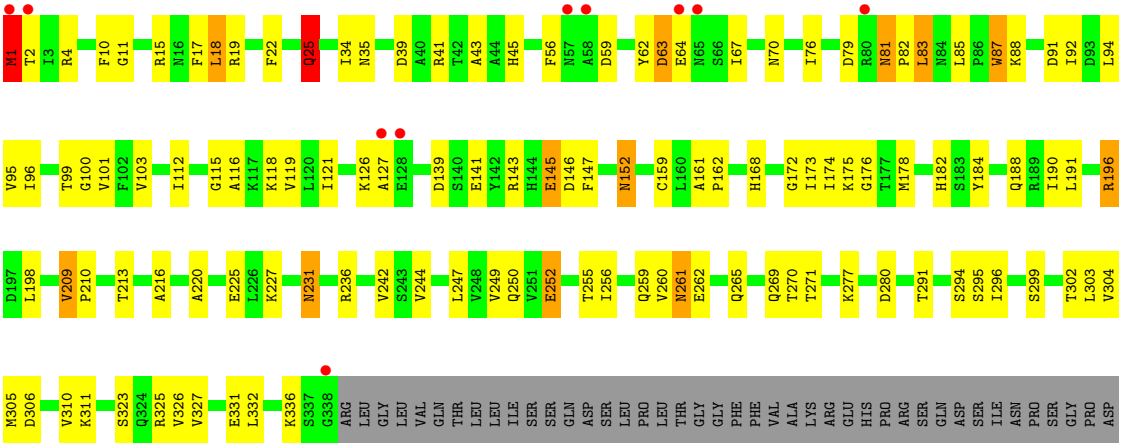
• Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

Chain O:



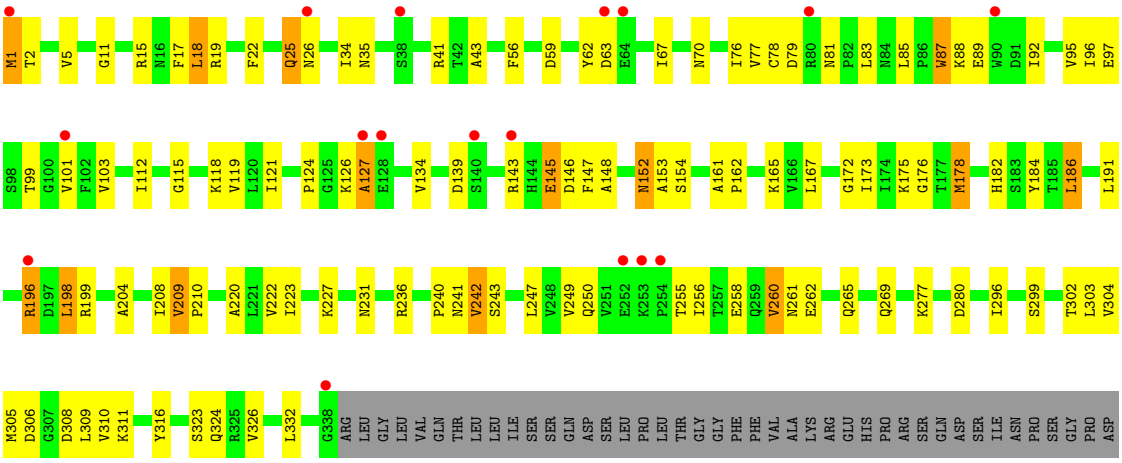
- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

Chain P:



- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

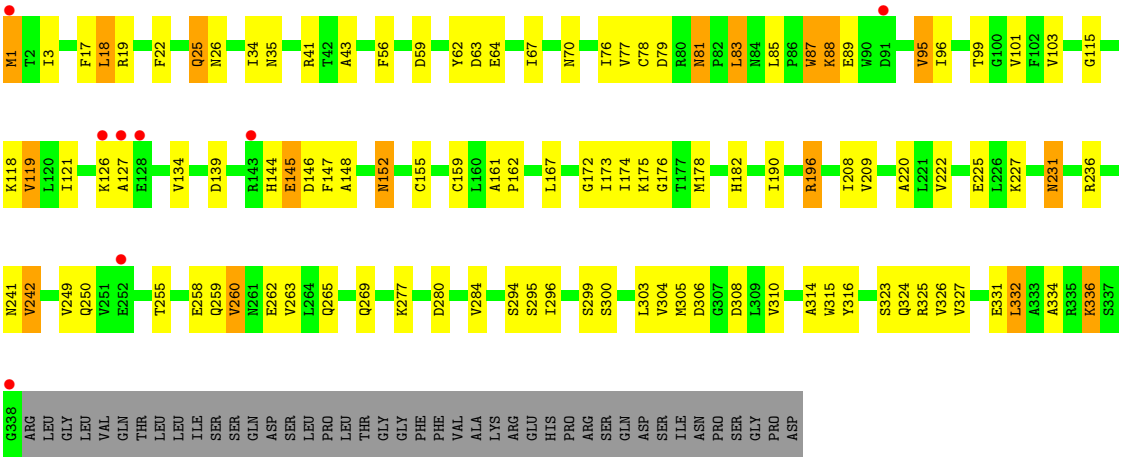
Chain Q:



- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

Chain R:

2%
61%
24%
11%


M1 T2 I3 F17 L18 R19 F22 Q25 N26 I34 N35 R41 T42 A43 F56 D59 Y62 D63 E64 I67 N70 I76 V77 C78 D79 R80 N81 P82 L83 N84 I85 P86 W87 K88 E89 W90 D91 V95 I96 T99 G100 V101 F102 V103 G115
K118 V119 L120 I121 K126 A127 E128 V134 D139 R143 H144 E145 D146 F147 A148 N152 C155 C159 L160 A161 P162 L167 G172 I173 I174 K175 G176 T177 M178 H182 I190 R196 I208 V209 A220 L221 V222 E225 L226 K227 N231 R236
N241 V242 V249 Q250 V251 E252 T255 E258 Q259 V260 N261 E262 V263 L264 Q265 Q269 K277 D280 V284 S294 S295 I296 S299 S300 L303 V304 M305 D306 G307 D308 L309 V310 A314 W315 Y316 S323 Q324 R325 V326 V327 E331 L332 A333 A334 R335 K336 S337
G338 ARG LEU GLY LEU VAL GLN THR LEU LEU ILE SER SER GLN ASP SER LEU PRO LEU THR GLY GLY PHE PHE VAL ALA LYS ARG GLU HIS PRO ARG SER GLN ASP SER ILE ASN PRO SER GLY PRO ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.01Å 79.59Å 206.16Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.9 (19.96-2.50) 86.0 (19.95-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.240 0.185 , 0.234	Depositor DCC
R_{free} test set	7199 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	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	16415	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.61	0/2629	0.87	4/3575 (0.1%)
1	B	0.63	0/2629	0.88	1/3575 (0.0%)
1	O	0.61	0/2629	0.81	3/3575 (0.1%)
1	P	0.73	7/2629 (0.3%)	0.80	2/3575 (0.1%)
1	Q	0.50	0/2629	0.72	1/3575 (0.0%)
1	R	0.60	5/2629 (0.2%)	0.75	1/3575 (0.0%)
All	All	0.62	12/15774 (0.1%)	0.81	12/21450 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	25	GLN	C-O	11.80	1.45	1.23
1	P	25	GLN	CB-CG	9.79	1.78	1.52
1	R	89	GLU	CB-CG	-8.74	1.35	1.52
1	R	89	GLU	CG-CD	-7.77	1.40	1.51
1	P	25	GLN	CA-CB	-7.67	1.37	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	25	GLN	CB-CA-C	-8.27	93.85	110.40
1	A	208	ILE	N-CA-C	-7.20	91.56	111.00
1	A	335	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	335	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	208	ILE	N-CA-C	-6.50	93.44	111.00

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	2588	0	2615	114	0
1	B	2588	0	2615	97	0
1	O	2588	0	2615	83	0
1	P	2588	0	2615	121	0
1	Q	2588	0	2615	102	0
1	R	2588	0	2615	84	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	O	10	0	0	0	0
2	P	10	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	0	0
3	O	48	0	25	0	0
3	P	48	0	25	3	0
3	Q	48	0	25	1	0
3	R	48	0	25	0	0
4	A	107	0	0	13	0
4	B	142	0	0	7	0
4	O	86	0	0	5	0
4	P	82	0	0	5	0
4	Q	47	0	0	3	0
4	R	75	0	0	2	0
All	All	16415	0	15840	568	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 18.

The worst 5 of 568 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:P:25:GLN:CG	1:P:25:GLN:CB	1.79	1.61
1:A:324:GLN:HE21	1:A:324:GLN:HA	1.11	1.14
1:P:25:GLN:H	1:P:25:GLN:HG3	1.14	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:MET:HE2	1:O:1:MET:O	1.52	1.08
1:A:80:ARG:HH11	1:A:80:ARG:HG2	1.13	1.07

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	336/380 (88%)	308 (92%)	22 (6%)	6 (2%)	8	14
1	B	336/380 (88%)	308 (92%)	22 (6%)	6 (2%)	8	14
1	O	336/380 (88%)	313 (93%)	20 (6%)	3 (1%)	17	31
1	P	336/380 (88%)	318 (95%)	16 (5%)	2 (1%)	25	43
1	Q	336/380 (88%)	314 (94%)	18 (5%)	4 (1%)	13	24
1	R	336/380 (88%)	313 (93%)	21 (6%)	2 (1%)	25	43
All	All	2016/2280 (88%)	1874 (93%)	119 (6%)	23 (1%)	14	26

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	LYS
1	A	242	VAL
1	B	242	VAL
1	B	336	LYS
1	O	242	VAL

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	284/321 (88%)	254 (89%)	30 (11%)	6 13
1	B	284/321 (88%)	256 (90%)	28 (10%)	8 15
1	O	284/321 (88%)	262 (92%)	22 (8%)	13 25
1	P	284/321 (88%)	260 (92%)	24 (8%)	10 21
1	Q	284/321 (88%)	264 (93%)	20 (7%)	15 29
1	R	284/321 (88%)	262 (92%)	22 (8%)	13 25
All	All	1704/1926 (88%)	1558 (91%)	146 (9%)	10 20

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	152	ASN
1	R	316	TYR
1	Q	209	VAL
1	R	83	LEU
1	B	209	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	259	GLN
1	R	265	GLN
1	Q	265	GLN
1	R	113	GLN
1	O	70	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)

18 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	$\#\|Z\| > 2$
3	NAP	A	1341	-	46,52,52	2.39	18 (39%)	61,80,80	1.72	14 (22%)
2	SO4	A	1340	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	2340	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	B	2339	-	4,4,4	0.31	0	6,6,6	0.25	0
2	SO4	O	3340	-	4,4,4	0.39	0	6,6,6	0.27	0
2	SO4	P	4339	-	4,4,4	0.25	0	6,6,6	0.39	0
3	NAP	O	3341	-	46,52,52	2.25	13 (28%)	61,80,80	1.63	14 (22%)
3	NAP	R	6341	-	46,52,52	2.10	12 (26%)	61,80,80	1.66	15 (24%)
2	SO4	Q	5340	-	4,4,4	0.27	0	6,6,6	0.22	0
3	NAP	Q	5341	-	46,52,52	2.21	11 (23%)	61,80,80	1.61	13 (21%)
2	SO4	R	6339	-	4,4,4	0.39	0	6,6,6	0.15	0
2	SO4	A	1339	-	4,4,4	0.39	0	6,6,6	0.37	0
2	SO4	P	4340	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	Q	5339	-	4,4,4	0.33	0	6,6,6	0.17	0
3	NAP	P	4341	-	46,52,52	2.29	12 (26%)	61,80,80	1.51	13 (21%)
2	SO4	R	6340	-	4,4,4	0.27	0	6,6,6	0.29	0
3	NAP	B	2341	-	46,52,52	2.04	9 (19%)	61,80,80	1.66	11 (18%)
2	SO4	O	3339	-	4,4,4	0.40	0	6,6,6	0.25	0

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
3	NAP	A	1341	-	-	7/31/67/67	0/5/5/5
3	NAP	O	3341	-	-	10/31/67/67	0/5/5/5
3	NAP	R	6341	-	-	6/31/67/67	0/5/5/5
3	NAP	Q	5341	-	-	8/31/67/67	0/5/5/5
3	NAP	P	4341	-	-	8/31/67/67	0/5/5/5
3	NAP	B	2341	-	-	12/31/67/67	0/5/5/5

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1341	NAP	C2N-N1N	7.63	1.43	1.35
3	P	4341	NAP	C2N-N1N	7.24	1.42	1.35
3	Q	5341	NAP	C2N-N1N	6.94	1.42	1.35
3	O	3341	NAP	C2N-N1N	6.81	1.42	1.35
3	R	6341	NAP	C2N-N1N	6.17	1.41	1.35

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	6341	NAP	C5A-C6A-N6A	4.70	127.47	120.31
3	Q	5341	NAP	C5A-C6A-N6A	4.66	127.41	120.31
3	A	1341	NAP	N3A-C2A-N1A	-4.39	122.71	128.67
3	O	3341	NAP	C5A-C6A-N6A	4.29	126.84	120.31
3	B	2341	NAP	N3A-C2A-N1A	-4.24	122.91	128.67

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1341	NAP	C5B-O5B-PA-O1A
3	A	1341	NAP	PN-O3-PA-O5B
3	A	1341	NAP	O4D-C1D-N1N-C2N
3	B	2341	NAP	C5B-O5B-PA-O1A
3	B	2341	NAP	C5B-O5B-PA-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1341	NAP	2	0

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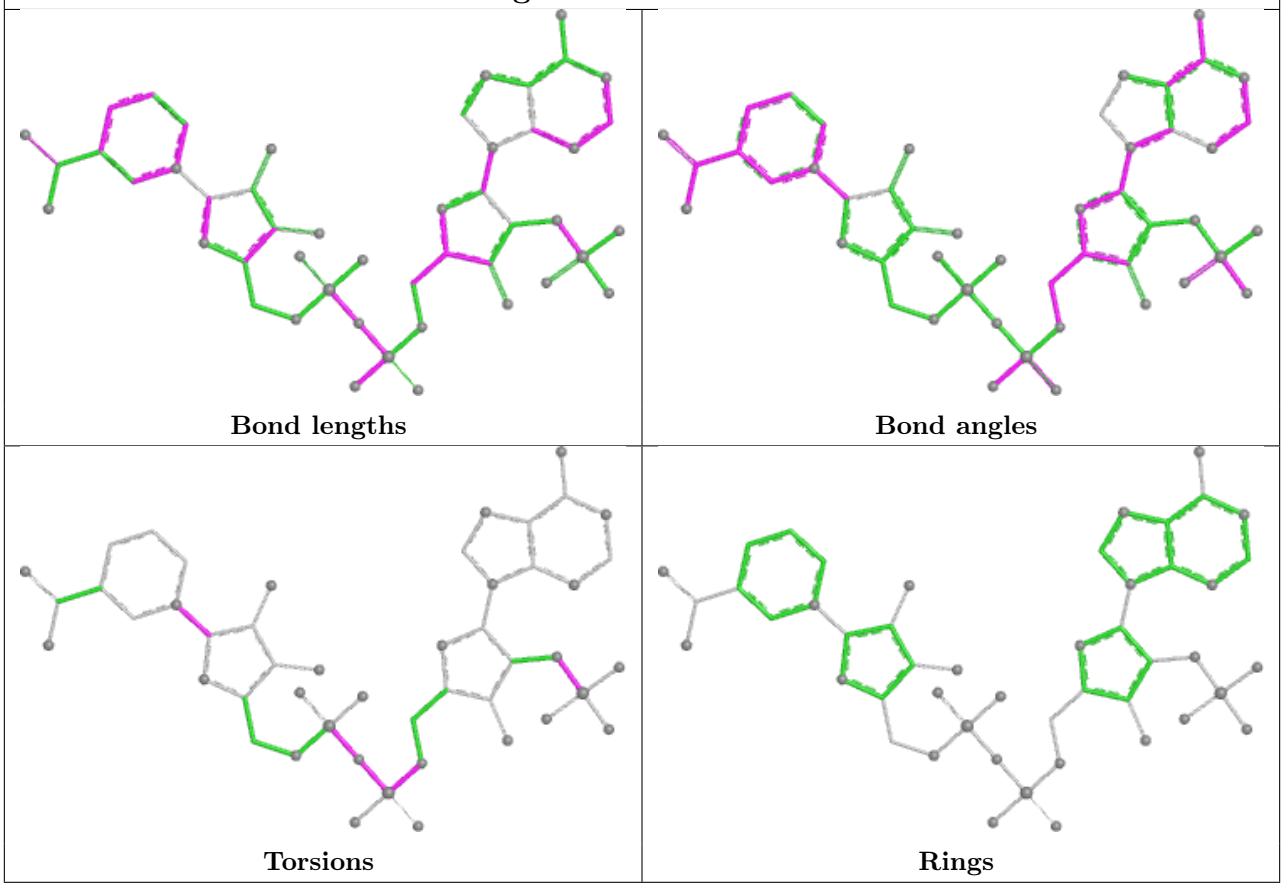
Continued from previous page...

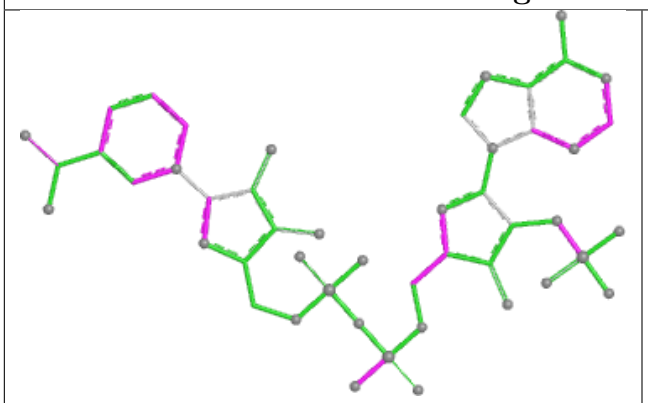
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	4339	SO4	1	0
3	Q	5341	NAP	1	0
3	P	4341	NAP	3	0

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

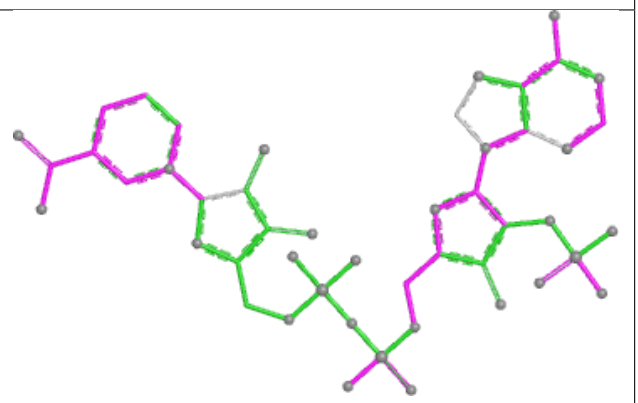
Ligand NAP A 1341



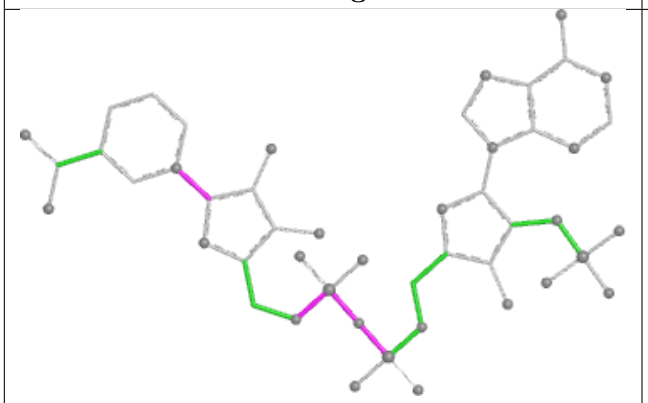
Ligand NAP O 3341



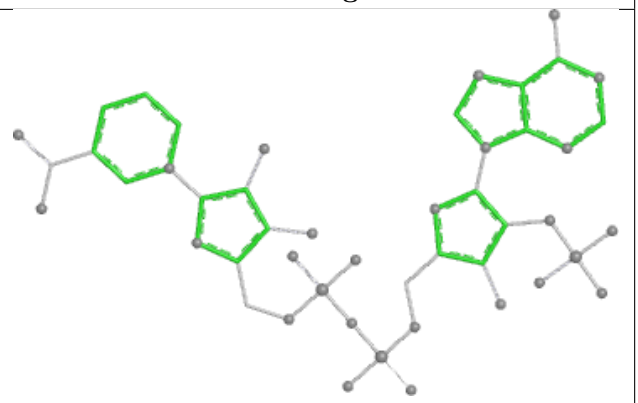
Bond lengths



Bond angles

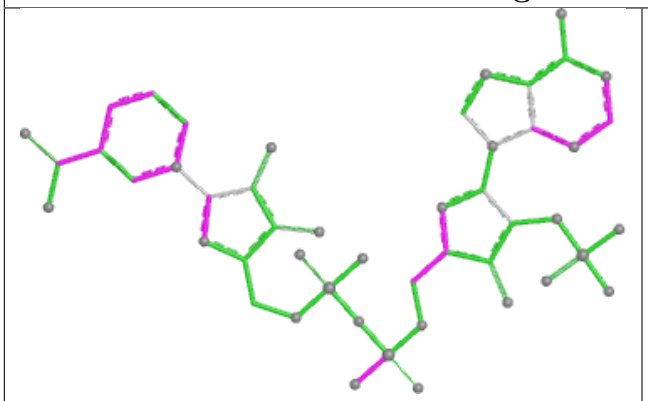


Torsions

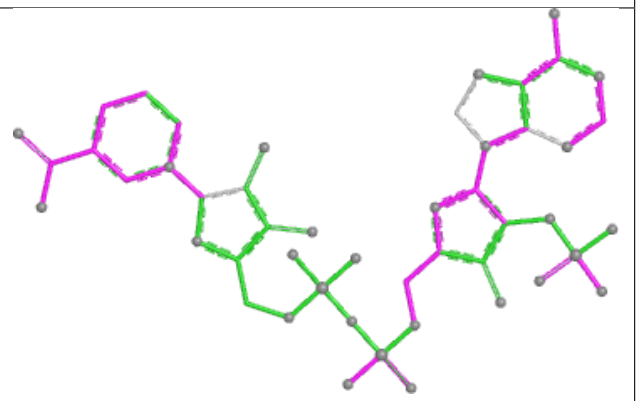


Rings

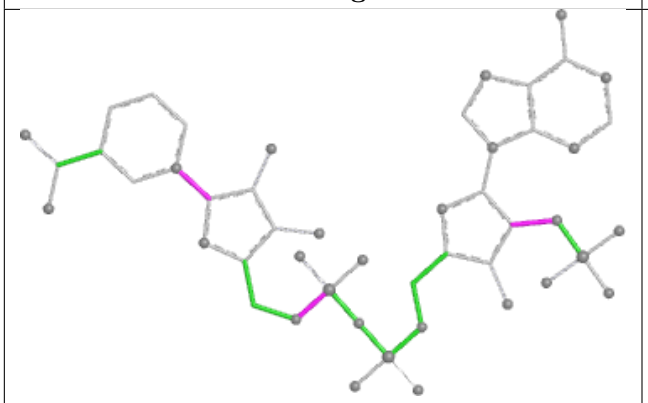
Ligand NAP R 6341



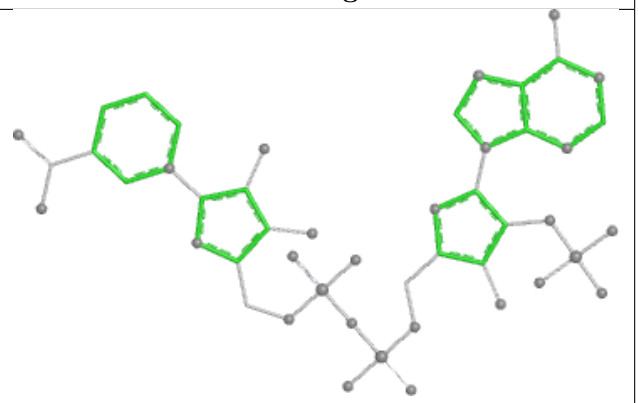
Bond lengths



Bond angles

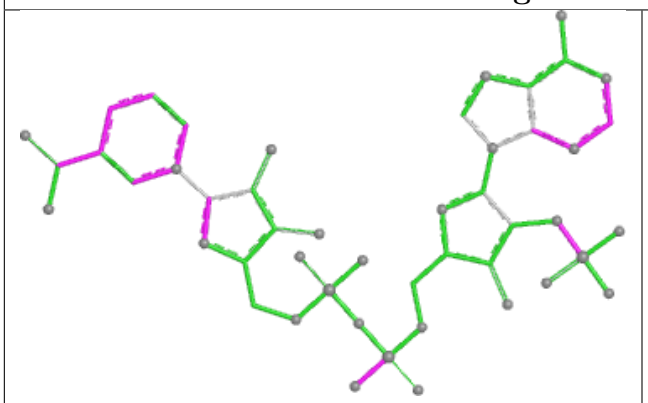


Torsions

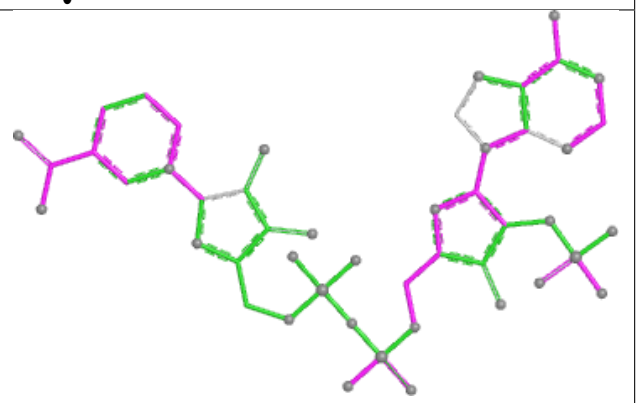


Rings

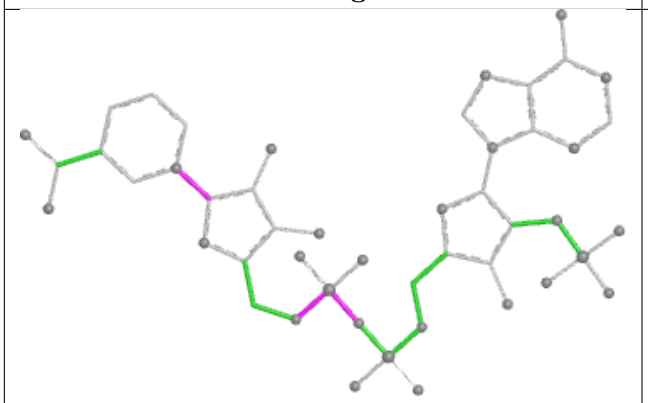
Ligand NAP Q 5341



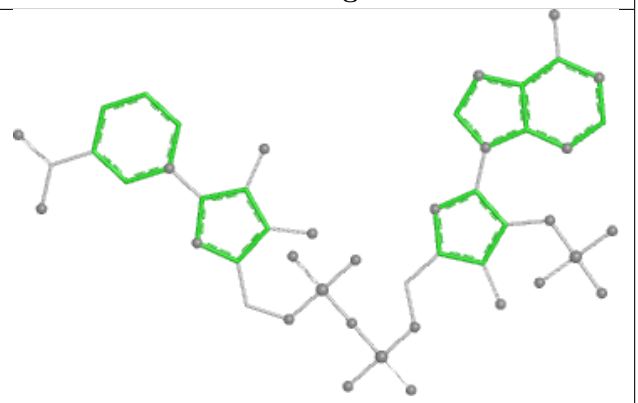
Bond lengths



Bond angles

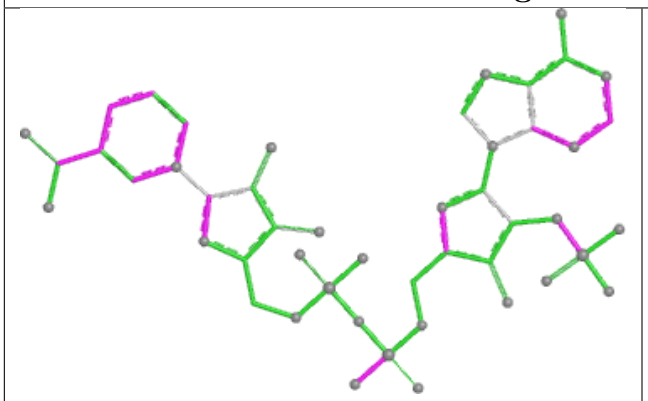


Torsions

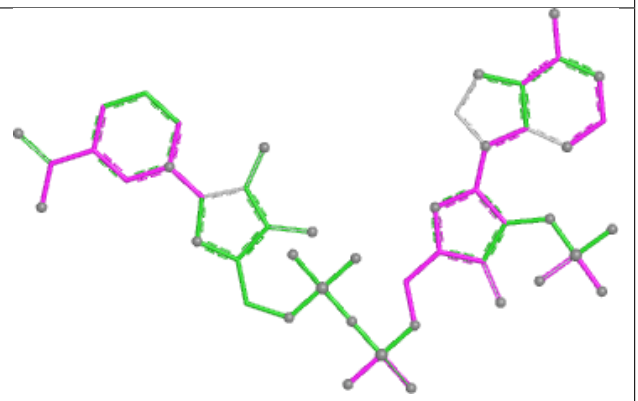


Rings

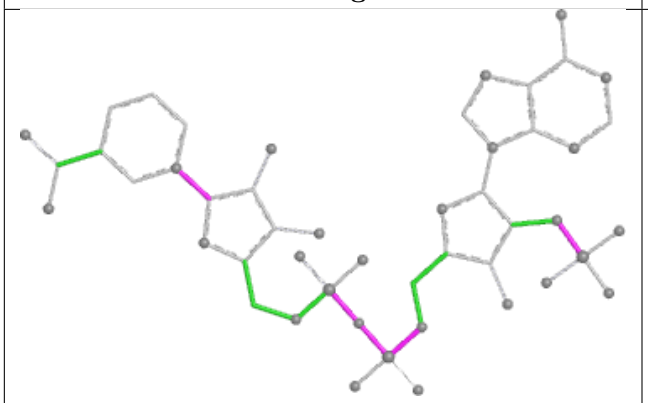
Ligand NAP P 4341



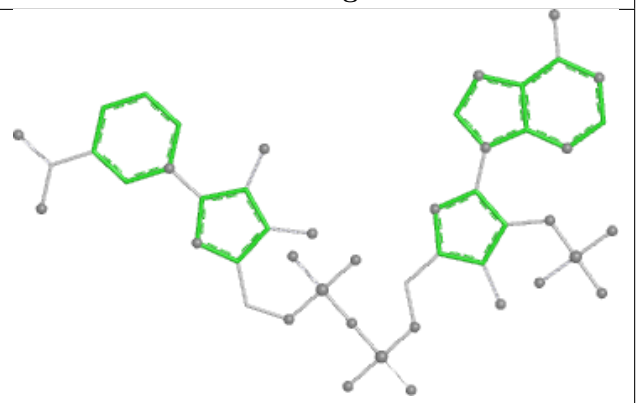
Bond lengths



Bond angles

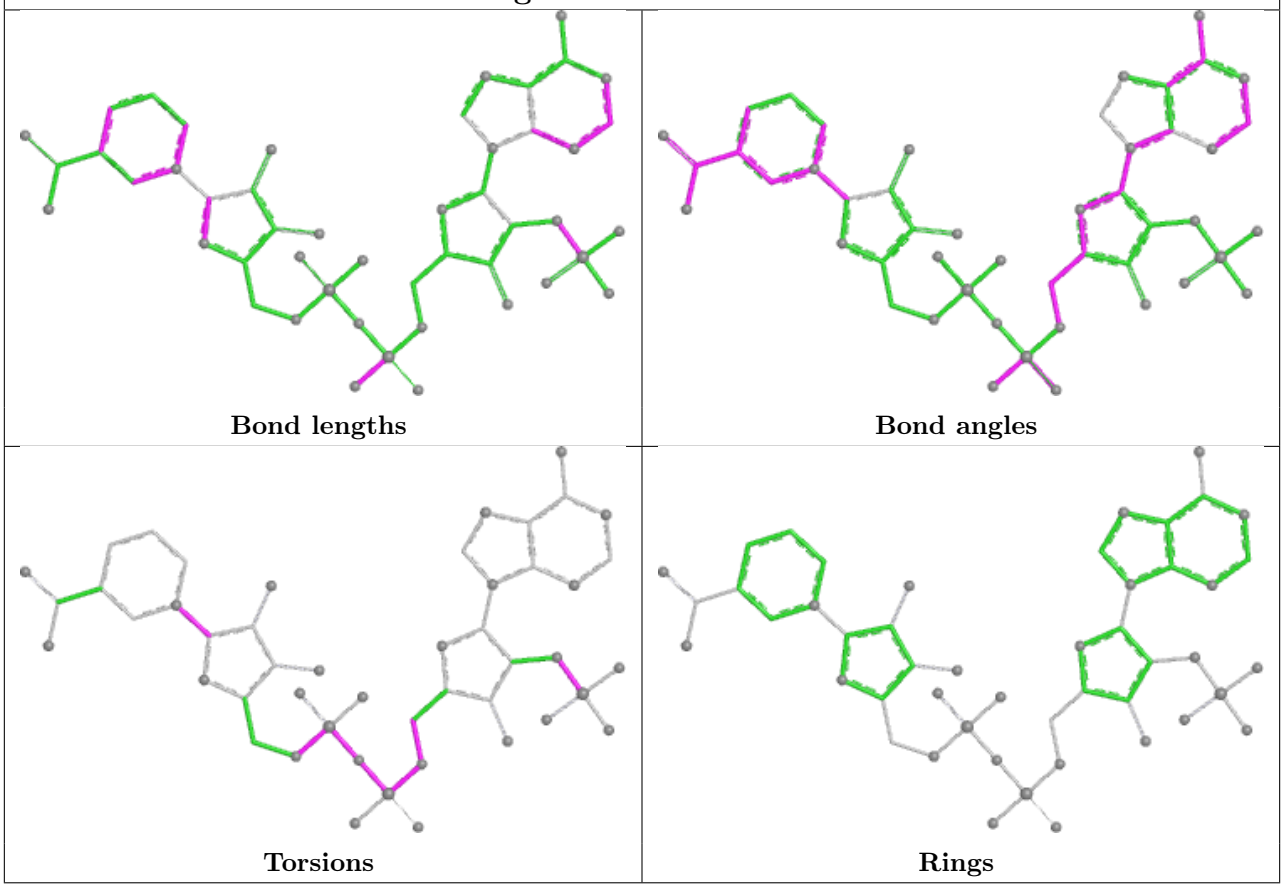


Torsions



Rings

Ligand NAP B 2341



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	338/380 (88%)	-0.46	3 (0%)	84	86	11, 25, 45, 77	0
1	B	338/380 (88%)	-0.60	3 (0%)	84	86	11, 21, 39, 81	0
1	O	338/380 (88%)	-0.45	3 (0%)	84	86	13, 27, 47, 81	0
1	P	338/380 (88%)	-0.31	10 (2%)	50	53	16, 31, 57, 89	0
1	Q	338/380 (88%)	-0.08	17 (5%)	28	30	22, 40, 62, 83	0
1	R	338/380 (88%)	-0.24	8 (2%)	59	62	19, 36, 56, 84	0
All	All	2028/2280 (88%)	-0.36	44 (2%)	62	65	11, 30, 55, 89	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	1	MET	11.2
1	B	1	MET	10.6
1	P	1	MET	8.9
1	A	1	MET	8.4
1	Q	1	MET	6.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

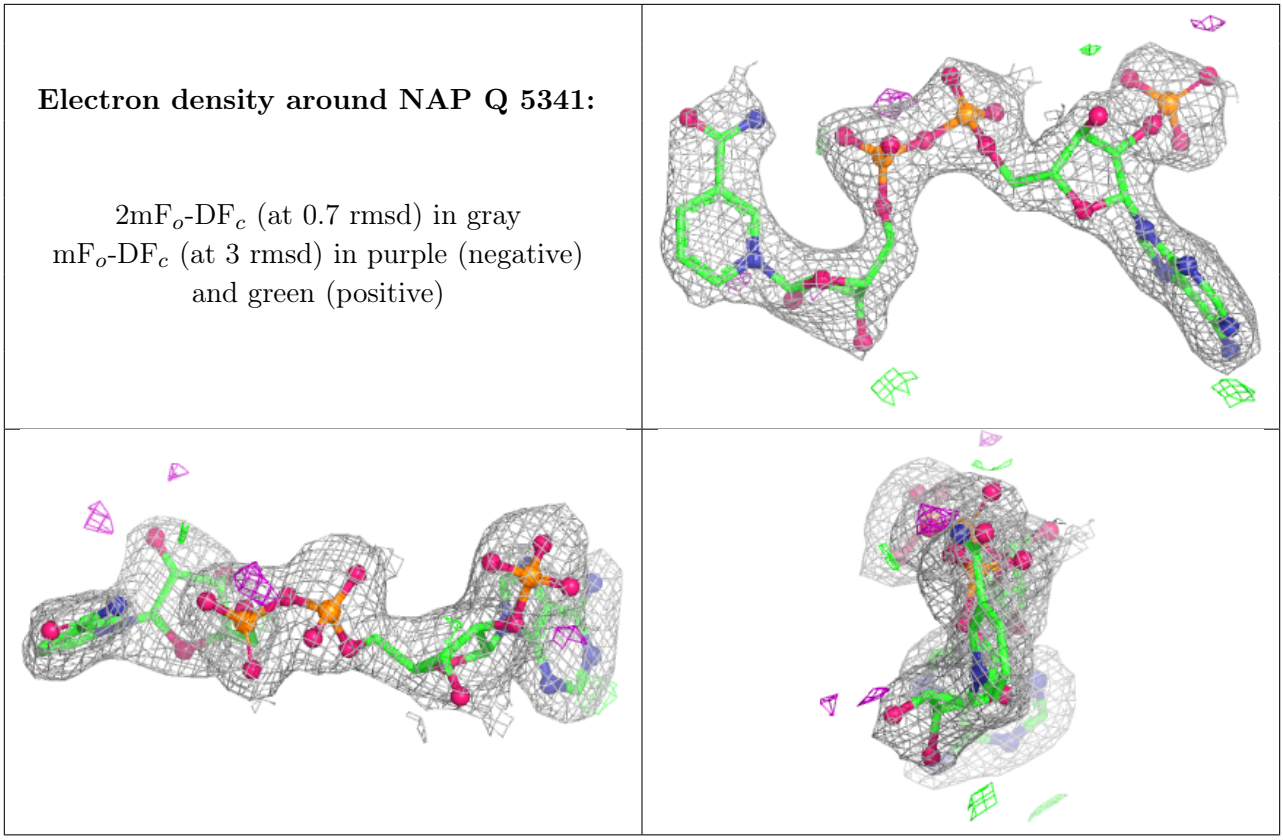
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	P	4339	5/5	0.88	0.23	39,41,44,44	5
3	NAP	Q	5341	48/48	0.95	0.14	36,43,53,58	0
3	NAP	R	6341	48/48	0.95	0.13	31,43,51,56	0
2	SO4	R	6339	5/5	0.96	0.16	35,36,37,40	5
3	NAP	O	3341	48/48	0.96	0.12	19,38,56,58	0
3	NAP	P	4341	48/48	0.96	0.13	25,39,48,52	0
2	SO4	O	3340	5/5	0.96	0.19	22,26,30,30	5
2	SO4	O	3339	5/5	0.96	0.18	33,35,36,37	5
2	SO4	Q	5339	5/5	0.97	0.12	45,45,47,49	5
2	SO4	R	6340	5/5	0.97	0.17	25,27,33,35	5
3	NAP	A	1341	48/48	0.97	0.11	16,27,42,47	0
3	NAP	B	2341	48/48	0.97	0.10	11,25,42,45	0
2	SO4	A	1339	5/5	0.98	0.12	14,16,19,23	5
2	SO4	Q	5340	5/5	0.98	0.13	27,29,34,34	5
2	SO4	B	2339	5/5	0.98	0.12	17,21,22,25	5
2	SO4	B	2340	5/5	0.98	0.16	16,22,23,24	5
2	SO4	P	4340	5/5	0.98	0.11	28,31,34,36	5
2	SO4	A	1340	5/5	0.99	0.13	24,27,29,31	5

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.

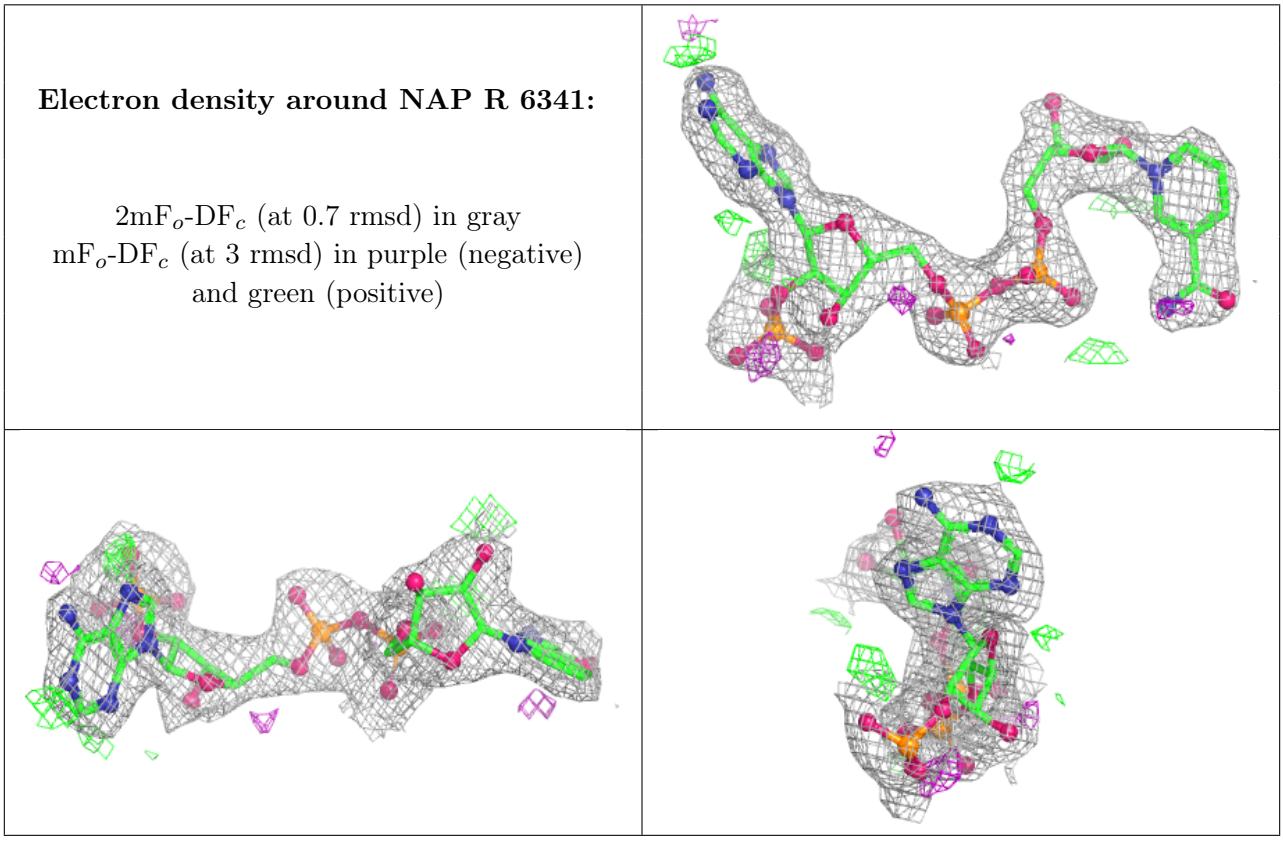
Electron density around NAP Q 5341:

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



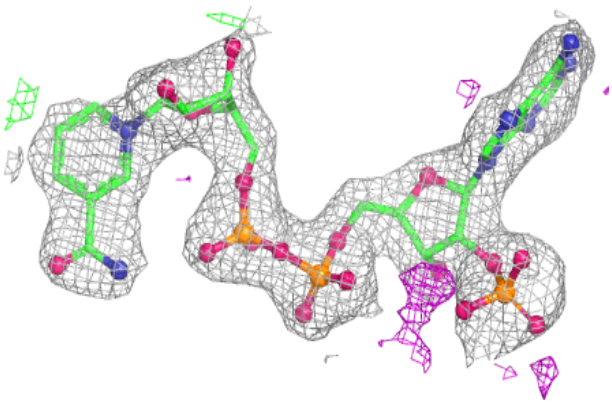
Electron density around NAP R 6341:

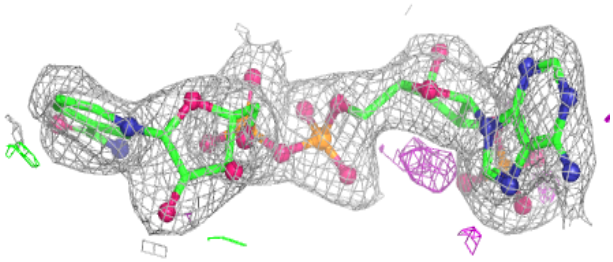
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

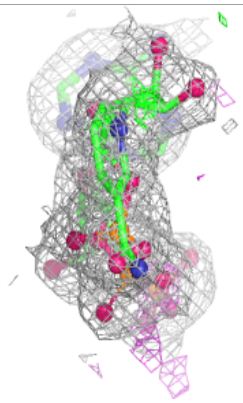


Electron density around NAP O 3341:

$2mF_o$-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 P 4341:

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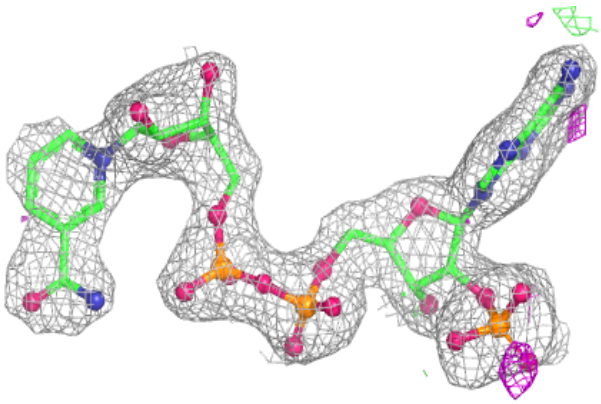
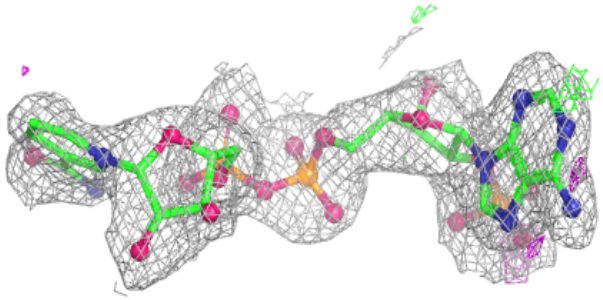
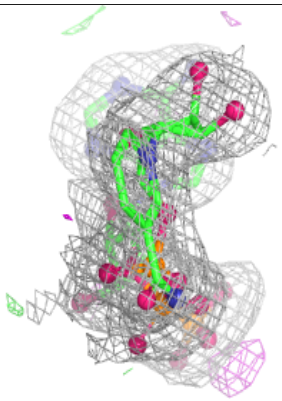
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAP A 1341:

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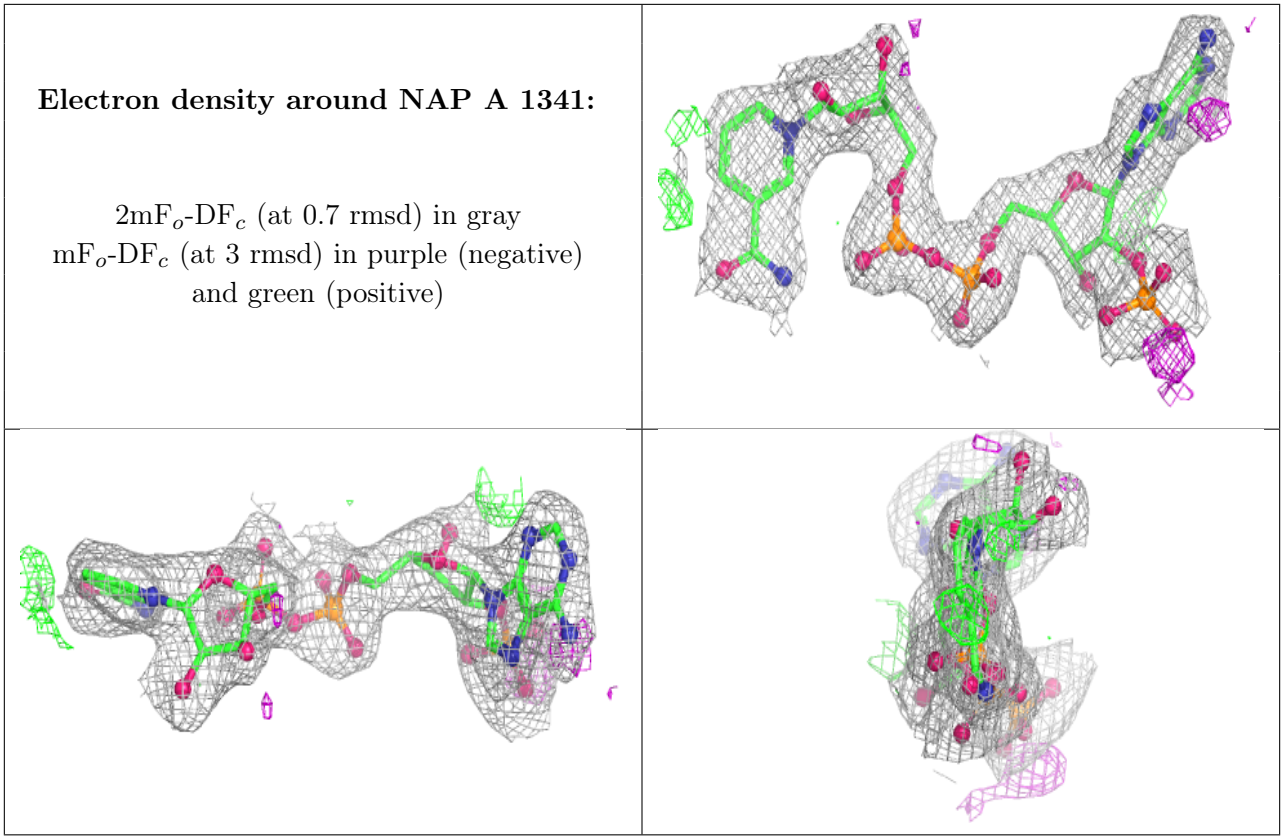
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAP B 2341:

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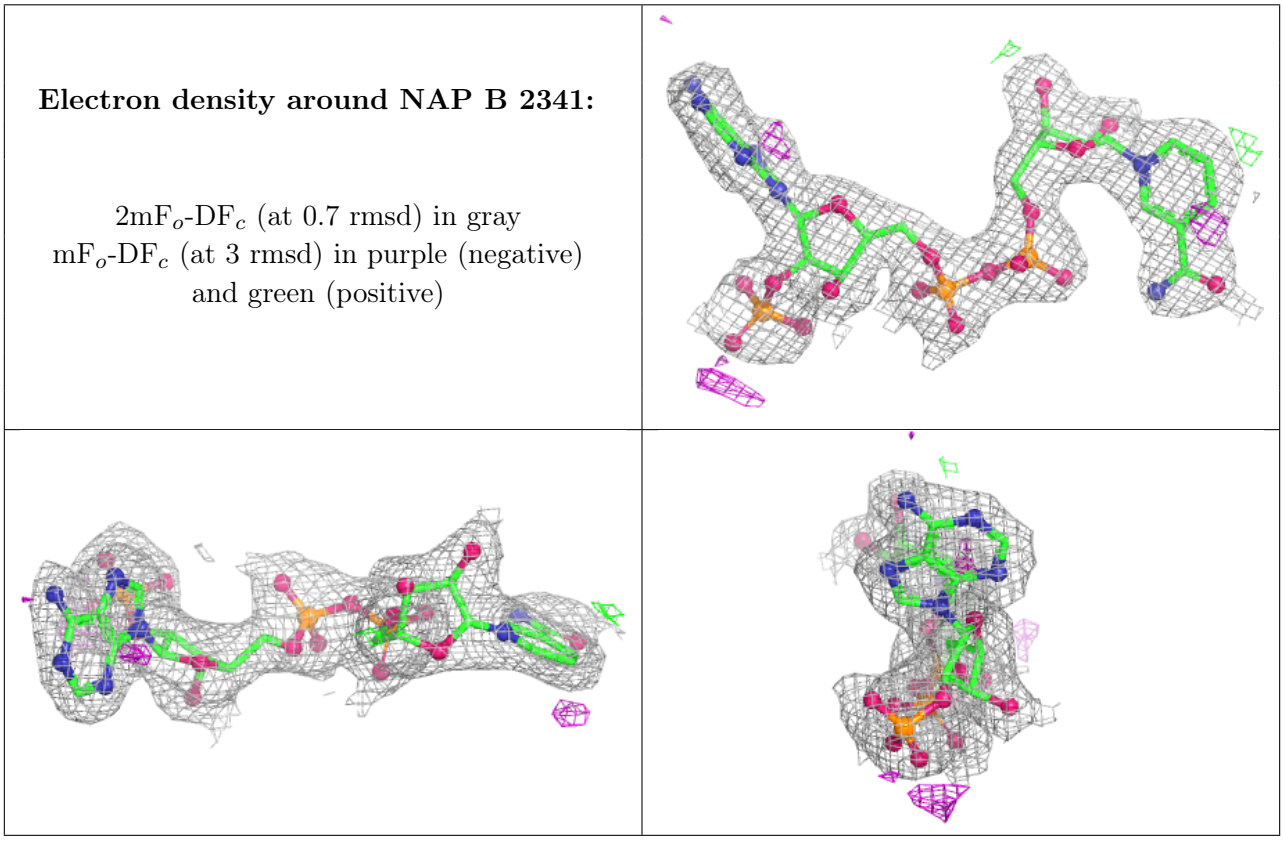
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.