



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 01:52 PM EST

PDB ID : 2QFX
Title : Crystal structure of *Saccharomyces cerevesiae* mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with NADPH, α -ketoglutarate and $\text{Ca}(2+)$
Authors : Peng, Y.J.; Ding, J.P.
Deposited on : 2007-06-28
Resolution : 2.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

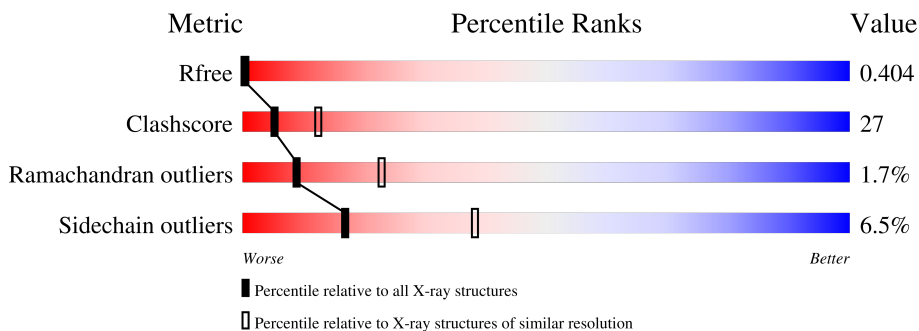
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	427	19% 71% 6% .
1	B	427	19% 70% 6% .
1	C	427	26% 65% 5% .
1	D	427	18% 72% 6% .
1	E	427	15% 75% 7% .
1	F	427	27% 63% 6% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDP	A	1101	-	-	X	-
3	NDP	B	1201	-	-	X	-
3	NDP	D	1401	-	-	X	-
3	NDP	F	1601	-	-	X	-
4	AKG	A	1102	-	-	X	-
4	AKG	B	1202	-	-	X	-
4	AKG	C	1302	-	-	X	-
4	AKG	D	1402	-	-	X	-
4	AKG	E	1502	-	-	X	-
4	AKG	F	1602	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20069 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].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3248	2070	550	616	12	0	0	0
1	B	410	3248	2070	550	616	12	0	0	0
1	C	410	3248	2070	550	616	12	0	0	0
1	D	410	3248	2070	550	616	12	0	0	0
1	E	410	3248	2070	550	616	12	0	0	0
1	F	410	3248	2070	550	616	12	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P21954
A	-12	HIS	-	expression tag	UNP P21954
A	-11	HIS	-	expression tag	UNP P21954
A	-10	HIS	-	expression tag	UNP P21954
A	-9	HIS	-	expression tag	UNP P21954
A	-8	HIS	-	expression tag	UNP P21954
A	-7	HIS	-	expression tag	UNP P21954
A	-6	ALA	-	expression tag	UNP P21954
A	-5	MET	-	expression tag	UNP P21954
A	-4	GLY	-	expression tag	UNP P21954
A	-3	ILE	-	expression tag	UNP P21954
A	-2	PRO	-	expression tag	UNP P21954
A	-1	GLY	-	expression tag	UNP P21954
A	0	HIS	-	expression tag	UNP P21954
B	-13	MET	-	expression tag	UNP P21954
B	-12	HIS	-	expression tag	UNP P21954
B	-11	HIS	-	expression tag	UNP P21954

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP P21954
B	-9	HIS	-	expression tag	UNP P21954
B	-8	HIS	-	expression tag	UNP P21954
B	-7	HIS	-	expression tag	UNP P21954
B	-6	ALA	-	expression tag	UNP P21954
B	-5	MET	-	expression tag	UNP P21954
B	-4	GLY	-	expression tag	UNP P21954
B	-3	ILE	-	expression tag	UNP P21954
B	-2	PRO	-	expression tag	UNP P21954
B	-1	GLY	-	expression tag	UNP P21954
B	0	HIS	-	expression tag	UNP P21954
C	-13	MET	-	expression tag	UNP P21954
C	-12	HIS	-	expression tag	UNP P21954
C	-11	HIS	-	expression tag	UNP P21954
C	-10	HIS	-	expression tag	UNP P21954
C	-9	HIS	-	expression tag	UNP P21954
C	-8	HIS	-	expression tag	UNP P21954
C	-7	HIS	-	expression tag	UNP P21954
C	-6	ALA	-	expression tag	UNP P21954
C	-5	MET	-	expression tag	UNP P21954
C	-4	GLY	-	expression tag	UNP P21954
C	-3	ILE	-	expression tag	UNP P21954
C	-2	PRO	-	expression tag	UNP P21954
C	-1	GLY	-	expression tag	UNP P21954
C	0	HIS	-	expression tag	UNP P21954
D	-13	MET	-	expression tag	UNP P21954
D	-12	HIS	-	expression tag	UNP P21954
D	-11	HIS	-	expression tag	UNP P21954
D	-10	HIS	-	expression tag	UNP P21954
D	-9	HIS	-	expression tag	UNP P21954
D	-8	HIS	-	expression tag	UNP P21954
D	-7	HIS	-	expression tag	UNP P21954
D	-6	ALA	-	expression tag	UNP P21954
D	-5	MET	-	expression tag	UNP P21954
D	-4	GLY	-	expression tag	UNP P21954
D	-3	ILE	-	expression tag	UNP P21954
D	-2	PRO	-	expression tag	UNP P21954
D	-1	GLY	-	expression tag	UNP P21954
D	0	HIS	-	expression tag	UNP P21954
E	-13	MET	-	expression tag	UNP P21954
E	-12	HIS	-	expression tag	UNP P21954
E	-11	HIS	-	expression tag	UNP P21954

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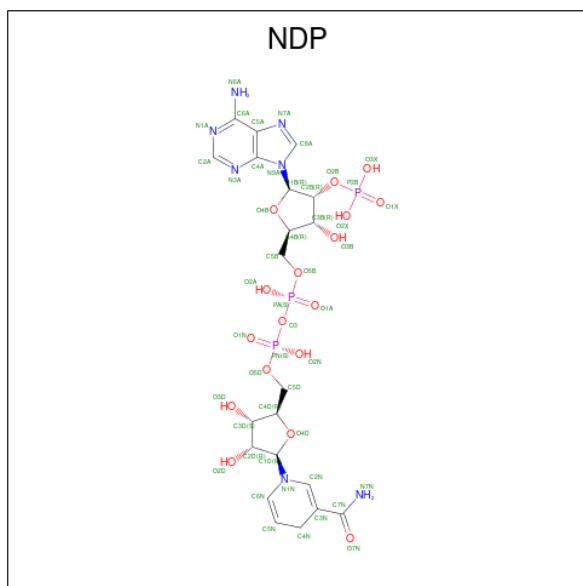
Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P21954
E	-9	HIS	-	expression tag	UNP P21954
E	-8	HIS	-	expression tag	UNP P21954
E	-7	HIS	-	expression tag	UNP P21954
E	-6	ALA	-	expression tag	UNP P21954
E	-5	MET	-	expression tag	UNP P21954
E	-4	GLY	-	expression tag	UNP P21954
E	-3	ILE	-	expression tag	UNP P21954
E	-2	PRO	-	expression tag	UNP P21954
E	-1	GLY	-	expression tag	UNP P21954
E	0	HIS	-	expression tag	UNP P21954
F	-13	MET	-	expression tag	UNP P21954
F	-12	HIS	-	expression tag	UNP P21954
F	-11	HIS	-	expression tag	UNP P21954
F	-10	HIS	-	expression tag	UNP P21954
F	-9	HIS	-	expression tag	UNP P21954
F	-8	HIS	-	expression tag	UNP P21954
F	-7	HIS	-	expression tag	UNP P21954
F	-6	ALA	-	expression tag	UNP P21954
F	-5	MET	-	expression tag	UNP P21954
F	-4	GLY	-	expression tag	UNP P21954
F	-3	ILE	-	expression tag	UNP P21954
F	-2	PRO	-	expression tag	UNP P21954
F	-1	GLY	-	expression tag	UNP P21954
F	0	HIS	-	expression tag	UNP P21954

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

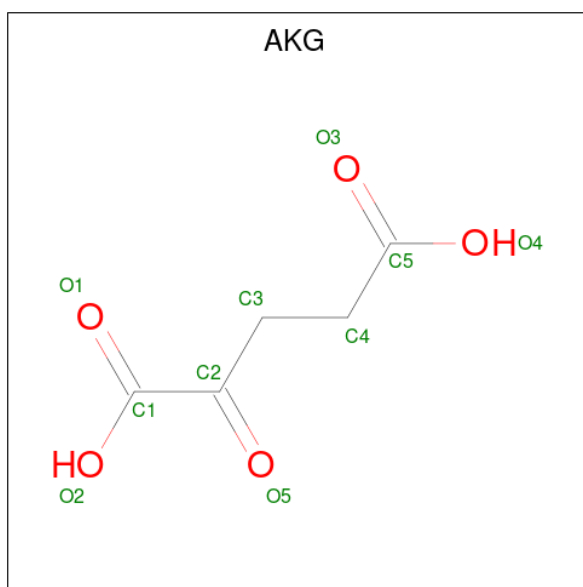
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

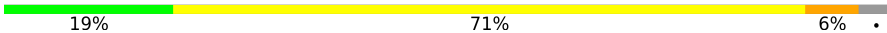
- Molecule 5 is water.

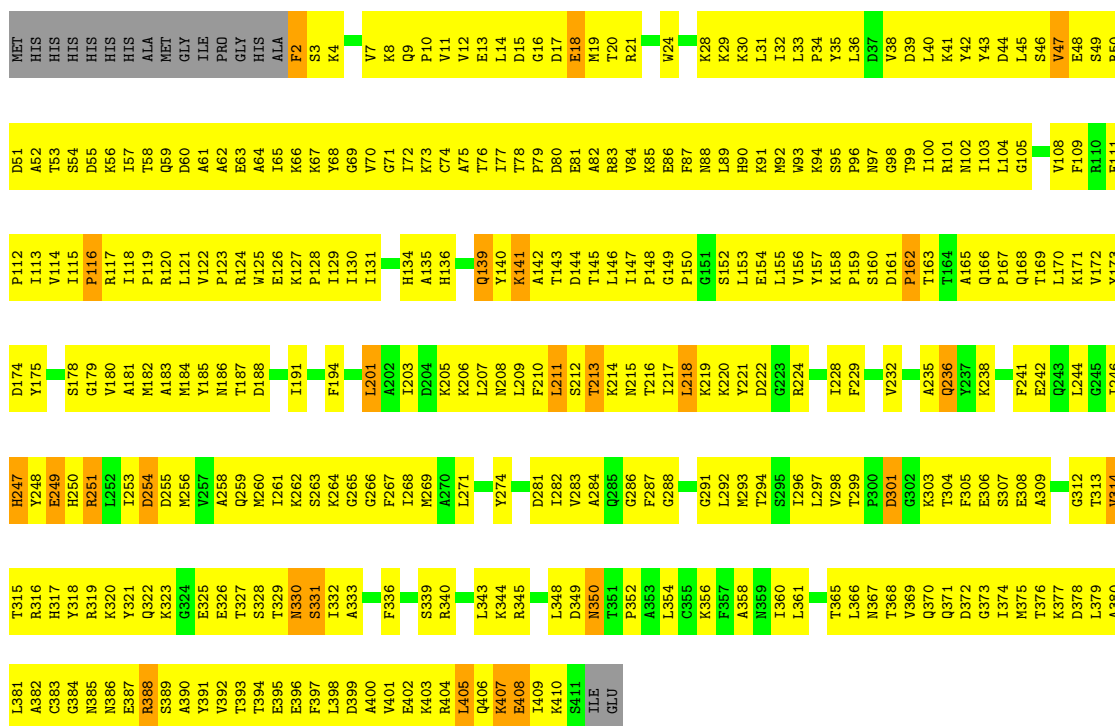
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	22	Total	O	0	0
			22	22		
5	C	47	Total	O	0	0
			47	47		
5	D	49	Total	O	0	0
			49	49		
5	E	30	Total	O	0	0
			30	30		
5	F	53	Total	O	0	0
			53	53		

3 Residue-property plots

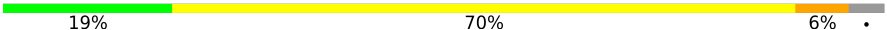
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

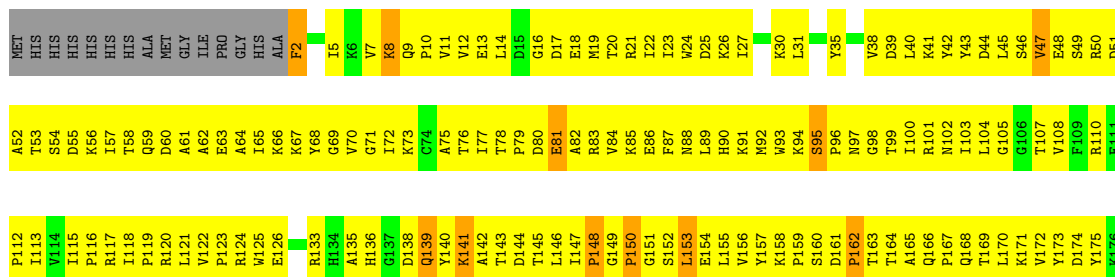
- Molecule 1: Isocitrate dehydrogenase [NADP]

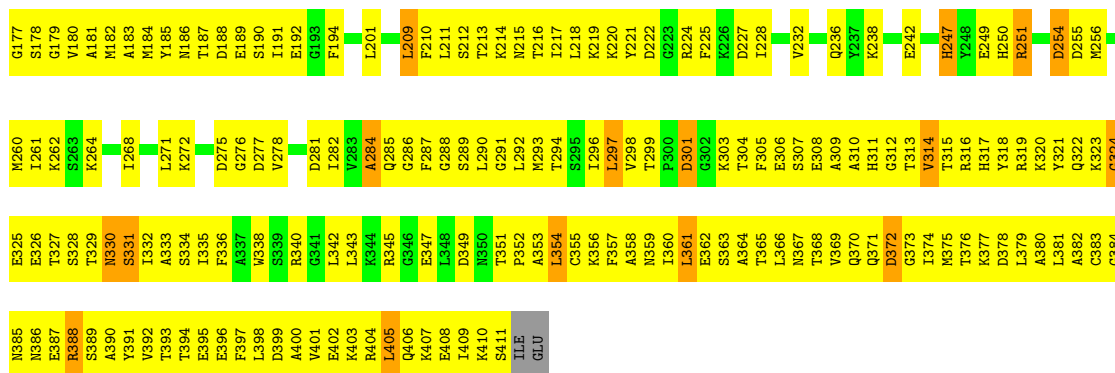
Chain A: 



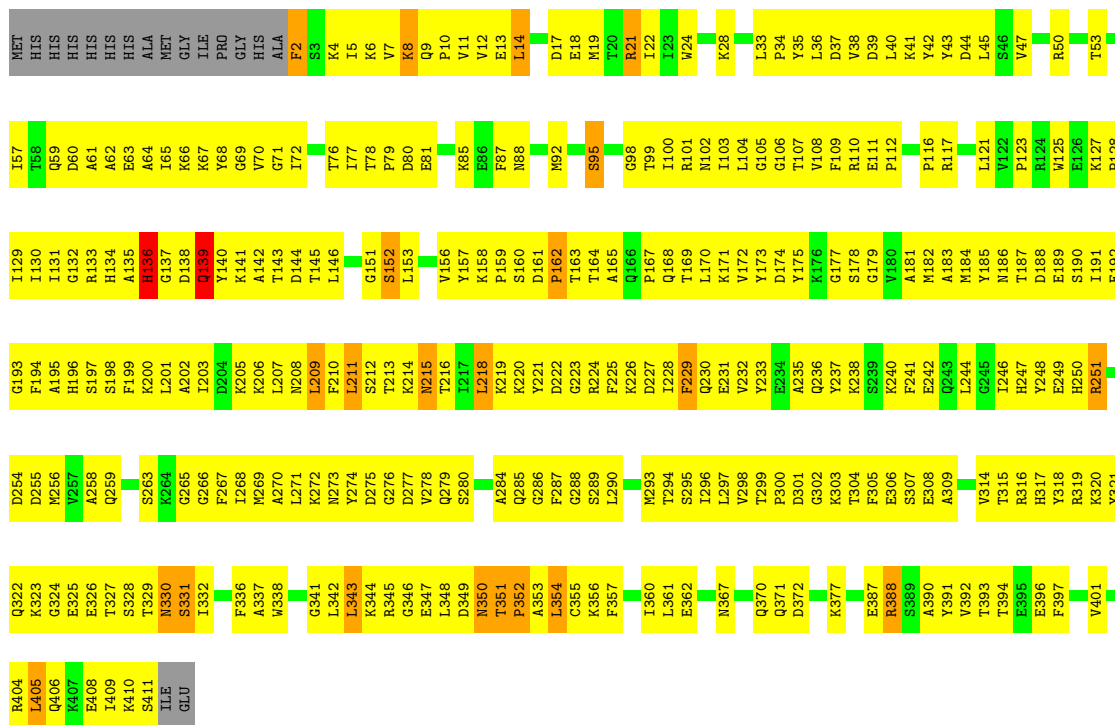
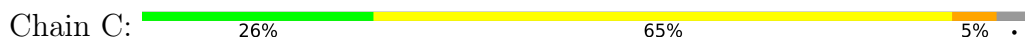
- Molecule 1: Isocitrate dehydrogenase [NADP]

Chain B: 

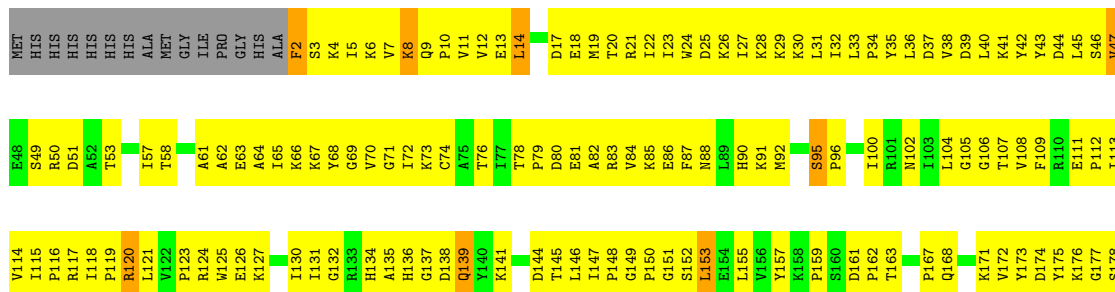
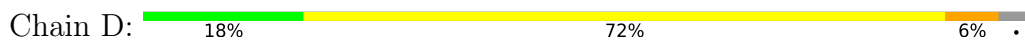


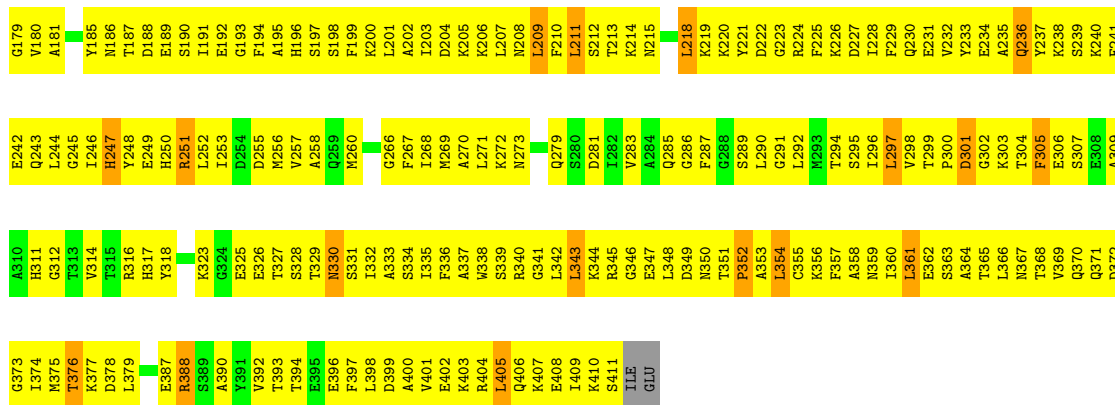


• Molecule 1: Isocitrate dehydrogenase [NADP]

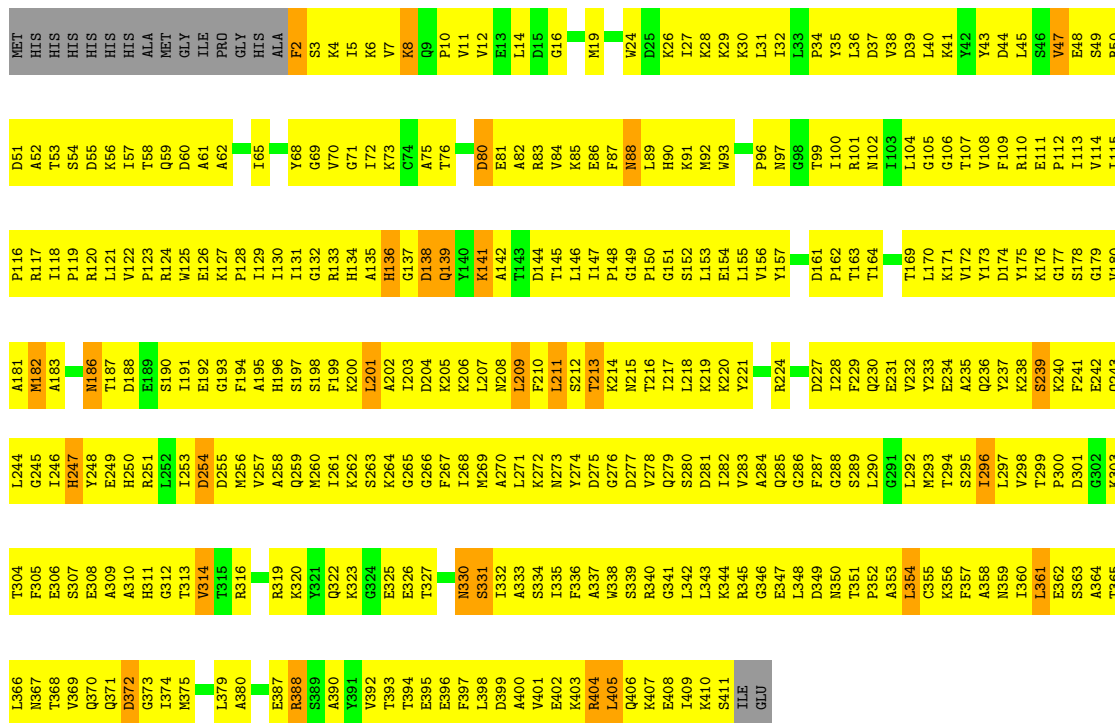


• Molecule 1: Isocitrate dehydrogenase [NADP]

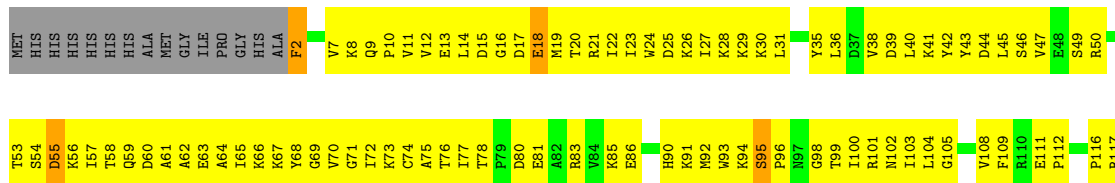




• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.42Å 99.63Å 129.95Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	49.73 – 2.70 49.73 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.73-2.70) 98.1 (49.73-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.69Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.285 0.406 , 0.404	Depositor DCC
R_{free} test set	3723 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtrriage
Anisotropy	0.412	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	20069	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NDP, 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	0.36	0/3311	0.67	1/4466 (0.0%)
1	B	0.37	0/3311	0.66	1/4466 (0.0%)
1	C	0.39	0/3311	0.68	1/4466 (0.0%)
1	D	0.39	0/3311	0.68	0/4466
1	E	0.37	0/3311	0.66	1/4466 (0.0%)
1	F	0.38	0/3311	0.68	1/4466 (0.0%)
All	All	0.38	0/19866	0.67	5/26796 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	HIS	N-CA-C	6.19	127.72	111.00
1	B	136	HIS	N-CA-C	6.15	127.60	111.00
1	F	136	HIS	N-CA-C	5.86	126.81	111.00
1	E	136	HIS	N-CA-C	5.44	125.69	111.00
1	C	136	HIS	N-CA-C	5.27	125.24	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	3248	0	3291	176	3143
1	B	3248	0	3291	188	4212
1	C	3248	0	3291	187	2384
1	D	3248	0	3291	180	3911
1	E	3248	0	3291	178	4218
1	F	3248	0	3291	179	2554
2	A	1	0	0	0	0
2	B	1	0	0	0	1
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	48	0	26	13	54
3	B	48	0	26	13	10
3	C	48	0	26	12	4
3	D	48	0	26	12	12
3	E	48	0	26	12	0
3	F	48	0	26	11	109
4	A	10	0	4	7	4
4	B	10	0	4	6	5
4	C	10	0	4	6	4
4	D	10	0	4	5	0
4	E	10	0	4	6	1
4	F	10	0	4	5	0
5	A	26	0	0	4	33
5	B	22	0	0	2	29
5	C	47	0	0	1	30
5	D	49	0	0	4	38
5	E	30	0	0	4	44
5	F	53	0	0	9	41
All	All	20069	0	19926	1056	10959

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 27.

The worst 5 of 1056 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:7:VAL:HG21	1:E:38:VAL:HG12	1.39	1.02
1:F:213:THR:HG23	1:F:215:ASN:H	1.27	0.98
1:E:53:THR:HG21	1:E:57:ILE:HG22	1.48	0.96
1:C:301:ASP:HB3	1:C:303:LYS:HG2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD12	1:E:172:VAL:HB	1.47	0.95

The worst 5 of 10959 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:CA	1:A:157:TYR:CZ[2_757]	0.07	2.13
1:B:49:SER:O	1:E:340:ARG:CD[2_757]	0.09	2.11
1:A:380:ALA:CB	1:F:12:VAL:CA[2_657]	0.12	2.08
1:A:48:GLU:CG	1:A:173:TYR:CD2[2_757]	0.14	2.06
1:A:367:ASN:CB	1:F:55:ASP:CG[2_657]	0.14	2.06

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	408/427 (96%)	365 (90%)	35 (9%)	8 (2%)	7	19
1	B	408/427 (96%)	368 (90%)	32 (8%)	8 (2%)	7	19
1	C	408/427 (96%)	364 (89%)	35 (9%)	9 (2%)	6	17
1	D	408/427 (96%)	359 (88%)	43 (10%)	6 (2%)	10	26
1	E	408/427 (96%)	364 (89%)	39 (10%)	5 (1%)	13	32
1	F	408/427 (96%)	361 (88%)	41 (10%)	6 (2%)	10	26
All	All	2448/2562 (96%)	2181 (89%)	225 (9%)	42 (2%)	9	23

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	236	GLN
1	B	8	LYS

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Mol	Chain	Res	Type
1	D	8	LYS
1	E	8	LYS

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	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	B	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	C	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	D	354/367 (96%)	331 (94%)	23 (6%)	17	38
1	E	354/367 (96%)	330 (93%)	24 (7%)	16	36
1	F	354/367 (96%)	330 (93%)	24 (7%)	16	36
All	All	2124/2202 (96%)	1987 (94%)	137 (6%)	17	38

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	55	ASP
1	F	161	ASP
1	F	331	SER
1	C	95	SER
1	C	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	370	GLN
1	F	90	HIS
1	E	59	GLN
1	E	322	GLN
1	F	236	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	NDP	C	1301	-	45,52,52	1.27	5 (11%)	53,80,80	1.02	2 (3%)
4	AKG	D	1402	-	9,9,9	1.22	1 (11%)	11,11,11	1.45	2 (18%)
3	NDP	D	1401	-	45,52,52	1.27	5 (11%)	53,80,80	1.09	3 (5%)
3	NDP	A	1101	-	45,52,52	1.27	5 (11%)	53,80,80	1.02	4 (7%)
4	AKG	E	1502	-	9,9,9	1.20	0	11,11,11	1.55	2 (18%)
3	NDP	F	1601	-	45,52,52	1.27	5 (11%)	53,80,80	1.09	3 (5%)
4	AKG	F	1602	-	9,9,9	1.23	1 (11%)	11,11,11	1.43	3 (27%)
4	AKG	C	1302	-	9,9,9	1.22	1 (11%)	11,11,11	1.42	1 (9%)
3	NDP	B	1201	-	45,52,52	1.28	5 (11%)	53,80,80	0.99	2 (3%)
3	NDP	E	1501	-	45,52,52	1.28	5 (11%)	53,80,80	1.11	3 (5%)
4	AKG	A	1102	-	9,9,9	1.24	1 (11%)	11,11,11	1.42	2 (18%)
4	AKG	B	1202	-	9,9,9	1.23	1 (11%)	11,11,11	1.41	2 (18%)

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	NDP	C	1301	-	-	12/30/77/77	0/5/5/5
4	AKG	D	1402	-	-	4/9/9/9	-
3	NDP	D	1401	-	-	12/30/77/77	0/5/5/5
3	NDP	A	1101	-	-	13/30/77/77	0/5/5/5
4	AKG	E	1502	-	-	3/9/9/9	-
3	NDP	F	1601	-	-	13/30/77/77	0/5/5/5
4	AKG	F	1602	-	-	3/9/9/9	-
4	AKG	C	1302	-	-	5/9/9/9	-
3	NDP	B	1201	-	-	12/30/77/77	0/5/5/5
3	NDP	E	1501	-	-	10/30/77/77	0/5/5/5
4	AKG	A	1102	-	-	3/9/9/9	-
4	AKG	B	1202	-	-	3/9/9/9	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	NDP	C4N-C5N	-3.64	1.39	1.48
3	C	1301	NDP	C4N-C5N	-3.57	1.39	1.48
3	D	1401	NDP	C4N-C5N	-3.55	1.39	1.48
3	A	1101	NDP	C4N-C5N	-3.54	1.39	1.48
3	E	1501	NDP	C4N-C5N	-3.54	1.39	1.48

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1501	NDP	N3A-C2A-N1A	-4.54	121.58	128.68
3	B	1201	NDP	N3A-C2A-N1A	-4.38	121.84	128.68
3	D	1401	NDP	N3A-C2A-N1A	-4.37	121.86	128.68
3	C	1301	NDP	N3A-C2A-N1A	-4.34	121.89	128.68
3	A	1101	NDP	N3A-C2A-N1A	-4.26	122.02	128.68

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	NDP	C5B-O5B-PA-O1A
3	A	1101	NDP	C5B-O5B-PA-O2A

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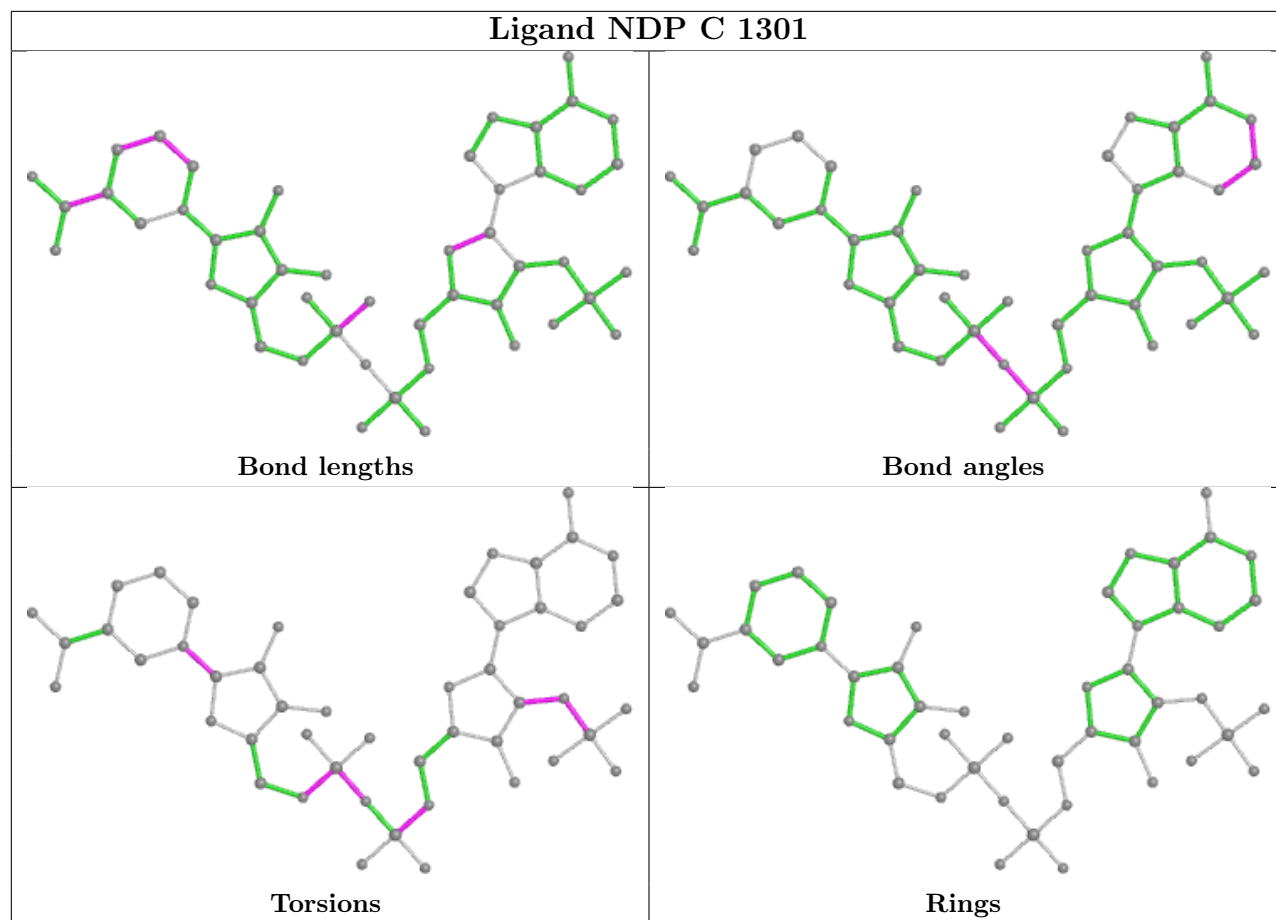
Mol	Chain	Res	Type	Atoms
3	A	1101	NDP	C3B-C2B-O2B-P2B
3	A	1101	NDP	C5D-O5D-PN-O1N
3	B	1201	NDP	C5B-O5B-PA-O1A

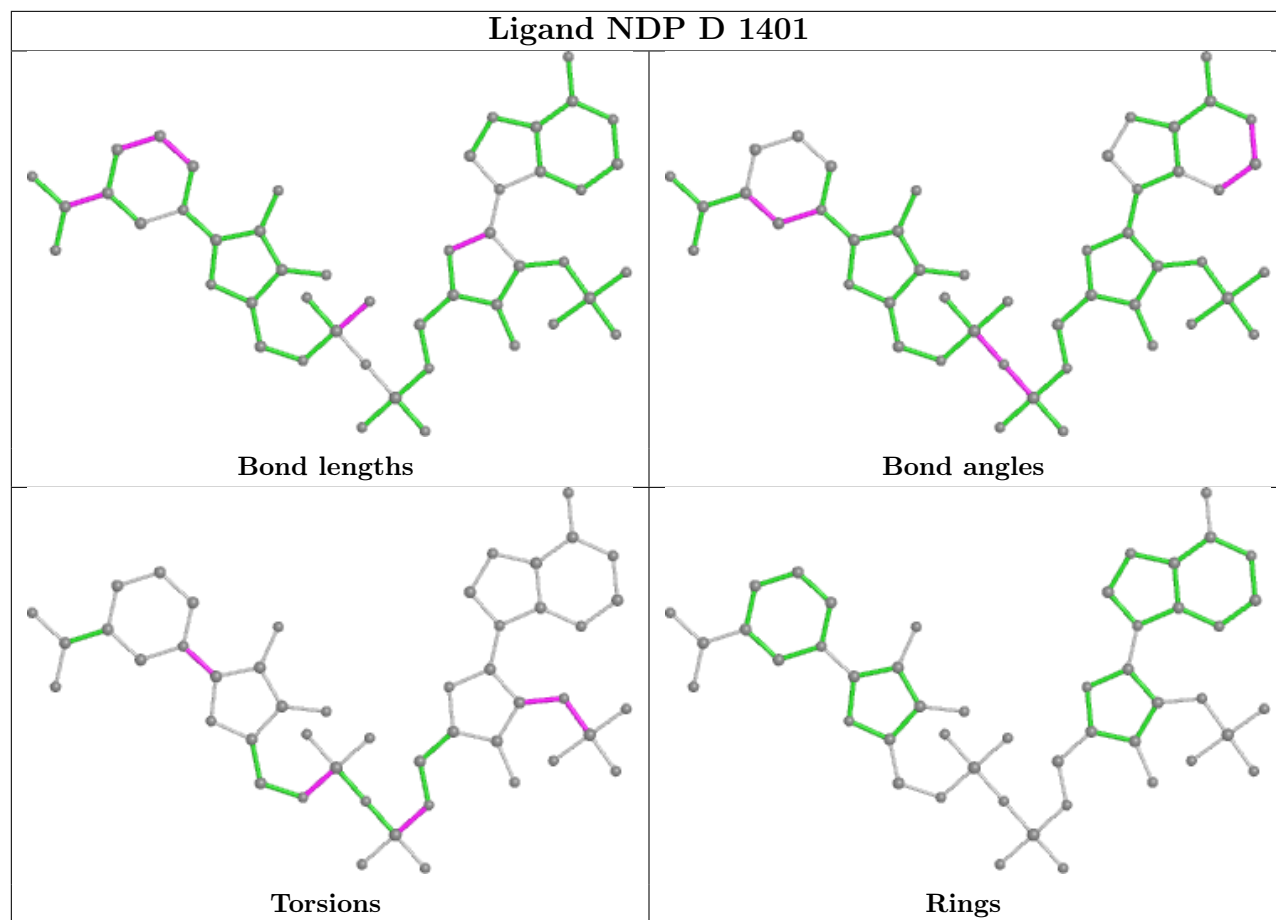
There are no ring outliers.

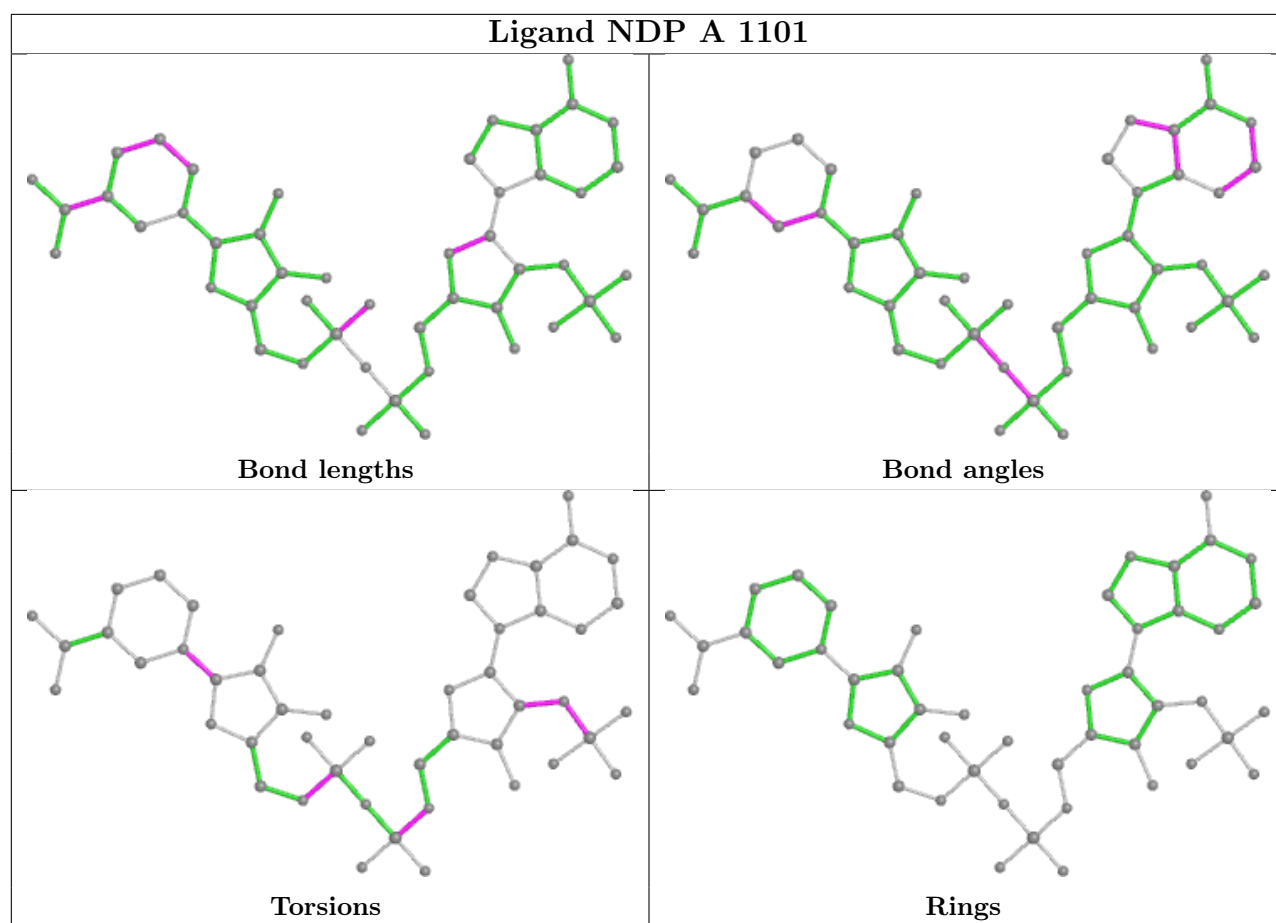
12 monomers are involved in 277 short contacts:

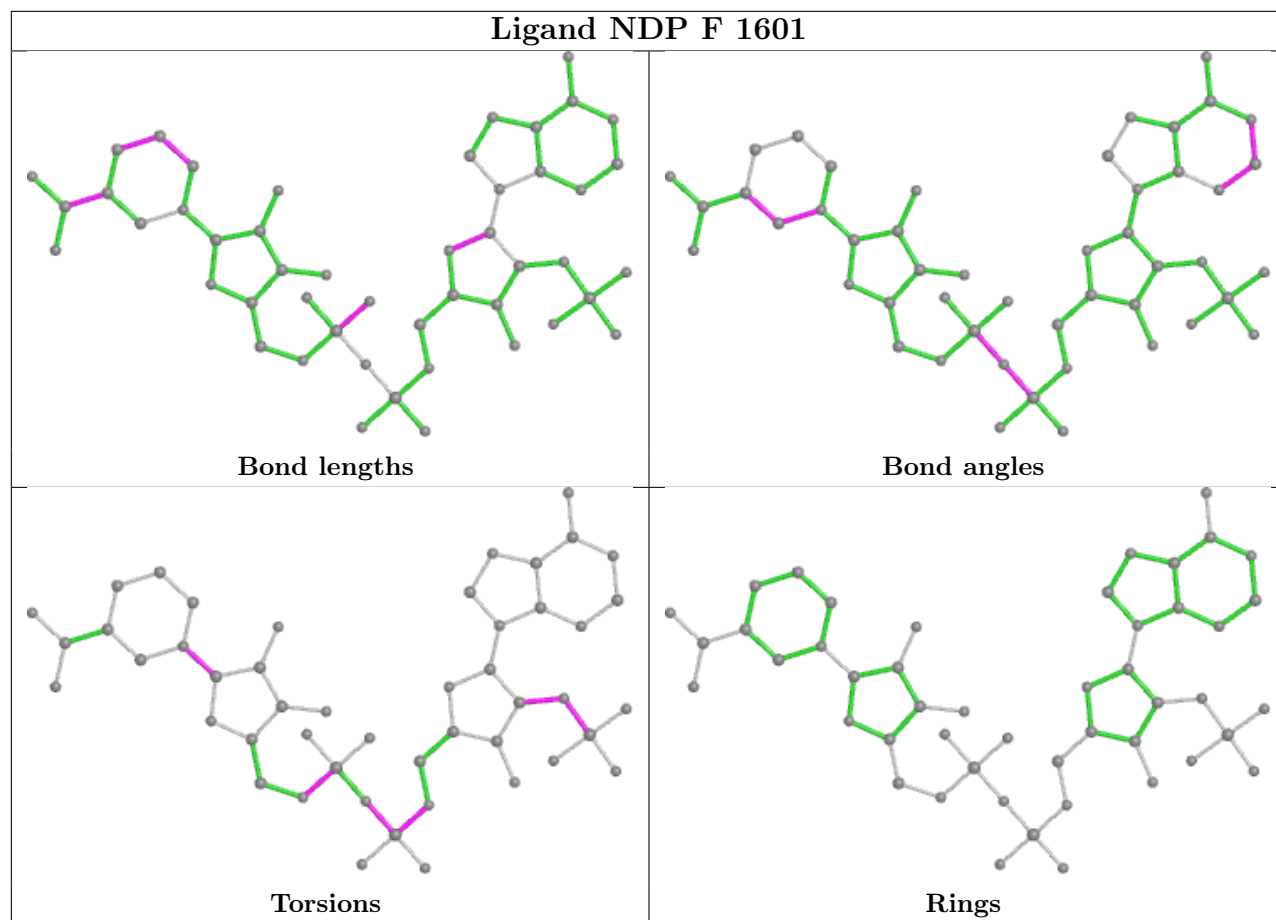
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	NDP	12	4
4	D	1402	AKG	5	0
3	D	1401	NDP	12	12
3	A	1101	NDP	13	54
4	E	1502	AKG	6	1
3	F	1601	NDP	11	109
4	F	1602	AKG	5	0
4	C	1302	AKG	6	4
3	B	1201	NDP	13	10
3	E	1501	NDP	12	0
4	A	1102	AKG	7	4
4	B	1202	AKG	6	5

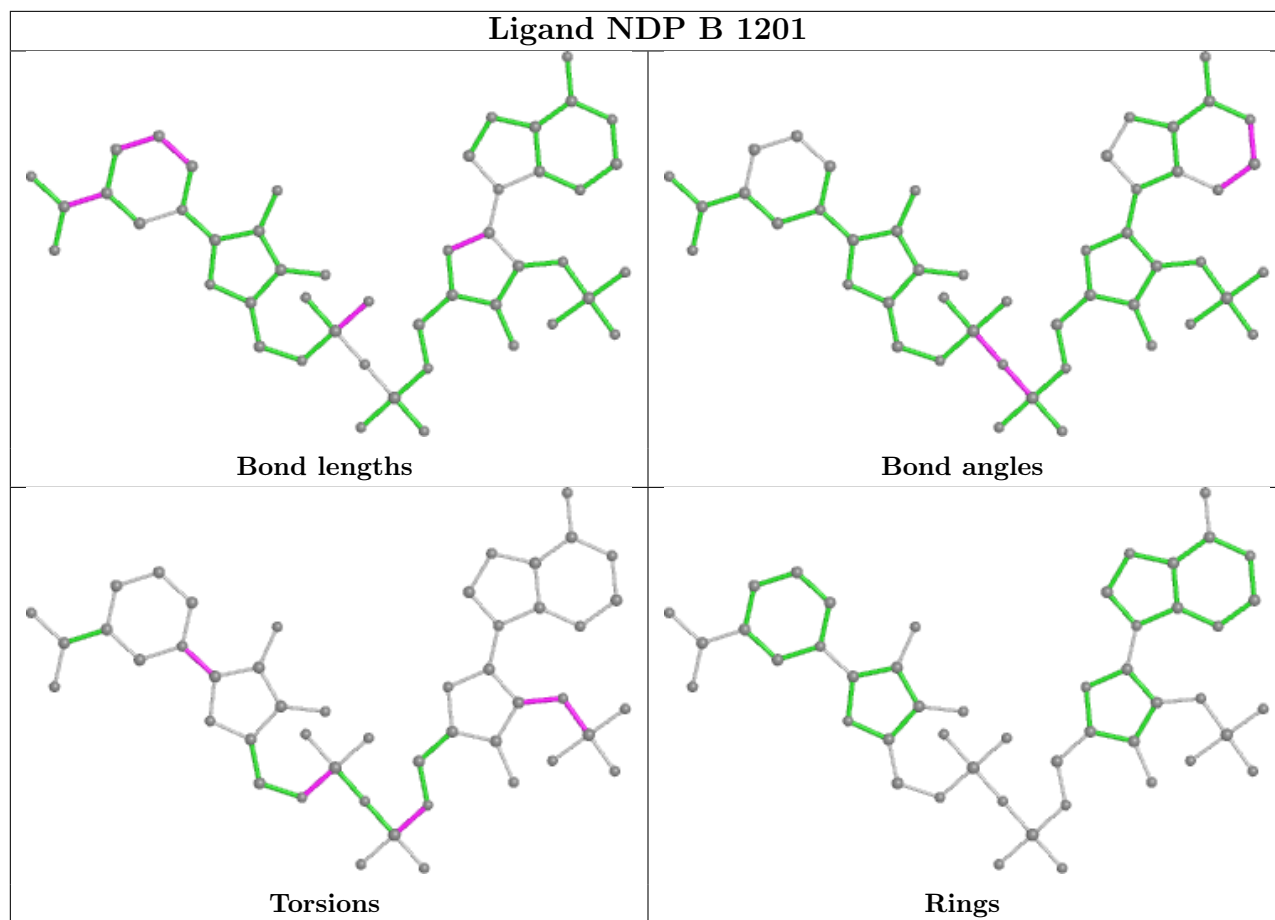
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

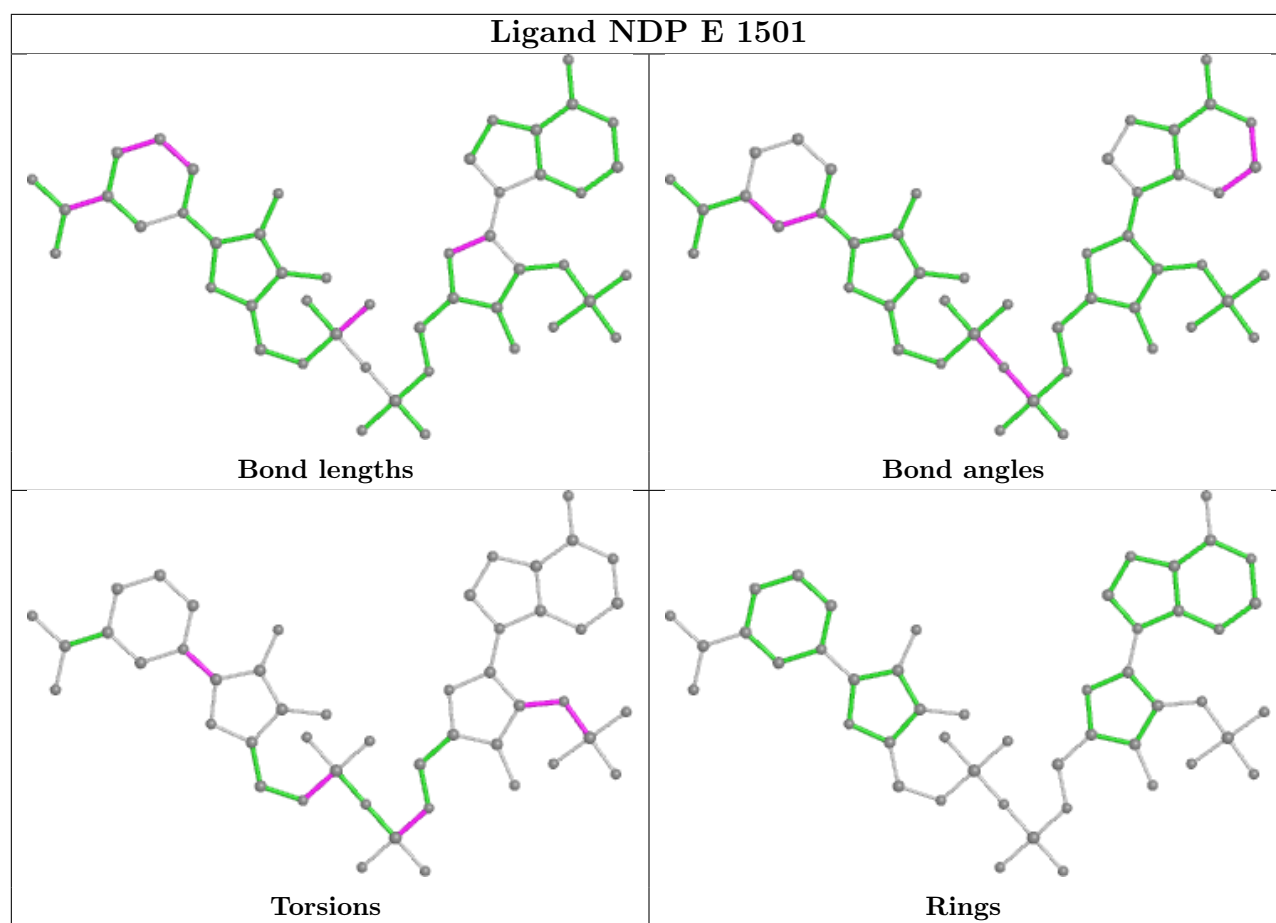












5.7 Other polymers [\(i\)](#)

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 [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

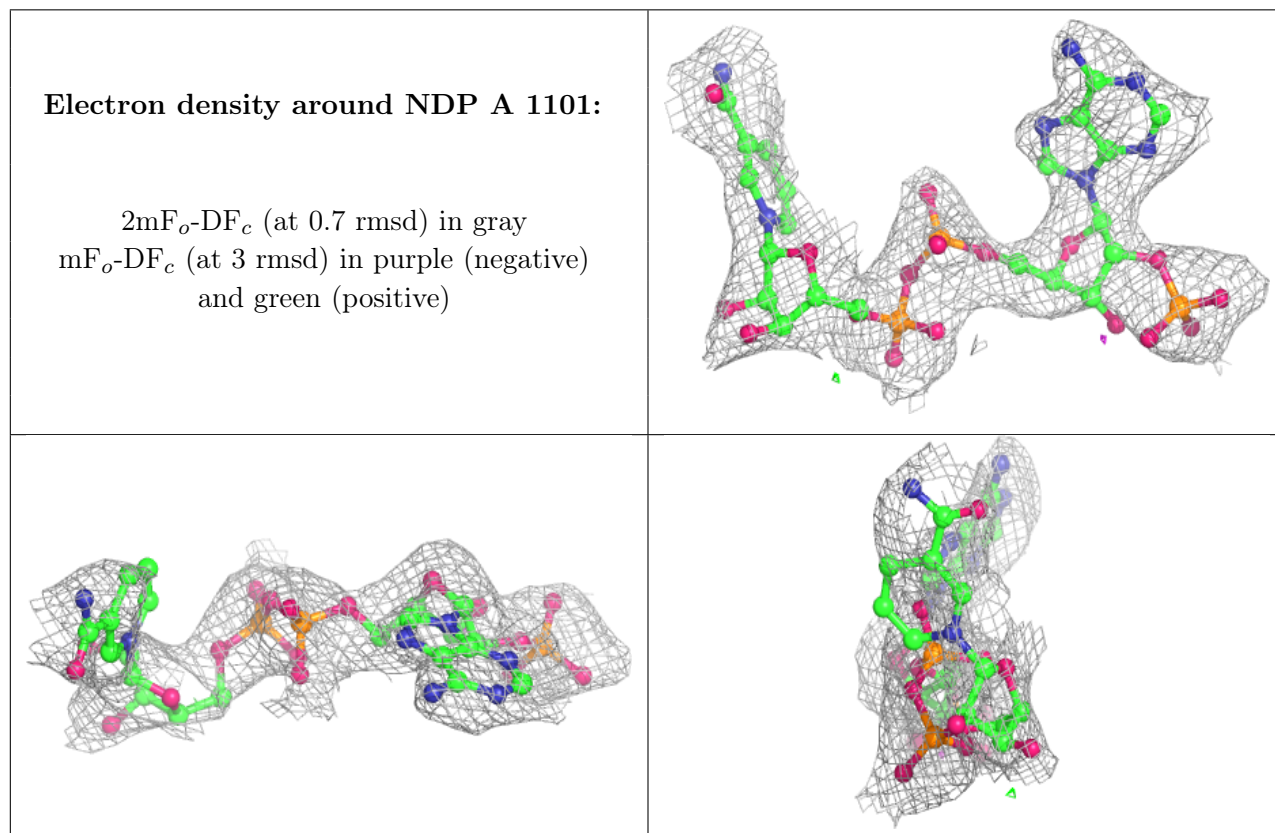
6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

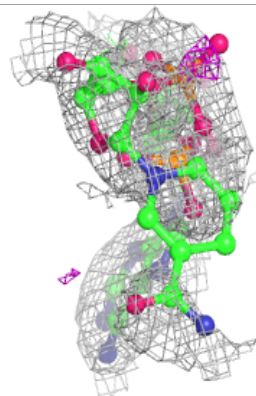
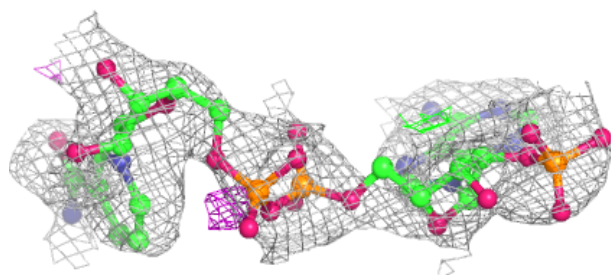
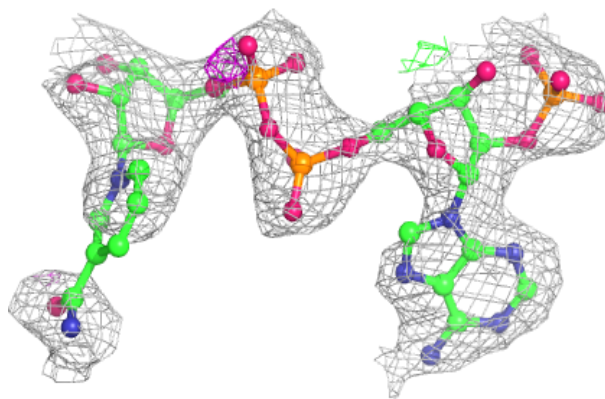
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

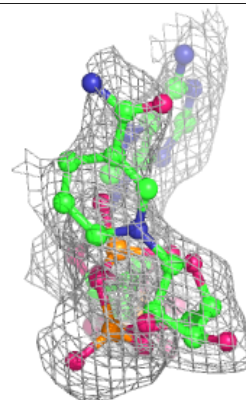
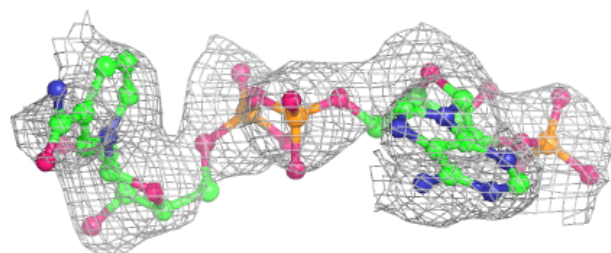
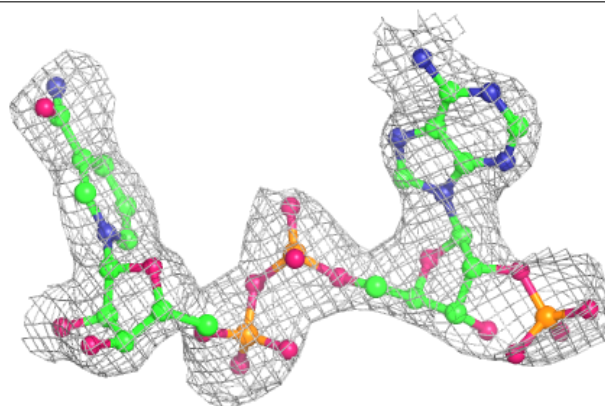


Electron density around NDP B 1201:

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

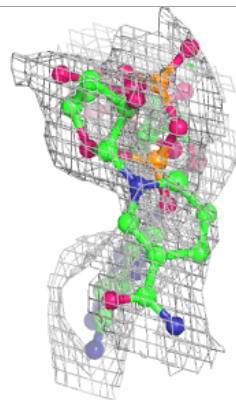
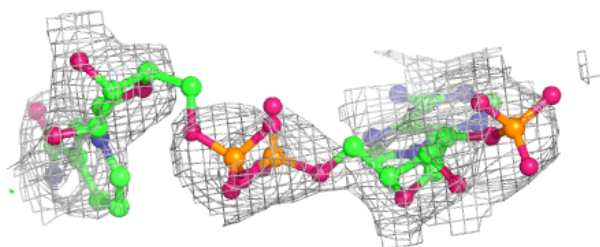
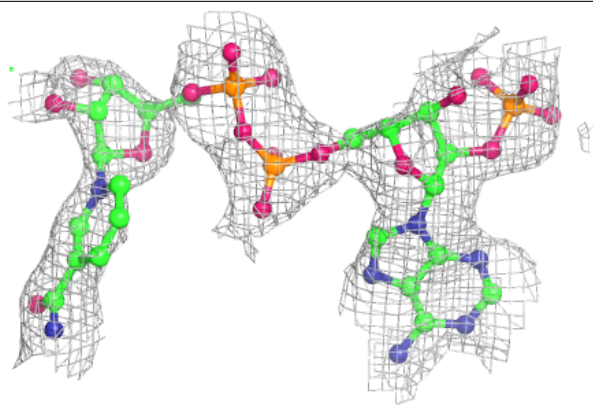
**Electron density around NDP C 1301:**

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

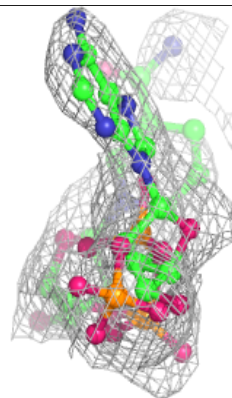
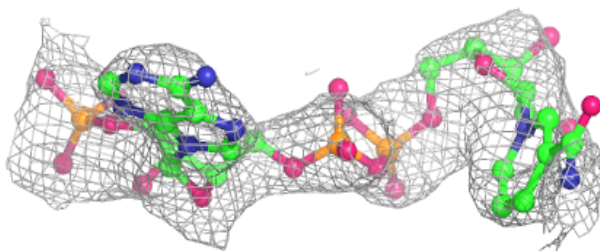
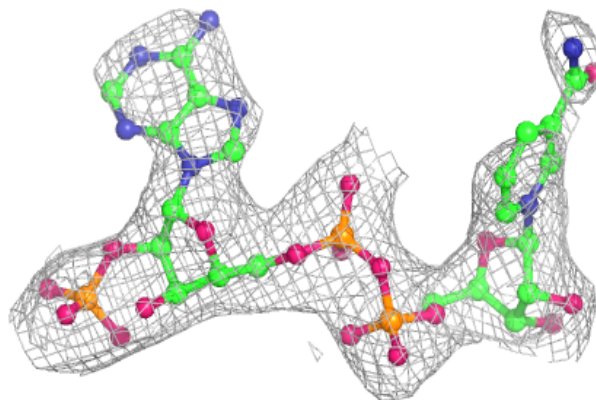


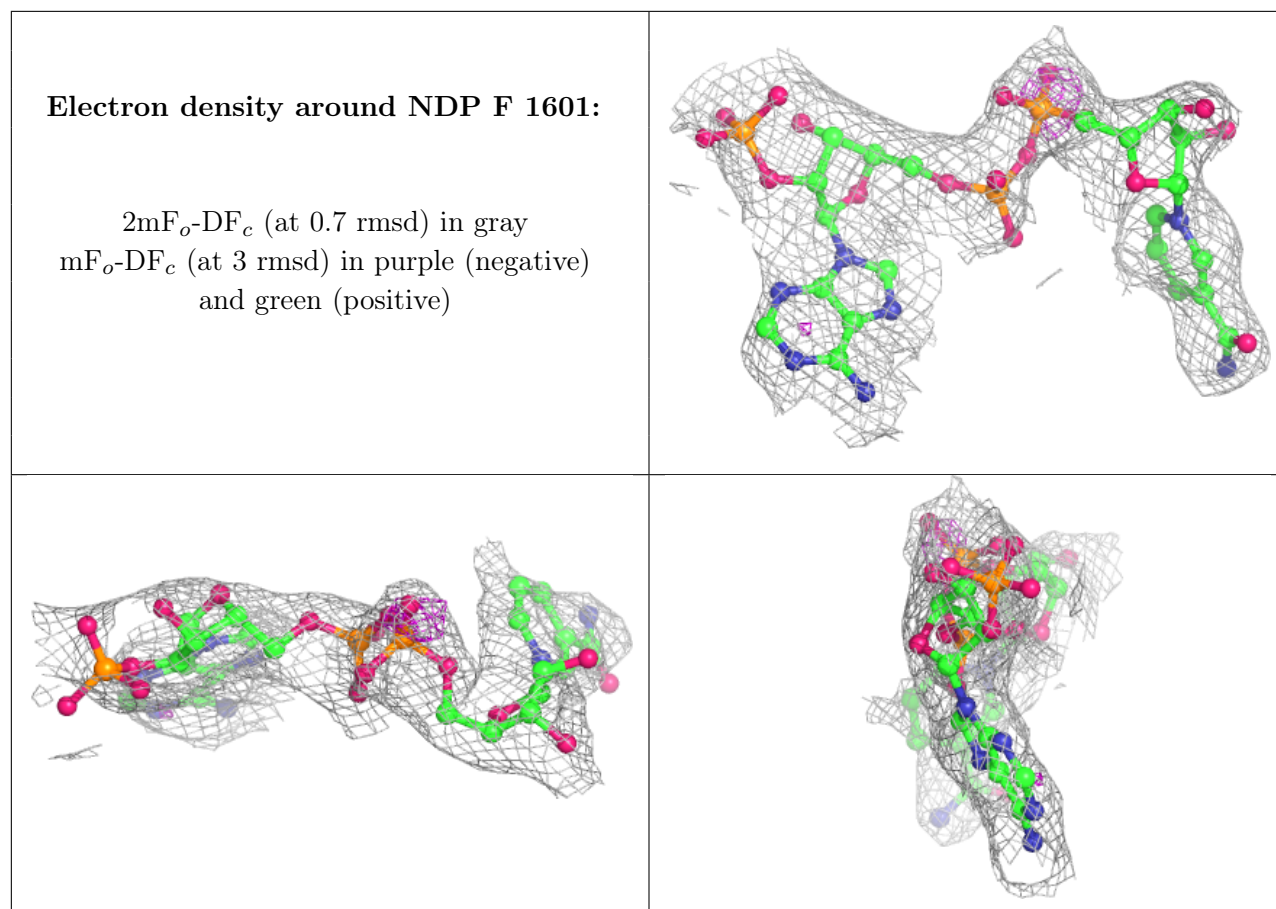
Electron density around NDP D 1401:

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

**Electron density around NDP E 1501:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.