WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2024 – 06:54 AM EST

PDB ID	:	4L06
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	:	2.28 Å(reported)

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

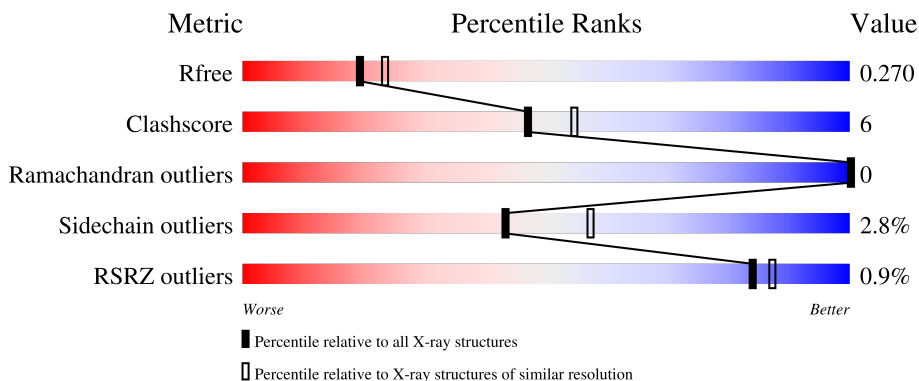|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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.
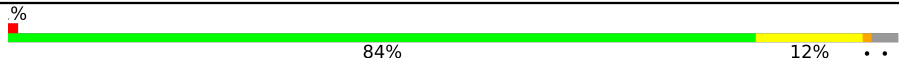
Metric	Percentile Ranks	Value
Rfree		0.270
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.8%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	80% 16% •
1	B	425	.% 84% 12% • •
1	C	425	82% 14% • •
1	D	425	2% 75% 20% • •
1	E	425	81% 16% •

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Mol	Chain	Length	Quality of chain
1	F	425	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19823 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
1	A	413	Total	C	N	O	S	0	1	0
			3231	2050	548	615	18			
1	B	412	Total	C	N	O	S	0	2	0
			3220	2046	545	611	18			
1	C	411	Total	C	N	O	S	0	0	0
			3234	2052	549	615	18			
1	D	411	Total	C	N	O	S	0	1	0
			3168	2006	541	603	18			
1	E	413	Total	C	N	O	S	0	1	0
			3232	2051	547	616	18			
1	F	412	Total	C	N	O	S	0	1	0
			3255	2068	552	617	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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	139	ASP	TYR	engineered mutation	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

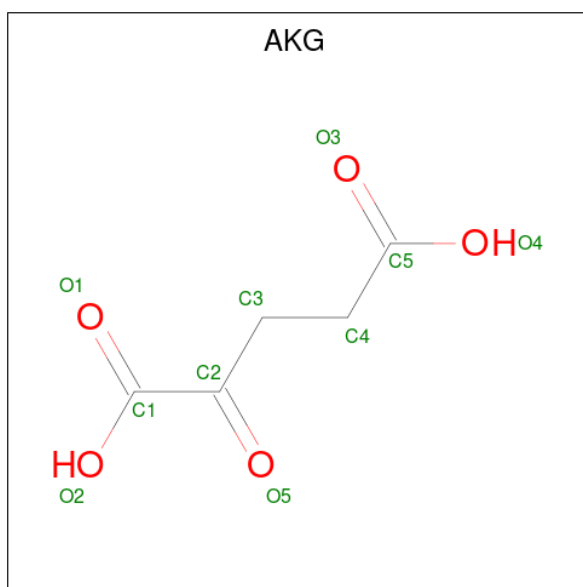- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	E	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 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
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: $C_5H_6O_5$).

AKG

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total 47	O 47	0	0
5	B	14	Total 14	O 14	0	0
5	C	16	Total 16	O 16	0	0
5	D	6	Total 6	O 6	0	0
5	E	25	Total 25	O 25	0	0
5	F	21	Total 21	O 21	0	0

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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 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

Chain A:

• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:

• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:

• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:

• 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	96.22Å 116.55Å 275.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.17 – 2.28 72.17 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.17-2.28) 99.9 (72.17-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.224 , 0.270 0.224 , 0.270	Depositor DCC
R_{free} test set	7083 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.0	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19823	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 67.21 % 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 5.3413e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.35	0/3301	0.55	0/4462
1	B	0.31	0/3293	0.51	0/4451
1	C	0.34	0/3301	0.53	0/4456
1	D	0.32	0/3237	0.54	0/4383
1	E	0.35	0/3302	0.54	0/4463
1	F	0.33	0/3325	0.53	1/4486 (0.0%)
All	All	0.33	0/19759	0.53	1/26701 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	F	381	LYS	C-N-CA	6.42	135.79	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3231	0	3149	41	0
1	B	3220	0	3139	31	0
1	C	3234	0	3175	36	0
1	D	3168	0	3043	64	0
1	E	3232	0	3149	41	0
1	F	3255	0	3217	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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	25	2	0
3	B	48	0	25	3	0
3	C	48	0	25	2	0
3	D	48	0	25	6	0
3	E	48	0	25	0	0
3	F	48	0	25	1	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
4	C	10	0	4	1	0
4	D	10	0	4	0	0
4	E	10	0	4	0	0
4	F	10	0	4	0	0
5	A	47	0	0	2	0
5	B	14	0	0	0	0
5	C	16	0	0	0	0
5	D	6	0	0	0	0
5	E	25	0	0	0	0
5	F	21	0	0	2	0
All	All	19823	0	19046	239	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 6.

The worst 5 of 239 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:D:29:LYS:NZ	1:D:399:ASP:OD1	2.04	0.90
1:C:3:LYS:N	1:C:33:PRO:O	2.12	0.82
1:F:324:GLU:OE1	1:F:388:ARG:NH1	2.13	0.81
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.65	0.77
1:D:340:LEU:HD22	1:D:352:LEU:HD11	1.66	0.76

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	412/425 (97%)	404 (98%)	8 (2%)	0	100	100
1	B	412/425 (97%)	398 (97%)	14 (3%)	0	100	100
1	C	409/425 (96%)	401 (98%)	8 (2%)	0	100	100
1	D	410/425 (96%)	397 (97%)	13 (3%)	0	100	100
1	E	412/425 (97%)	397 (96%)	15 (4%)	0	100	100
1	F	411/425 (97%)	399 (97%)	12 (3%)	0	100	100
All	All	2466/2550 (97%)	2396 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	339/361 (94%)	330 (97%)	9 (3%)	44	59
1	B	336/361 (93%)	329 (98%)	7 (2%)	53	68
1	C	342/361 (95%)	333 (97%)	9 (3%)	46	60
1	D	325/361 (90%)	311 (96%)	14 (4%)	29	38
1	E	339/361 (94%)	332 (98%)	7 (2%)	53	68
1	F	346/361 (96%)	336 (97%)	10 (3%)	42	56
All	All	2027/2166 (94%)	1971 (97%)	56 (3%)	43	57

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	287	SER
1	F	414	LEU
1	D	363	SER
1	F	388	ARG
1	F	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	96	ASN
1	E	96	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NAP	E	502	-	45,52,52	1.72	3 (6%)	56,80,80	1.11	2 (3%)
3	NAP	A	502	-	45,52,52	1.69	3 (6%)	56,80,80	1.08	2 (3%)
3	NAP	F	502	-	45,52,52	1.67	3 (6%)	56,80,80	1.05	1 (1%)
4	AKG	A	503	2	9,9,9	1.87	1 (11%)	11,11,11	1.68	5 (45%)
3	NAP	B	502	-	45,52,52	1.70	3 (6%)	56,80,80	1.06	1 (1%)
4	AKG	D	503	2	9,9,9	1.97	1 (11%)	11,11,11	1.80	5 (45%)
4	AKG	C	503	2	9,9,9	1.90	1 (11%)	11,11,11	1.80	5 (45%)
3	NAP	C	502	-	45,52,52	1.66	3 (6%)	56,80,80	1.20	5 (8%)
4	AKG	B	503	2	9,9,9	1.99	1 (11%)	11,11,11	1.70	3 (27%)
4	AKG	E	503	2	9,9,9	1.95	1 (11%)	11,11,11	1.79	4 (36%)
4	AKG	F	503	2	9,9,9	1.98	1 (11%)	11,11,11	1.84	3 (27%)
3	NAP	D	502	-	45,52,52	1.69	3 (6%)	56,80,80	1.20	6 (10%)

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	E	502	-	-	11/31/67/67	0/5/5/5
3	NAP	A	502	-	-	12/31/67/67	0/5/5/5
3	NAP	F	502	-	-	10/31/67/67	0/5/5/5
4	AKG	A	503	2	-	0/9/9/9	-
3	NAP	B	502	-	-	17/31/67/67	0/5/5/5
4	AKG	D	503	2	-	1/9/9/9	-
4	AKG	C	503	2	-	0/9/9/9	-
3	NAP	C	502	-	-	12/31/67/67	0/5/5/5
4	AKG	B	503	2	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	E	503	2	-	0/9/9/9	-
4	AKG	F	503	2	-	0/9/9/9	-
3	NAP	D	502	-	-	13/31/67/67	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	NAP	O7N-C7N	9.28	1.41	1.24
3	A	502	NAP	O7N-C7N	9.01	1.41	1.24
3	B	502	NAP	O7N-C7N	8.89	1.41	1.24
3	D	502	NAP	O7N-C7N	8.89	1.41	1.24
3	F	502	NAP	O7N-C7N	8.83	1.41	1.24

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	502	NAP	N3A-C2A-N1A	-5.32	120.37	128.68
3	E	502	NAP	N3A-C2A-N1A	-5.23	120.51	128.68
3	B	502	NAP	N3A-C2A-N1A	-4.96	120.93	128.68
3	A	502	NAP	N3A-C2A-N1A	-4.95	120.94	128.68
3	D	502	NAP	N3A-C2A-N1A	-4.91	121.00	128.68

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C5D-O5D-PN-O2N
3	A	502	NAP	O4D-C1D-N1N-C2N
3	A	502	NAP	O4D-C1D-N1N-C6N
3	B	502	NAP	C5B-O5B-PA-O1A
3	B	502	NAP	C5B-O5B-PA-O2A

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAP	2	0
3	F	502	NAP	1	0
3	B	502	NAP	3	0
4	C	503	AKG	1	0
3	C	502	NAP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	NAP	6	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 E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 502

Bond lengths

Bond angles

Torsions

Rings
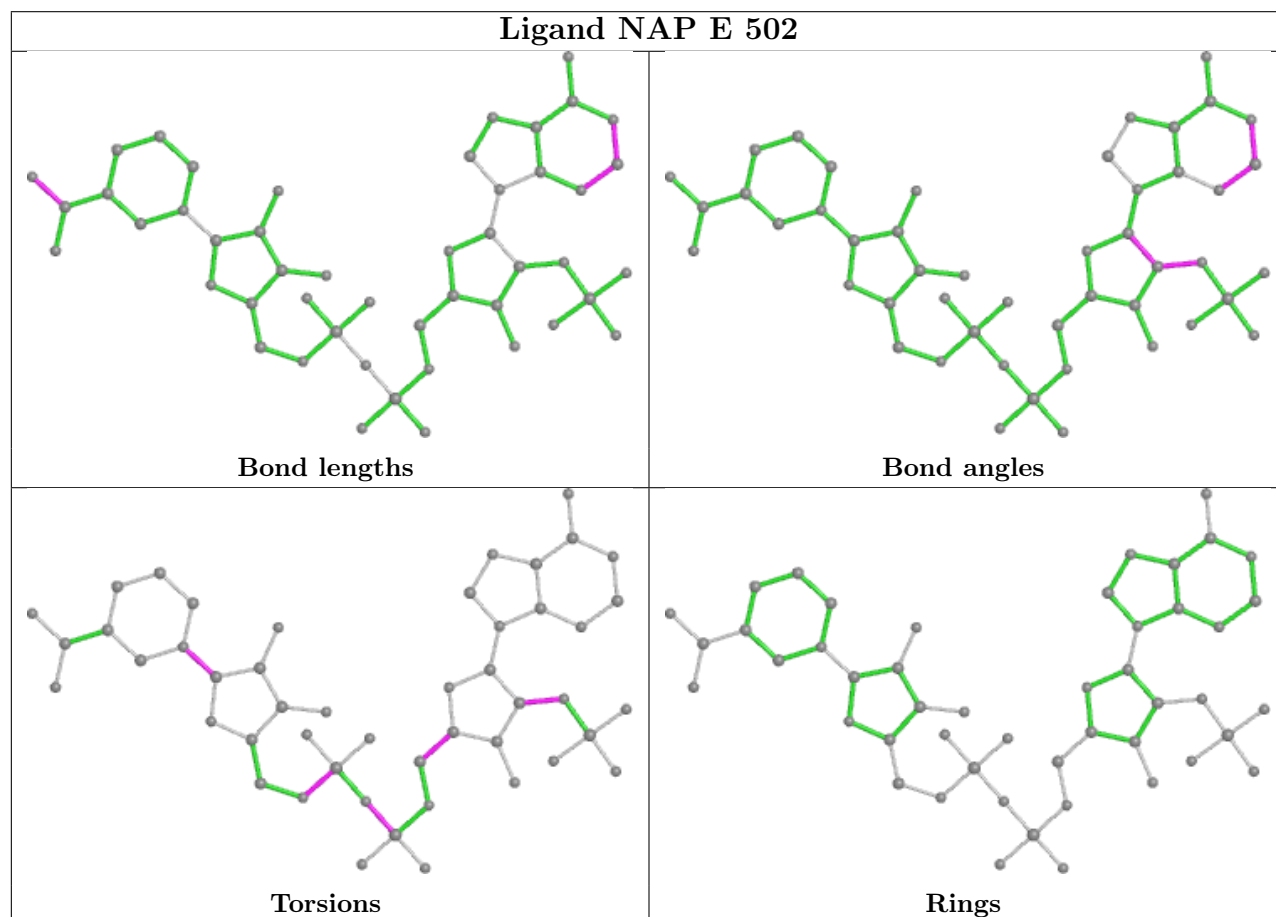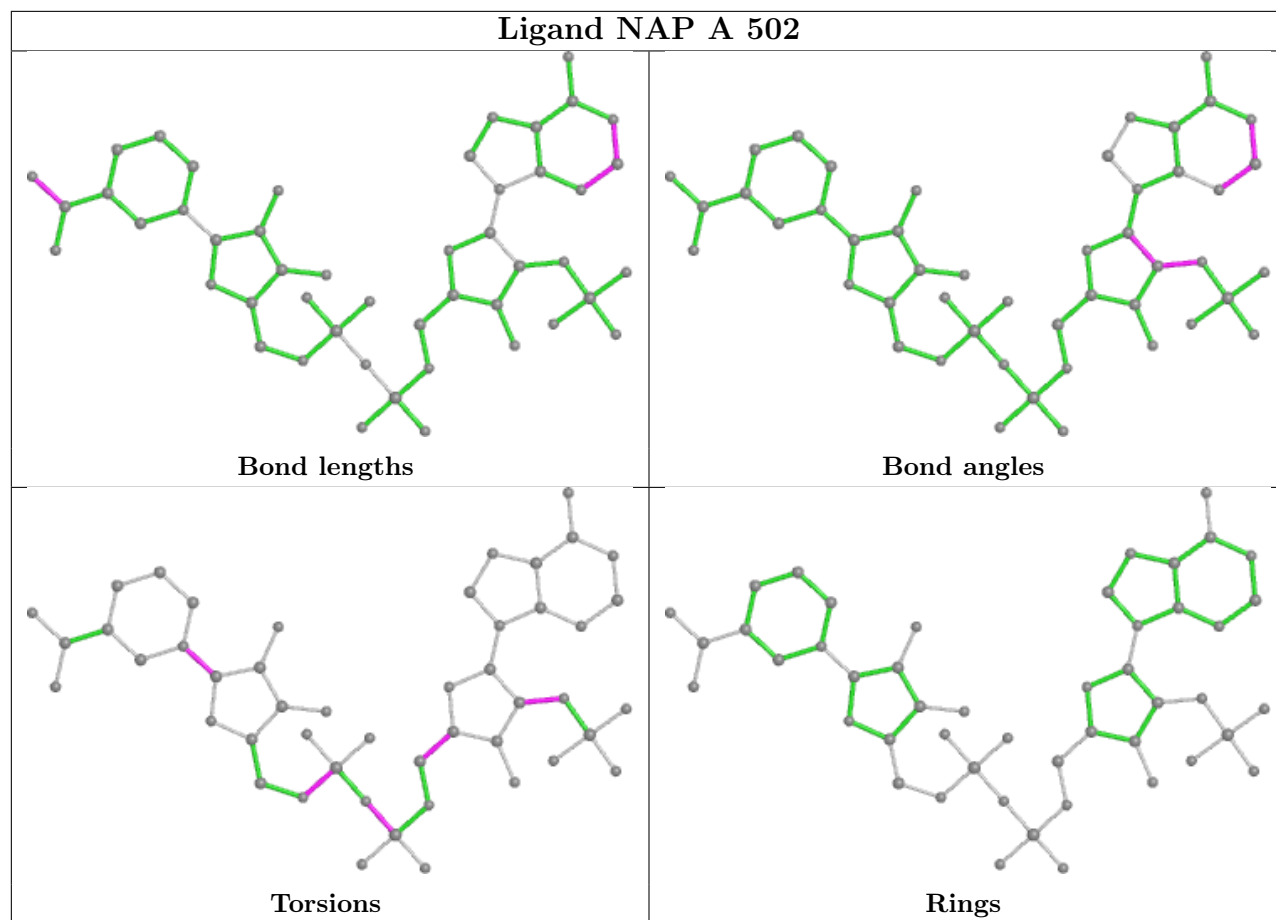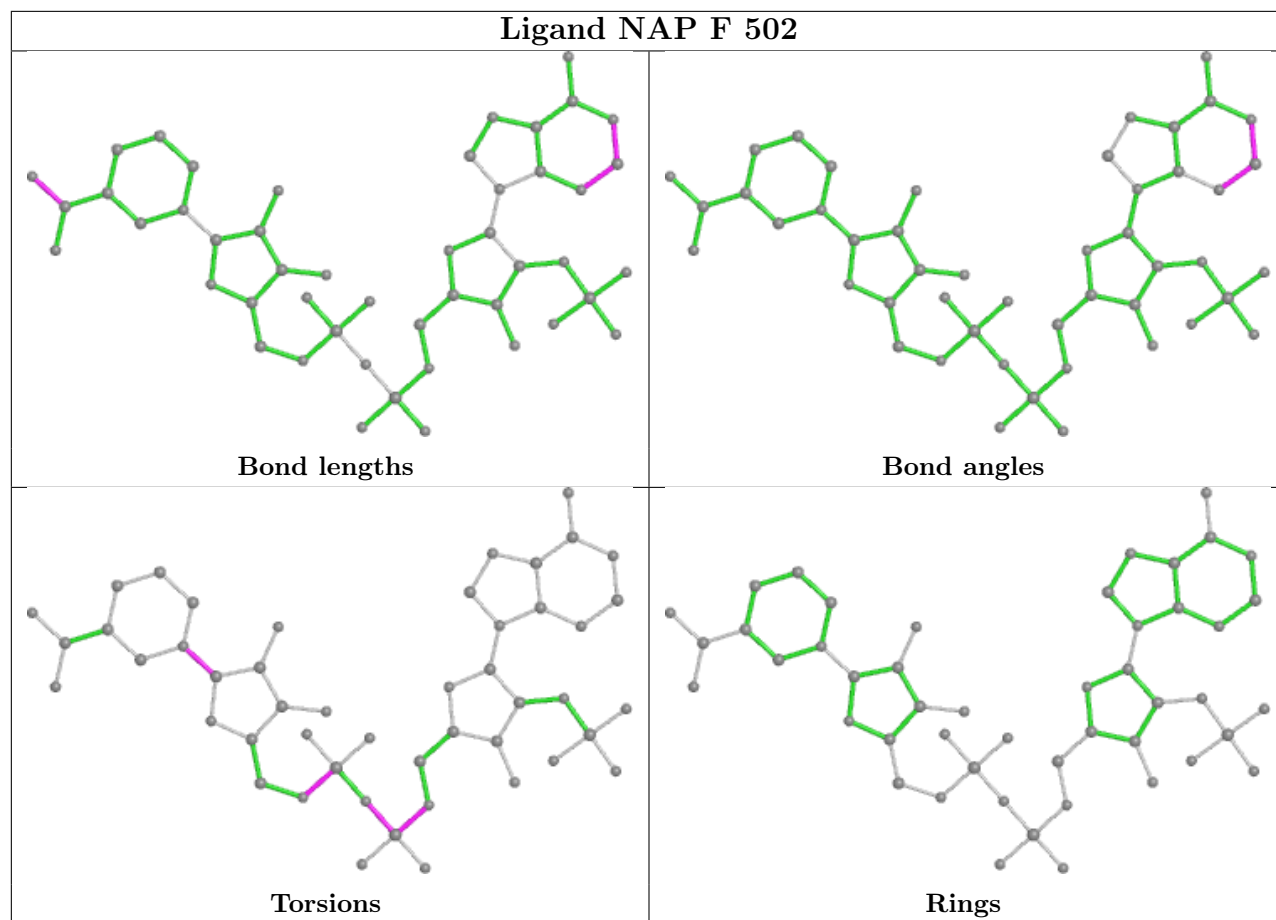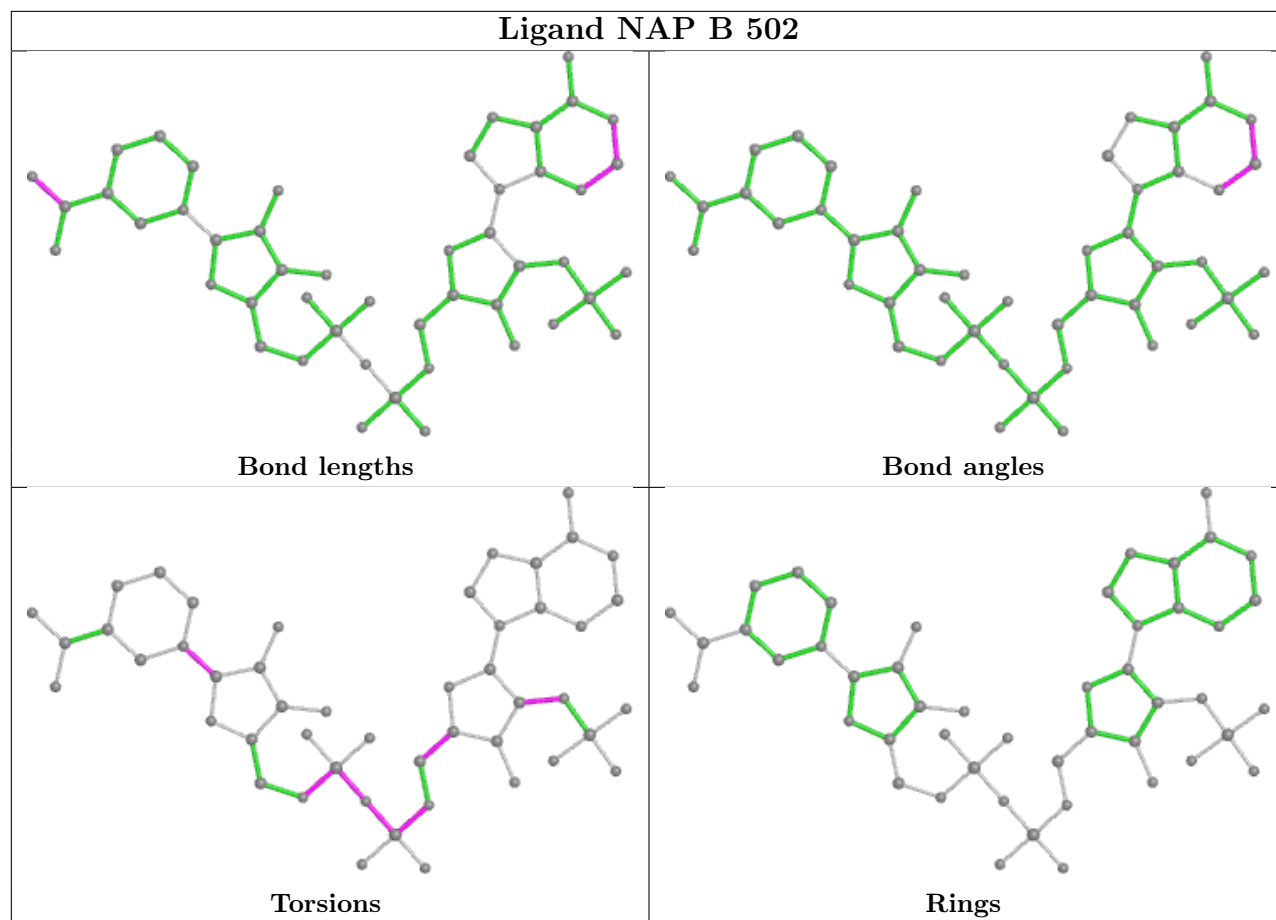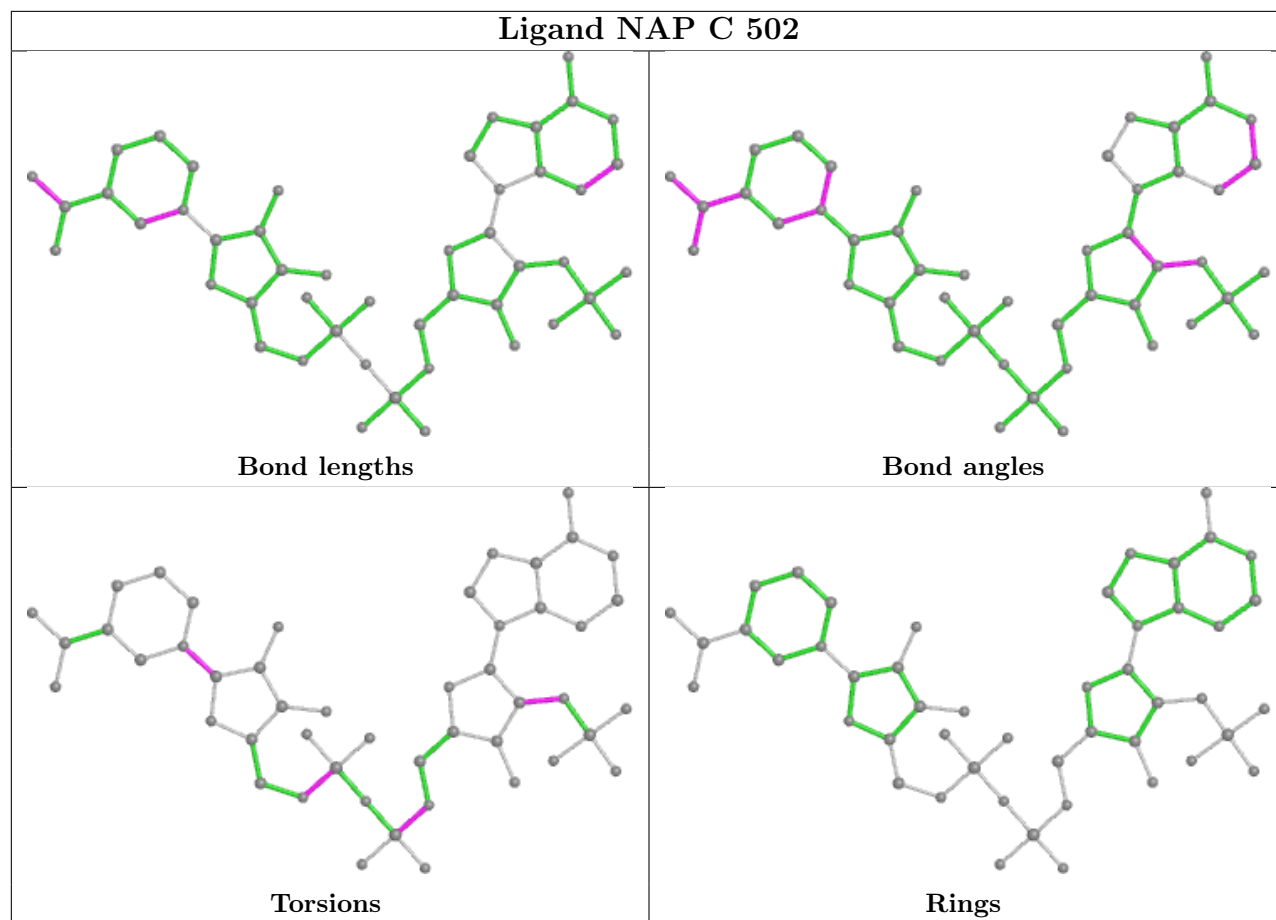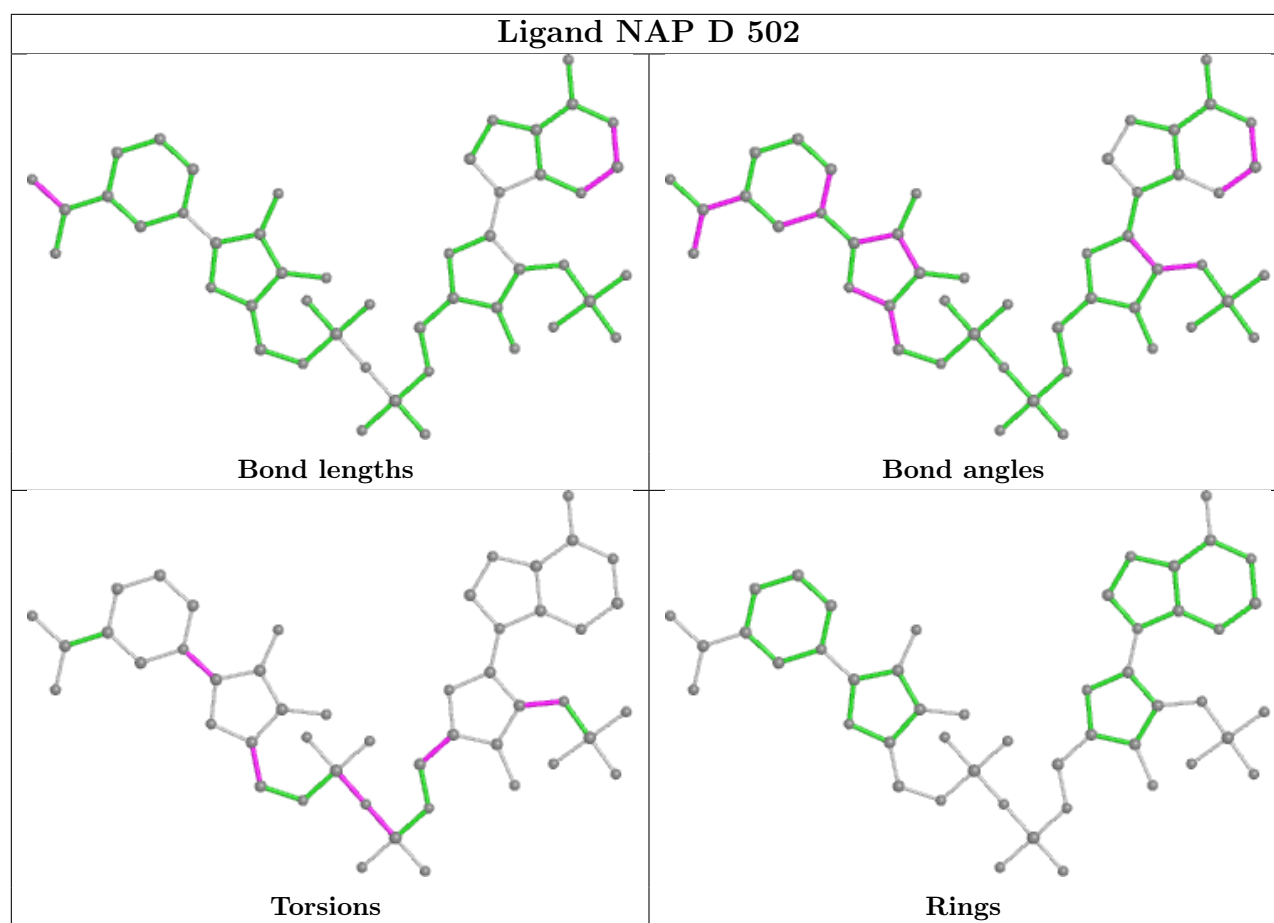
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	413/425 (97%)	-0.12	0	100	100	12, 32, 55, 67	0
1	B	412/425 (96%)	0.03	4 (0%)	82	86	16, 40, 65, 92	0
1	C	411/425 (96%)	-0.11	1 (0%)	95	96	15, 31, 54, 73	0
1	D	411/425 (96%)	0.22	10 (2%)	59	65	18, 45, 77, 96	0
1	E	413/425 (97%)	-0.13	2 (0%)	91	93	12, 33, 56, 65	0
1	F	412/425 (96%)	0.00	6 (1%)	73	78	12, 35, 58, 80	0
All	All	2472/2550 (96%)	-0.02	23 (0%)	84	87	12, 36, 62, 96	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	413	LYS	4.3
1	F	414	LEU	4.0
1	D	319	TYR	3.8
1	F	412	ALA	3.7
1	E	3	LYS	3.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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	AKG	F	503	10/10	0.83	0.14	42,61,75,77	0
4	AKG	D	503	10/10	0.84	0.15	61,69,76,76	0
4	AKG	B	503	10/10	0.86	0.15	70,77,81,82	0
2	CA	C	501	1/1	0.92	0.18	42,42,42,42	0
4	AKG	C	503	10/10	0.92	0.12	42,48,51,52	0
4	AKG	E	503	10/10	0.93	0.12	41,51,58,62	0
2	CA	B	501	1/1	0.94	0.12	49,49,49,49	0
4	AKG	A	503	10/10	0.95	0.14	32,42,45,48	0
3	NAP	B	502	48/48	0.95	0.12	18,44,53,57	0
3	NAP	D	502	48/48	0.95	0.15	12,35,50,111	0
2	CA	E	501	1/1	0.96	0.08	35,35,35,35	0
3	NAP	F	502	48/48	0.96	0.13	11,37,47,54	0
3	NAP	E	502	48/48	0.97	0.11	7,23,35,74	0
2	CA	A	501	1/1	0.97	0.09	34,34,34,34	0
3	NAP	C	502	48/48	0.97	0.14	5,19,27,41	0
3	NAP	A	502	48/48	0.97	0.11	6,20,32,60	0
2	CA	D	501	1/1	0.98	0.17	55,55,55,55	0
2	CA	F	501	1/1	0.98	0.07	39,39,39,39	0

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

Electron density around NAP B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
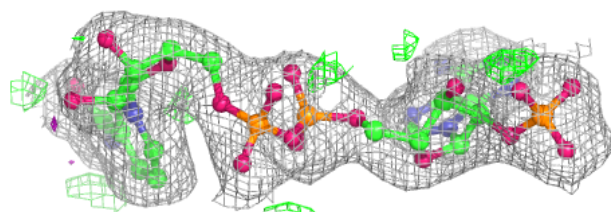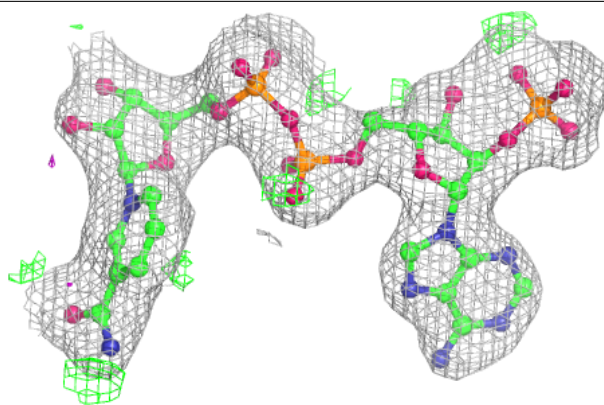
Electron density around NAP D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
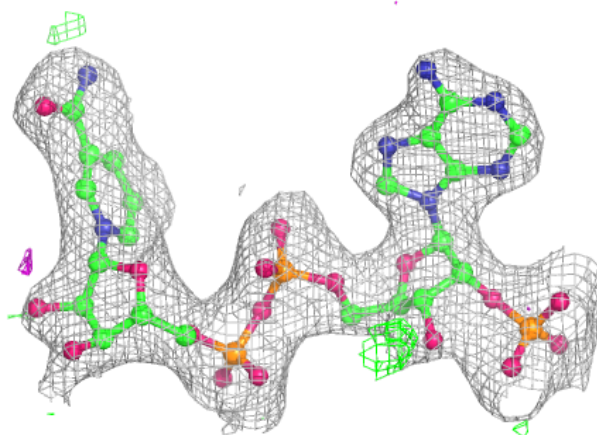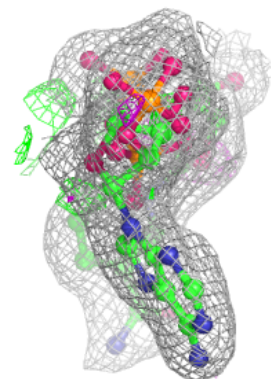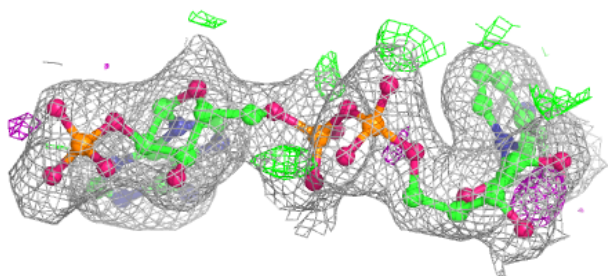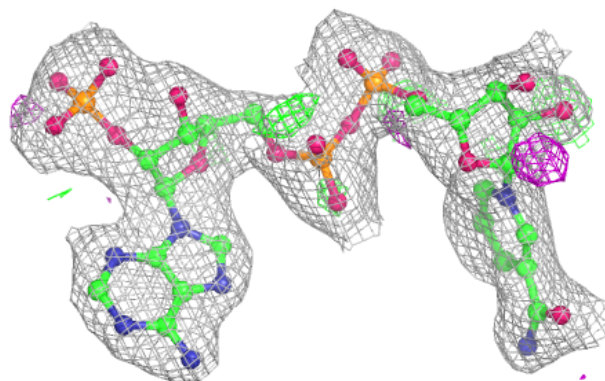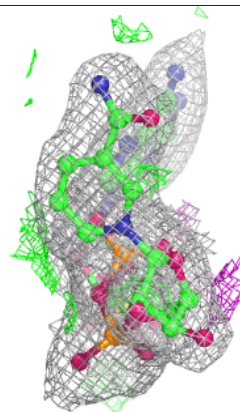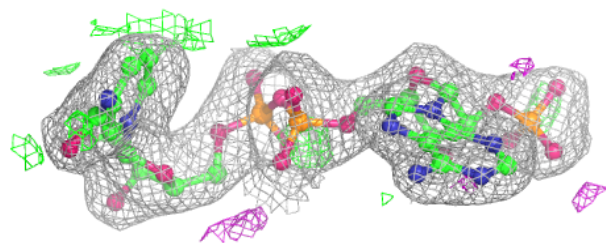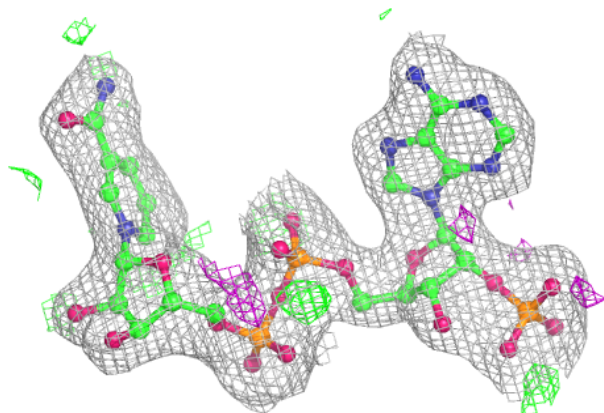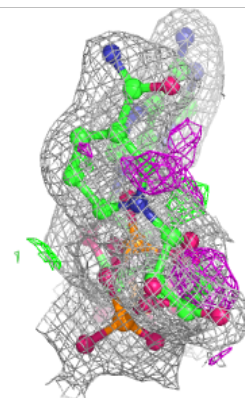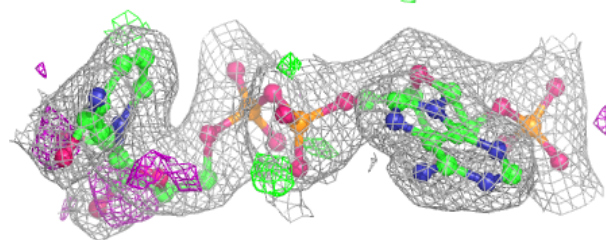$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
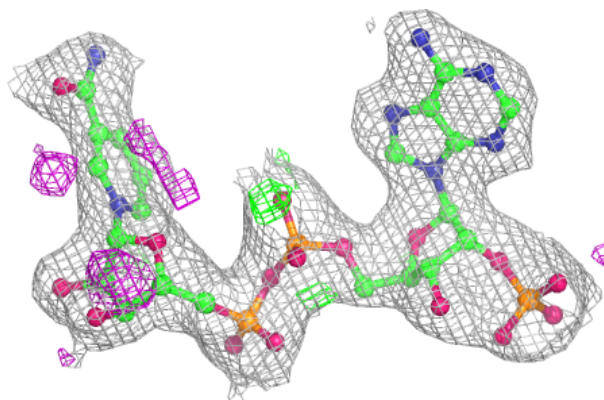and green (positive)
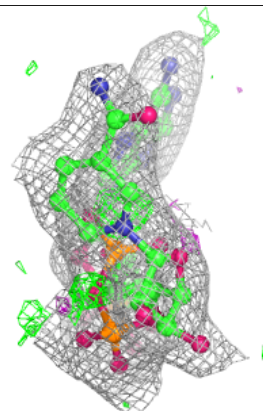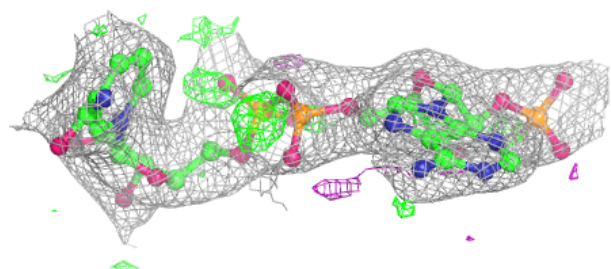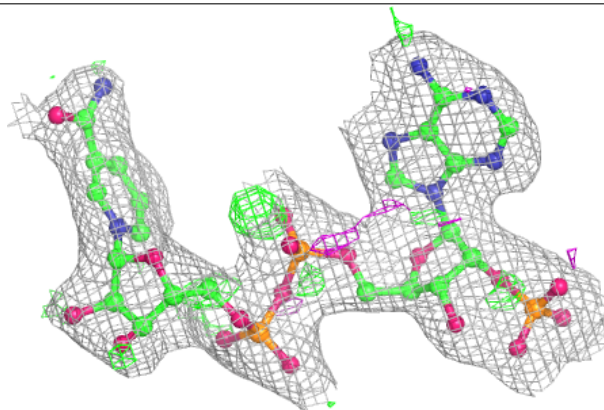
Electron density around NAP F 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
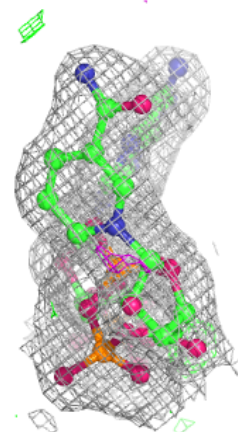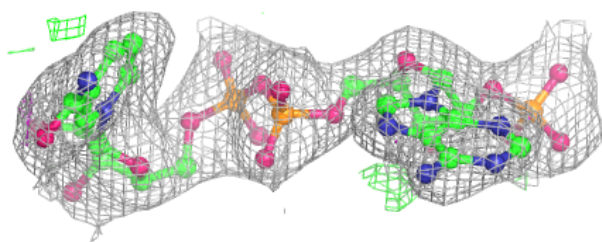
Electron density around NAP E 502:

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 502:

$2mF_o$-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 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 ⓘ

There are no such residues in this entry.