



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:47 PM UTC

PDB ID : 8VHB / pdb_00008vhb
Title : Crystal Structure of Human IDH1 R132Q in complex with NADPH and Alpha-Ketoglutarate
Authors : Mealka, M.; Sohl, C.D.; Huxford, T.
Deposited on : 2023-12-31
Resolution : 1.89 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

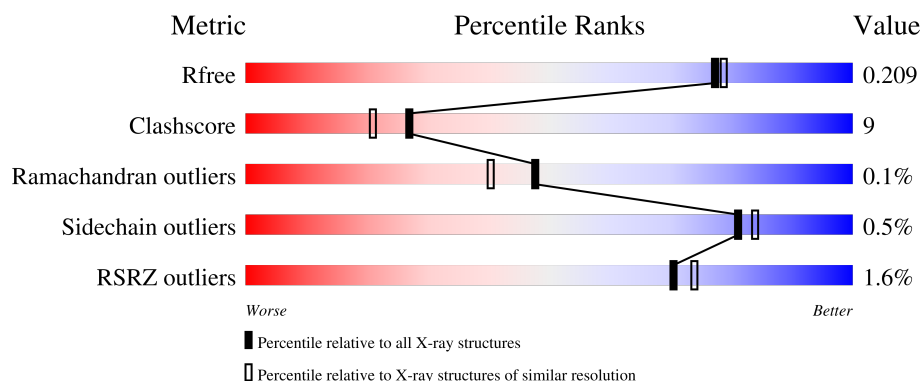
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	430	
1	B	430	
1	C	430	
1	D	430	

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
4	GOL	D	504	-	-	X	-
5	SCN	D	507	-	-	X	-
6	CL	D	508	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14665 atoms, of which 64 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	411	Total	C	N	O	S	0	3	0
			3278	2084	552	623	19			
1	B	412	Total	C	N	O	S	0	4	0
			3294	2093	558	624	19			
1	C	417	Total	C	N	O	S	0	0	0
			3291	2090	558	625	18			
1	D	413	Total	C	N	O	S	0	2	0
			3285	2087	555	624	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP O75874
A	-14	HIS	-	expression tag	UNP O75874
A	-13	HIS	-	expression tag	UNP O75874
A	-12	HIS	-	expression tag	UNP O75874
A	-11	HIS	-	expression tag	UNP O75874
A	-10	HIS	-	expression tag	UNP O75874
A	-9	SER	-	expression tag	UNP O75874
A	-8	SER	-	expression tag	UNP O75874
A	-7	GLY	-	expression tag	UNP O75874
A	-6	LEU	-	expression tag	UNP O75874
A	-5	VAL	-	expression tag	UNP O75874
A	-4	PRO	-	expression tag	UNP O75874
A	-3	ARG	-	expression tag	UNP O75874
A	-2	GLY	-	expression tag	UNP O75874
A	-1	SER	-	expression tag	UNP O75874
A	0	HIS	-	expression tag	UNP O75874
A	132	GLN	ARG	engineered mutation	UNP O75874
B	-15	HIS	-	expression tag	UNP O75874
B	-14	HIS	-	expression tag	UNP O75874
B	-13	HIS	-	expression tag	UNP O75874
B	-12	HIS	-	expression tag	UNP O75874

Continued on next page...

Continued from previous page...

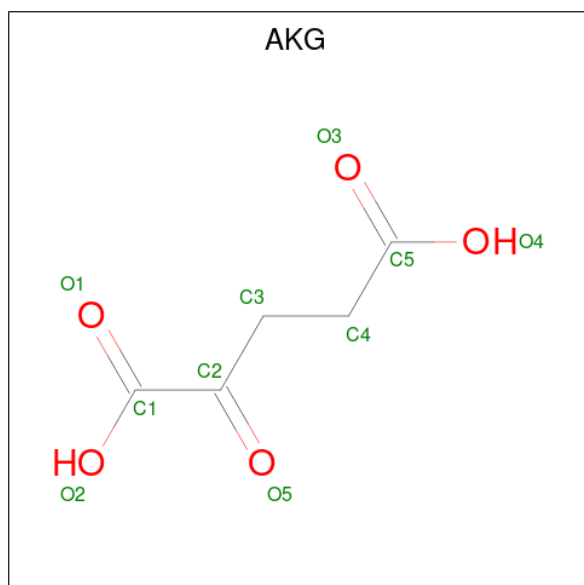
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP O75874
B	-10	HIS	-	expression tag	UNP O75874
B	-9	SER	-	expression tag	UNP O75874
B	-8	SER	-	expression tag	UNP O75874
B	-7	GLY	-	expression tag	UNP O75874
B	-6	LEU	-	expression tag	UNP O75874
B	-5	VAL	-	expression tag	UNP O75874
B	-4	PRO	-	expression tag	UNP O75874
B	-3	ARG	-	expression tag	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	SER	-	expression tag	UNP O75874
B	0	HIS	-	expression tag	UNP O75874
B	132	GLN	ARG	engineered mutation	UNP O75874
C	-15	HIS	-	expression tag	UNP O75874
C	-14	HIS	-	expression tag	UNP O75874
C	-13	HIS	-	expression tag	UNP O75874
C	-12	HIS	-	expression tag	UNP O75874
C	-11	HIS	-	expression tag	UNP O75874
C	-10	HIS	-	expression tag	UNP O75874
C	-9	SER	-	expression tag	UNP O75874
C	-8	SER	-	expression tag	UNP O75874
C	-7	GLY	-	expression tag	UNP O75874
C	-6	LEU	-	expression tag	UNP O75874
C	-5	VAL	-	expression tag	UNP O75874
C	-4	PRO	-	expression tag	UNP O75874
C	-3	ARG	-	expression tag	UNP O75874
C	-2	GLY	-	expression tag	UNP O75874
C	-1	SER	-	expression tag	UNP O75874
C	0	HIS	-	expression tag	UNP O75874
C	132	GLN	ARG	engineered mutation	UNP O75874
D	-15	HIS	-	expression tag	UNP O75874
D	-14	HIS	-	expression tag	UNP O75874
D	-13	HIS	-	expression tag	UNP O75874
D	-12	HIS	-	expression tag	UNP O75874
D	-11	HIS	-	expression tag	UNP O75874
D	-10	HIS	-	expression tag	UNP O75874
D	-9	SER	-	expression tag	UNP O75874
D	-8	SER	-	expression tag	UNP O75874
D	-7	GLY	-	expression tag	UNP O75874
D	-6	LEU	-	expression tag	UNP O75874
D	-5	VAL	-	expression tag	UNP O75874
D	-4	PRO	-	expression tag	UNP O75874

Continued on next page...

Continued from previous page...

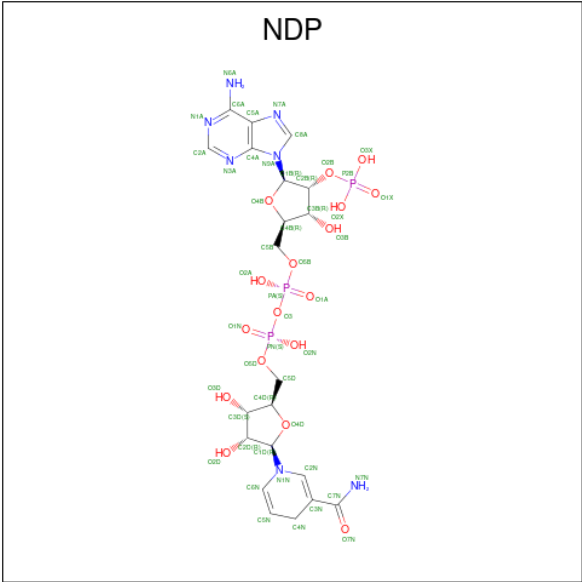
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP O75874
D	-2	GLY	-	expression tag	UNP O75874
D	-1	SER	-	expression tag	UNP O75874
D	0	HIS	-	expression tag	UNP O75874
D	132	GLN	ARG	engineered mutation	UNP O75874

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



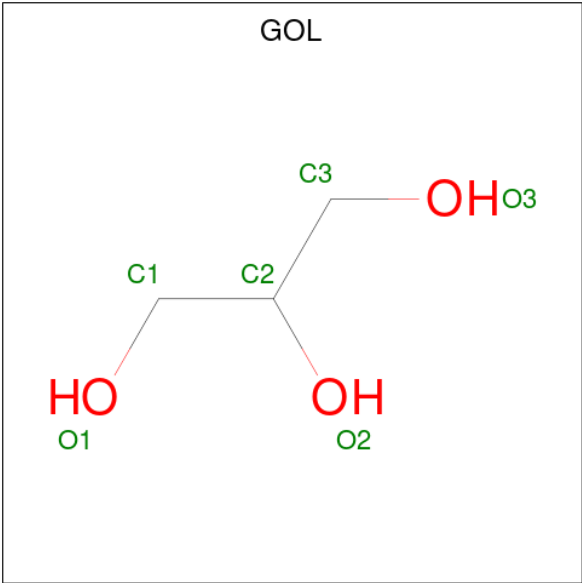
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		
3	C	1	Total	C	H	N	O	P	0	0
			59	15	19	6	16	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



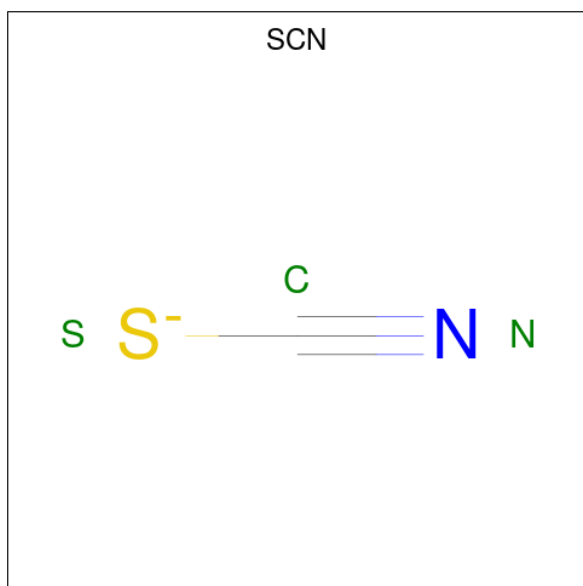
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	H	O	0
			14	3	8	3	0
4	C	1	Total	C	H	O	0
			14	3	8	3	0
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	S	0
			3	1	1	1	0
5	A	1	Total	C	N	S	0
			3	1	1	1	0
5	A	1	Total	C	N	S	0
			3	1	1	1	0
5	A	1	Total	C	N	S	0
			3	1	1	1	0
5	B	1	Total	C	N	S	0
			3	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	C	1	Total 3	C 1	N 1	S 1	0	0
5	C	1	Total 3	C 1	N 1	S 1	0	0
5	D	1	Total 3	C 1	N 1	S 1	0	0
5	D	1	Total 3	C 1	N 1	S 1	0	0
5	D	1	Total 3	C 1	N 1	S 1	0	0

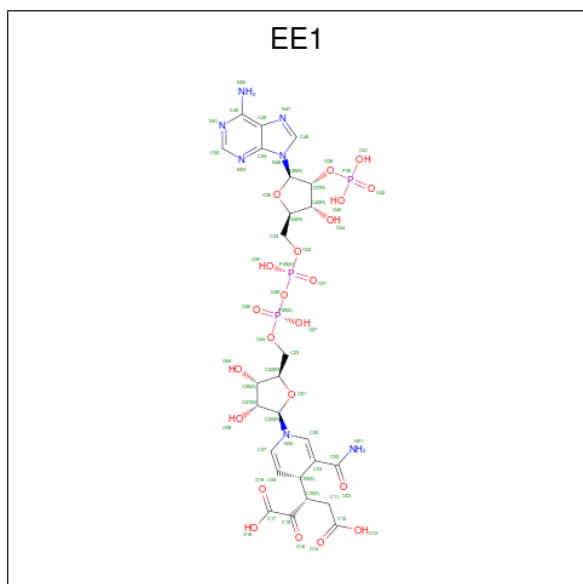
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0
6	B	1	Total 1	Cl 1	0	0
6	C	1	Total 1	Cl 1	0	0
6	D	1	Total 1	Cl 1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

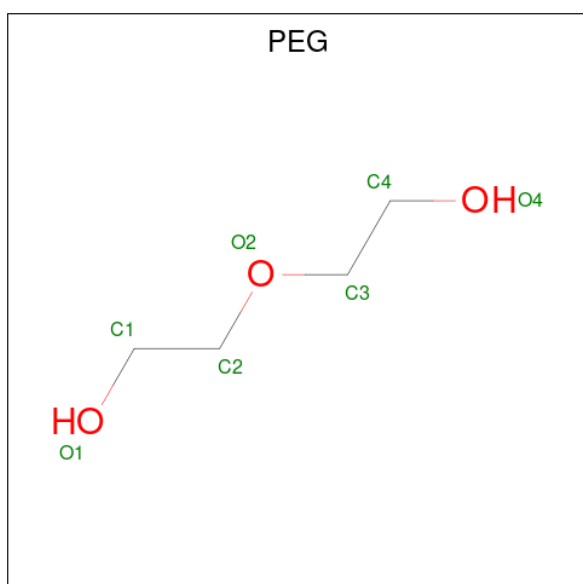
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Ca 2	0	0
7	C	1	Total 1	Ca 1	0	0
7	D	1	Total 1	Ca 1	0	0

- Molecule 8 is (3 {S})-3-[(4 {S})-3-aminocarbonyl-1-[(2 {R},3 {R},4 {S},5 {R})-5-[[[(2 {R},3 {R},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3-oxidanyl-4-phosphonooxy-oxolan-2-yl] methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-3,4-bis(oxidanyl)oxolan-2-yl]-4 {H}-pyridin-4-yl]-2-oxidanylidene-pentanedioic acid (CCD ID: EE1) (formula: $C_{26}H_{34}N_7O_{22}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			58	26	7	22	3		
8	D	1	Total	C	N	O	P	0	1
			116	52	14	44	6		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	297	Total	O	0	0
			297	297		
10	B	348	Total	O	0	0
			348	348		
10	C	187	Total	O	0	0
			187	187		
10	D	239	Total	O	0	0
			239	239		

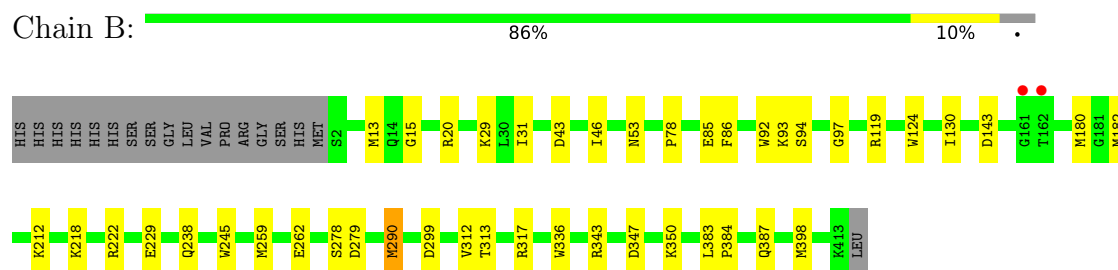
3 Residue-property plots

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.

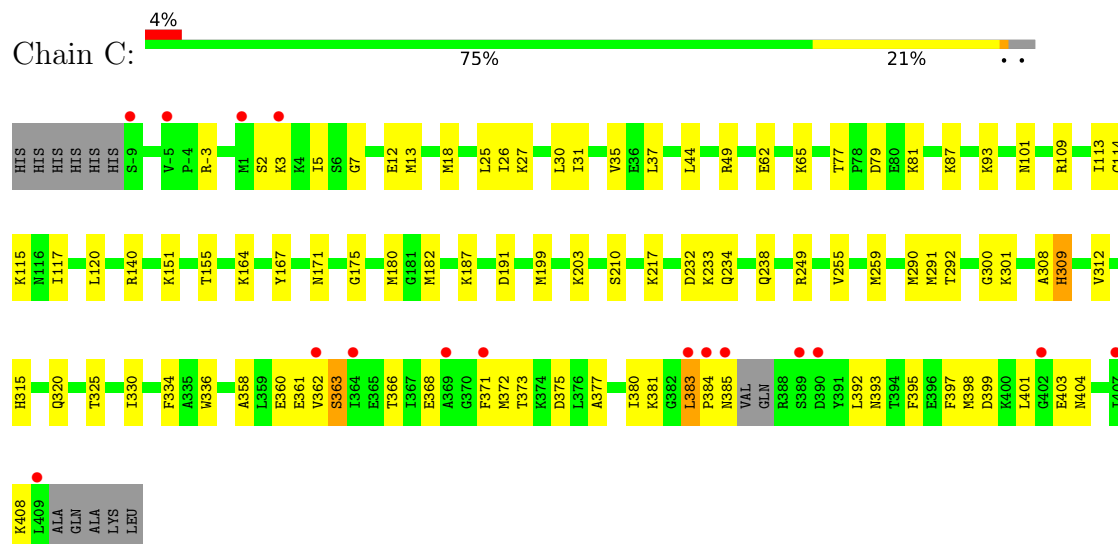
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



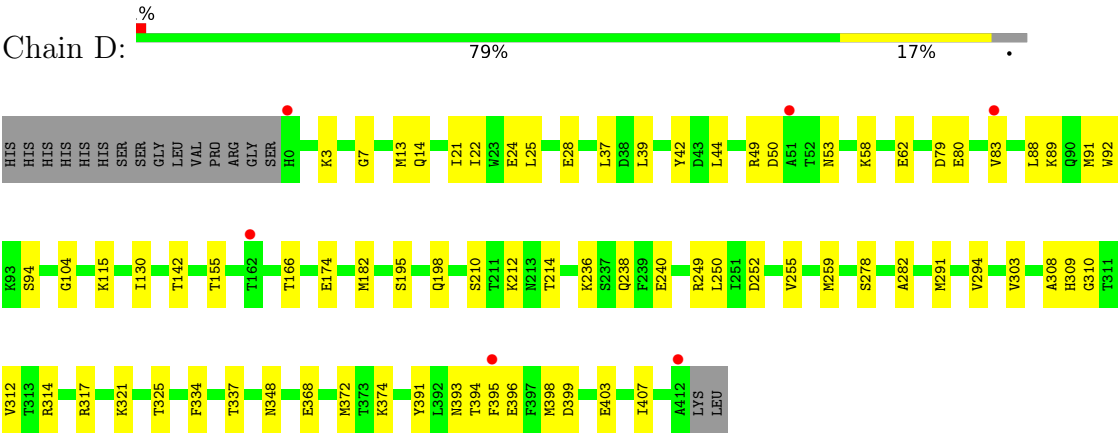
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



● Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.40Å 105.81Å 109.78Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	39.63 – 1.89 39.63 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.63-1.89) 97.1 (39.63-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.206 (Not available) , 0.209	Depositor DCC
R_{free} test set	7518 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14665	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: CL, EE1, CA, SCN, PEG, GOL, AKG, NDP

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	0.33	0/3346	0.51	0/4513
1	B	0.37	0/3362	0.55	1/4533 (0.0%)
1	C	0.30	0/3360	0.48	0/4530
1	D	0.32	0/3354	0.49	0/4524
All	All	0.33	0/13422	0.51	1/18100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	MET	CB-CG-SD	-5.09	97.43	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3278	0	3238	53	0
1	B	3294	0	3257	41	0
1	C	3291	0	3247	83	0
1	D	3285	0	3240	69	0
2	A	10	0	4	0	0
2	C	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	40	19	19	6	0
3	C	40	19	17	3	0
4	A	12	0	16	2	0
4	B	18	8	24	4	0
4	C	6	8	8	2	0
4	D	12	0	16	7	0
5	A	12	0	0	0	0
5	B	18	0	0	1	0
5	C	6	0	0	1	0
5	D	9	0	0	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	2	0
7	A	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	58	0	0	4	0
8	D	116	0	0	13	0
9	D	7	10	10	1	0
10	A	297	0	0	6	0
10	B	348	0	0	8	0
10	C	187	0	0	5	0
10	D	239	0	0	7	0
All	All	14601	64	13100	246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 246 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:195:SER:HA	4:D:504:GOL:H11	1.23	1.10
1:C:372:MET:HE3	1:C:377:ALA:HA	1.34	1.07
1:C:372:MET:HE3	1:C:377:ALA:CA	1.97	0.93
1:C:180:MET:HE2	1:C:182:MET:HE2	1.52	0.91
1:A:77:THR:N	3:A:502:NDP:O2D	2.04	0.90

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	412/430 (96%)	399 (97%)	12 (3%)	1 (0%)	43	36
1	B	414/430 (96%)	402 (97%)	12 (3%)	0	100	100
1	C	413/430 (96%)	398 (96%)	14 (3%)	1 (0%)	43	36
1	D	413/430 (96%)	399 (97%)	14 (3%)	0	100	100
All	All	1652/1720 (96%)	1598 (97%)	52 (3%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	C	309	HIS

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	350/364 (96%)	349 (100%)	1 (0%)	86	88
1	B	351/364 (96%)	350 (100%)	1 (0%)	86	88
1	C	351/364 (96%)	346 (99%)	5 (1%)	59	59
1	D	350/364 (96%)	350 (100%)	0	100	100
All	All	1402/1456 (96%)	1395 (100%)	7 (0%)	81	84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	LYS
1	C	312	VAL
1	C	383	LEU
1	C	363	SER
1	C	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	ASN
1	D	53	ASN
1	D	213	ASN
1	D	185	GLN
1	B	213	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 8 are monoatomic - leaving 31 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
5	SCN	B	510	-	1,2,2	0.75	0	0,1,1	-	-
5	SCN	B	502	-	1,2,2	0.92	0	0,1,1	-	-
5	SCN	D	502	-	1,2,2	1.02	0	0,1,1	-	-
3	NDP	C	502	-	42,43,52	2.50	12 (28%)	62,67,80	1.64	14 (22%)
5	SCN	B	508	-	1,2,2	0.80	0	0,1,1	-	-
4	GOL	C	505	-	5,5,5	0.61	0	5,5,5	1.35	1 (20%)
5	SCN	A	505	-	1,2,2	0.82	0	0,1,1	-	-
4	GOL	A	504	-	5,5,5	0.81	0	5,5,5	1.10	0
4	GOL	A	503	-	5,5,5	1.07	0	5,5,5	1.06	0
5	SCN	C	503	-	1,2,2	1.00	0	0,1,1	-	-
5	SCN	D	507	-	1,2,2	0.86	0	0,1,1	-	-
5	SCN	A	506	-	1,2,2	1.03	0	0,1,1	-	-
4	GOL	B	504	-	5,5,5	0.82	0	5,5,5	1.13	0
4	GOL	B	503	-	5,5,5	0.33	0	5,5,5	1.65	1 (20%)
8	EE1	D	501[A]	7	60,62,62	2.03	14 (23%)	81,95,95	1.66	14 (17%)
5	SCN	C	504	-	1,2,2	0.90	0	0,1,1	-	-
5	SCN	B	506	-	1,2,2	0.97	0	0,1,1	-	-
5	SCN	B	507	-	1,2,2	0.71	0	0,1,1	-	-
2	AKG	C	501	7	9,9,9	0.12	0	11,11,11	0.51	0
8	EE1	B	501	7	60,62,62	2.29	14 (23%)	81,95,95	1.65	14 (17%)
5	SCN	D	505	-	1,2,2	0.67	0	0,1,1	-	-
9	PEG	D	506	-	6,6,6	0.20	0	5,5,5	0.19	0
4	GOL	B	509	-	5,5,5	0.83	0	5,5,5	1.18	1 (20%)
5	SCN	A	507	-	1,2,2	0.88	0	0,1,1	-	-
4	GOL	D	504	-	5,5,5	1.15	0	5,5,5	1.08	1 (20%)
8	EE1	D	501[B]	7	60,62,62	2.16	12 (20%)	81,95,95	1.69	13 (16%)
5	SCN	B	505	-	1,2,2	0.74	0	0,1,1	-	-
5	SCN	A	508	-	1,2,2	1.13	0	0,1,1	-	-
3	NDP	A	502	-	42,43,52	2.56	15 (35%)	62,67,80	1.66	13 (20%)
2	AKG	A	501	7	9,9,9	0.30	0	11,11,11	0.61	0
4	GOL	D	503	-	5,5,5	1.02	0	5,5,5	1.00	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
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	B	504	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	503	-	-	3/4/4/4	-
3	NDP	C	502	-	-	6/27/59/77	0/4/4/5
4	GOL	D	504	-	-	3/4/4/4	-
8	EE1	D	501[A]	7	-	16/49/96/96	0/5/5/5
8	EE1	D	501[B]	7	-	8/49/96/96	0/5/5/5
4	GOL	C	505	-	-	3/4/4/4	-
9	PEG	D	506	-	-	1/4/4/4	-
4	GOL	B	509	-	-	2/4/4/4	-
8	EE1	B	501	7	-	10/49/96/96	0/5/5/5
2	AKG	C	501	7	-	0/9/9/9	-
4	GOL	A	504	-	-	2/4/4/4	-
3	NDP	A	502	-	-	7/27/59/77	0/4/4/5
2	AKG	A	501	7	-	0/9/9/9	-
4	GOL	D	503	-	-	4/4/4/4	-

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NDP	P2B-O2B	11.21	1.79	1.59
3	C	502	NDP	P2B-O2B	10.21	1.77	1.59
8	D	501[B]	EE1	P39-O38	10.17	1.77	1.59
8	B	501	EE1	P39-O38	9.36	1.75	1.59
8	D	501[A]	EE1	P39-O38	8.96	1.75	1.59

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501[B]	EE1	C07-N06-C05	-6.41	112.46	119.32
8	D	501[A]	EE1	C07-N06-C05	-6.10	112.79	119.32
8	B	501	EE1	C07-N06-C05	-5.53	113.40	119.32
8	B	501	EE1	O19-C17-C15	-4.50	116.42	122.15
8	D	501[B]	EE1	O21-C20-N06	4.38	116.43	108.08

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NDP	C5D-O5D-PN-O3
3	A	502	NDP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

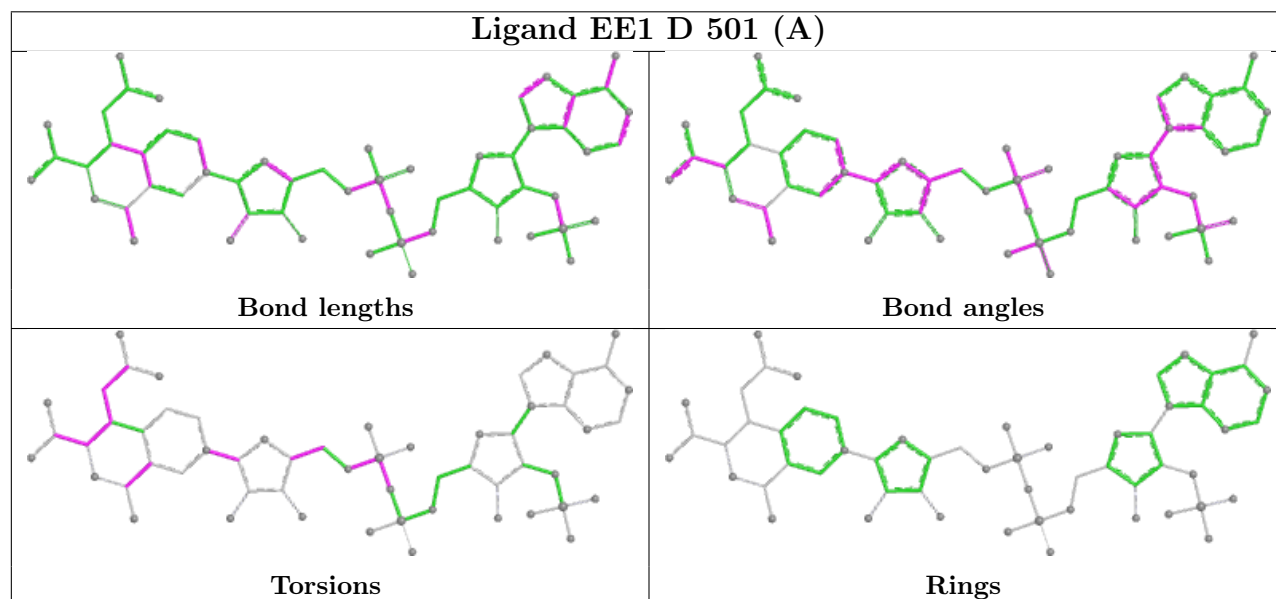
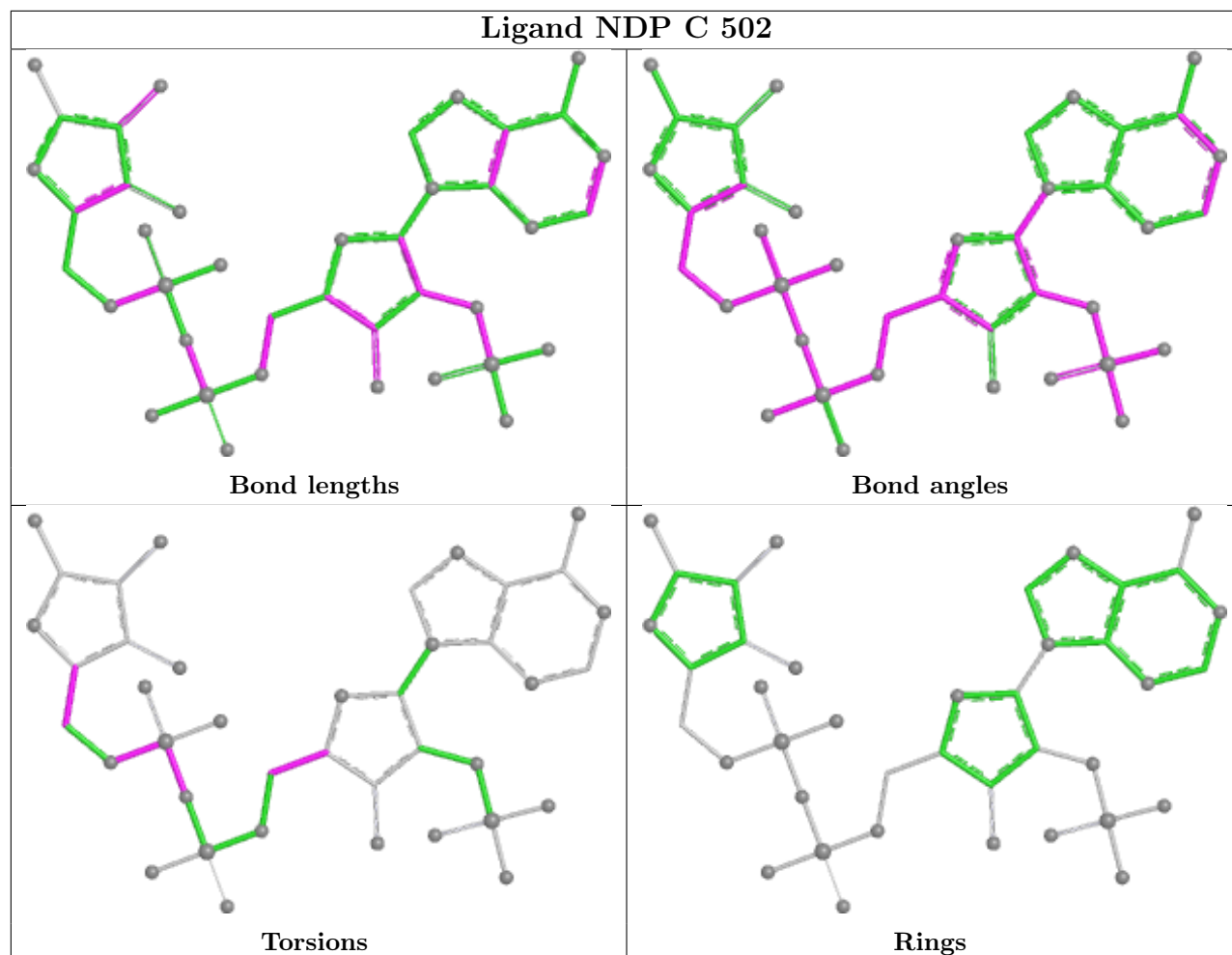
Mol	Chain	Res	Type	Atoms
3	A	502	NDP	C5D-O5D-PN-O2N
3	A	502	NDP	O4D-C4D-C5D-O5D
4	A	504	GOL	C1-C2-C3-O3

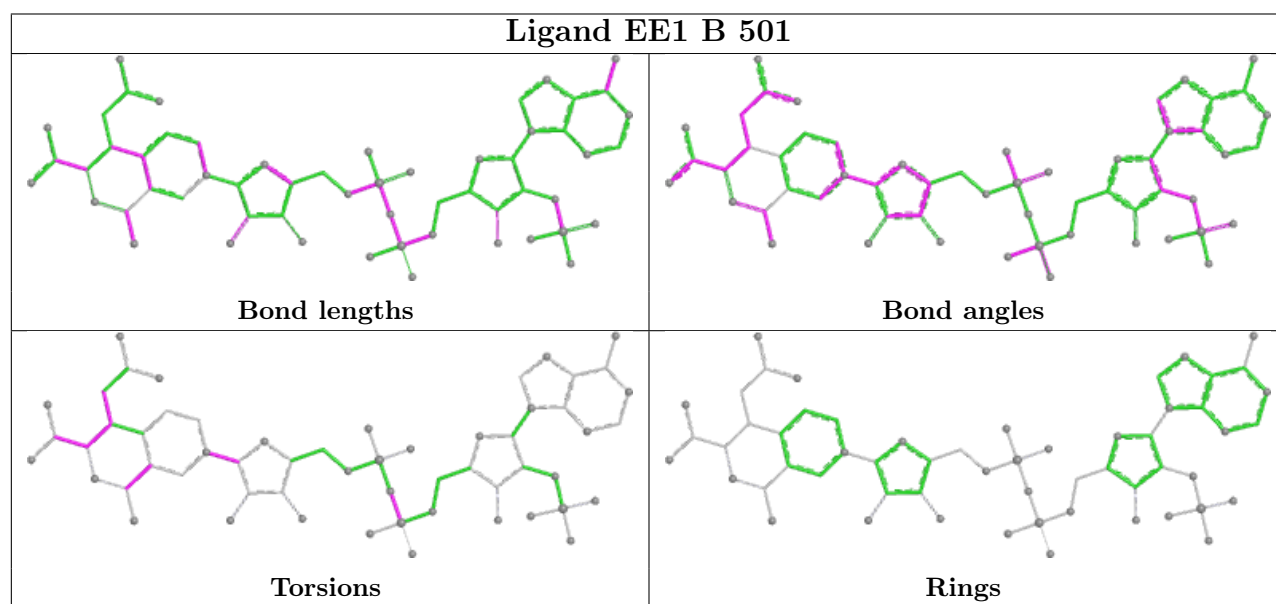
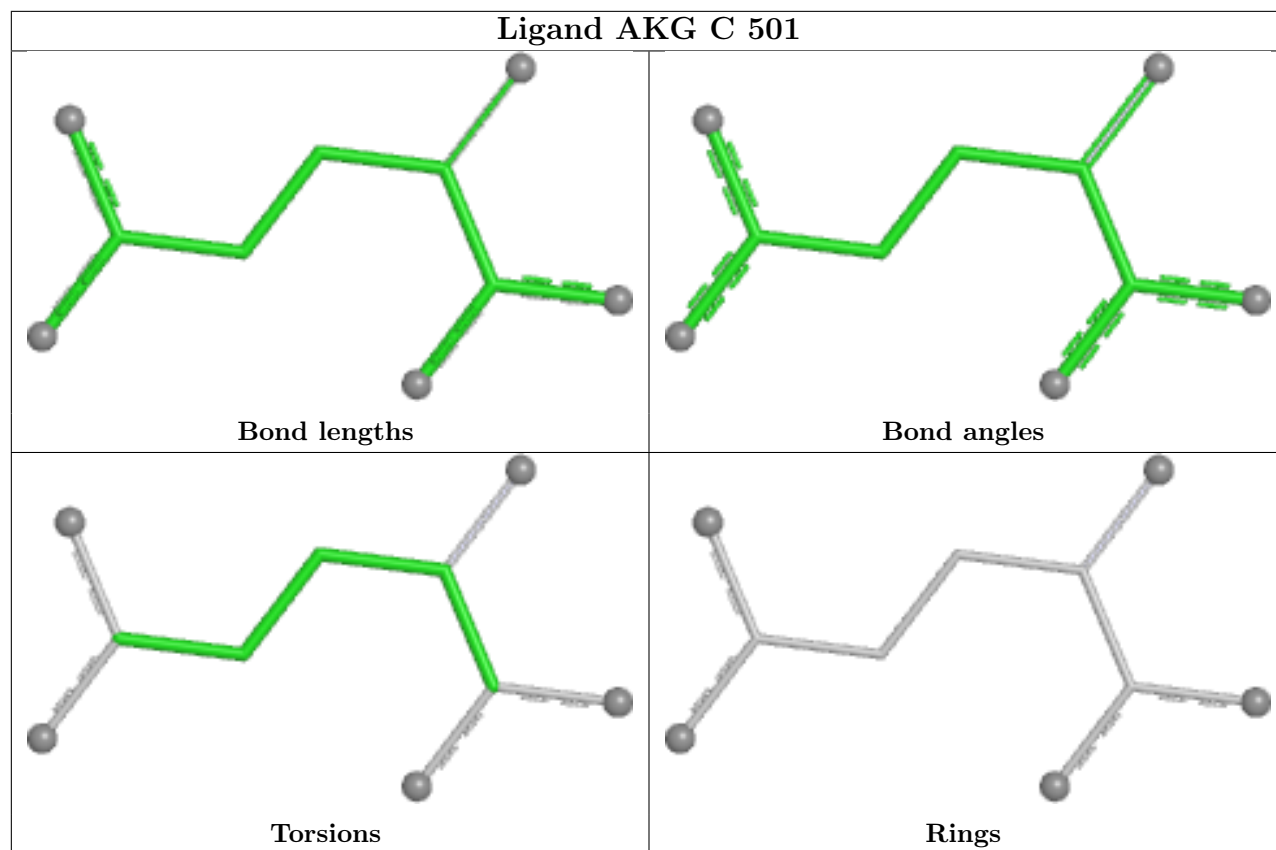
There are no ring outliers.

16 monomers are involved in 46 short contacts:

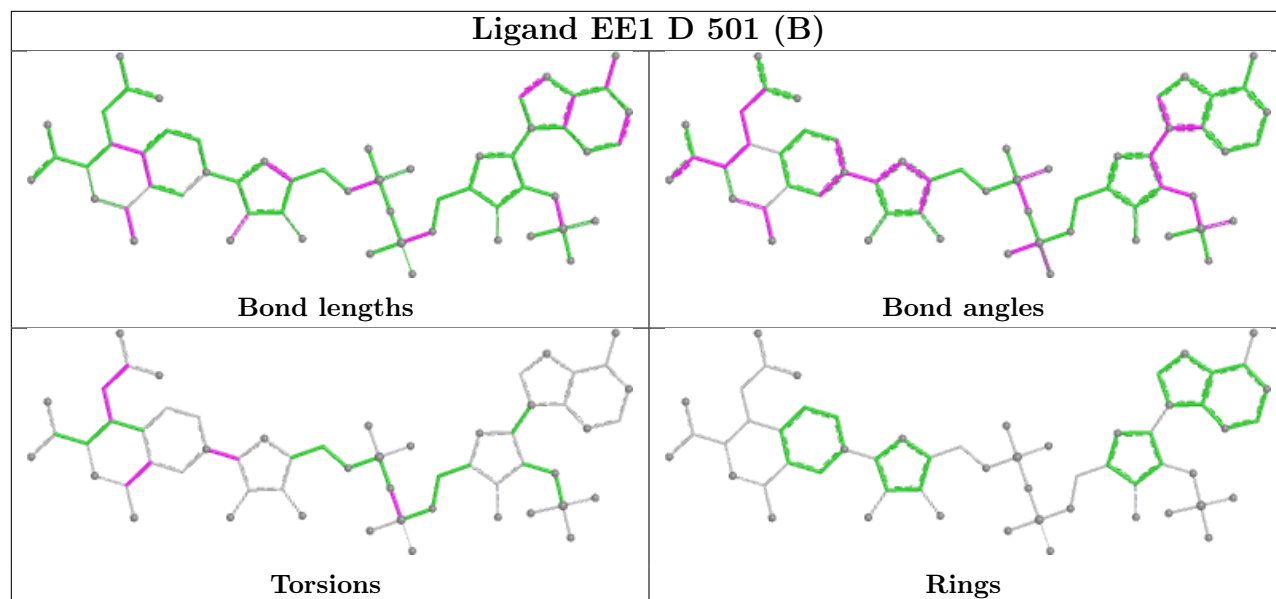
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	SCN	1	0
3	C	502	NDP	3	0
4	C	505	GOL	2	0
4	A	504	GOL	1	0
4	A	503	GOL	1	0
5	C	503	SCN	1	0
5	D	507	SCN	2	0
4	B	504	GOL	1	0
4	B	503	GOL	2	0
8	D	501[A]	EE1	4	0
8	B	501	EE1	4	0
9	D	506	PEG	1	0
4	B	509	GOL	1	0
4	D	504	GOL	7	0
8	D	501[B]	EE1	9	0
3	A	502	NDP	6	0

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 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.

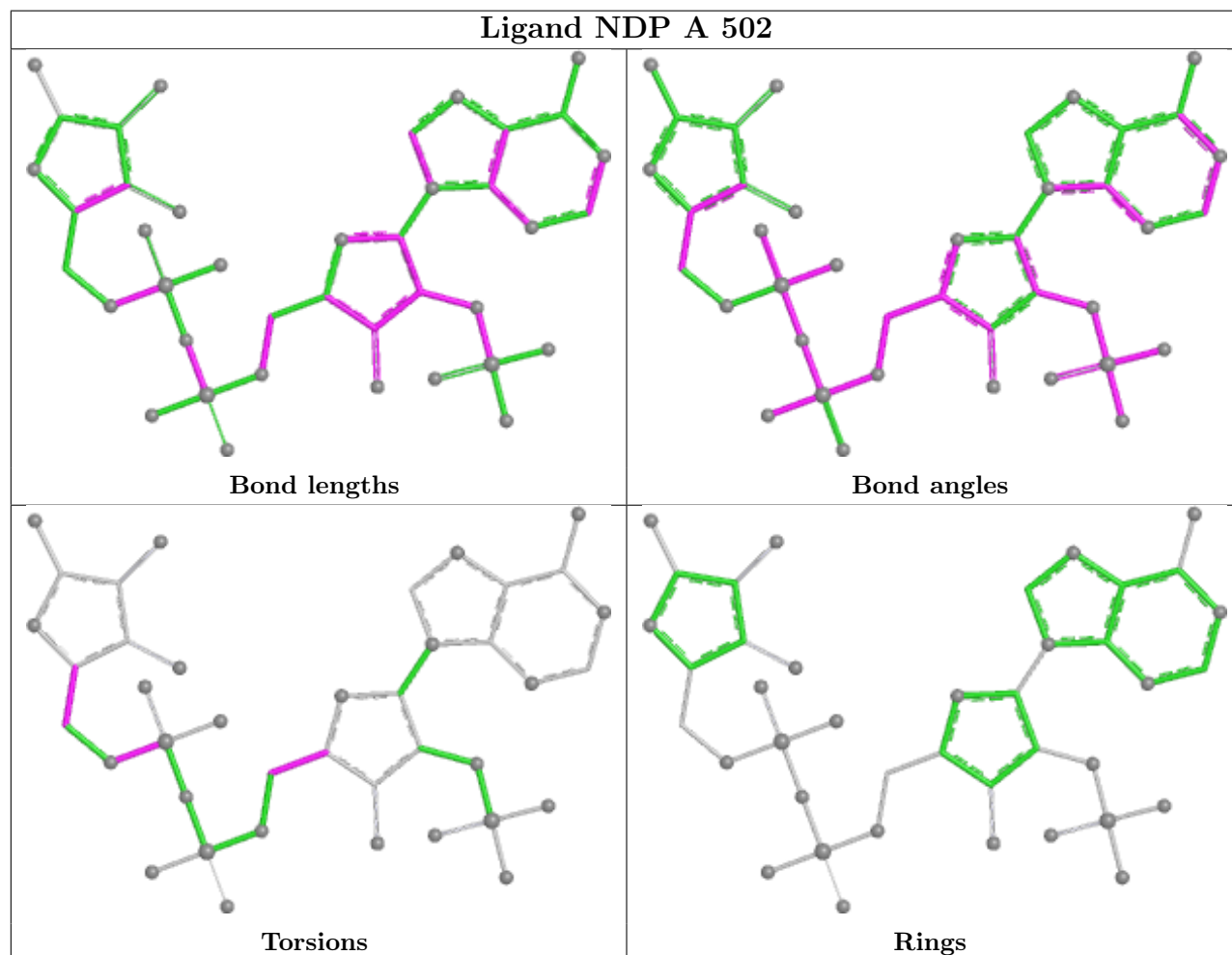


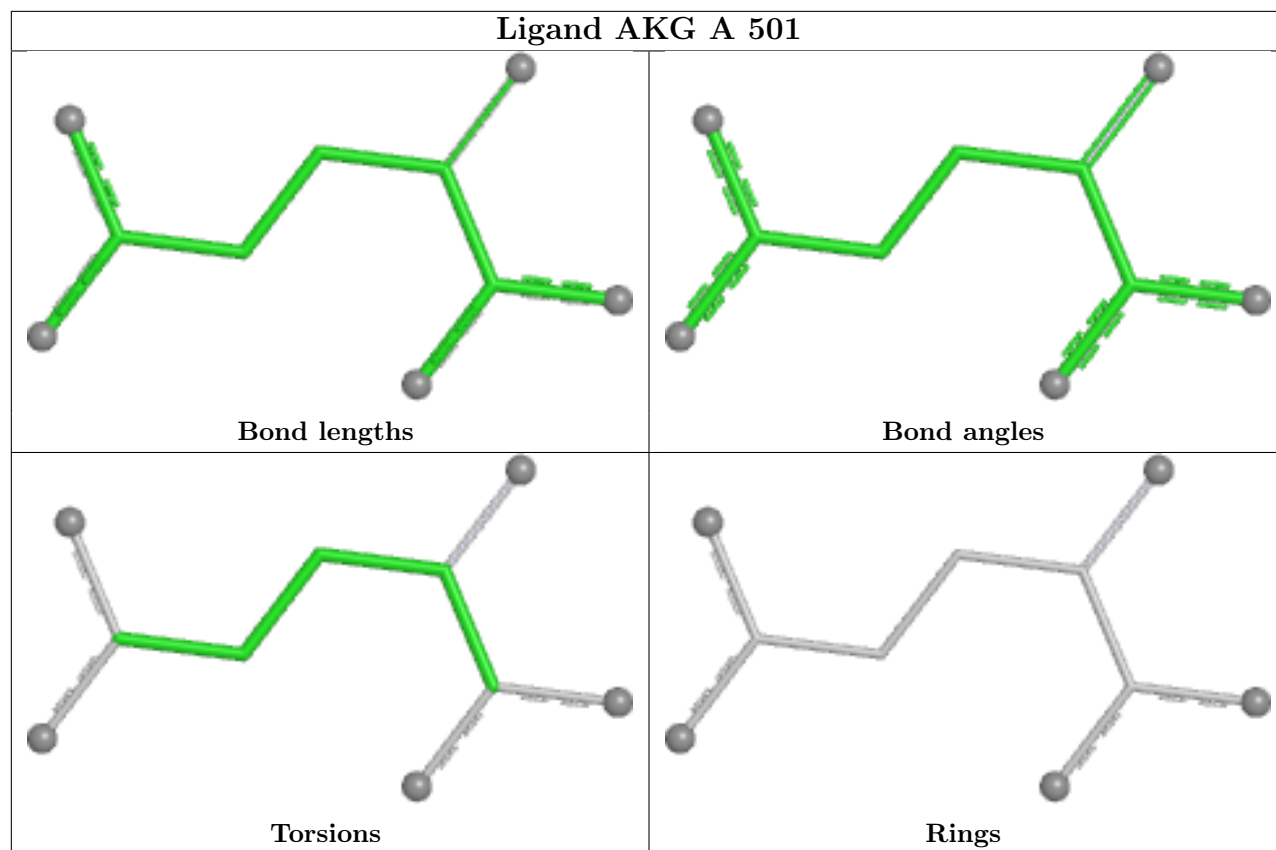


Ligand EE1 D 501 (B)



Ligand NDP A 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/430 (95%)	-0.29	3 (0%) 84 86	12, 33, 49, 95	3 (0%)
1	B	412/430 (95%)	-0.42	2 (0%) 87 89	13, 28, 46, 78	4 (0%)
1	C	417/430 (96%)	0.30	16 (3%) 44 47	20, 44, 75, 91	0
1	D	413/430 (96%)	-0.09	6 (1%) 72 75	12, 37, 65, 98	2 (0%)
All	All	1653/1720 (96%)	-0.12	27 (1%) 70 74	12, 35, 64, 98	9 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	LEU	3.9
1	C	385	ASN	3.8
1	C	409	LEU	3.5
1	D	395	PHE	3.4
1	D	0	HIS	3.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

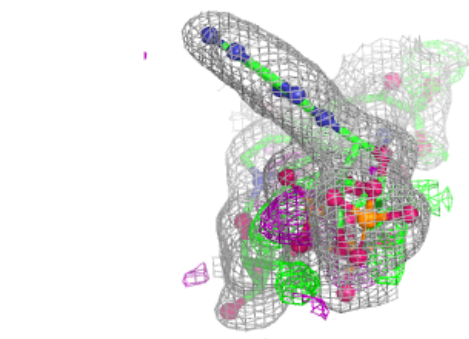
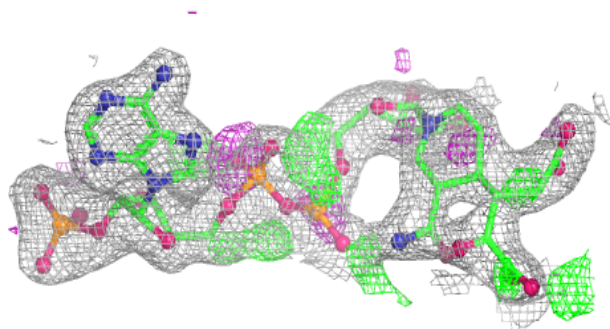
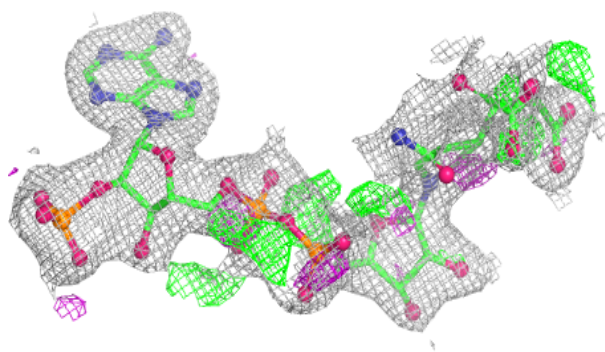
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SCN	B	502	3/3	0.75	0.22	45,45,63,73	0
9	PEG	D	506	7/7	0.75	0.14	45,58,69,72	0
5	SCN	D	502	3/3	0.77	0.23	54,54,56,76	0
4	GOL	A	504	6/6	0.77	0.11	52,57,61,68	0
4	GOL	B	509	6/6	0.81	0.10	53,64,73,77	0
5	SCN	B	508	3/3	0.82	0.24	42,42,43,60	0
8	EE1	D	501[A]	58/58	0.82	0.13	36,47,55,63	58
8	EE1	D	501[B]	58/58	0.82	0.13	34,45,55,60	58
5	SCN	C	504	3/3	0.82	0.15	59,59,64,68	0
4	GOL	C	505	6/6	0.83	0.12	37,48,62,65	0
5	SCN	A	505	3/3	0.83	0.15	55,55,56,60	0
6	CL	D	508	1/1	0.83	0.16	56,56,56,56	0
5	SCN	A	508	3/3	0.84	0.15	47,47,57,75	0
5	SCN	B	510	3/3	0.84	0.19	48,48,51,68	0
5	SCN	B	506	3/3	0.85	0.23	49,49,52,72	0
5	SCN	D	505	3/3	0.85	0.15	44,44,55,74	0
4	GOL	D	503	6/6	0.85	0.12	44,53,55,66	0
5	SCN	C	503	3/3	0.87	0.24	39,39,41,65	0
5	SCN	D	507	3/3	0.87	0.19	40,40,41,67	0
4	GOL	A	503	6/6	0.88	0.11	44,46,51,56	0
5	SCN	A	507	3/3	0.88	0.12	45,45,55,69	0
5	SCN	B	507	3/3	0.89	0.17	41,41,49,62	0
4	GOL	D	504	6/6	0.89	0.11	36,44,51,55	0
4	GOL	B	503	6/6	0.90	0.14	27,35,39,39	0
3	NDP	A	502	40/48	0.91	0.10	27,43,74,90	0
5	SCN	A	506	3/3	0.91	0.13	58,58,59,64	0
2	AKG	A	501	10/10	0.92	0.08	34,41,46,48	0
2	AKG	C	501	10/10	0.92	0.09	40,49,53,54	0
3	NDP	C	502	40/48	0.93	0.10	36,48,81,91	0
8	EE1	B	501	58/58	0.94	0.08	22,33,52,74	0
6	CL	C	506	1/1	0.94	0.09	49,49,49,49	0
4	GOL	B	504	6/6	0.95	0.07	36,41,46,50	0
5	SCN	B	505	3/3	0.96	0.11	38,38,41,42	0
6	CL	B	511	1/1	0.98	0.06	40,40,40,40	0
7	CA	A	511	1/1	0.98	0.07	37,37,37,37	0
7	CA	A	510	1/1	0.99	0.03	29,29,29,29	0
6	CL	A	509	1/1	0.99	0.08	41,41,41,41	0
7	CA	C	507	1/1	0.99	0.06	33,33,33,33	0
7	CA	D	509	1/1	0.99	0.04	32,32,32,32	0

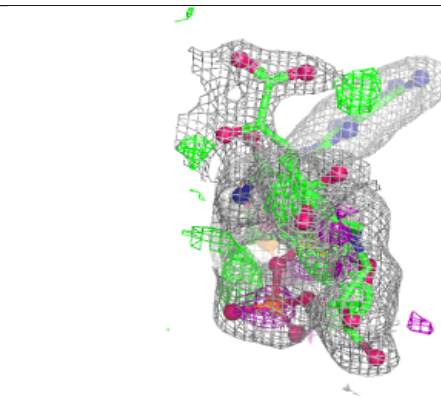
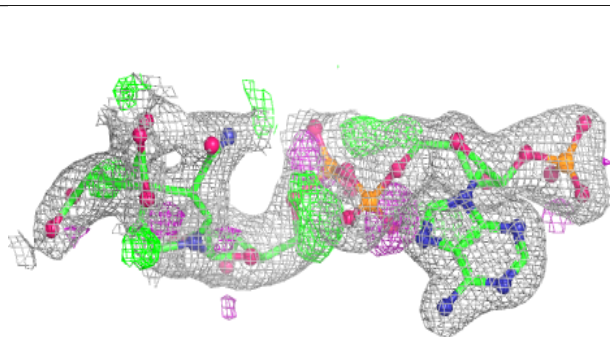
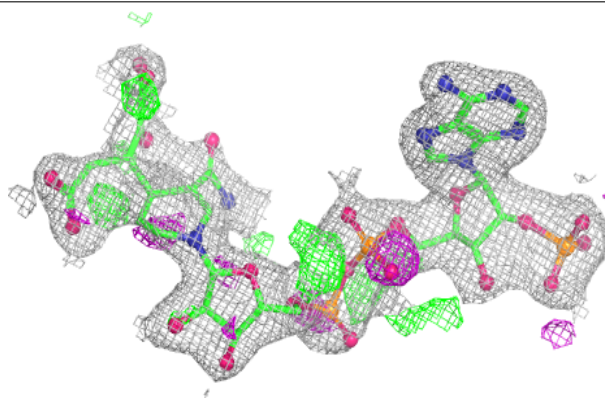
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EE1 D 501 (A):

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

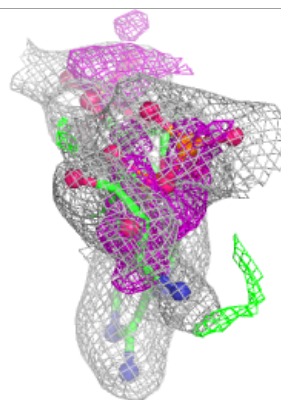
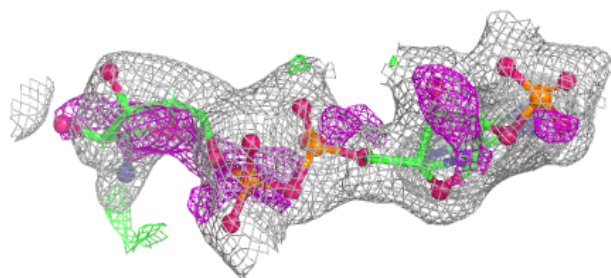
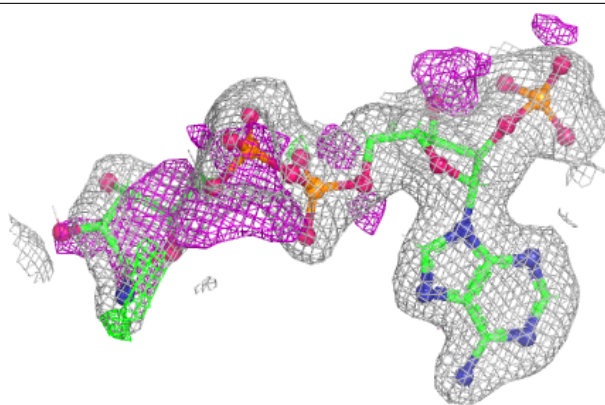
**Electron density around EE1 D 501 (B):**

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

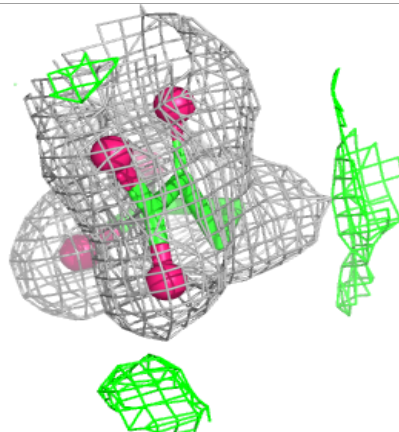
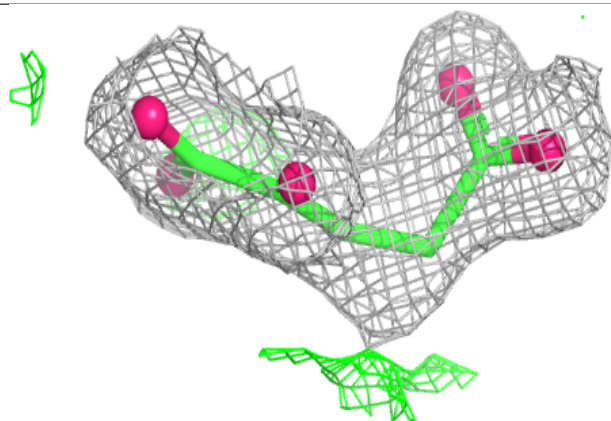
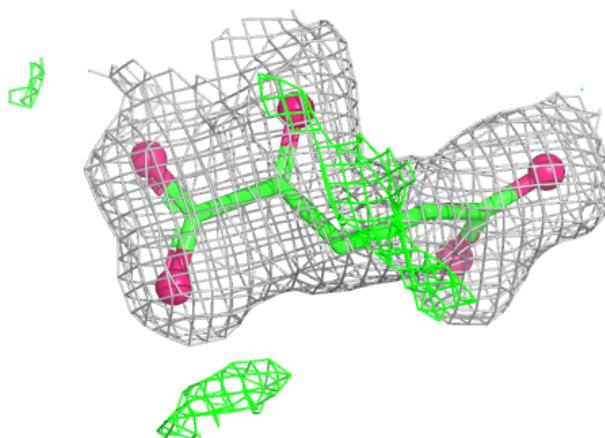


Electron density around NDP A 502:

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

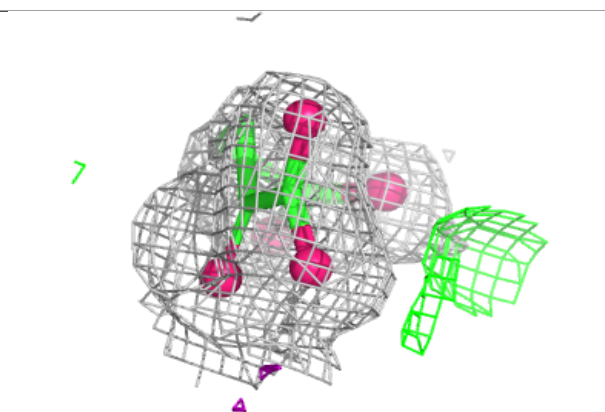
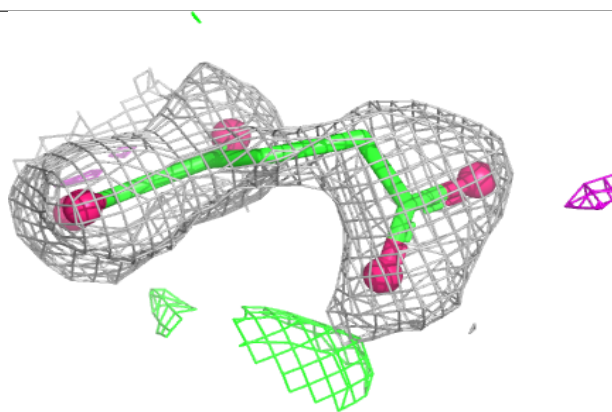
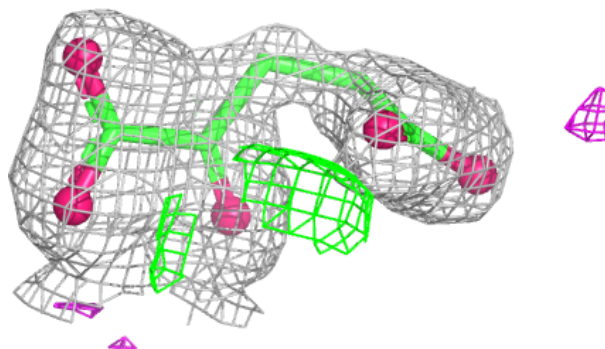
**Electron density around AKG A 501:**

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

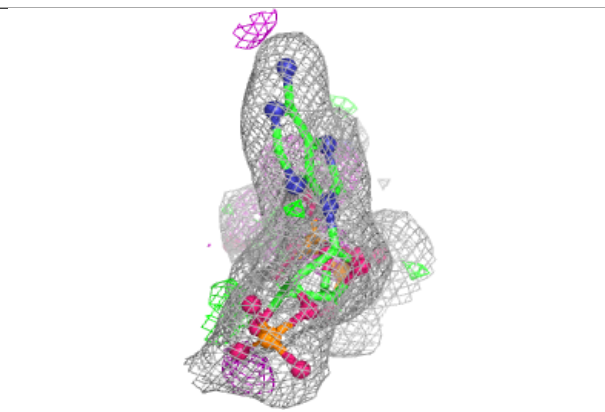
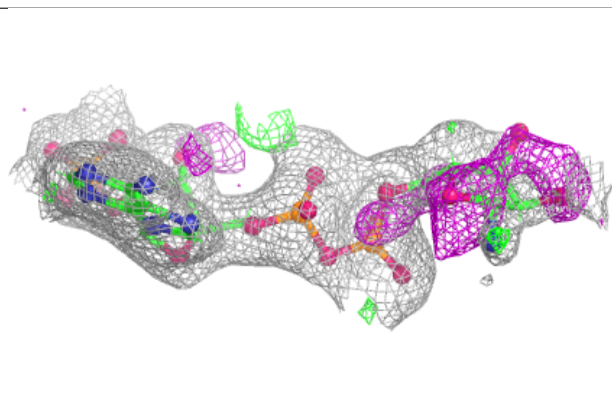
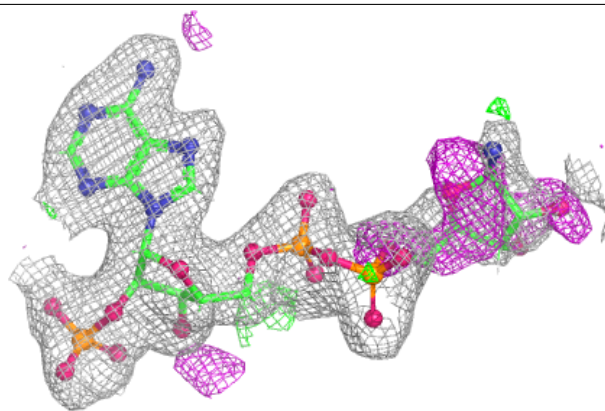


Electron density around AKG C 501:

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

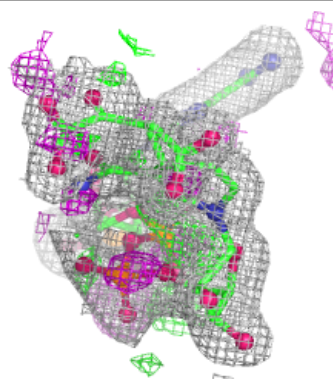
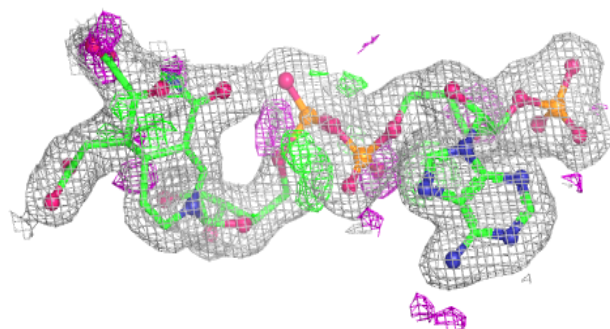
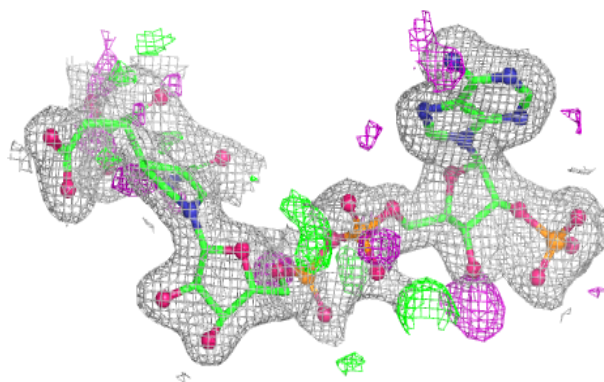
**Electron density around NDP C 502:**

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



Electron density around EE1 B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.