



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 4L2O / pdb_00004l2o
Title : Crystal structure of human ALDH3A1 with its selective inhibitor 1-(4-fluorophenyl)sulfonyl-2-methylbenzimidazole
Authors : Hurley, T.D.; Parajuli, B.
Deposited on : 2013-06-04
Resolution : 1.94 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

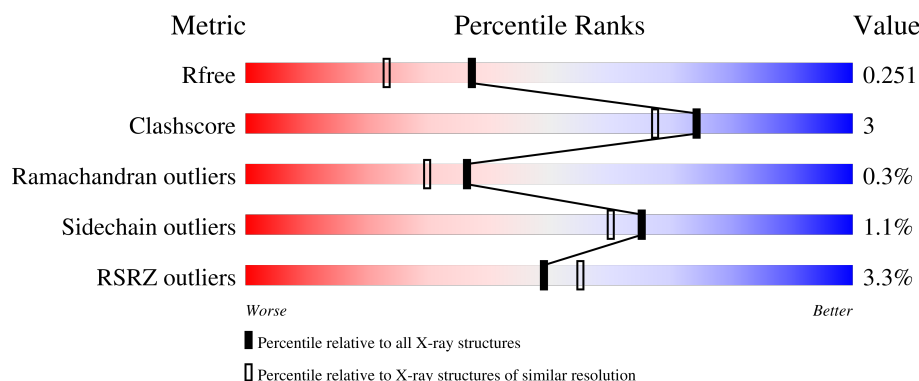
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

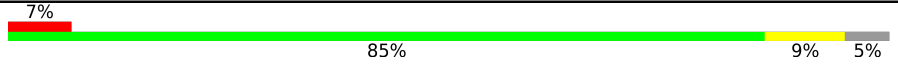
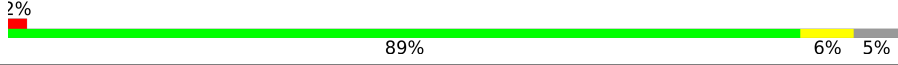
The reported resolution of this entry is 1.94 Å.

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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	469	
1	B	469	
1	E	469	
1	G	469	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15234 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	6	0
			3519	2242	598	661	18			
1	B	447	Total	C	N	O	S	0	2	0
			3498	2230	593	657	18			
1	E	447	Total	C	N	O	S	0	6	0
			3521	2244	598	661	18			
1	G	447	Total	C	N	O	S	0	5	0
			3509	2236	594	661	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP P30838
A	-15	HIS	-	expression tag	UNP P30838
A	-14	HIS	-	expression tag	UNP P30838
A	-13	HIS	-	expression tag	UNP P30838
A	-12	HIS	-	expression tag	UNP P30838
A	-11	HIS	-	expression tag	UNP P30838
A	-10	SER	-	expression tag	UNP P30838
A	-9	SER	-	expression tag	UNP P30838
A	-8	GLY	-	expression tag	UNP P30838
A	-7	LEU	-	expression tag	UNP P30838
A	-6	VAL	-	expression tag	UNP P30838
A	-5	PRO	-	expression tag	UNP P30838
A	-4	ARG	-	expression tag	UNP P30838
A	-3	GLY	-	expression tag	UNP P30838
A	-2	SER	-	expression tag	UNP P30838
A	-1	HIS	-	expression tag	UNP P30838
A	133	ALA	SER	variant	UNP P30838
B	-16	HIS	-	expression tag	UNP P30838
B	-15	HIS	-	expression tag	UNP P30838
B	-14	HIS	-	expression tag	UNP P30838
B	-13	HIS	-	expression tag	UNP P30838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P30838
B	-11	HIS	-	expression tag	UNP P30838
B	-10	SER	-	expression tag	UNP P30838
B	-9	SER	-	expression tag	UNP P30838
B	-8	GLY	-	expression tag	UNP P30838
B	-7	LEU	-	expression tag	UNP P30838
B	-6	VAL	-	expression tag	UNP P30838
B	-5	PRO	-	expression tag	UNP P30838
B	-4	ARG	-	expression tag	UNP P30838
B	-3	GLY	-	expression tag	UNP P30838
B	-2	SER	-	expression tag	UNP P30838
B	-1	HIS	-	expression tag	UNP P30838
B	133	ALA	SER	variant	UNP P30838
E	-16	HIS	-	expression tag	UNP P30838
E	-15	HIS	-	expression tag	UNP P30838
E	-14	HIS	-	expression tag	UNP P30838
E	-13	HIS	-	expression tag	UNP P30838
E	-12	HIS	-	expression tag	UNP P30838
E	-11	HIS	-	expression tag	UNP P30838
E	-10	SER	-	expression tag	UNP P30838
E	-9	SER	-	expression tag	UNP P30838
E	-8	GLY	-	expression tag	UNP P30838
E	-7	LEU	-	expression tag	UNP P30838
E	-6	VAL	-	expression tag	UNP P30838
E	-5	PRO	-	expression tag	UNP P30838
E	-4	ARG	-	expression tag	UNP P30838
E	-3	GLY	-	expression tag	UNP P30838
E	-2	SER	-	expression tag	UNP P30838
E	-1	HIS	-	expression tag	UNP P30838
E	133	ALA	SER	variant	UNP P30838
G	-16	HIS	-	expression tag	UNP P30838
G	-15	HIS	-	expression tag	UNP P30838
G	-14	HIS	-	expression tag	UNP P30838
G	-13	HIS	-	expression tag	UNP P30838
G	-12	HIS	-	expression tag	UNP P30838
G	-11	HIS	-	expression tag	UNP P30838
G	-10	SER	-	expression tag	UNP P30838
G	-9	SER	-	expression tag	UNP P30838
G	-8	GLY	-	expression tag	UNP P30838
G	-7	LEU	-	expression tag	UNP P30838
G	-6	VAL	-	expression tag	UNP P30838
G	-5	PRO	-	expression tag	UNP P30838

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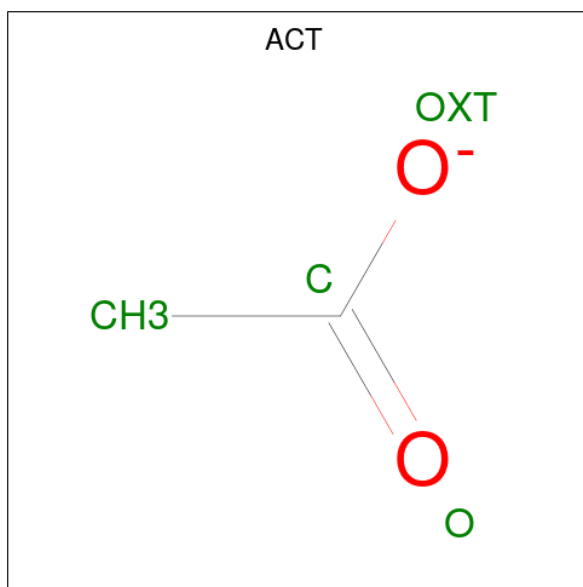
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ARG	-	expression tag	UNP P30838
G	-3	GLY	-	expression tag	UNP P30838
G	-2	SER	-	expression tag	UNP P30838
G	-1	HIS	-	expression tag	UNP P30838
G	133	ALA	SER	variant	UNP P30838

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	B	2	Total K 2 2	0	0
2	E	1	Total K 1 1	0	0
2	G	2	Total K 2 2	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



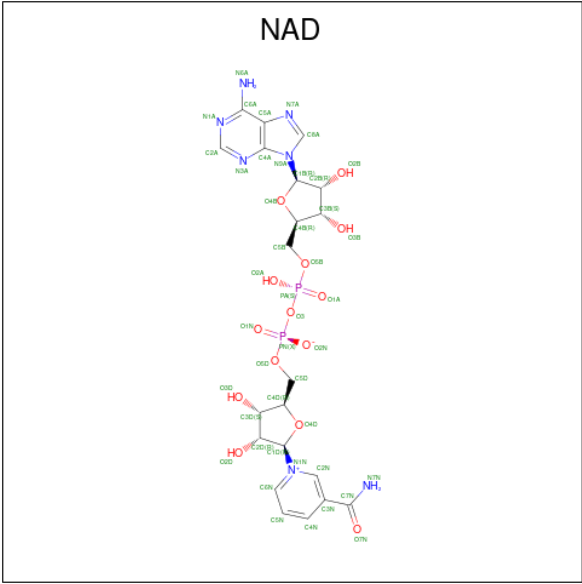
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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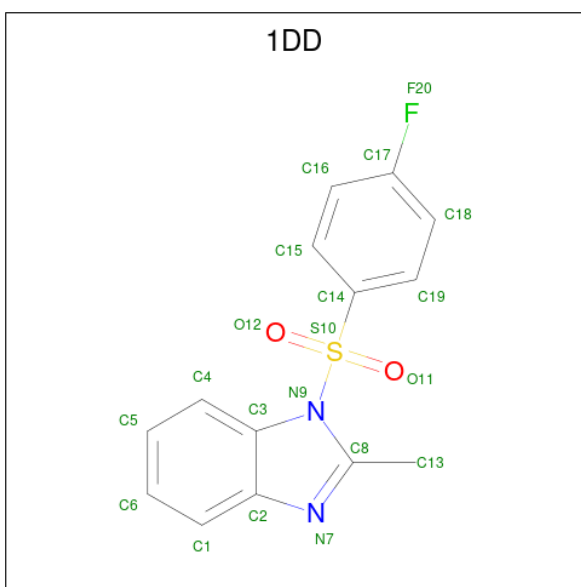
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is 1-[(4-fluorophenyl)sulfonyl]-2-methyl-1H-benzimidazole (CCD ID: 1DD) (formula: C₁₄H₁₁FN₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	S	
			20	14	1	2	2	1	0
5	B	1	Total	C	F	N	O	S	
			20	14	1	2	2	1	0
5	E	1	Total	C	F	N	O	S	
			20	14	1	2	2	1	0
5	G	1	Total	C	F	N	O	S	
			20	14	1	2	2	1	0

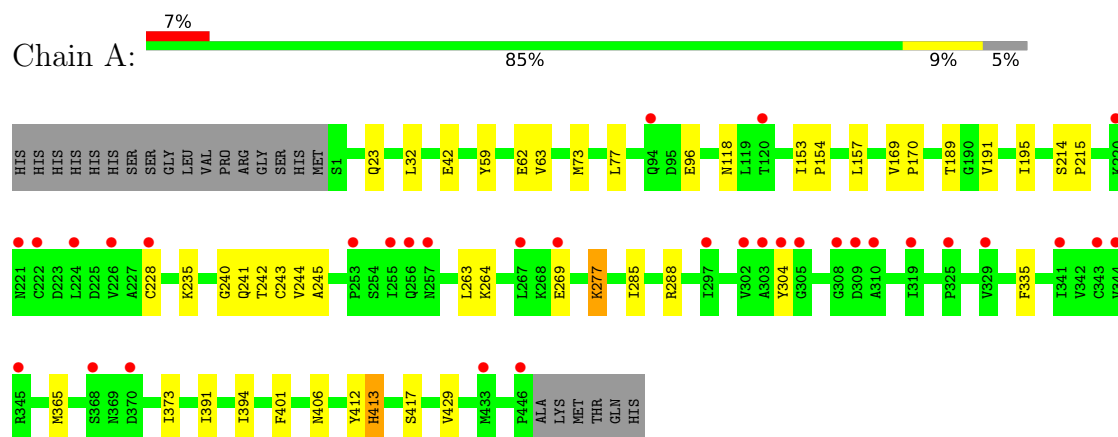
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O		
			212	212	0	0
6	B	256	Total	O		
			256	256	0	0
6	E	235	Total	O		
			235	235	0	0
6	G	205	Total	O		
			205	205	0	0

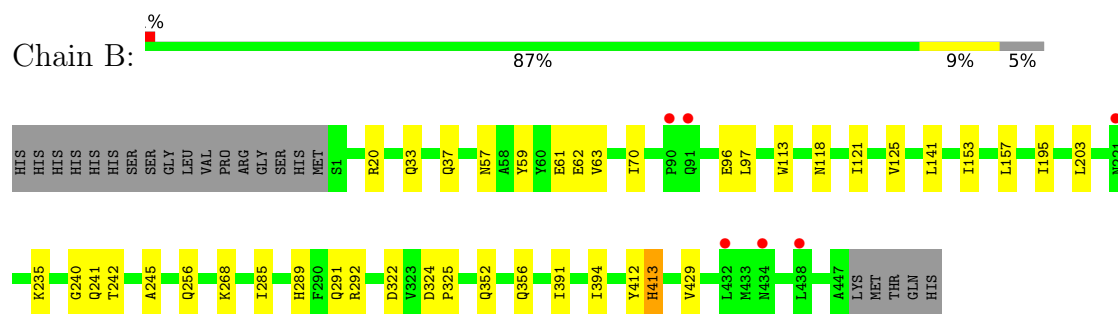
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

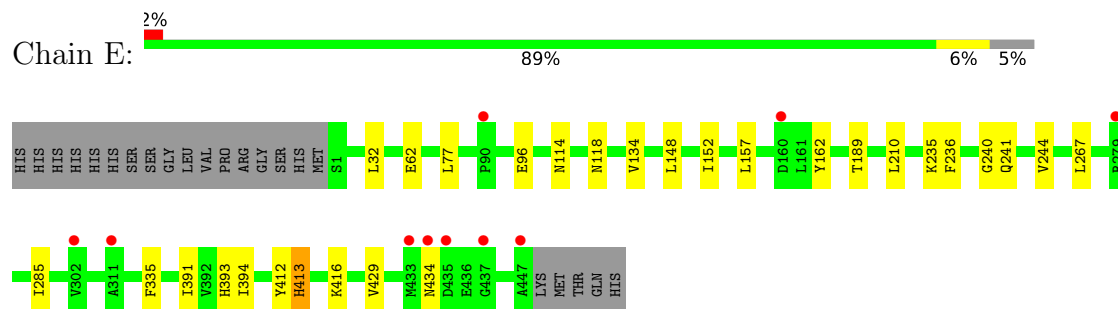
- Molecule 1: Aldehyde dehydrogenase



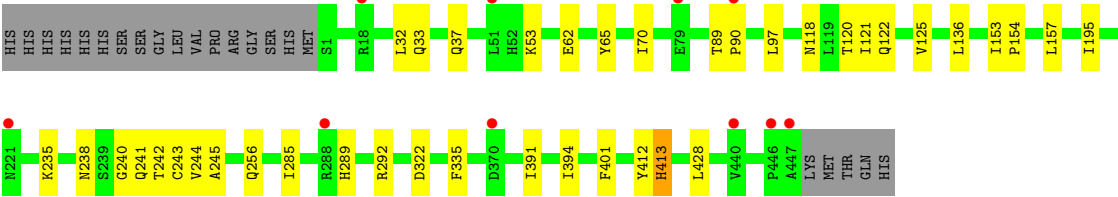
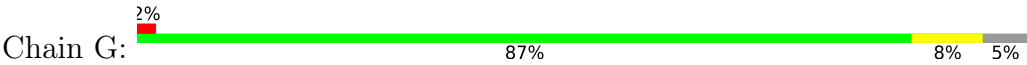
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.22Å 90.92Å 117.92Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	40.00 – 1.94 40.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-1.94) 95.7 (40.00-1.94)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.215 , 0.250 0.215 , 0.251	Depositor DCC
R_{free} test set	6935 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15234	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 22.66 % 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 5.4431e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: K, 1DD, ACT, NAD

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	0.69	2/3604 (0.1%)	0.76	0/4885
1	B	0.53	0/3577	0.76	0/4850
1	E	0.54	0/3609	0.77	0/4892
1	G	0.52	0/3594	0.77	0/4873
All	All	0.58	2/14384 (0.0%)	0.76	0/19500

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLU	C-O	-5.54	1.17	1.24
1	A	288	ARG	C-O	-5.15	1.18	1.24

There are no bond angle outliers.

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	3519	0	3559	26	0
1	B	3498	0	3535	21	0
1	E	3521	0	3565	17	0
1	G	3509	0	3547	26	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	E	1	0	0	0	0
2	G	2	0	0	0	0
3	A	8	0	6	0	0
3	E	4	0	3	0	0
3	G	4	0	3	0	0
4	A	44	0	26	0	0
4	B	44	0	26	1	0
4	E	44	0	26	0	0
4	G	44	0	26	1	0
5	A	20	0	11	2	0
5	B	20	0	11	1	0
5	E	20	0	11	1	0
5	G	20	0	11	3	0
6	A	212	0	0	1	0
6	B	256	0	0	0	0
6	E	235	0	0	2	0
6	G	205	0	0	1	0
All	All	15234	0	14366	89	0

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

The worst 5 of 89 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:G:256:GLN:HE22	1:G:322:ASP:H	1.19	0.91
1:B:256:GLN:HE22	1:B:322:ASP:H	1.26	0.83
1:B:289:HIS:HD2	1:B:292:ARG:HE	1.42	0.67
1:G:412:TYR:O	1:G:413:HIS:HB2	1.94	0.67
1:G:289:HIS:HD2	1:G:292:ARG:HE	1.44	0.64

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	450/469 (96%)	440 (98%)	9 (2%)	1 (0%)	43	37
1	B	447/469 (95%)	436 (98%)	10 (2%)	1 (0%)	43	37
1	E	451/469 (96%)	444 (98%)	5 (1%)	2 (0%)	30	22
1	G	450/469 (96%)	444 (99%)	5 (1%)	1 (0%)	43	37
All	All	1798/1876 (96%)	1764 (98%)	29 (2%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	B	413	HIS
1	E	413	HIS
1	G	413	HIS
1	E	434	ASN

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	386/400 (96%)	381 (99%)	5 (1%)	61	54
1	B	382/400 (96%)	376 (98%)	6 (2%)	55	46
1	E	386/400 (96%)	384 (100%)	2 (0%)	81	82
1	G	385/400 (96%)	381 (99%)	4 (1%)	68	64
All	All	1539/1600 (96%)	1522 (99%)	17 (1%)	65	60

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	122	GLN
1	G	335	PHE
1	B	97	LEU

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Mol	Chain	Res	Type
1	B	195	ILE
1	B	268	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	393	HIS
1	G	75	GLN
1	E	406	ASN
1	G	27	GLN
1	G	166	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 19 ligands modelled in this entry, 7 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	$\# Z > 2$
5	1DD	G	505	-	22,22,22	3.76	6 (27%)	30,33,33	2.34	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1DD	A	506	-	22,22,22	3.77	6 (27%)	30,33,33	2.38	10 (33%)
5	1DD	E	504	-	22,22,22	3.78	6 (27%)	30,33,33	2.33	10 (33%)
4	NAD	G	504	-	46,48,48	1.23	7 (15%)	64,73,73	1.54	9 (14%)
3	ACT	A	503	-	3,3,3	0.83	0	3,3,3	0.71	0
3	ACT	A	504	-	3,3,3	0.81	0	3,3,3	0.75	0
3	ACT	G	503	-	3,3,3	0.81	0	3,3,3	0.72	0
4	NAD	B	503	-	46,48,48	1.21	4 (8%)	64,73,73	1.54	11 (17%)
4	NAD	A	505	-	46,48,48	1.22	5 (10%)	64,73,73	1.49	10 (15%)
3	ACT	E	502	-	3,3,3	0.80	0	3,3,3	0.69	0
4	NAD	E	503	-	46,48,48	1.21	5 (10%)	64,73,73	1.55	9 (14%)
5	1DD	B	504	-	22,22,22	3.77	6 (27%)	30,33,33	2.34	11 (36%)

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
5	1DD	G	505	-	-	1/12/12/12	0/3/3/3
5	1DD	A	506	-	-	1/12/12/12	0/3/3/3
4	NAD	B	503	-	-	5/30/62/62	0/5/5/5
4	NAD	G	504	-	-	7/30/62/62	0/5/5/5
5	1DD	E	504	-	-	0/12/12/12	0/3/3/3
4	NAD	E	503	-	-	5/30/62/62	0/5/5/5
4	NAD	A	505	-	-	7/30/62/62	0/5/5/5
5	1DD	B	504	-	-	0/12/12/12	0/3/3/3

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	504	1DD	C14-S10	-12.35	1.59	1.76
5	A	506	1DD	C14-S10	-12.31	1.59	1.76
5	G	505	1DD	C14-S10	-12.30	1.59	1.76
5	B	504	1DD	C14-S10	-12.23	1.60	1.76
5	B	504	1DD	C3-N9	-7.98	1.32	1.42

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	1DD	O12-S10-O11	-6.66	109.20	119.59

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	505	1DD	O12-S10-O11	-6.61	109.28	119.59
5	B	504	1DD	O12-S10-O11	-6.59	109.30	119.59
5	E	504	1DD	O12-S10-O11	-6.51	109.44	119.59
5	A	506	1DD	C14-S10-N9	5.84	112.18	104.90

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	NAD	C5B-O5B-PA-O2A
4	A	505	NAD	C5B-O5B-PA-O3
4	G	504	NAD	C5B-O5B-PA-O2A
4	G	504	NAD	PN-O3-PA-O5B
4	A	505	NAD	O4B-C4B-C5B-O5B

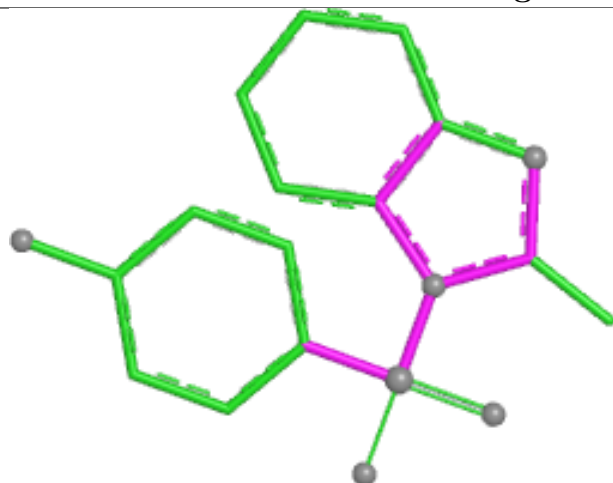
There are no ring outliers.

6 monomers are involved in 9 short contacts:

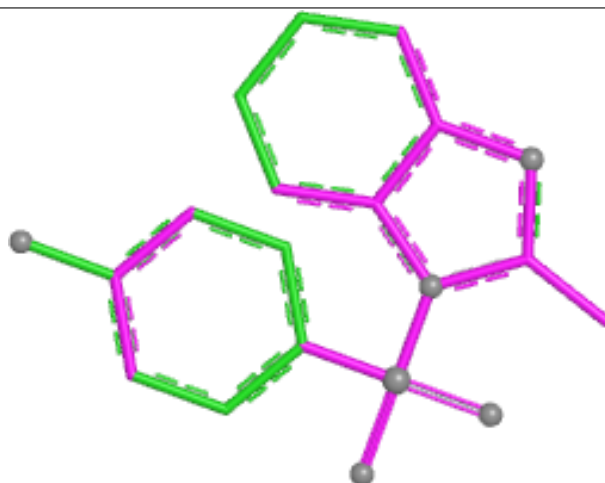
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	505	1DD	3	0
5	A	506	1DD	2	0
5	E	504	1DD	1	0
4	G	504	NAD	1	0
4	B	503	NAD	1	0
5	B	504	1DD	1	0

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

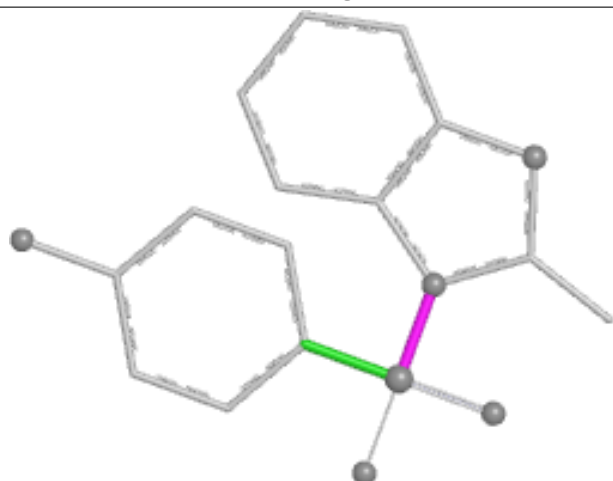
Ligand 1DD G 505



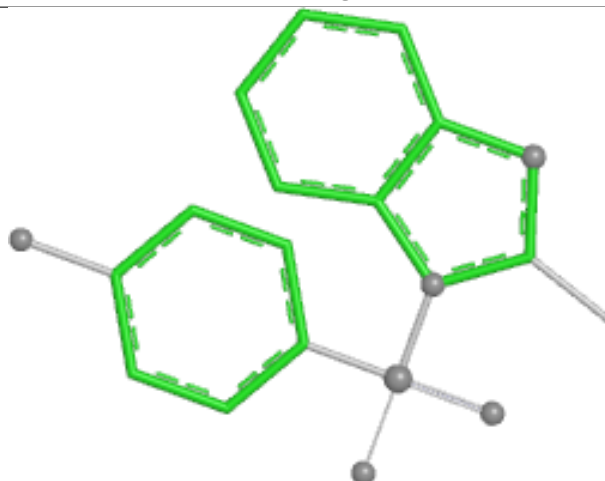
Bond lengths



Bond angles

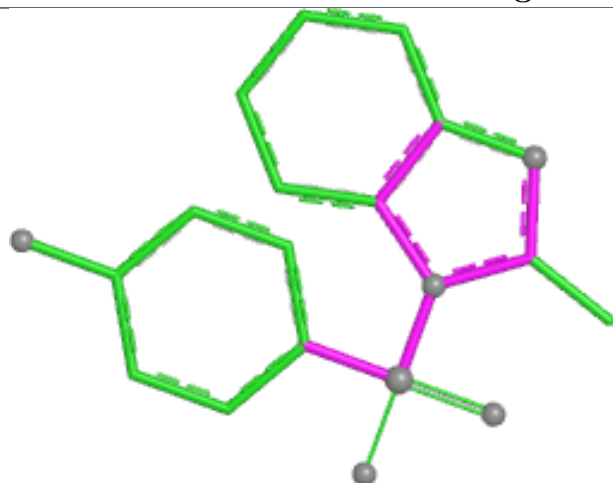


Torsions

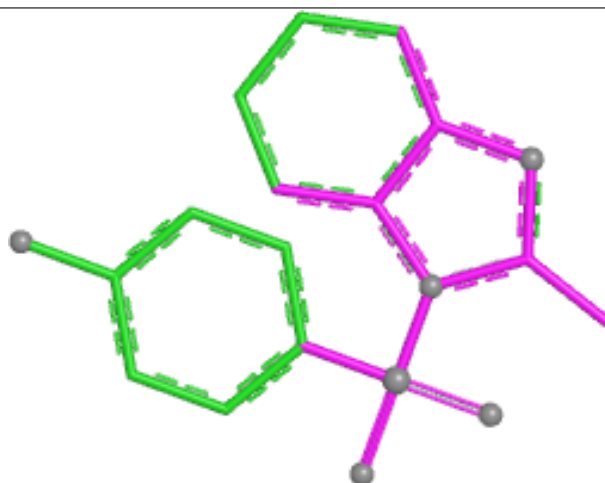


Rings

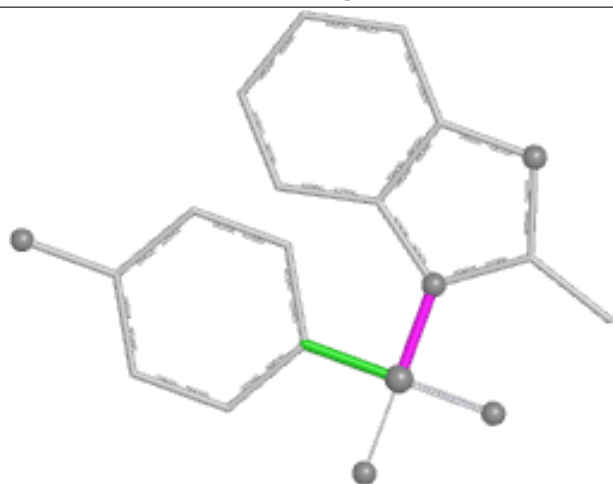
Ligand 1DD A 506



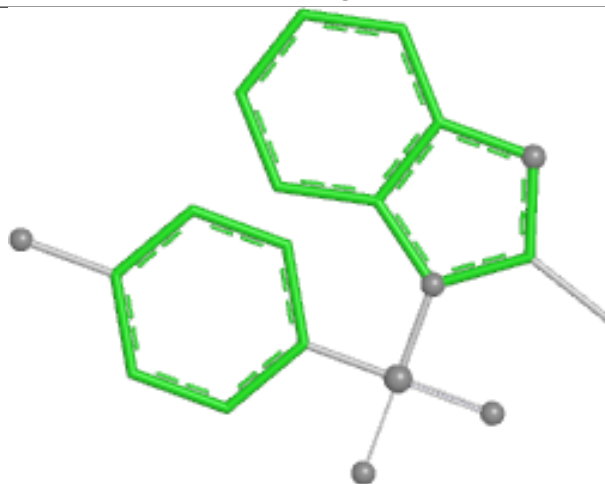
Bond lengths



Bond angles

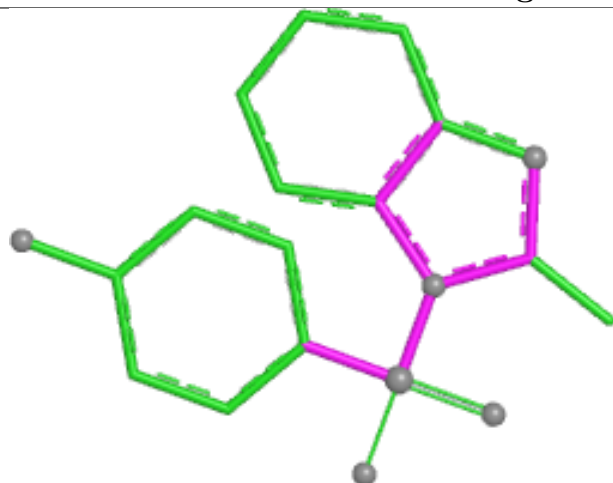


Torsions

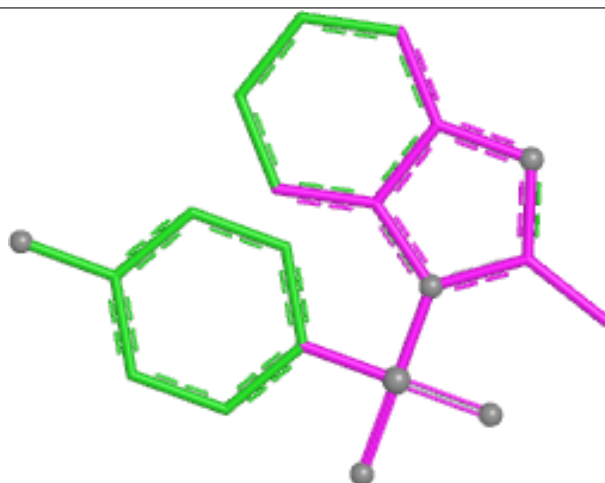


Rings

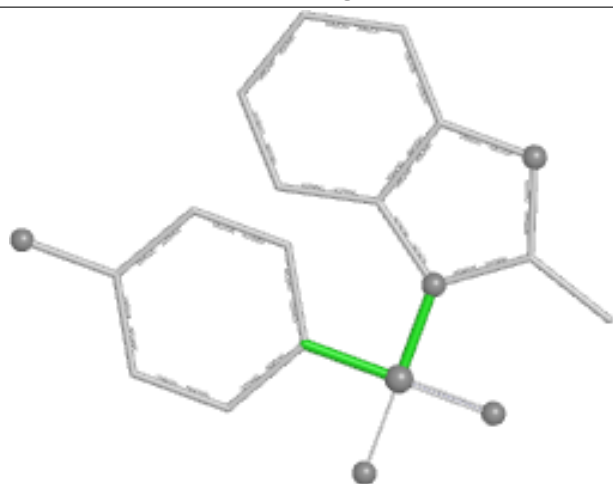
Ligand 1DD E 504



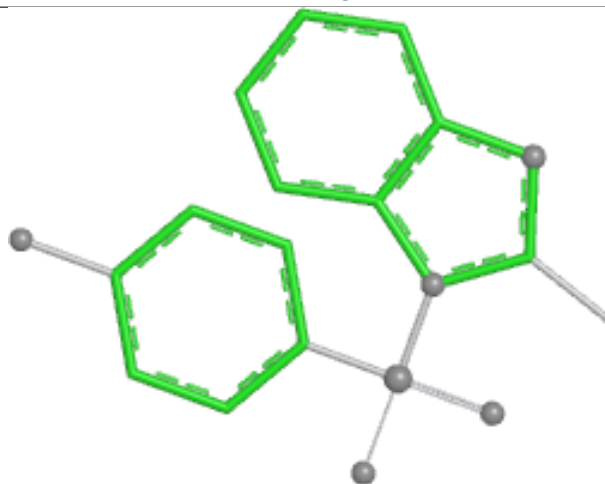
Bond lengths



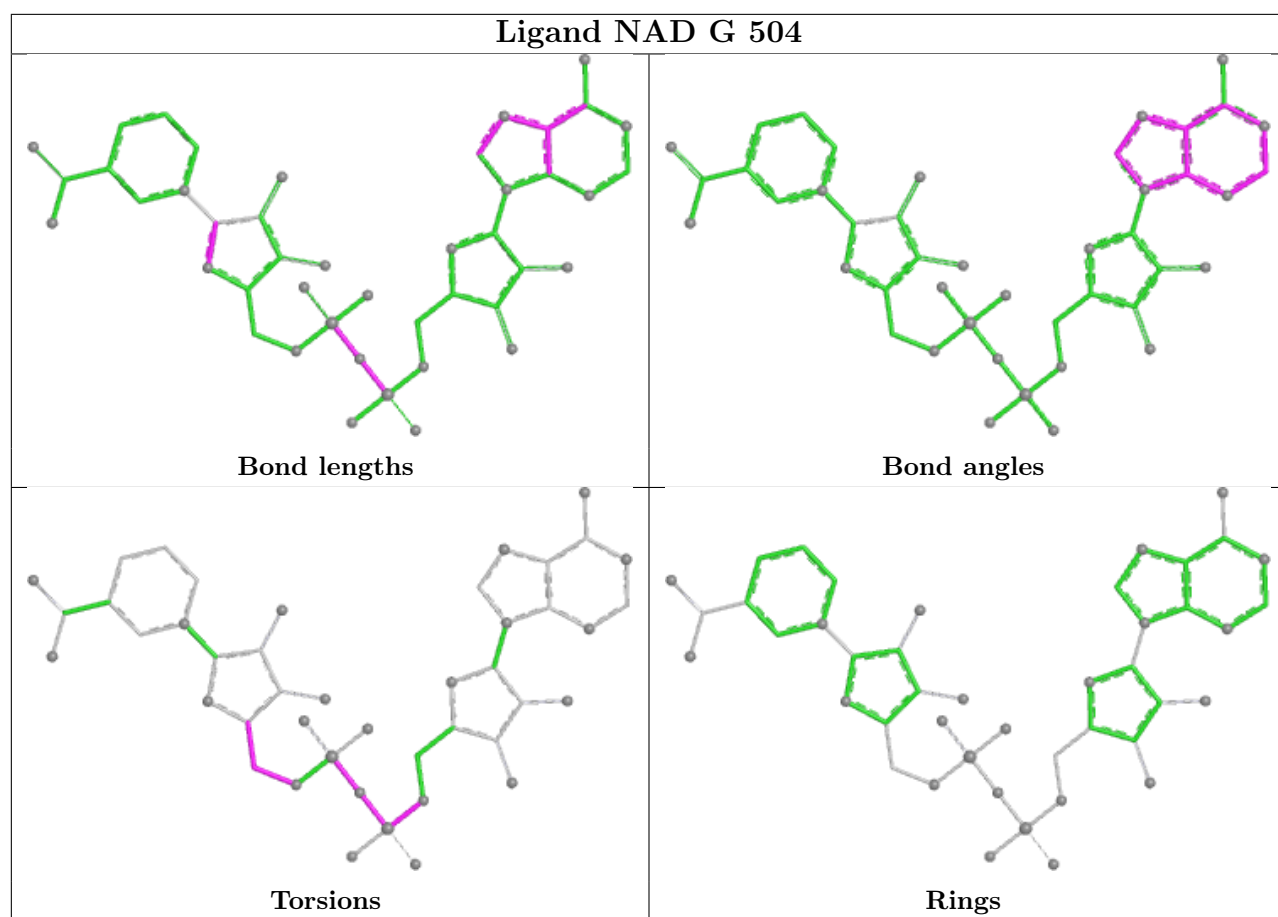
Bond angles

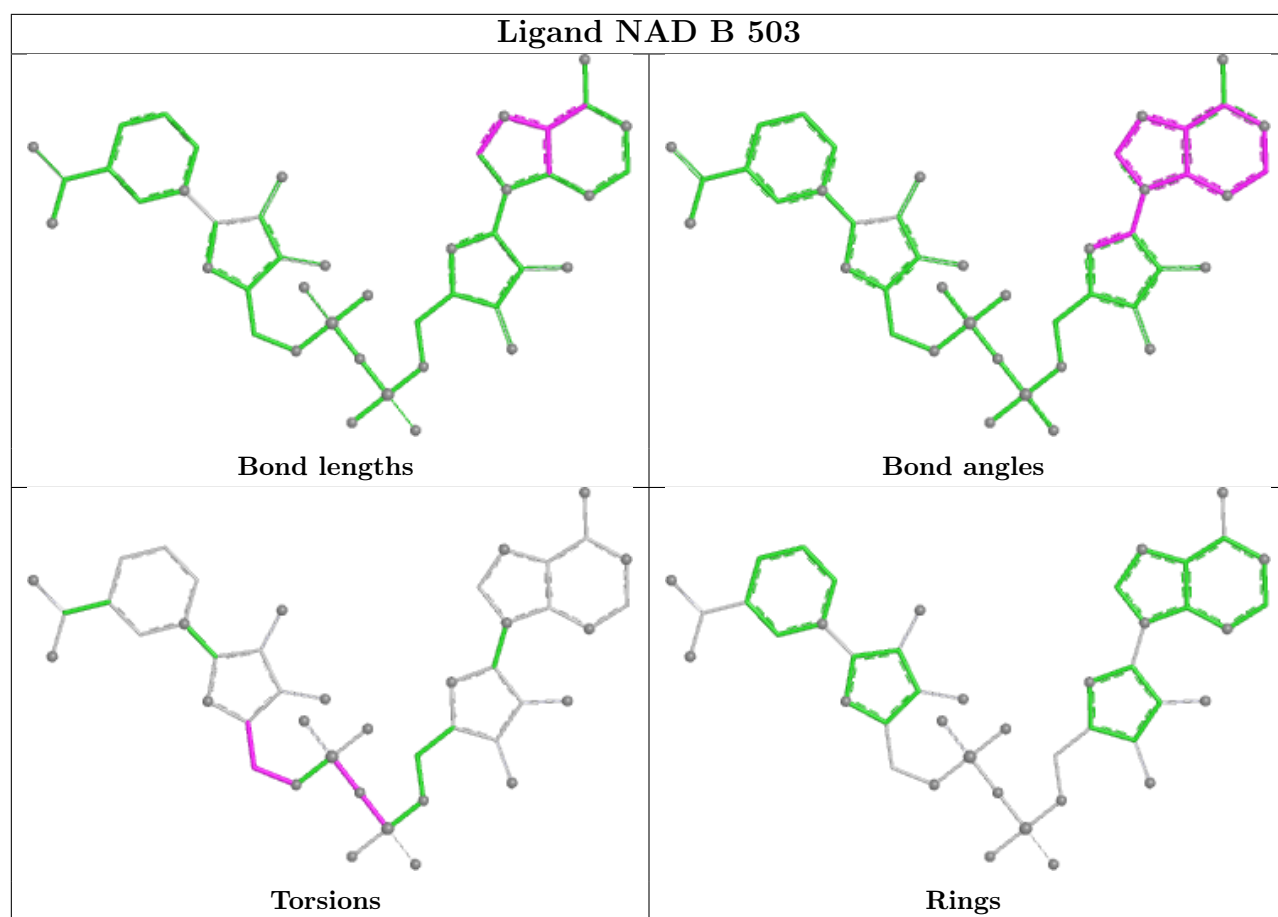


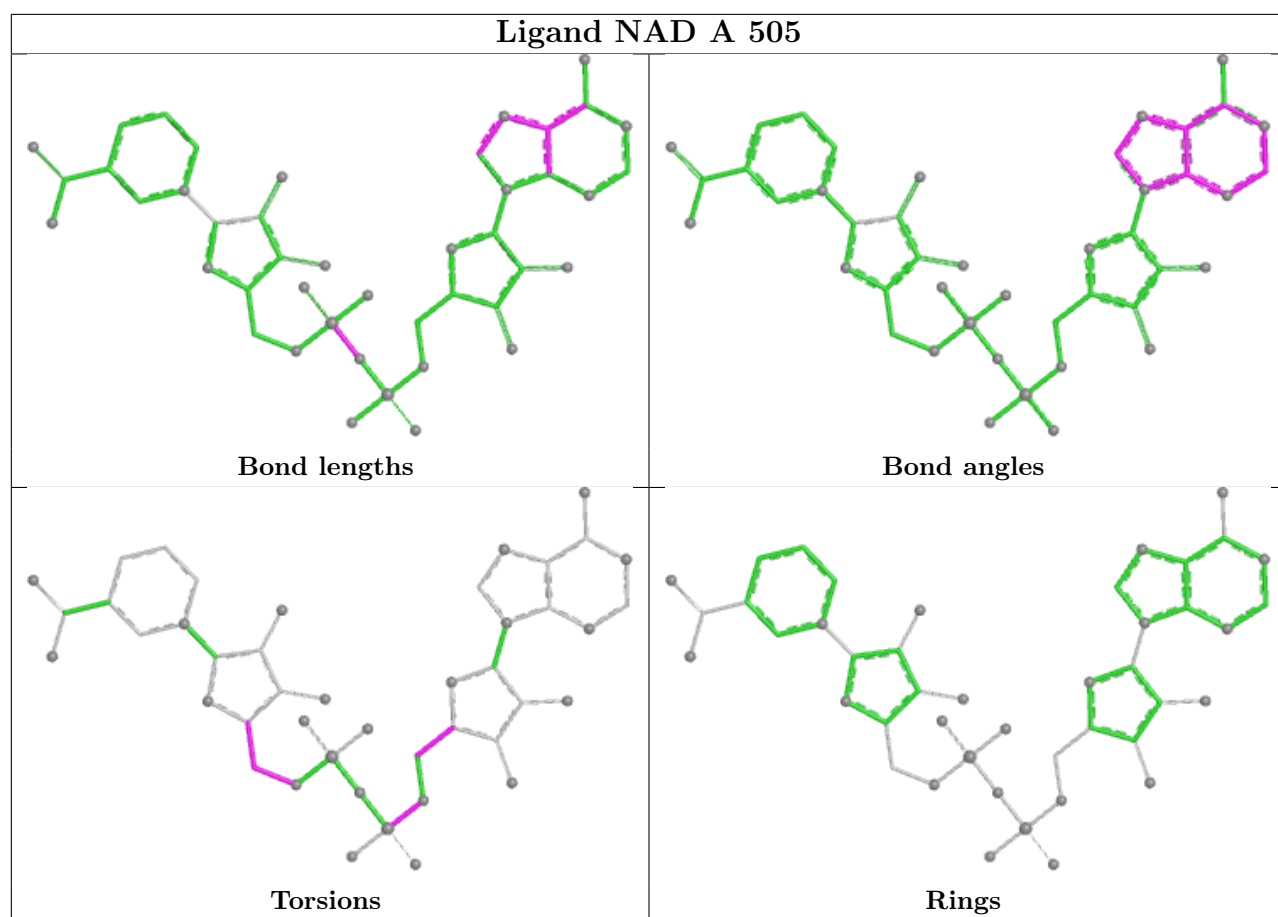
Torsions

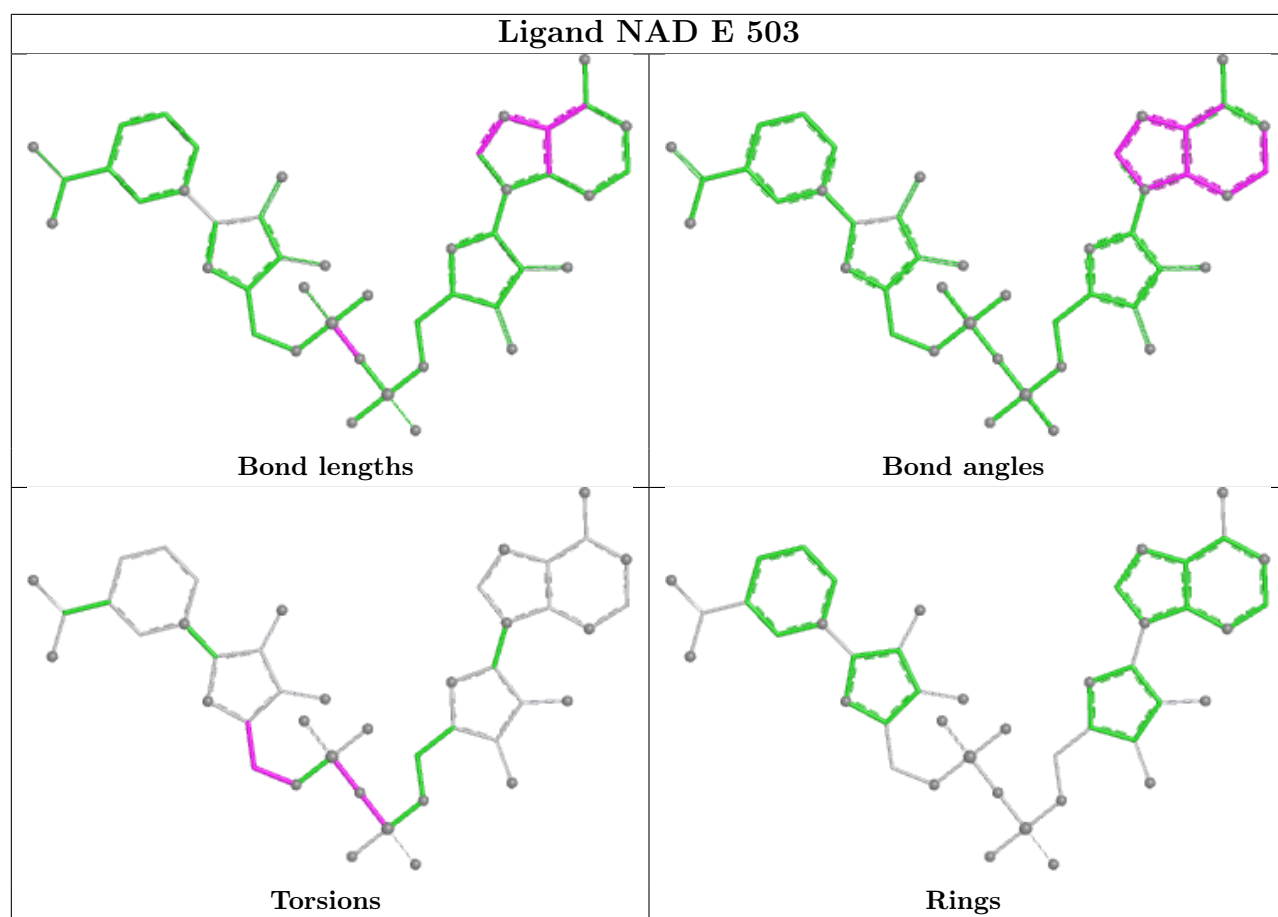


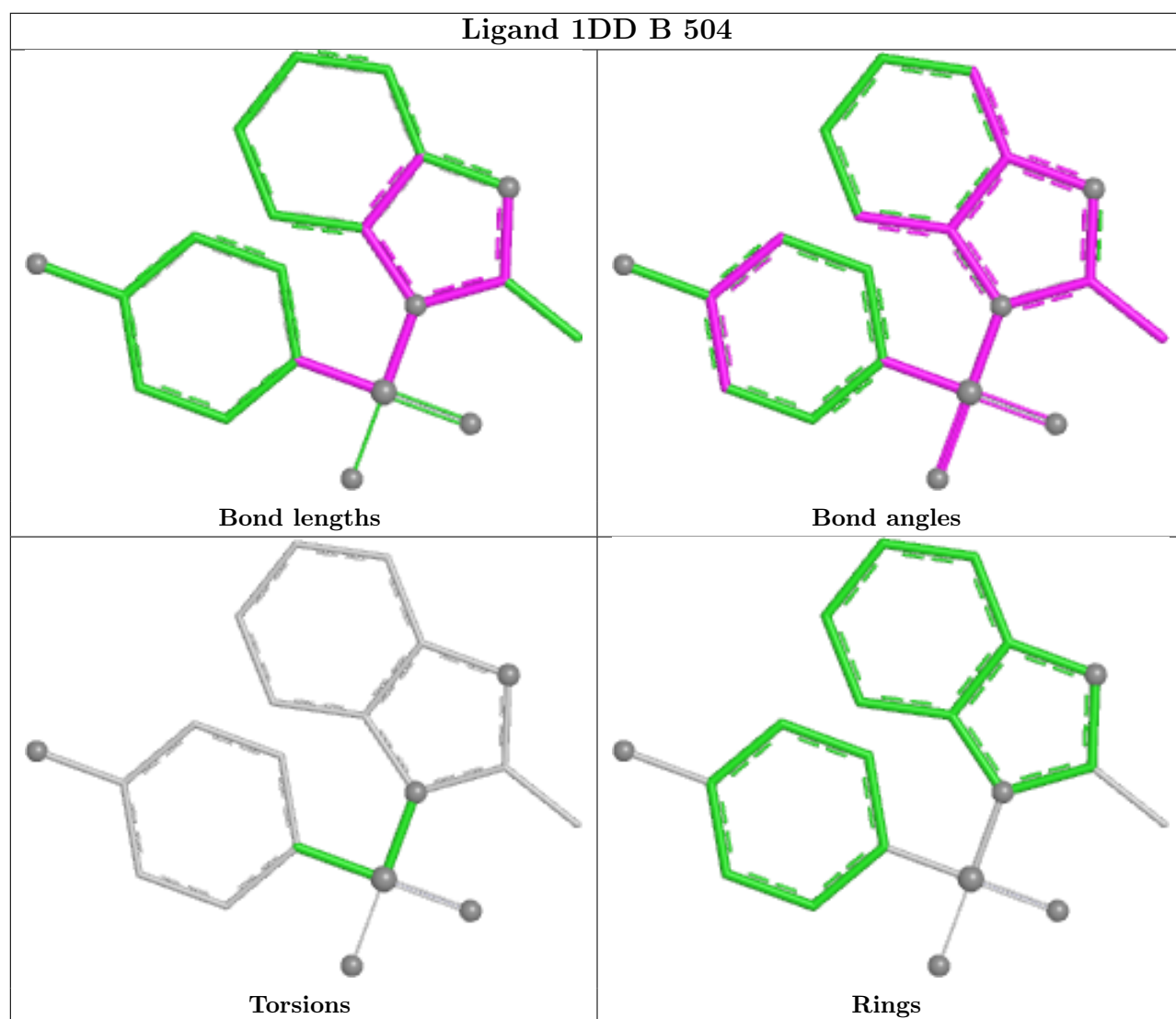
Rings











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	446/469 (95%)	0.65	33 (7%)	20 23	12, 32, 49, 55	8 (1%)
1	B	447/469 (95%)	0.36	6 (1%)	75 80	15, 30, 41, 57	2 (0%)
1	E	447/469 (95%)	0.39	10 (2%)	62 69	14, 30, 39, 54	6 (1%)
1	G	447/469 (95%)	0.44	10 (2%)	62 69	17, 31, 42, 53	6 (1%)
All	All	1787/1876 (95%)	0.46	59 (3%)	49 55	12, 31, 44, 57	22 (1%)

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	LYS	4.7
1	G	18	ARG	4.0
1	A	303	ALA	3.9
1	E	434	ASN	3.7
1	G	447	ALA	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](#)

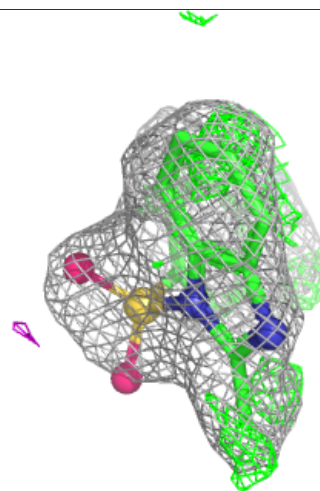
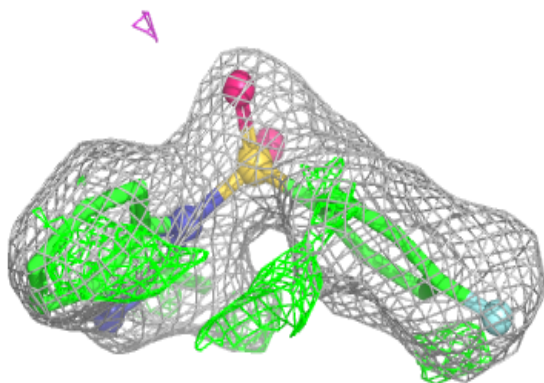
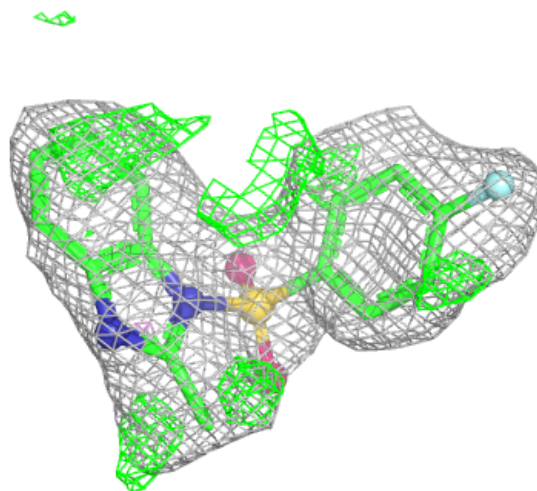
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
2	K	A	502	1/1	0.66	0.18	62,62,62,62	0
2	K	G	502	1/1	0.72	0.17	64,64,64,64	0
5	1DD	E	504	20/20	0.73	0.22	34,35,35,36	20
2	K	B	502	1/1	0.74	0.16	61,61,61,61	0
2	K	B	501	1/1	0.75	0.28	51,51,51,51	0
5	1DD	G	505	20/20	0.75	0.23	35,35,36,36	20
2	K	A	501	1/1	0.77	0.12	67,67,67,67	0
5	1DD	B	504	20/20	0.78	0.21	33,33,34,34	20
5	1DD	A	506	20/20	0.79	0.21	34,34,35,35	20
2	K	G	501	1/1	0.79	0.22	53,53,53,53	0
2	K	E	501	1/1	0.83	0.17	48,48,48,48	0
3	ACT	A	504	4/4	0.87	0.10	44,45,45,45	0
3	ACT	E	502	4/4	0.88	0.14	37,39,39,39	0
4	NAD	A	505	44/44	0.88	0.10	32,35,43,44	0
4	NAD	G	504	44/44	0.92	0.09	28,36,38,39	0
3	ACT	G	503	4/4	0.92	0.11	38,38,38,39	0
3	ACT	A	503	4/4	0.92	0.10	46,46,46,47	0
4	NAD	B	503	44/44	0.92	0.08	27,31,34,35	0
4	NAD	E	503	44/44	0.92	0.09	30,37,39,40	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.

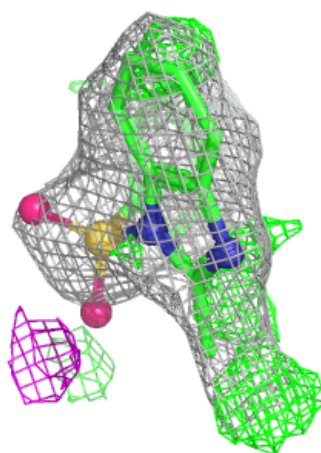
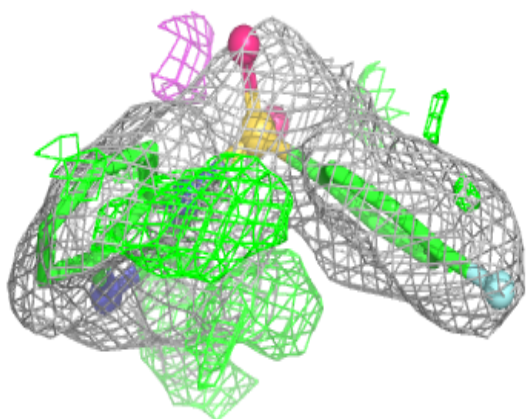
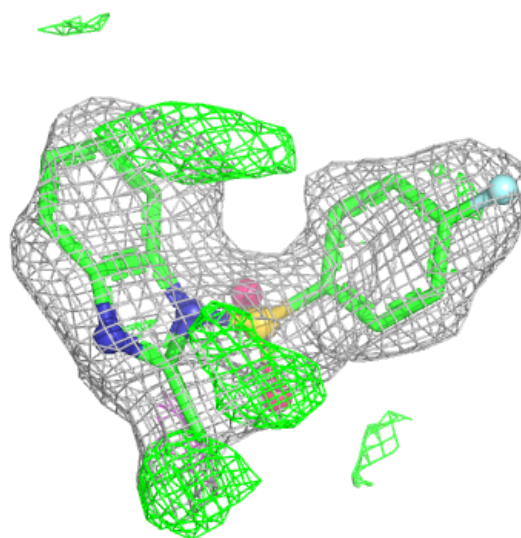
Electron density around 1DD E 504:

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



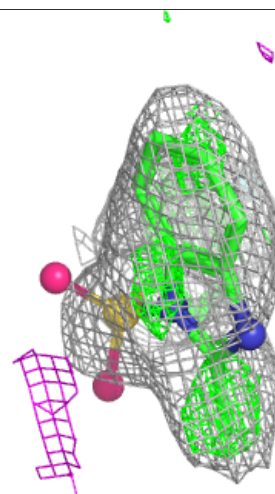
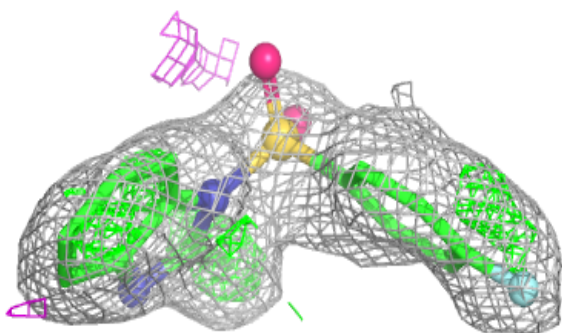
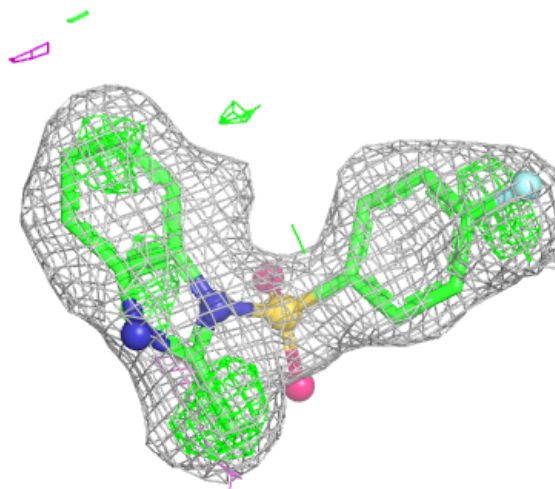
Electron density around 1DD G 505:

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



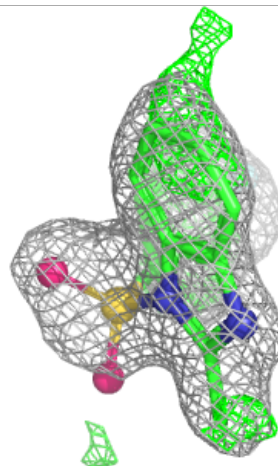
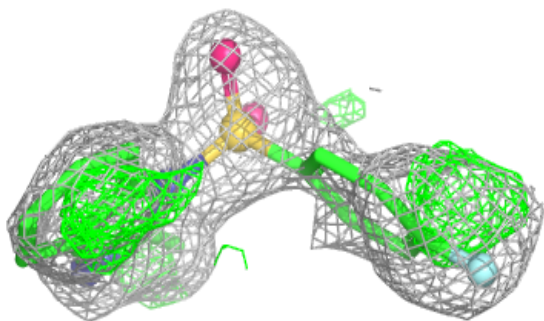
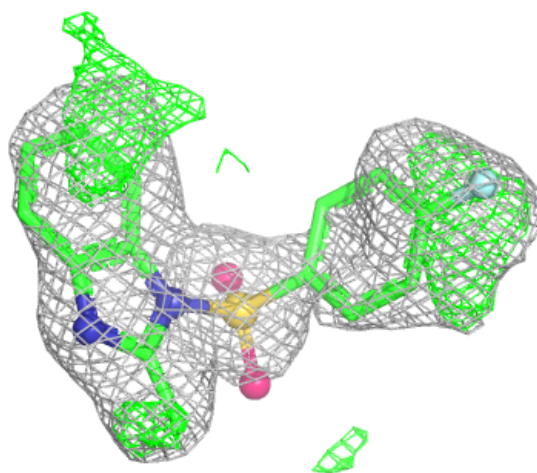
Electron density around 1DD B 504:

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



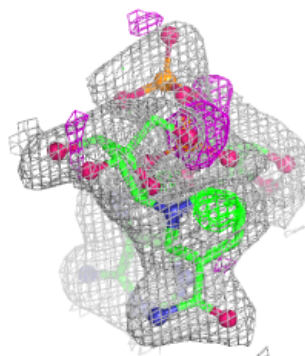
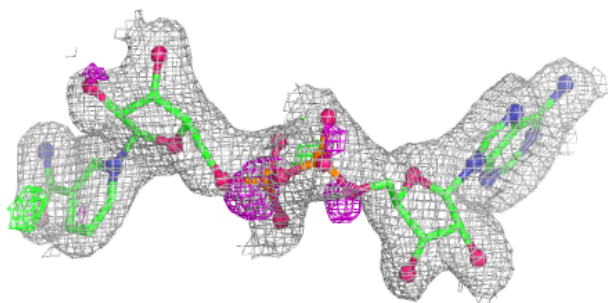
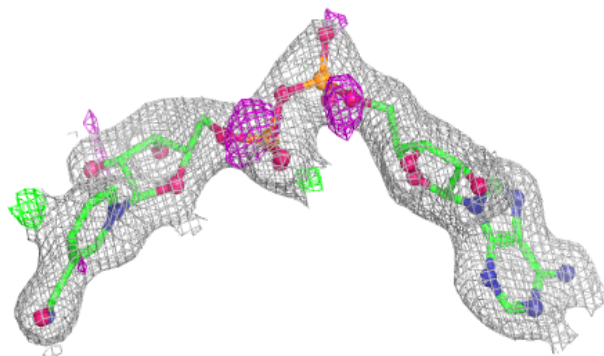
Electron density around 1DD A 506:

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

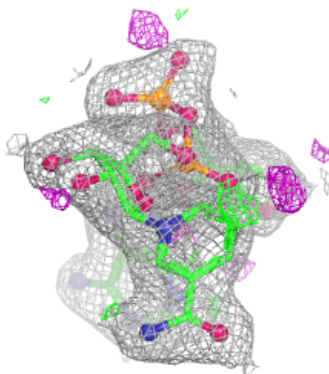
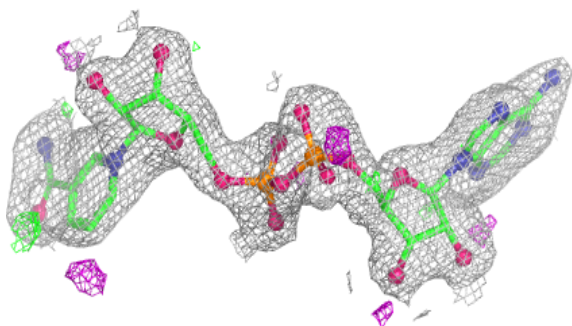
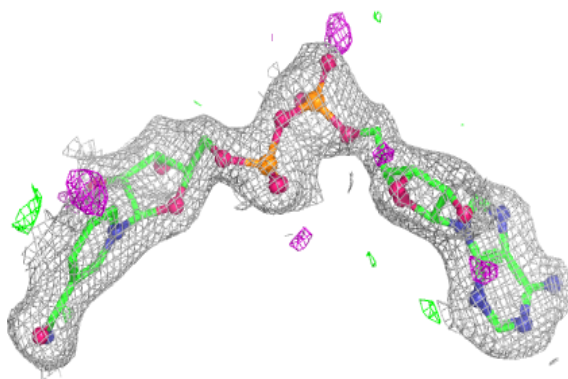


Electron density around NAD A 505:

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and green (positive)

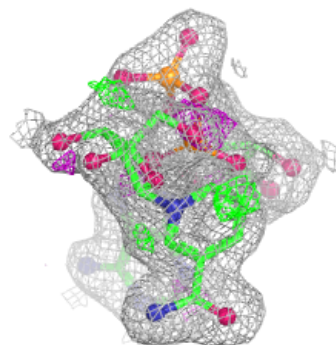
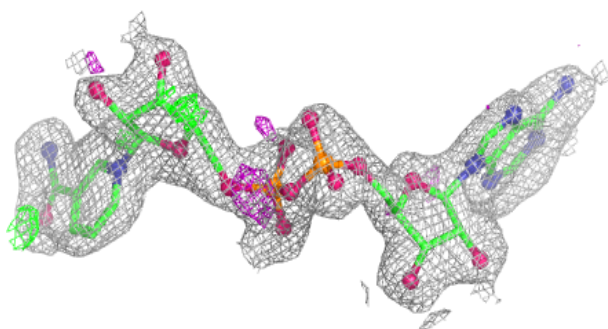
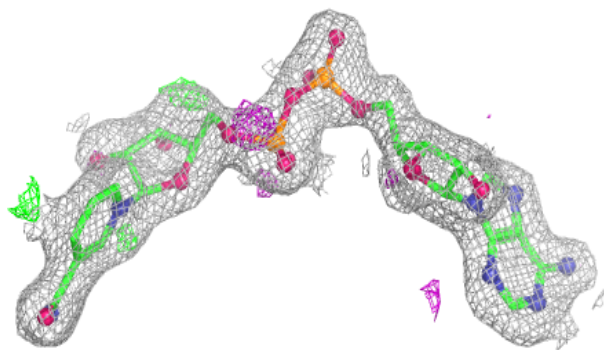
**Electron density around NAD G 504:**

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and green (positive)

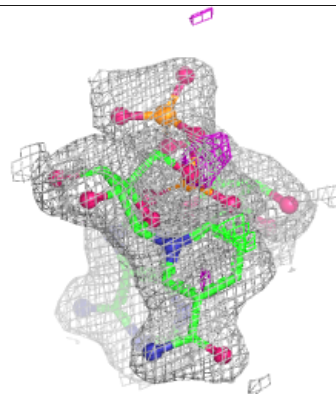
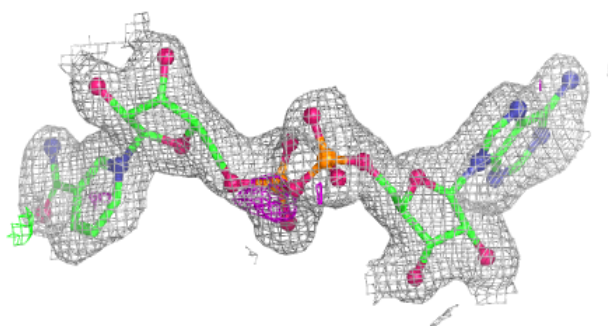
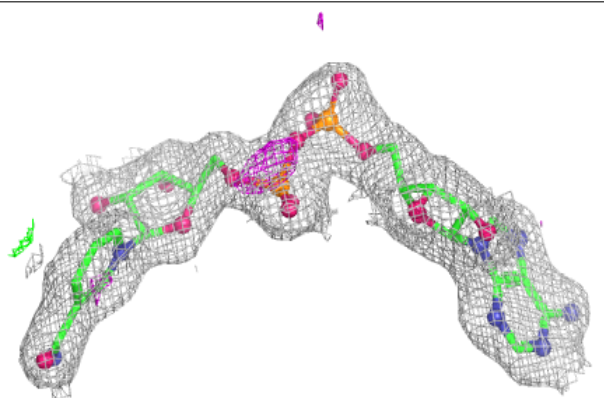


Electron density around NAD B 503:

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

**Electron density around NAD E 503:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.