



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:09 PM UTC

PDB ID : 9B81 / pdb_00009b81
Title : Crystal structure of wild type IDH1 bound to compound 4
Authors : Lu, J.; Abeywickrema, P.; Heo, M.R.; Parthasarathy, G.; McCoy, M.; Soisson, S.M.
Deposited on : 2024-03-28
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

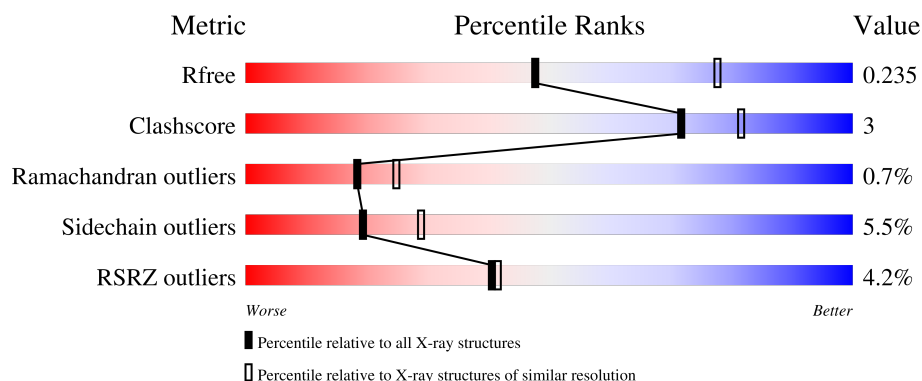
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	424	6% 79% 11% 8%
1	B	424	6% 79% 11% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6244 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.

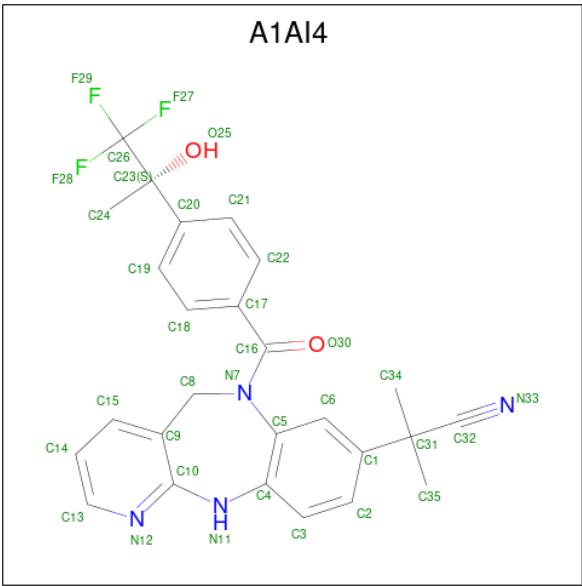
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3023	1929	509	567	18			
1	B	390	Total	C	N	O	S	0	0	0
			3002	1914	509	561	18			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	variant	UNP O75874
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	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
B	132	HIS	ARG	variant	UNP O75874
B	415	LEU	-	expression tag	UNP O75874
B	416	GLU	-	expression tag	UNP O75874
B	417	HIS	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
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

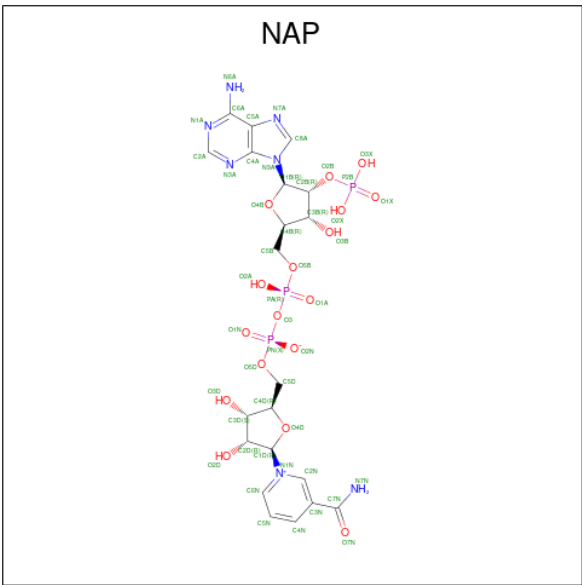
- Molecule 2 is 2-methyl-2-(6-{4-[(2S)-1,1,1-trifluoro-2-hydroxypropan-2-yl]benzoyl}-6,11-dihydro-5H-pyrido[2,3-b][1,5]benzodiazepin-8-yl)propanenitrile (CCD ID: A1AI4) (formula:

C₂₆H₂₃F₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



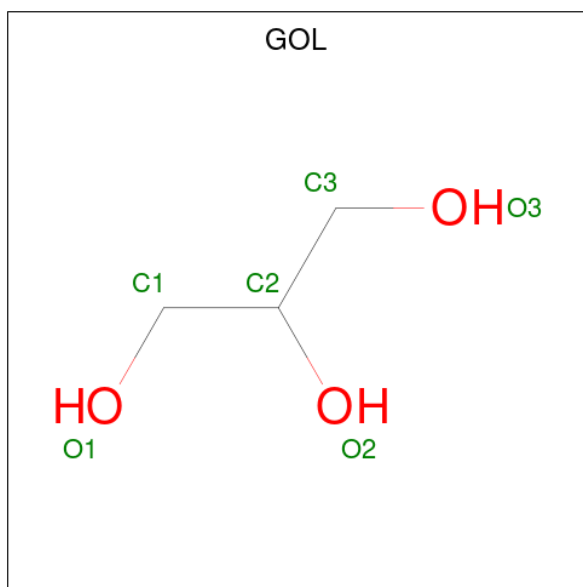
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	26	3	4	2		
2	B	1	Total	C	F	N	O	0	0
			35	26	3	4	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

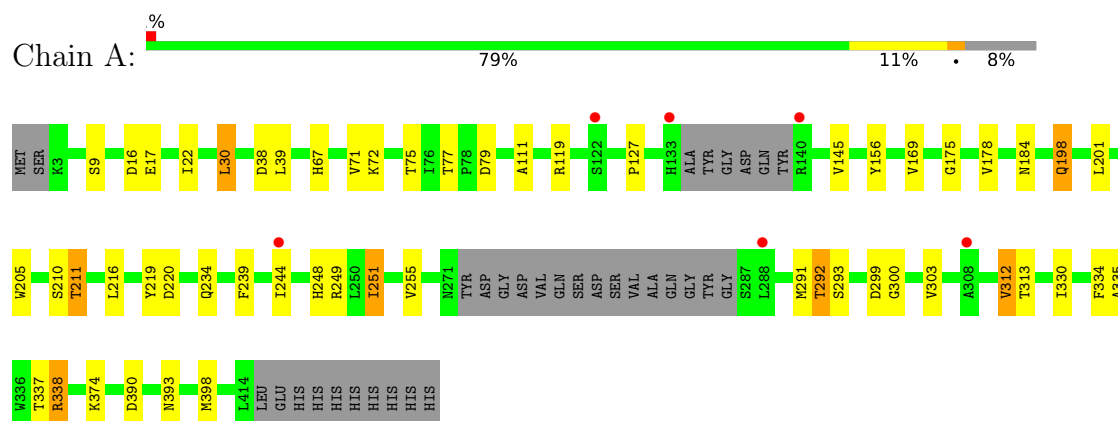
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O		
			26	26	0	0
5	B	21	Total	O		
			21	21	0	0

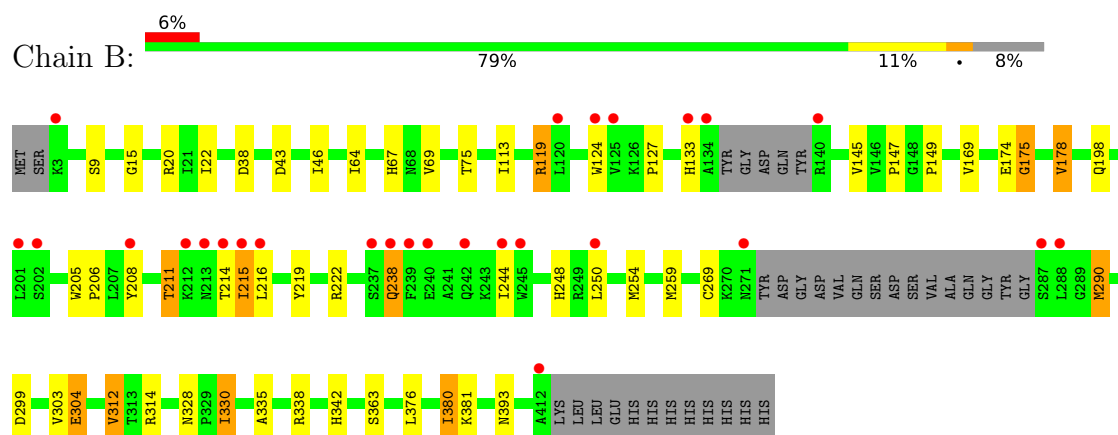
3 Residue-property plots [i](#)

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: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.79Å 82.79Å 302.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.06 – 2.56 35.06 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.06-2.56) 99.9 (35.06-2.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.57Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.201 , 0.233 0.202 , 0.235	Depositor DCC
R_{free} test set	1758 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6244	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AI4, GOL, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/3086	1.41	20/4176 (0.5%)
1	B	0.86	1/3065 (0.0%)	1.42	14/4151 (0.3%)
All	All	0.84	1/6151 (0.0%)	1.41	34/8327 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	MET	SD-CE	-11.25	1.51	1.79

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	VAL	N-CA-C	-8.43	102.64	110.82
1	B	174	GLU	N-CA-C	-8.06	103.33	113.01
1	B	38	ASP	N-CA-C	-7.16	96.09	108.56
1	A	67	HIS	N-CA-C	6.45	121.15	113.28
1	B	335	ALA	N-CA-C	-6.24	104.40	111.14
1	A	335	ALA	N-CA-C	-6.18	104.46	111.14
1	A	9	SER	N-CA-C	6.15	118.20	108.67
1	A	39	LEU	N-CA-C	6.13	118.64	109.25
1	B	214	THR	N-CA-C	-6.01	104.10	112.45
1	A	374	LYS	N-CA-C	5.90	118.19	111.11
1	A	72	LYS	N-CA-C	5.72	118.72	109.40
1	B	330	ILE	N-CA-C	5.69	116.33	110.36
1	B	380	ILE	CA-C-N	5.63	128.29	120.29
1	B	380	ILE	C-N-CA	5.63	128.29	120.29
1	B	46	ILE	N-CA-C	5.63	116.27	110.36
1	B	381	LYS	N-CA-C	5.58	117.44	111.36
1	A	169	VAL	N-CA-C	-5.54	105.44	110.82
1	B	9	SER	N-CA-C	5.51	117.20	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLN	N-CA-C	5.47	120.63	113.30
1	A	38	ASP	N-CA-C	-5.43	99.11	108.56
1	A	299	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	393	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	201	LEU	CA-C-N	5.27	127.60	120.38
1	A	201	LEU	C-N-CA	5.27	127.60	120.38
1	A	79	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	71	VAL	N-CA-CB	5.18	118.38	111.64
1	A	17	GLU	N-CA-C	5.17	116.81	108.08
1	B	133	HIS	N-CA-C	5.16	117.95	110.42
1	A	330	ILE	N-CA-CB	5.16	116.03	110.62
1	B	67	HIS	N-CA-C	5.15	119.56	113.28
1	A	16	ASP	N-CA-C	5.08	117.88	109.85
1	B	393	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	77	THR	N-CA-C	-5.05	99.59	108.69
1	A	390	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

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	3023	0	2933	19	0
1	B	3002	0	2889	25	0
2	A	35	0	0	0	0
2	B	35	0	0	1	0
3	A	48	0	25	3	0
3	B	48	0	25	2	0
4	A	6	0	8	0	0
5	A	26	0	0	0	0
5	B	21	0	0	0	0
All	All	6244	0	5880	40	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.

All (40) 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:B:208:TYR:HB3	1:B:254:MET:HE1	1.54	0.89
1:B:290:MET:HE2	1:B:328:ASN:HD21	1.39	0.88
1:A:178:VAL:HG21	1:B:219:TYR:HA	1.60	0.84
1:A:219:TYR:HA	1:B:178:VAL:HG21	1.67	0.77
1:B:290:MET:CE	1:B:328:ASN:HD21	2.05	0.69
1:B:75:THR:O	3:B:501:NAP:H2N	1.98	0.63
1:B:290:MET:HE3	1:B:376:LEU:HD11	1.84	0.59
1:A:211:THR:CG2	1:A:248:HIS:HE1	2.17	0.58
1:B:290:MET:HE2	1:B:328:ASN:ND2	2.15	0.58
1:A:211:THR:HG23	1:A:220:ASP:HB3	1.86	0.57
1:A:219:TYR:HA	1:B:178:VAL:CG2	2.35	0.54
1:A:292:THR:HG21	1:A:338:ARG:HH21	1.72	0.54
1:A:111:ALA:HB2	1:A:291:MET:HE2	1.91	0.53
1:A:211:THR:HG22	1:A:248:HIS:HE1	1.73	0.52
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.90	0.52
1:B:20:ARG:NH2	1:B:43:ASP:OD1	2.39	0.50
1:B:127:PRO:HD2	1:B:205:TRP:CH2	2.47	0.49
1:B:64:ILE:HD13	1:B:304:GLU:HG3	1.94	0.49
1:A:312:VAL:HG13	3:A:502:NAP:H3B	1.95	0.48
1:B:290:MET:HE3	1:B:376:LEU:HD21	1.96	0.48
1:A:239:PHE:CD2	1:A:244:ILE:HG22	2.50	0.47
1:B:211:THR:HG22	1:B:248:HIS:HE1	1.80	0.47
1:B:312:VAL:HG13	3:B:501:NAP:H3B	1.99	0.45
1:A:334:PHE:HA	1:A:337:THR:OG1	2.17	0.45
1:A:211:THR:HG22	1:A:248:HIS:CE1	2.51	0.44
1:A:313:THR:OG1	3:A:502:NAP:H51N	2.17	0.44
1:B:113:ILE:HD11	2:B:500:A1AI4:C14	2.47	0.43
1:A:75:THR:O	3:A:502:NAP:H2N	2.18	0.43
1:A:127:PRO:HD2	1:A:205:TRP:HH2	1.84	0.43
1:B:119:ARG:HD2	1:B:124:TRP:O	2.18	0.43
1:A:30:LEU:HD22	1:A:398:MET:HE1	2.01	0.42
1:A:210:SER:HA	1:A:249:ARG:O	2.20	0.42
1:A:198:GLN:HG2	1:A:300:GLY:HA2	2.02	0.42
1:B:206:PRO:HA	1:B:244:ILE:HG23	2.02	0.41
1:B:238:GLN:H	1:B:238:GLN:HG2	1.60	0.41
1:A:156:TYR:CE1	1:B:147:PRO:HD2	2.56	0.41
1:B:69:VAL:HG22	1:B:342:HIS:HD2	1.85	0.41
1:B:149:PRO:HG3	1:B:175:GLY:HA3	2.03	0.41
1:B:15:GLY:O	1:B:20:ARG:NE	2.54	0.41
1:B:211:THR:CG2	1:B:248:HIS:HE1	2.34	0.40

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	385/424 (91%)	371 (96%)	12 (3%)	2 (0%)	24	33
1	B	384/424 (91%)	361 (94%)	20 (5%)	3 (1%)	16	22
All	All	769/848 (91%)	732 (95%)	32 (4%)	5 (1%)	18	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	GLY
1	A	175	GLY
1	A	251	ILE
1	B	215	ILE
1	B	380	ILE

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	313/360 (87%)	298 (95%)	15 (5%)	23	34
1	B	306/360 (85%)	287 (94%)	19 (6%)	16	24
All	All	619/720 (86%)	585 (94%)	34 (6%)	19	29

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	30	LEU
1	A	119	ARG
1	A	145	VAL
1	A	184	ASN
1	A	198	GLN
1	A	211	THR
1	A	216	LEU
1	A	251	ILE
1	A	255	VAL
1	A	292	THR
1	A	293	SER
1	A	303	VAL
1	A	312	VAL
1	A	338	ARG
1	B	22	ILE
1	B	119	ARG
1	B	145	VAL
1	B	178	VAL
1	B	198	GLN
1	B	211	THR
1	B	215	ILE
1	B	216	LEU
1	B	222	ARG
1	B	238	GLN
1	B	250	LEU
1	B	259	MET
1	B	269	CYS
1	B	299	ASP
1	B	303	VAL
1	B	304	GLU
1	B	312	VAL
1	B	314	ARG
1	B	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	53	ASN
1	A	101	ASN
1	A	132	HIS
1	A	228	GLN

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Mol	Chain	Res	Type
1	A	248	HIS
1	A	328	ASN
1	B	40	HIS
1	B	96	ASN
1	B	132	HIS
1	B	133	HIS
1	B	213	ASN
1	B	248	HIS
1	B	257	GLN
1	B	328	ASN
1	B	404	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1AI4	B	500	-	38,38,38	1.28	3 (7%)	52,59,59	1.38	8 (15%)
3	NAP	B	501	-	50,52,52	2.56	10 (20%)	71,80,80	1.51	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	503	-	5,5,5	1.01	0	5,5,5	0.49	0
2	A1AI4	A	501	-	38,38,38	1.28	4 (10%)	52,59,59	1.29	6 (11%)
3	NAP	A	502	-	50,52,52	2.62	8 (16%)	71,80,80	1.52	15 (21%)

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
2	A1AI4	B	500	-	-	0/29/44/44	0/3/4/4
3	NAP	B	501	-	-	11/35/67/67	0/5/5/5
4	GOL	A	503	-	-	1/4/4/4	-
2	A1AI4	A	501	-	-	0/29/44/44	0/3/4/4
3	NAP	A	502	-	-	9/35/67/67	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAP	C4N-C3N	11.34	1.56	1.39
3	A	502	NAP	C4N-C3N	10.64	1.55	1.39
3	A	502	NAP	C5N-C4N	9.15	1.54	1.38
3	B	501	NAP	C5N-C4N	8.84	1.54	1.38
3	A	502	NAP	C2N-N1N	7.00	1.42	1.35
3	B	501	NAP	C2N-N1N	6.15	1.41	1.35
3	A	502	NAP	C6N-N1N	3.94	1.44	1.35
2	A	501	A1AI4	C8-N7	-3.82	1.43	1.47
3	B	501	NAP	C6N-N1N	3.67	1.43	1.35
3	B	501	NAP	O4D-C1D	3.63	1.45	1.40
2	B	500	A1AI4	C8-N7	-3.40	1.43	1.47
2	B	500	A1AI4	C31-C1	-3.32	1.51	1.53
3	A	502	NAP	O4D-C1D	3.05	1.44	1.40
2	A	501	A1AI4	C31-C1	-3.03	1.52	1.53
3	A	502	NAP	O4B-C1B	3.02	1.49	1.42
3	B	501	NAP	C4A-N3A	2.83	1.39	1.34
2	B	500	A1AI4	C16-N7	2.82	1.40	1.36
3	A	502	NAP	PN-O3	2.68	1.62	1.59
2	A	501	A1AI4	C16-N7	2.52	1.40	1.36
2	A	501	A1AI4	C34-C31	-2.19	1.51	1.54
3	B	501	NAP	O4B-C1B	2.17	1.47	1.42
3	A	502	NAP	C7N-N7N	2.16	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAP	C2A-N3A	2.11	1.37	1.33
3	B	501	NAP	PA-O2A	-2.05	1.45	1.55
3	B	501	NAP	O4B-C4B	2.02	1.49	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAP	C5N-C4N-C3N	-4.91	115.54	120.36
3	B	501	NAP	O7N-C7N-C3N	4.66	125.29	119.60
3	A	502	NAP	O7N-C7N-C3N	4.59	125.22	119.60
2	B	500	A1AI4	C24-C23-C26	3.84	114.13	109.04
2	A	501	A1AI4	C1-C31-C32	3.66	114.26	108.86
3	A	502	NAP	C5N-C4N-C3N	-3.59	116.83	120.36
3	B	501	NAP	C4D-O4D-C1D	-3.42	106.79	109.92
3	A	502	NAP	O7N-C7N-N7N	-3.07	118.18	122.62
3	A	502	NAP	O2N-PN-O3	3.06	115.54	107.27
3	A	502	NAP	O3-PN-O1N	-3.01	101.64	110.70
3	B	501	NAP	C6N-N1N-C2N	-2.83	119.47	121.88
2	B	500	A1AI4	O30-C16-N7	2.81	125.69	121.79
3	A	502	NAP	O3X-P2B-O2B	-2.67	95.46	105.85
2	B	500	A1AI4	C21-C20-C23	-2.66	118.51	121.43
3	A	502	NAP	C4D-O4D-C1D	-2.58	107.56	109.92
2	A	501	A1AI4	C22-C17-C18	2.58	121.85	118.57
2	A	501	A1AI4	O30-C16-N7	2.56	125.34	121.79
3	A	502	NAP	O2N-PN-O1N	2.54	124.26	112.44
3	B	501	NAP	O2A-PA-O1A	2.47	123.92	112.44
3	B	501	NAP	O7N-C7N-N7N	-2.46	119.07	122.62
2	B	500	A1AI4	C22-C17-C18	2.44	121.67	118.57
2	A	501	A1AI4	C24-C23-C26	2.42	112.24	109.04
3	A	502	NAP	O3D-C3D-C4D	2.39	117.95	111.08
3	A	502	NAP	C6N-N1N-C2N	-2.37	119.86	121.88
3	B	501	NAP	O4B-C1B-N9A	2.35	112.60	108.09
3	A	502	NAP	O4D-C4D-C3D	2.31	109.74	105.15
3	A	502	NAP	O4B-C1B-N9A	2.31	112.53	108.09
3	A	502	NAP	O3D-C3D-C2D	2.17	118.77	111.82
2	B	500	A1AI4	C19-C18-C17	-2.17	118.48	120.80
2	A	501	A1AI4	C21-C22-C17	-2.14	118.52	120.80
3	B	501	NAP	O4D-C4D-C3D	2.11	109.34	105.15
3	A	502	NAP	C6N-N1N-C1D	2.11	123.86	119.73
2	B	500	A1AI4	O25-C23-C24	-2.09	103.15	108.56
2	B	500	A1AI4	O30-C16-C17	-2.08	116.16	120.29
3	B	501	NAP	N3A-C2A-N1A	-2.06	125.47	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1AI4	C19-C18-C17	-2.05	118.61	120.80
2	B	500	A1AI4	C1-C31-C32	2.03	111.86	108.86
3	A	502	NAP	O2A-PA-O1A	2.01	121.82	112.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C5B-O5B-PA-O2A
3	A	502	NAP	C5D-O5D-PN-O1N
3	A	502	NAP	O4D-C4D-C5D-O5D
3	A	502	NAP	O4D-C1D-N1N-C2N
3	A	502	NAP	O4D-C1D-N1N-C6N
3	B	501	NAP	C5B-O5B-PA-O1A
3	B	501	NAP	C5D-O5D-PN-O3
3	B	501	NAP	O4D-C1D-N1N-C2N
3	B	501	NAP	O4D-C1D-N1N-C6N
3	A	502	NAP	C3D-C4D-C5D-O5D
3	B	501	NAP	O4D-C4D-C5D-O5D
3	B	501	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	C5B-O5B-PA-O1A
3	A	502	NAP	C5B-O5B-PA-O3
3	B	501	NAP	C5B-O5B-PA-O2A
3	B	501	NAP	C5B-O5B-PA-O3
3	B	501	NAP	C5D-O5D-PN-O1N
3	B	501	NAP	C2D-C1D-N1N-C2N
3	B	501	NAP	C2D-C1D-N1N-C6N
4	A	503	GOL	O1-C1-C2-O2
3	A	502	NAP	C2B-O2B-P2B-O3X

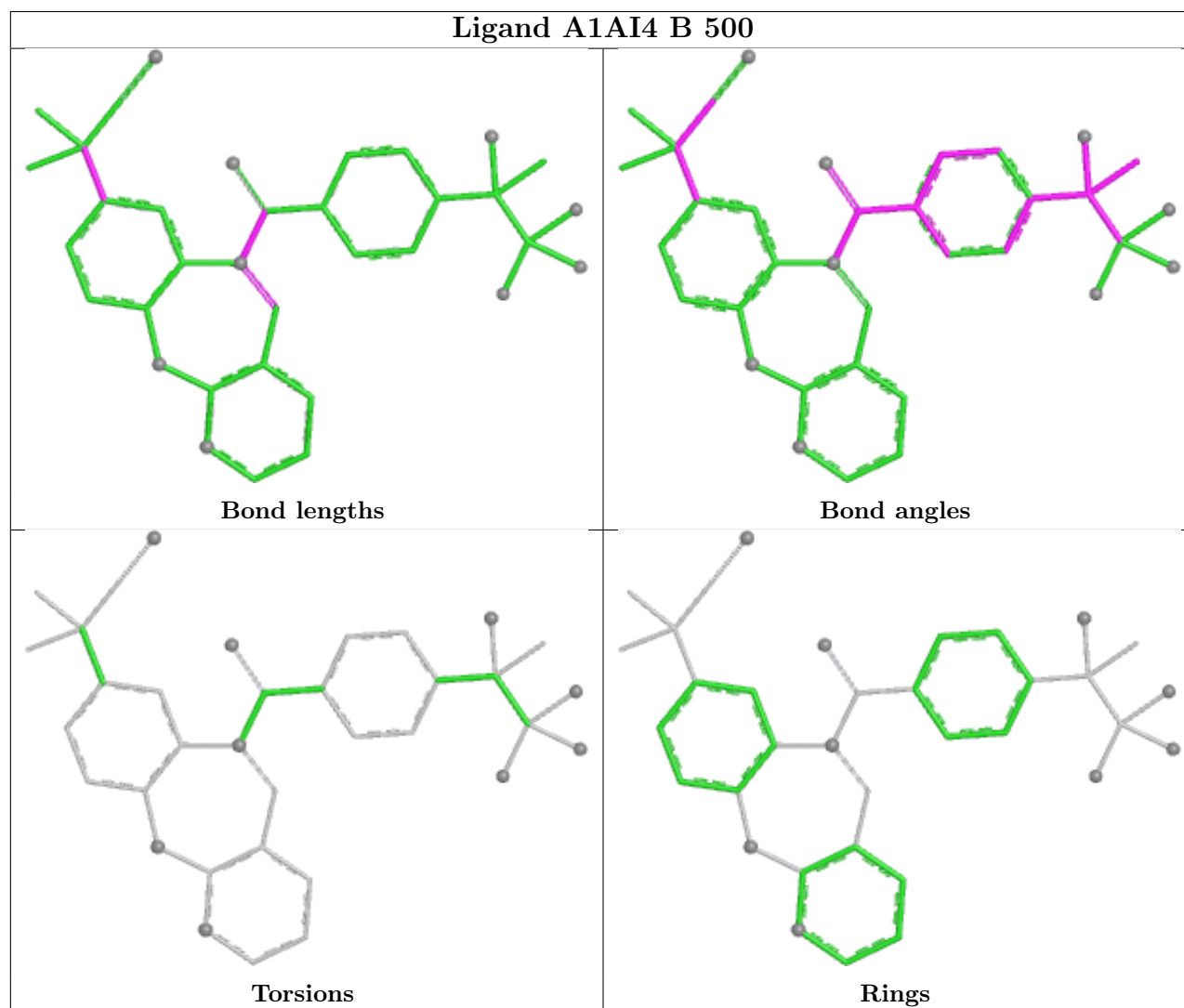
There are no ring outliers.

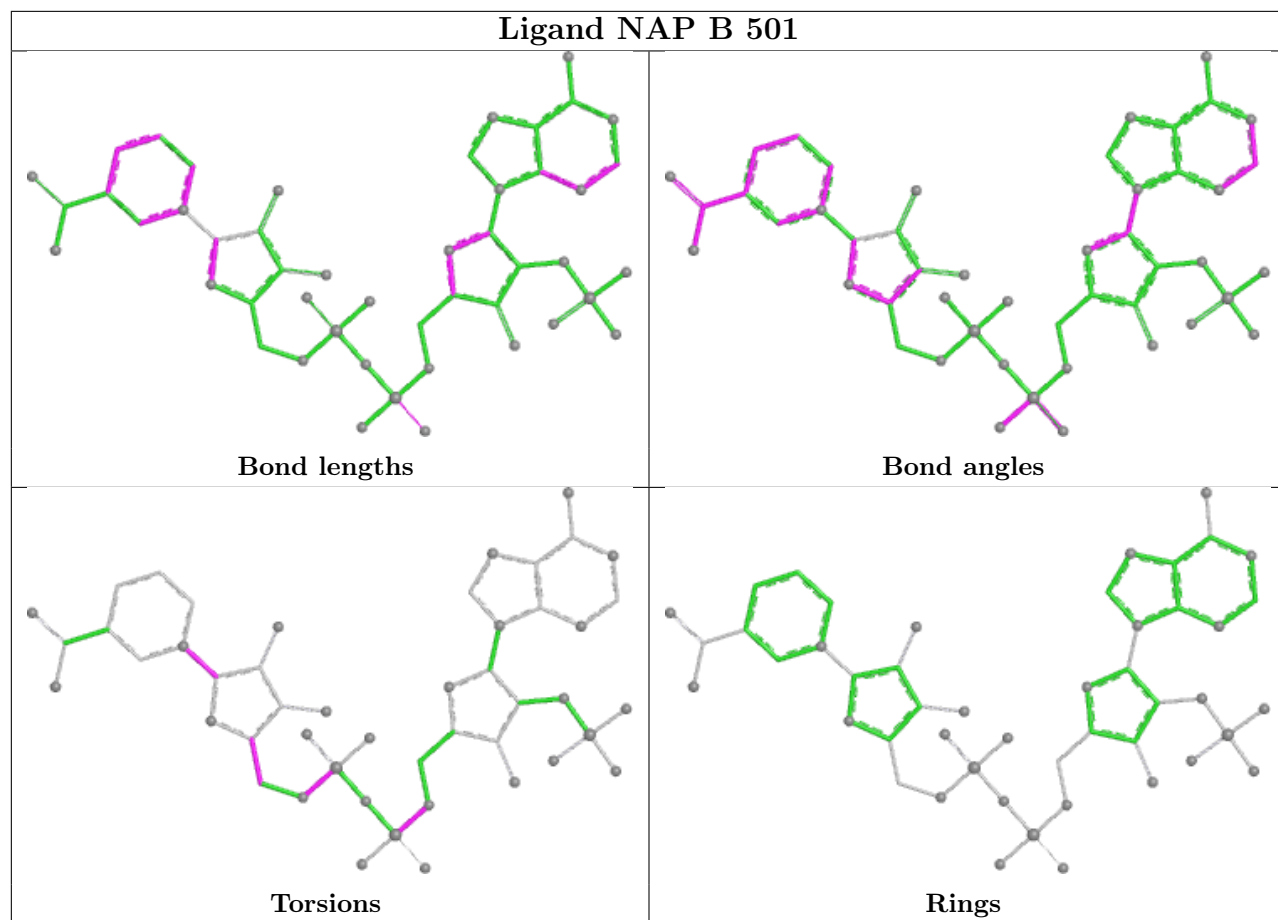
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	A1AI4	1	0
3	B	501	NAP	2	0
3	A	502	NAP	3	0

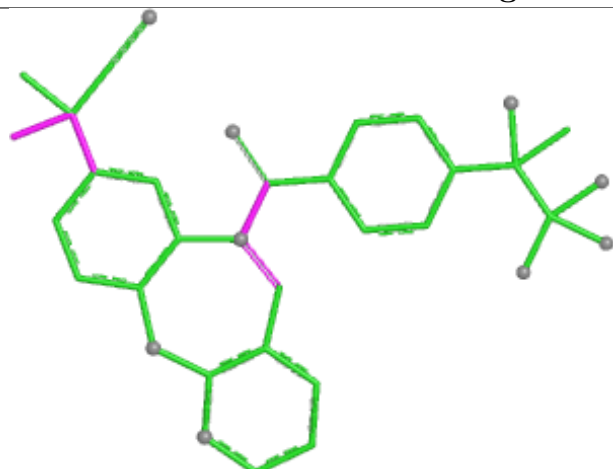
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

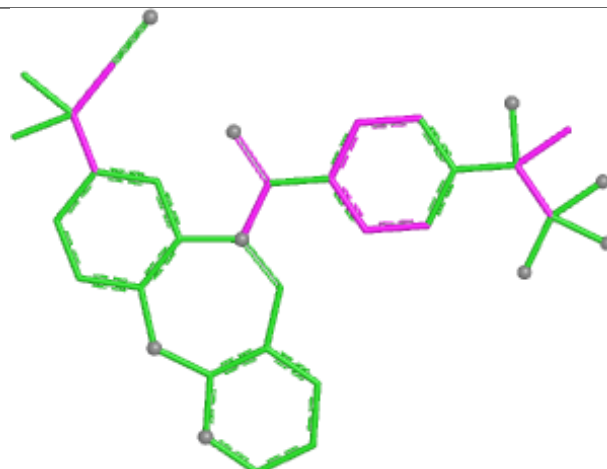




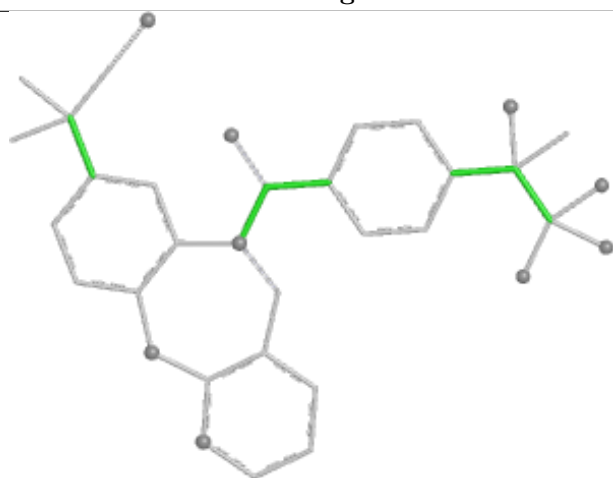
Ligand A1AI4 A 501



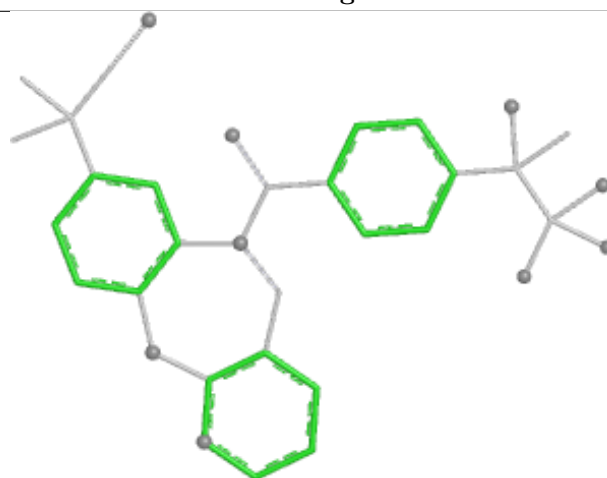
Bond lengths



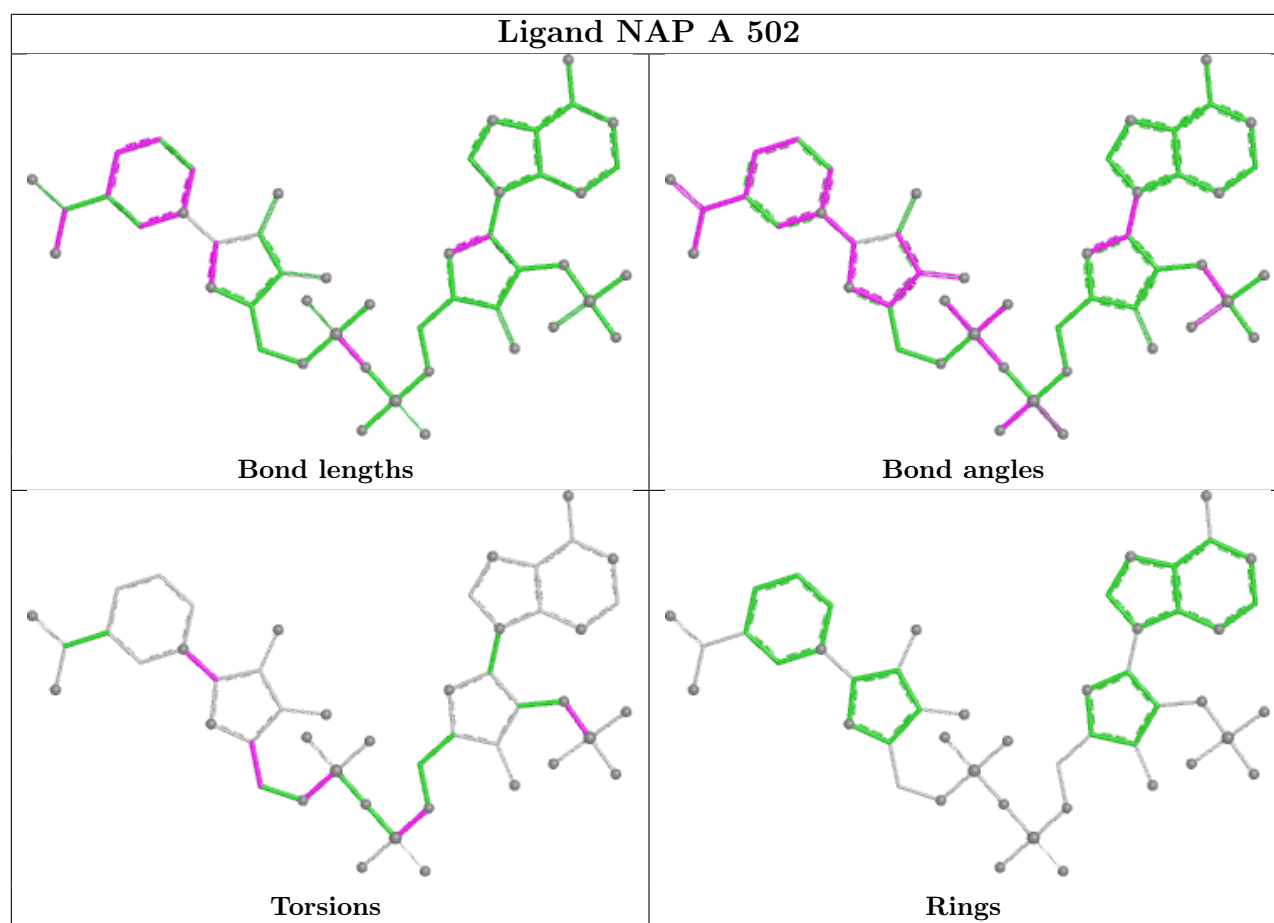
Bond angles



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

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	391/424 (92%)	0.06	6 (1%) 72 73	35, 50, 76, 97	0
1	B	390/424 (91%)	0.28	27 (6%) 23 22	33, 52, 88, 102	0
All	All	781/848 (92%)	0.17	33 (4%) 40 41	33, 51, 82, 102	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	ALA	7.3
1	B	244	ILE	4.9
1	B	134	ALA	4.8
1	A	308	ALA	4.3
1	A	133	HIS	4.2
1	B	240	GLU	4.0
1	B	140	ARG	3.7
1	A	244	ILE	3.4
1	B	215	ILE	3.4
1	B	214	THR	3.2
1	B	202	SER	3.2
1	B	288	LEU	3.1
1	A	140	ARG	2.9
1	B	239	PHE	2.7
1	A	288	LEU	2.7
1	B	133	HIS	2.7
1	B	125	VAL	2.6
1	B	271	ASN	2.6
1	A	122	SER	2.5
1	B	250	LEU	2.4
1	B	208	TYR	2.4
1	B	238	GLN	2.4
1	B	124	TRP	2.4
1	B	120	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	212	LYS	2.4
1	B	3	LYS	2.3
1	B	245	TRP	2.1
1	B	201	LEU	2.1
1	B	216	LEU	2.1
1	B	237	SER	2.1
1	B	287	SER	2.0
1	B	242	GLN	2.0
1	B	213	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

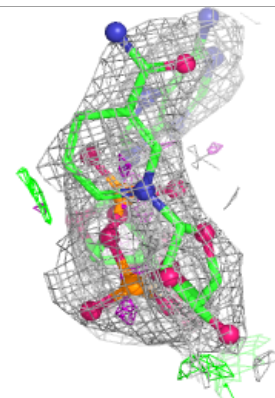
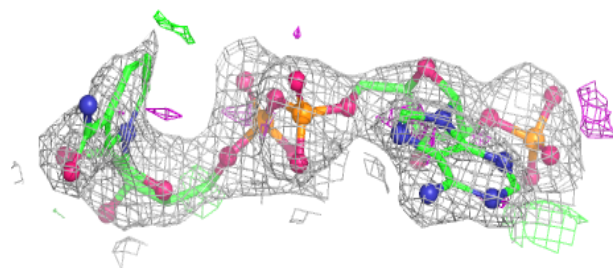
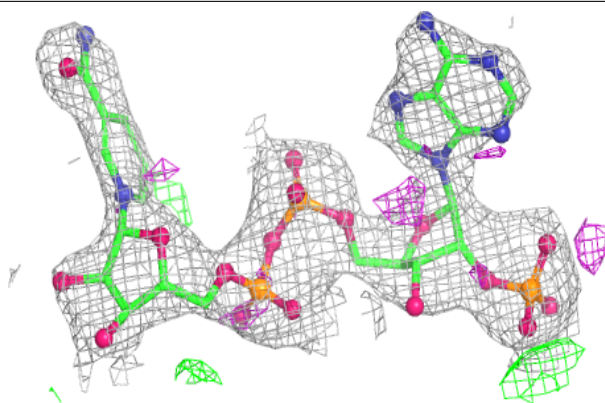
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAP	A	502	48/48	0.83	0.14	86,88,91,92	0
2	A1AI4	B	500	35/35	0.87	0.12	55,63,89,89	0
2	A1AI4	A	501	35/35	0.87	0.12	53,60,87,90	0
3	NAP	B	501	48/48	0.89	0.11	69,72,73,74	0
4	GOL	A	503	6/6	0.90	0.12	64,66,66,66	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.

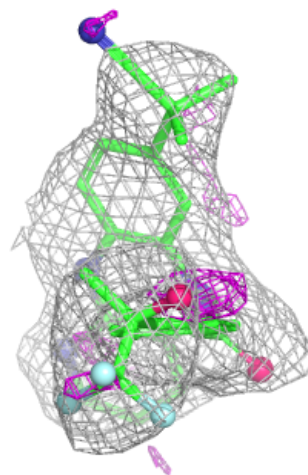
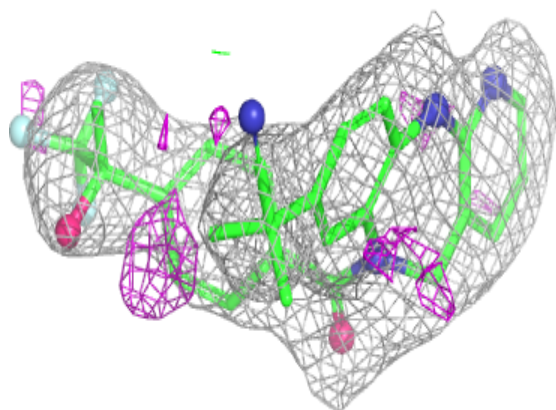
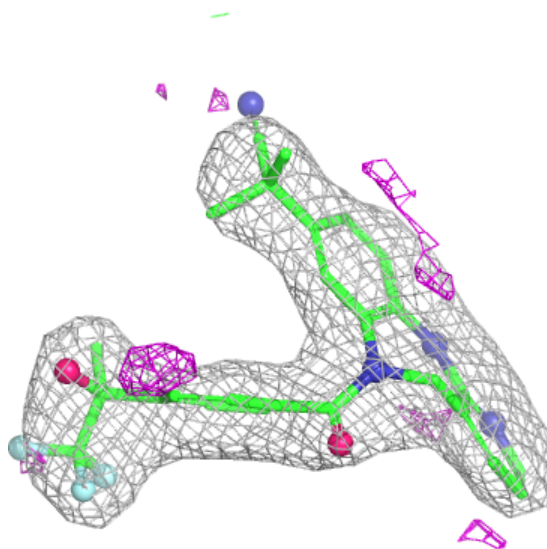
Electron density around NAP A 502:

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



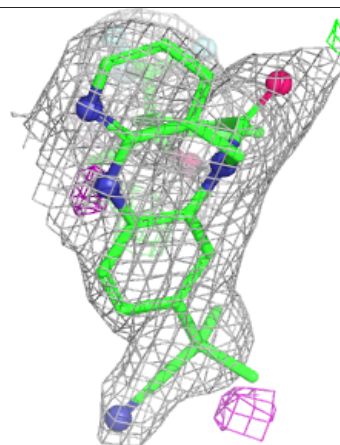
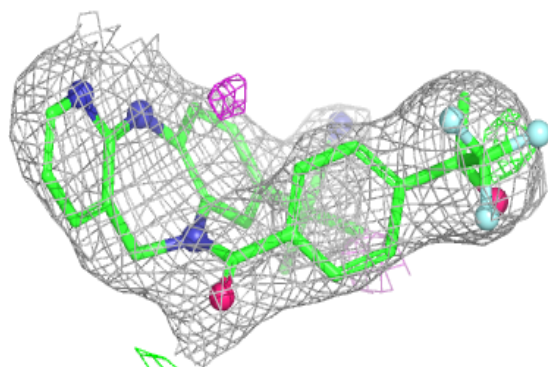
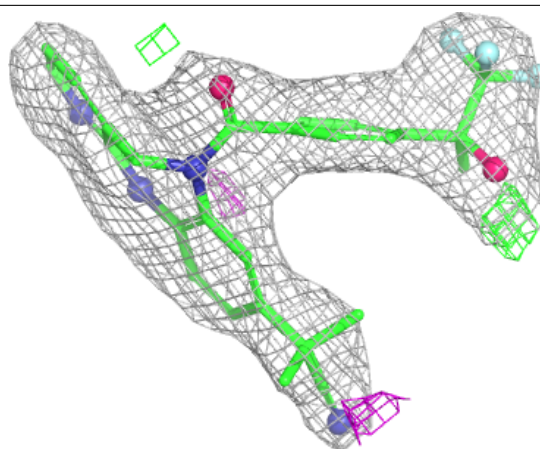
Electron density around A1AI4 B 500:

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



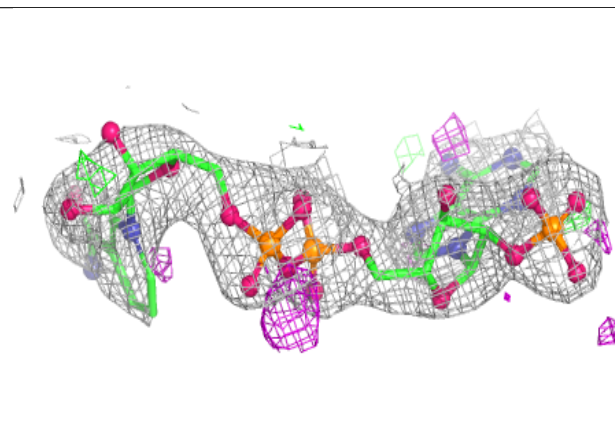
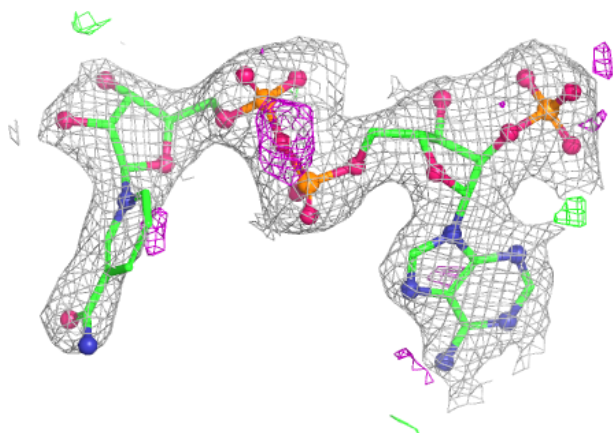
Electron density around A1AI4 A 501:

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



Electron density around NAP 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.