



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:41 PM UTC

PDB ID : 6BL0 / pdb_00006bl0
Title : Novel Modes of Inhibition of Wild-Type IDH1:Direct Covalent Modification of His315 with Cmpd11
Authors : Jakob, C.G.; Qiu, W.
Deposited on : 2017-11-09
Resolution : 2.17 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

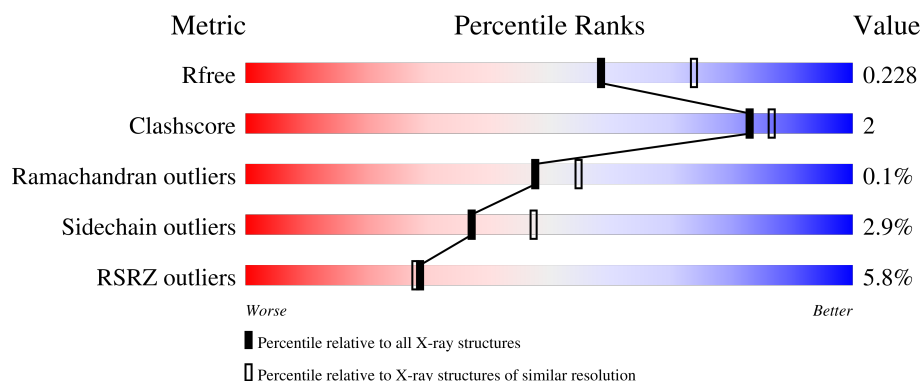
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	425	5% 89% 8% ..
1	B	425	8% 88% 9% ..
1	C	425	4% 89% 8% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10615 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	416	Total	C	N	O	S	0	0	0
			3288	2090	558	622	18			
1	B	416	Total	C	N	O	S	0	0	0
			3292	2093	559	622	18			
1	C	416	Total	C	N	O	S	0	0	0
			3292	2093	559	622	18			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874
B	425	HIS	-	expression tag	UNP O75874
C	415	SER	-	expression tag	UNP O75874

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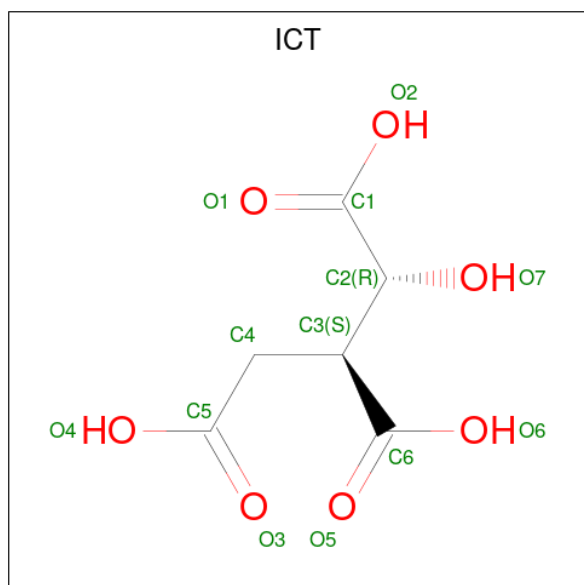
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Chain	Residue	Modelled	Actual	Comment	Reference
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



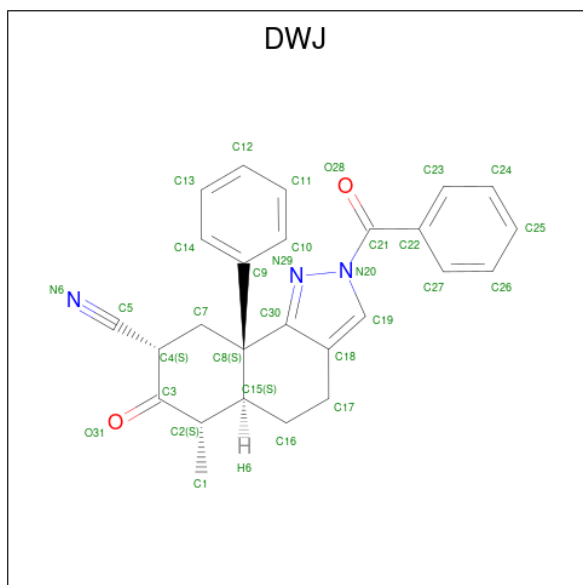
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	A	1	Total C O 13 6 7	0	0

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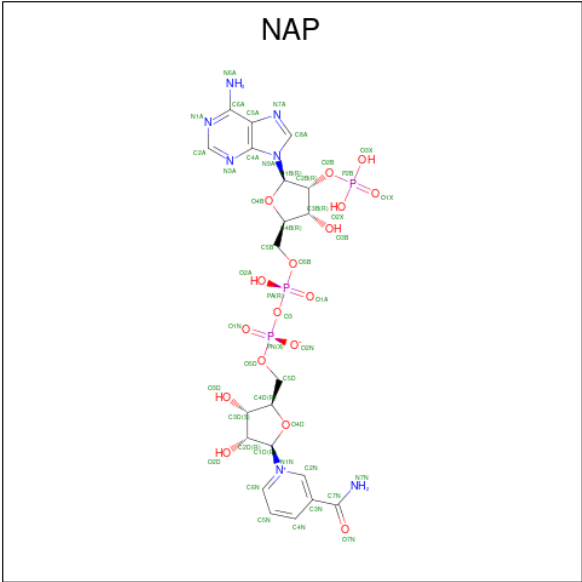
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is (5a*S*,6*S*,8*S*,9a*S*)-2-(benzenecarbonyl)-6-methyl-7-oxo-9a-phenyl-4,5,5a,6,7,8,9,9a-octahydro-2*H*-benzo[*g*]indazole-8-carbonitrile (CCD ID: DWJ) (formula: C₂₆H₂₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	26	3	2		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

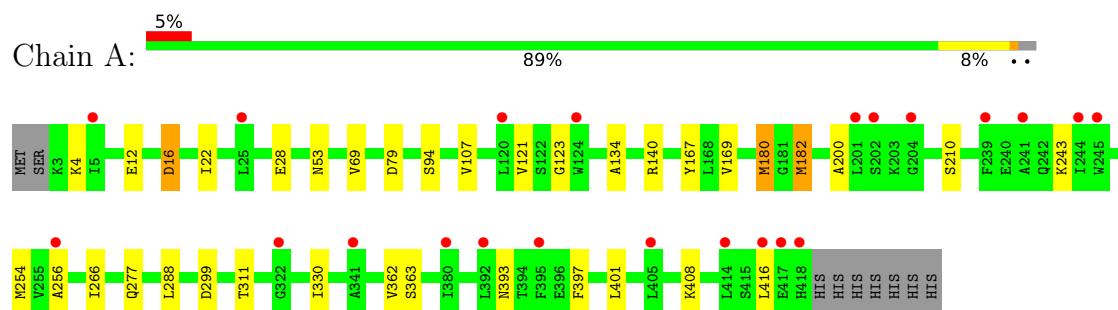
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	143	Total	O	0	0
			143	143		
6	B	173	Total	O	0	0
			173	173		
6	C	258	Total	O	0	0
			258	258		

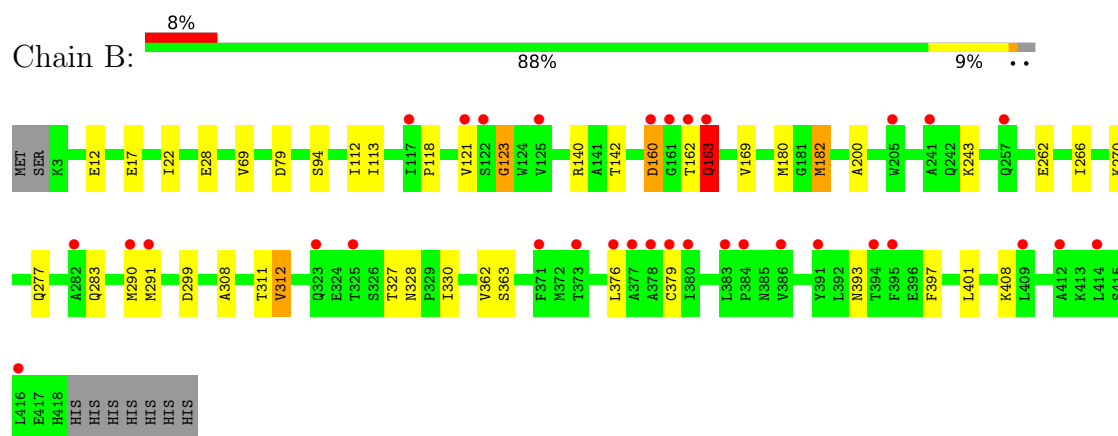
3 Residue-property plots [i](#)

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.

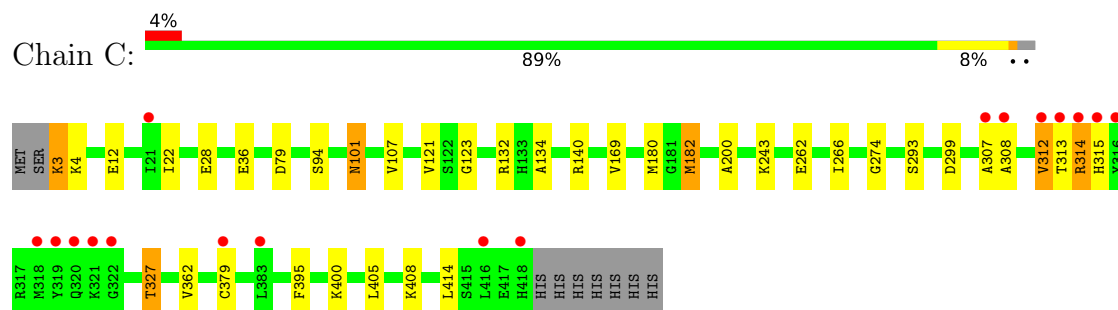
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.19Å 274.33Å 115.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.16 – 2.17 137.16 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (137.16-2.17) 99.9 (137.16-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.196 , 0.227 (Not available) , 0.228	Depositor DCC
R_{free} test set	4105 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10615	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: ICT, NAP, DWJ, MG

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	0.84	2/3357 (0.1%)	1.31	10/4529 (0.2%)
1	B	0.86	1/3361 (0.0%)	1.34	16/4533 (0.4%)
1	C	0.91	2/3361 (0.1%)	1.30	11/4533 (0.2%)
All	All	0.87	5/10079 (0.0%)	1.32	37/13595 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	182	MET	SD-CE	-8.56	1.58	1.79
1	B	182	MET	SD-CE	-6.32	1.63	1.79
1	A	182	MET	SD-CE	-5.97	1.64	1.79
1	A	180	MET	SD-CE	-5.40	1.66	1.79
1	C	101	ASN	CA-C	5.16	1.59	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-C	-7.44	104.53	111.45
1	C	169	VAL	N-CA-C	-6.84	105.09	111.45
1	B	270	LYS	N-CA-C	-6.01	102.59	110.53
1	B	162	THR	CA-C-N	5.98	132.96	121.54
1	B	162	THR	C-N-CA	5.98	132.96	121.54
1	C	313	THR	CA-C-N	5.80	129.52	120.82
1	C	313	THR	C-N-CA	5.80	129.52	120.82
1	C	307	ALA	CA-C-N	5.64	128.62	120.38
1	C	307	ALA	C-N-CA	5.64	128.62	120.38
1	B	169	VAL	N-CA-C	-5.63	105.36	110.82
1	B	160	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	79	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	113	ILE	N-CA-C	5.47	116.18	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	GLY	N-CA-C	5.47	120.68	114.67
1	B	121	VAL	CA-C-N	5.43	127.87	120.54
1	B	121	VAL	C-N-CA	5.43	127.87	120.54
1	A	416	LEU	CA-C-N	5.37	128.50	120.87
1	A	416	LEU	C-N-CA	5.37	128.50	120.87
1	B	312	VAL	CA-C-N	5.37	127.73	120.38
1	B	312	VAL	C-N-CA	5.37	127.73	120.38
1	B	299	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	163	GLN	CA-C-N	-5.32	113.36	121.66
1	B	163	GLN	C-N-CA	-5.32	113.36	121.66
1	C	121	VAL	CA-C-N	5.28	127.67	120.54
1	C	121	VAL	C-N-CA	5.28	127.67	120.54
1	A	121	VAL	CA-C-N	5.24	127.62	120.54
1	A	121	VAL	C-N-CA	5.24	127.62	120.54
1	C	79	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	16	ASP	N-CA-C	5.22	118.11	109.85
1	B	123	GLY	N-CA-C	5.15	120.34	114.67
1	A	393	ASN	CA-CB-CG	5.11	117.71	112.60
1	C	299	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	299	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	314	ARG	CA-C-N	5.05	129.21	120.58
1	C	314	ARG	C-N-CA	5.05	129.21	120.58
1	A	79	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	393	ASN	CA-CB-CG	5.01	117.61	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	3288	0	3244	13	0
1	B	3292	0	3255	21	0
1	C	3292	0	3255	15	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	26	0	8	1	0
3	C	13	0	4	1	0
4	A	31	0	0	0	0
5	B	48	0	25	1	0
5	C	48	0	25	2	0
6	A	143	0	0	0	0
6	B	173	0	0	0	0
6	C	258	0	0	2	0
All	All	10615	0	9816	47	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 2.

All (47) 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:C:101:ASN:HB3	6:C:790:HOH:O	1.35	1.23
1:B:291:MET:HE3	1:B:308:ALA:CB	2.11	0.80
1:C:180:MET:HE2	1:C:182:MET:HE2	1.65	0.78
1:B:180:MET:HE2	1:B:182:MET:HE2	1.69	0.75
1:A:180:MET:HE2	1:A:182:MET:HE2	1.69	0.73
1:B:291:MET:HE3	1:B:308:ALA:HB1	1.75	0.68
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.81	0.60
1:C:22:ILE:HD11	1:C:327:THR:HB	1.83	0.60
3:A:505:ICT:H2	5:B:501:NAP:C4N	2.32	0.60
1:C:4:LYS:HD2	1:C:36:GLU:HG3	1.86	0.57
1:A:277:GLN:HE22	1:B:277:GLN:HE22	1.54	0.55
1:C:180:MET:CE	1:C:182:MET:HE2	2.38	0.54
3:C:501:ICT:H2	5:C:502:NAP:C4N	2.37	0.53
1:B:291:MET:HE3	1:B:308:ALA:HB3	1.91	0.52
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.91	0.52
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.92	0.51
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.92	0.51
1:C:362:VAL:HG23	1:C:408:LYS:HD2	1.93	0.51
1:B:180:MET:CE	1:B:182:MET:HE2	2.41	0.49
1:B:112:ILE:HD13	1:B:330:ILE:HG22	1.95	0.48
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.96	0.48
1:B:397:PHE:CE2	1:B:401:LEU:HD11	2.48	0.48
1:A:180:MET:CE	1:A:182:MET:HE2	2.39	0.48
1:C:293:SER:HB2	1:C:308:ALA:HB2	1.96	0.48
1:C:200:ALA:HA	1:C:266:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:PHE:CE2	1:A:401:LEU:HD11	2.51	0.46
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.98	0.46
1:B:118:PRO:HD2	1:B:379:CYS:HB3	1.99	0.45
1:B:17:GLU:HB2	1:B:311:THR:HB	1.99	0.45
1:B:290:MET:HG3	1:B:376:LEU:HD21	1.99	0.45
1:A:200:ALA:HA	1:A:266:ILE:HG13	2.00	0.44
1:A:53:ASN:ND2	1:C:395:PHE:HB3	2.32	0.44
1:C:132:ARG:HG3	1:C:274:GLY:HA3	1.99	0.44
1:A:330:ILE:HD12	1:A:363:SER:HB3	2.00	0.43
1:B:328:ASN:OD1	1:B:330:ILE:HG12	2.18	0.43
1:B:163:GLN:CD	1:B:163:GLN:H	2.25	0.43
1:B:22:ILE:HD11	1:B:327:THR:HB	2.00	0.42
1:A:210:SER:HB3	1:A:254:MET:HG2	2.02	0.42
1:B:200:ALA:HA	1:B:266:ILE:HG13	2.01	0.42
1:C:123:GLY:O	1:C:262:GLU:HA	2.20	0.42
1:C:362:VAL:HG21	1:C:405:LEU:HA	2.02	0.42
1:B:123:GLY:O	1:B:262:GLU:HA	2.21	0.41
1:B:163:GLN:HB3	1:C:3:LYS:HB3	2.03	0.41
1:A:16:ASP:HB2	1:A:311:THR:HG21	2.03	0.40
1:A:256:ALA:O	1:B:283:GLN:HG2	2.21	0.40
5:C:502:NAP:C2A	6:C:698:HOH:O	2.69	0.40
1:C:312:VAL:HB	1:C:315:HIS:HB2	2.03	0.40

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	414/425 (97%)	401 (97%)	13 (3%)	0	100	100
1	B	414/425 (97%)	397 (96%)	16 (4%)	1 (0%)	43	49
1	C	414/425 (97%)	401 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1242/1275 (97%)	1199 (96%)	42 (3%)	1 (0%)	48 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	GLN

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	349/361 (97%)	340 (97%)	9 (3%)	40 51
1	B	350/361 (97%)	341 (97%)	9 (3%)	40 51
1	C	350/361 (97%)	338 (97%)	12 (3%)	32 41
All	All	1049/1083 (97%)	1019 (97%)	30 (3%)	37 47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	12	GLU
1	A	22	ILE
1	A	28	GLU
1	A	69	VAL
1	A	94	SER
1	A	140	ARG
1	A	243	LYS
1	A	288	LEU
1	B	12	GLU
1	B	28	GLU
1	B	69	VAL
1	B	94	SER
1	B	140	ARG
1	B	160	ASP

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	243	LYS
1	B	312	VAL
1	C	3	LYS
1	C	12	GLU
1	C	28	GLU
1	C	94	SER
1	C	140	ARG
1	C	243	LYS
1	C	312	VAL
1	C	314	ARG
1	C	327	THR
1	C	379	CYS
1	C	400	LYS
1	C	414	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	68	ASN
1	A	198	GLN
1	A	213	ASN
1	A	228	GLN
1	A	320	GLN
1	A	385	ASN
1	B	14	GLN
1	B	55	GLN
1	B	101	ASN
1	B	171	ASN
1	B	198	GLN
1	B	213	ASN
1	B	228	GLN
1	B	257	GLN
1	B	277	GLN
1	B	385	ASN
1	C	14	GLN
1	C	55	GLN
1	C	198	GLN
1	C	213	ASN
1	C	228	GLN
1	C	385	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ICT	C	501	2	12,12,12	1.13	0	13,16,16	2.20	6 (46%)
5	NAP	B	501	-	50,52,52	0.81	1 (2%)	71,80,80	0.86	4 (5%)
3	ICT	A	505	2	12,12,12	1.17	0	13,16,16	1.85	4 (30%)
3	ICT	A	502	2	12,12,12	1.19	0	13,16,16	1.75	5 (38%)
5	NAP	C	502	-	50,52,52	0.80	1 (2%)	71,80,80	0.95	7 (9%)
4	DWJ	A	504	1	33,35,35	0.72	0	37,52,52	1.99	5 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ICT	C	501	2	-	3/16/16/16	-
5	NAP	B	501	-	-	10/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ICT	A	505	2	-	1/16/16/16	-
3	ICT	A	502	2	-	5/16/16/16	-
5	NAP	C	502	-	-	9/35/67/67	0/5/5/5
4	DWJ	A	504	1	-	2/14/50/50	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	NAP	C2N-N1N	4.77	1.40	1.35
5	C	502	NAP	C2N-N1N	4.48	1.39	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	DWJ	C5-C4-C3	7.52	118.16	109.04
4	A	504	DWJ	O31-C3-C4	-4.77	118.38	123.07
4	A	504	DWJ	C2-C3-C4	3.90	121.33	113.67
3	C	501	ICT	O5-C6-C3	-3.34	115.12	123.01
3	C	501	ICT	O3-C5-C4	-3.21	112.99	122.84
4	A	504	DWJ	C7-C8-C9	3.16	116.93	111.01
3	A	505	ICT	O3-C5-C4	-3.15	113.17	122.84
3	C	501	ICT	O1-C1-C2	-3.07	113.44	121.62
4	A	504	DWJ	C22-C21-N20	2.91	124.20	118.58
5	C	502	NAP	C2B-C1B-N9A	2.90	118.52	113.75
3	A	502	ICT	O5-C6-C3	-2.75	116.52	123.01
3	A	502	ICT	C4-C3-C6	-2.65	107.04	111.25
5	B	501	NAP	C6N-N1N-C1D	2.63	124.88	119.73
3	C	501	ICT	C4-C3-C6	-2.56	107.18	111.25
3	A	505	ICT	O5-C6-C3	-2.52	117.06	123.01
5	C	502	NAP	C6N-N1N-C1D	2.49	124.61	119.73
5	C	502	NAP	C4D-O4D-C1D	2.45	112.17	109.92
3	A	505	ICT	O1-C1-C2	-2.43	115.16	121.62
3	A	502	ICT	O2-C1-O1	2.35	129.41	124.08
5	C	502	NAP	O2A-PA-O5B	-2.31	97.10	107.57
3	A	502	ICT	O4-C5-O3	2.27	129.18	123.33
3	C	501	ICT	O4-C5-O3	2.26	129.15	123.33
5	B	501	NAP	C2N-N1N-C1D	-2.25	114.17	119.13
3	A	502	ICT	C3-C4-C5	-2.21	109.81	113.95
3	A	505	ICT	O2-C1-O1	2.18	129.01	124.08
5	B	501	NAP	O3-PA-O1A	2.11	117.04	110.70
3	C	501	ICT	O2-C1-O1	2.08	128.81	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	NAP	C2N-N1N-C1D	-2.07	114.57	119.13
5	C	502	NAP	O3B-C3B-C2B	2.06	116.96	111.19
5	B	501	NAP	C2B-C1B-N9A	2.05	117.13	113.75
5	C	502	NAP	P2B-O2B-C2B	2.02	128.83	123.43

There are no chirality outliers.

All (30) torsion outliers are listed below:

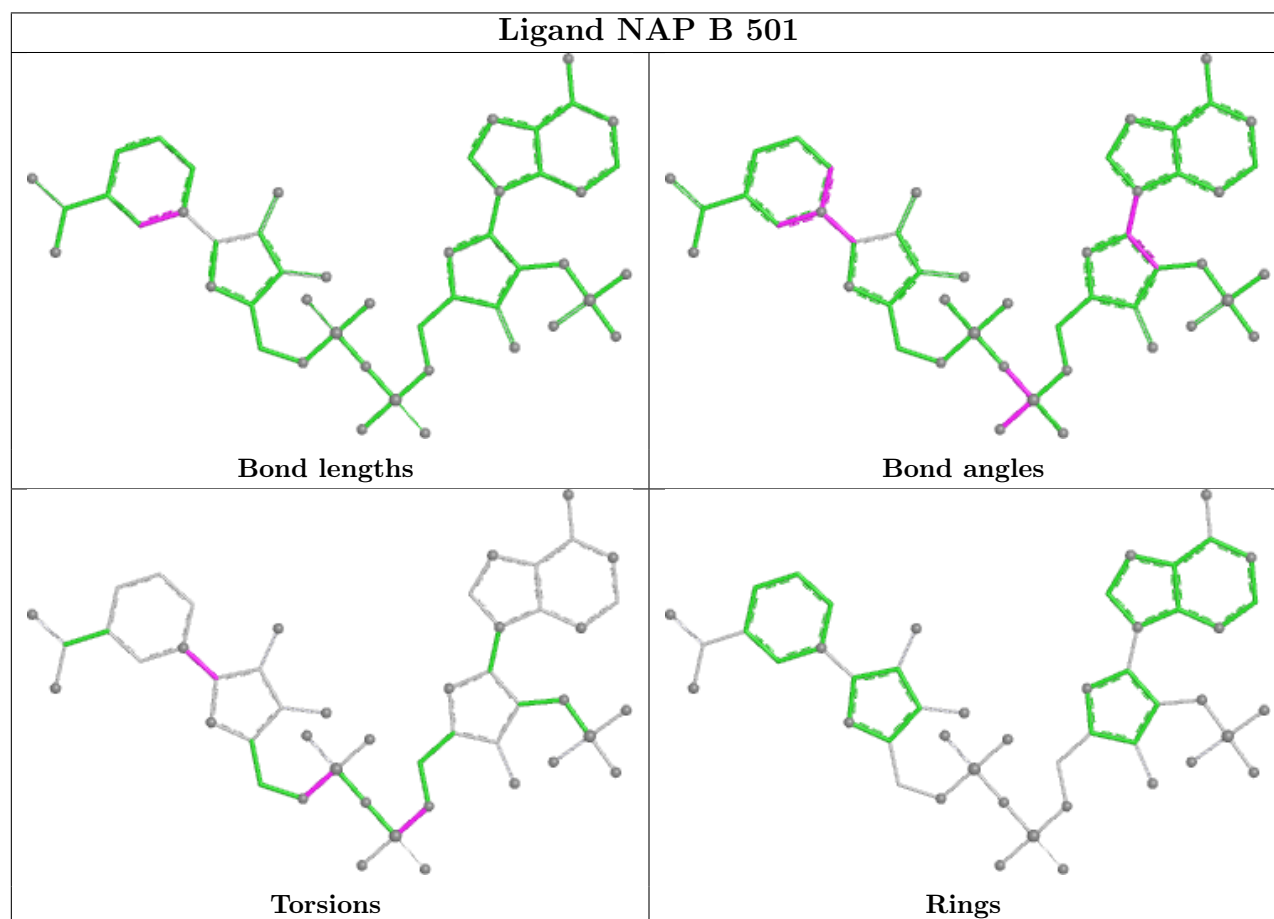
Mol	Chain	Res	Type	Atoms
4	A	504	DWJ	C22-C21-N20-N29
4	A	504	DWJ	O28-C21-N20-N29
5	B	501	NAP	C5B-O5B-PA-O3
5	B	501	NAP	C5D-O5D-PN-O3
5	B	501	NAP	C5D-O5D-PN-O1N
5	B	501	NAP	C5D-O5D-PN-O2N
5	B	501	NAP	O4D-C1D-N1N-C2N
5	B	501	NAP	O4D-C1D-N1N-C6N
5	B	501	NAP	C2D-C1D-N1N-C2N
5	C	502	NAP	C5B-O5B-PA-O1A
5	C	502	NAP	C5D-O5D-PN-O3
5	C	502	NAP	C5D-O5D-PN-O1N
5	C	502	NAP	C5D-O5D-PN-O2N
5	C	502	NAP	O4D-C1D-N1N-C2N
5	C	502	NAP	O4D-C1D-N1N-C6N
5	C	502	NAP	C2D-C1D-N1N-C2N
3	C	501	ICT	O1-C1-C2-C3
3	A	502	ICT	C4-C3-C6-O5
3	A	502	ICT	C4-C3-C6-O6
3	C	501	ICT	O2-C1-C2-C3
3	C	501	ICT	C1-C2-C3-C6
5	B	501	NAP	C5B-O5B-PA-O1A
5	B	501	NAP	C5B-O5B-PA-O2A
5	C	502	NAP	C5B-O5B-PA-O3
5	B	501	NAP	C2D-C1D-N1N-C6N
5	C	502	NAP	C2D-C1D-N1N-C6N
3	A	502	ICT	O2-C1-C2-C3
3	A	502	ICT	O1-C1-C2-C3
3	A	505	ICT	C3-C4-C5-O3
3	A	502	ICT	C1-C2-C3-C6

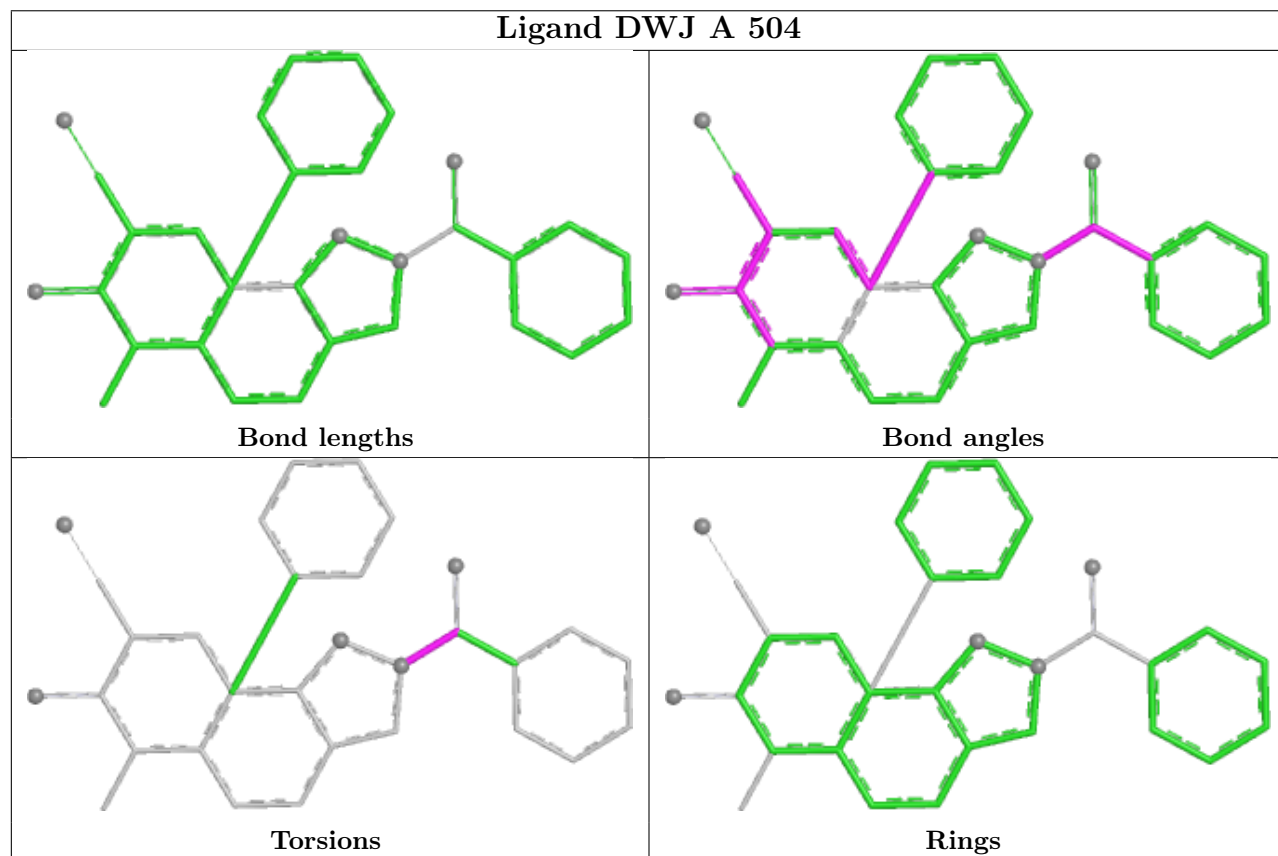
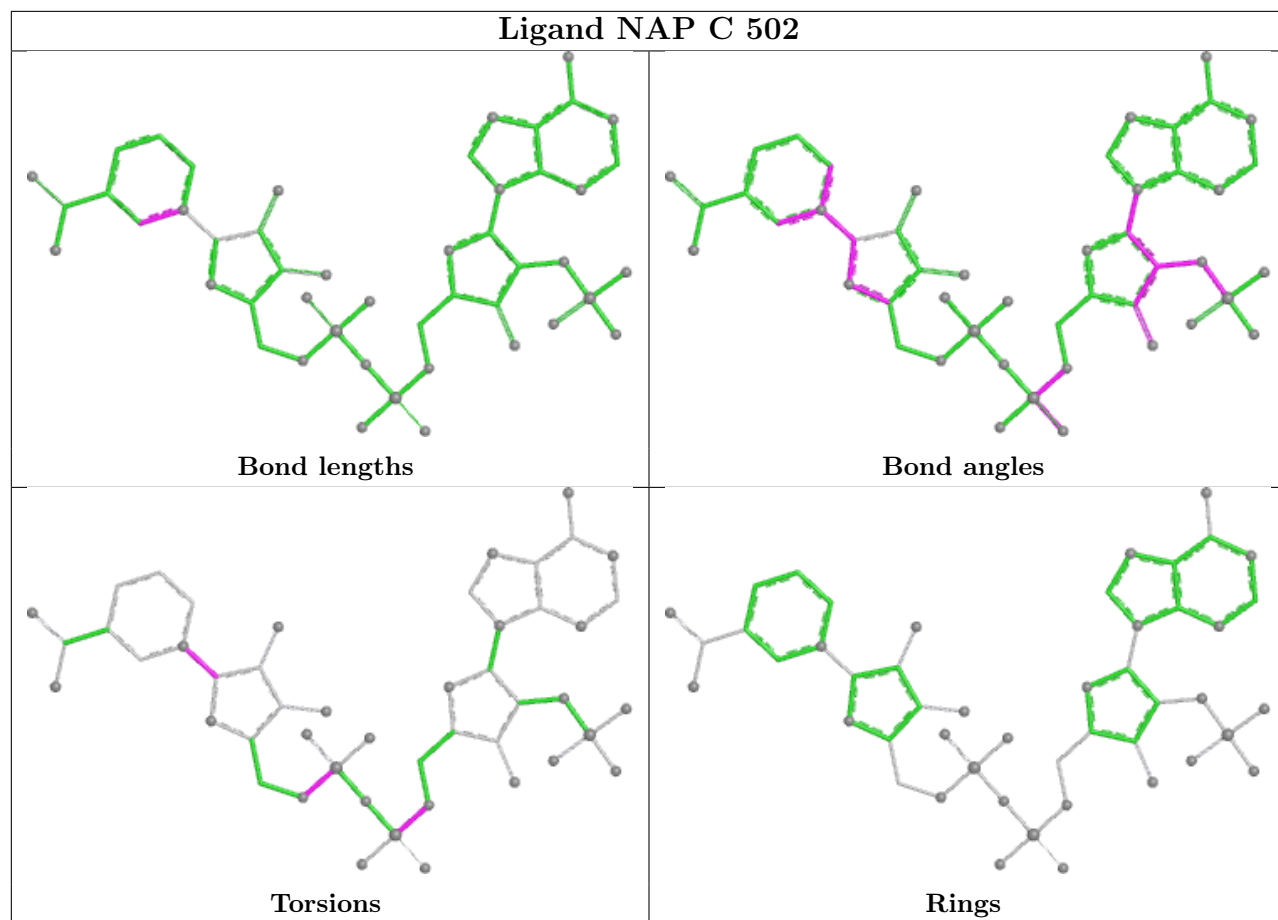
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	ICT	1	0
5	B	501	NAP	1	0
3	A	505	ICT	1	0
5	C	502	NAP	2	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.





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	416/425 (97%)	0.70	22 (5%)	32 31	33, 55, 82, 131	0
1	B	416/425 (97%)	0.60	33 (7%)	18 18	32, 54, 82, 170	0
1	C	416/425 (97%)	0.26	17 (4%)	41 41	28, 42, 74, 138	0
All	All	1248/1275 (97%)	0.52	72 (5%)	29 28	28, 51, 81, 170	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	4.3
1	A	418	HIS	4.2
1	B	416	LEU	3.7
1	C	315	HIS	3.7
1	B	162	THR	3.7
1	B	161	GLY	3.7
1	C	307	ALA	3.6
1	B	379	CYS	3.6
1	B	380	ILE	3.3
1	B	376	LEU	3.2
1	C	416	LEU	3.2
1	C	313	THR	3.2
1	C	418	HIS	3.2
1	C	318	MET	3.1
1	C	312	VAL	3.1
1	A	322	GLY	3.1
1	B	394	THR	3.0
1	A	5	ILE	3.0
1	B	325	THR	3.0
1	B	395	PHE	3.0
1	C	383	LEU	2.8
1	B	377	ALA	2.8
1	C	308	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	2.7
1	B	205	TRP	2.7
1	B	163	GLN	2.7
1	A	256	ALA	2.7
1	A	244	ILE	2.7
1	A	395	PHE	2.6
1	B	125	VAL	2.6
1	B	378	ALA	2.6
1	C	322	GLY	2.6
1	A	245	TRP	2.6
1	B	117	ILE	2.5
1	B	373	THR	2.5
1	C	314	ARG	2.5
1	B	241	ALA	2.5
1	B	383	LEU	2.5
1	B	160	ASP	2.5
1	A	405	LEU	2.4
1	C	21	ILE	2.4
1	A	202	SER	2.4
1	B	122	SER	2.4
1	A	241	ALA	2.4
1	B	391	TYR	2.3
1	C	316	TYR	2.3
1	B	414	LEU	2.3
1	C	320	GLN	2.3
1	A	414	LEU	2.3
1	A	239	PHE	2.3
1	B	282	ALA	2.3
1	A	380	ILE	2.3
1	A	201	LEU	2.3
1	B	412	ALA	2.2
1	A	120	LEU	2.2
1	B	257	GLN	2.2
1	B	291	MET	2.2
1	A	341	ALA	2.2
1	A	392	LEU	2.2
1	B	121	VAL	2.2
1	B	409	LEU	2.2
1	A	124	TRP	2.1
1	B	371	PHE	2.1
1	C	321	LYS	2.1
1	C	379	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	25	LEU	2.1
1	B	290	MET	2.1
1	A	204	GLY	2.1
1	A	417	GLU	2.0
1	B	386	VAL	2.0
1	B	323	GLN	2.0
1	B	384	PRO	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](#)

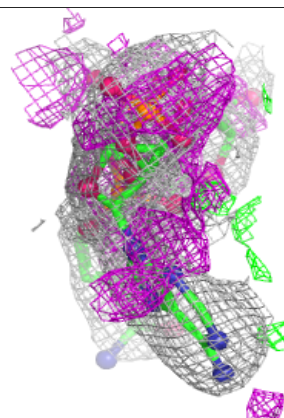
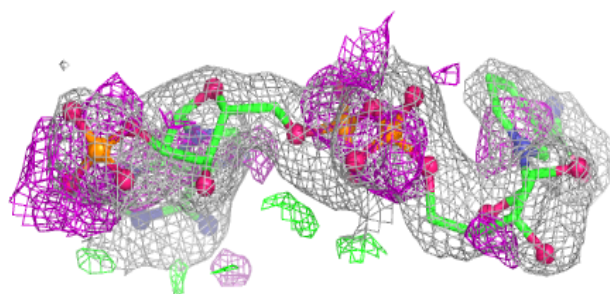
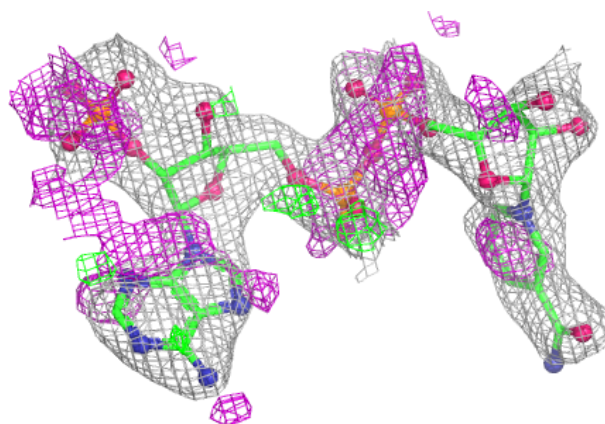
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	NAP	C	502	48/48	0.87	0.12	44,61,69,74	0
3	ICT	A	502	13/13	0.91	0.11	53,58,63,69	0
3	ICT	A	505	13/13	0.92	0.10	42,48,54,59	0
5	NAP	B	501	48/48	0.94	0.09	43,55,64,66	0
4	DWJ	A	504	31/31	0.94	0.09	55,58,64,64	0
3	ICT	C	501	13/13	0.95	0.07	40,46,55,64	0
2	MG	A	501	1/1	0.99	0.07	49,49,49,49	0
2	MG	A	503	1/1	0.99	0.03	42,42,42,42	0
2	MG	C	500	1/1	0.99	0.02	37,37,37,37	0

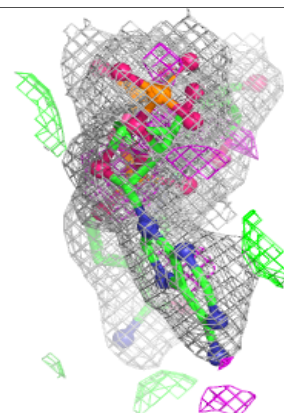
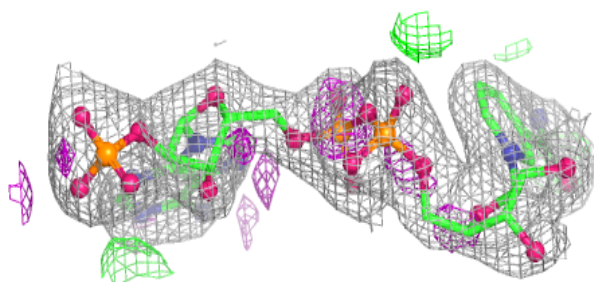
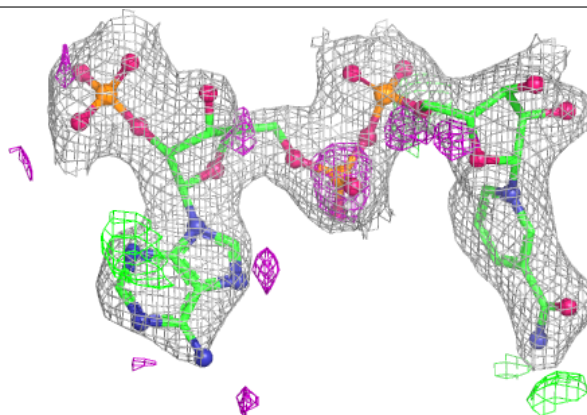
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 502:

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

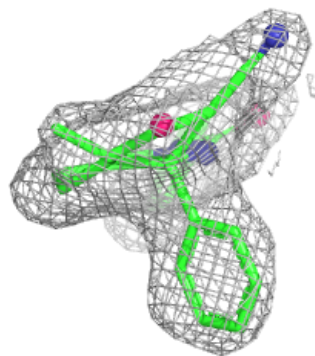
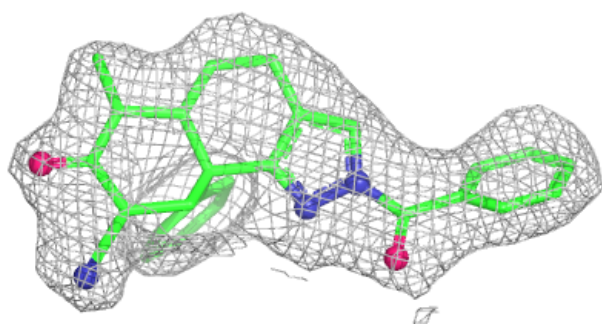
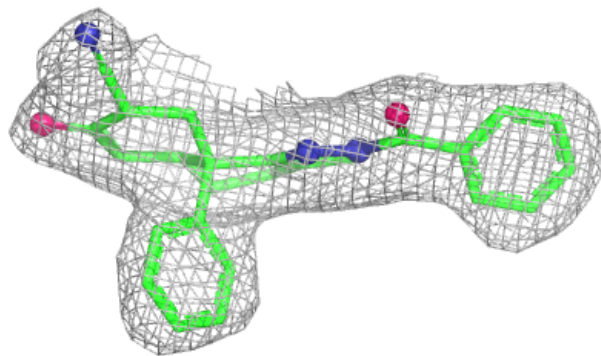
**Electron density around NAP B 501:**

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



Electron density around DWJ A 504:

$2mF_o-DF_c$ (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.