



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 AM UTC

PDB ID : 6BL1 / pdb_00006bl1
Title : Novel Modes of Inhibition of Wild-Type IDH1: Direct Covalent Modification of His315 with Cmpd13
Authors : Jakob, C.G.; Qiu, W.
Deposited on : 2017-11-09
Resolution : 2.02 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

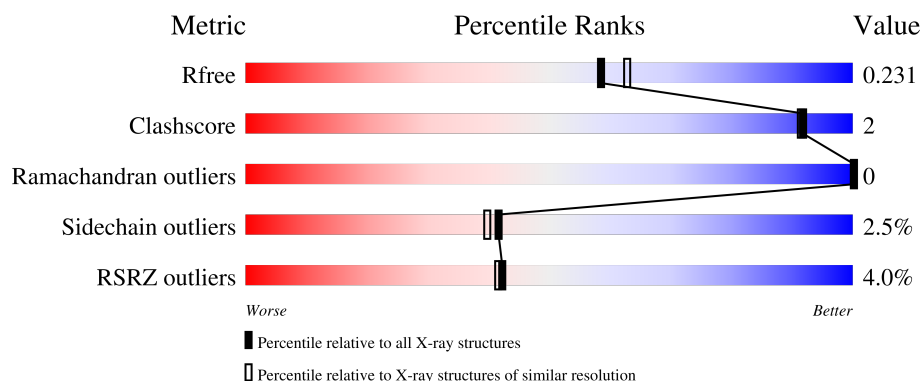
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	2% 93% 5%
1	B	425	8% 89% 8%
1	C	425	% 90% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10744 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	B	416	Total	C	N	O	S	0	2	0
			3303	2101	561	623	18			
1	C	416	Total	C	N	O	S	0	1	0
			3293	2093	559	623	18			
1	A	416	Total	C	N	O	S	0	2	0
			3303	2100	561	624	18			

There are 33 discrepancies between the modelled and reference sequences:

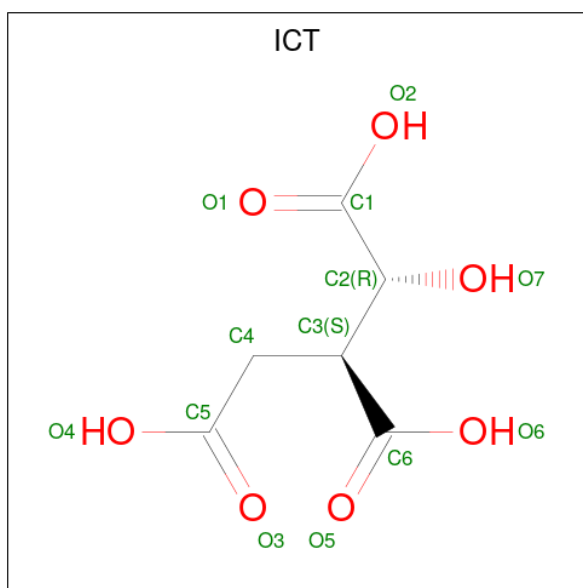
Chain	Residue	Modelled	Actual	Comment	Reference
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag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

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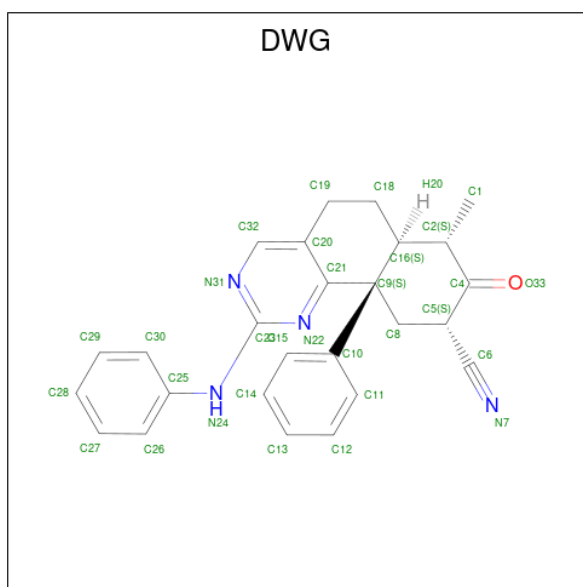
Chain	Residue	Modelled	Actual	Comment	Reference
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag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

- Molecule 2 is ISOCITRIC ACID (CCD ID: ICT) (formula: $C_6H_8O_7$).



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

- Molecule 3 is (6aS,7S,9S,10aS)-7-methyl-8-oxo-10a-phenyl-2-(phenylamino)-5,6,6a,7,8,9,10,10a-octahydrobenzo[h]quinazoline-9-carbonitrile (CCD ID: DWG) (formula: $C_{26}H_{24}N_4O$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	C	1	Total	Ca	0	0
			1	1		

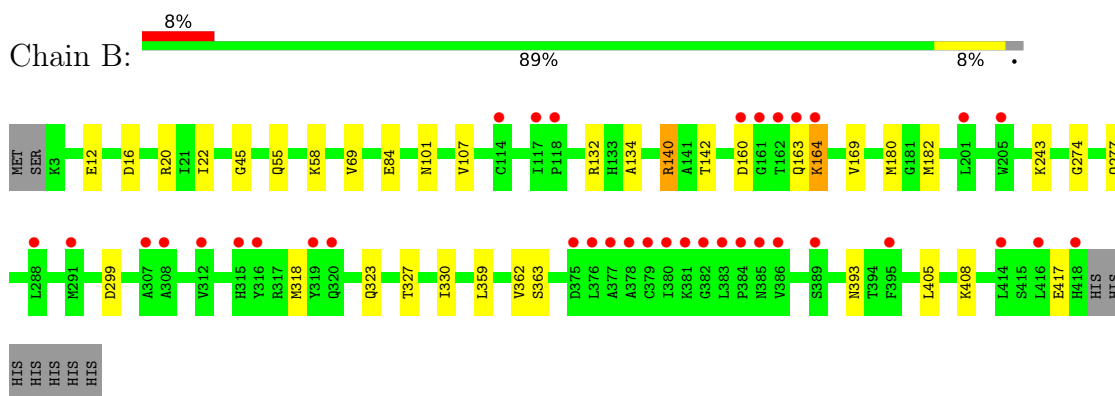
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	193	Total	O	0	0
			193	193		
5	C	313	Total	O	0	0
			313	313		
5	A	204	Total	O	0	0
			204	204		

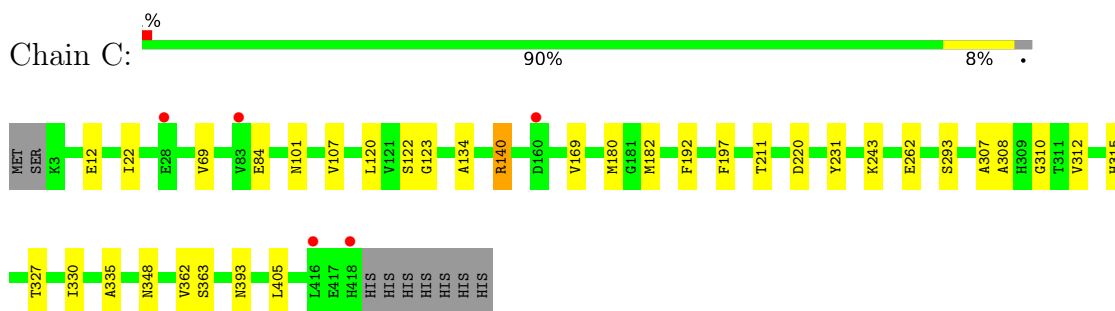
3 Residue-property plots

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

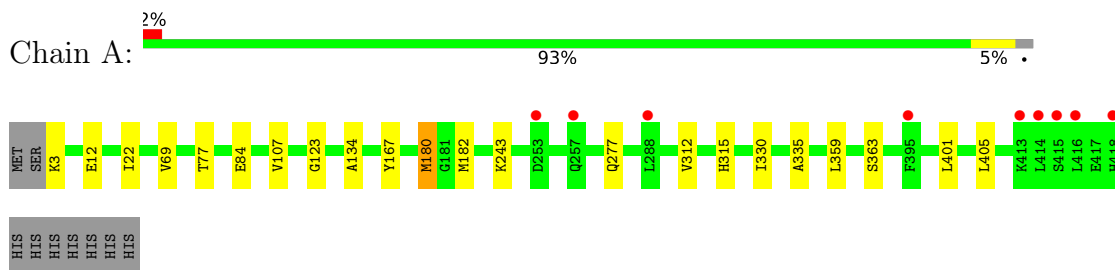
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



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- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.61Å 273.81Å 114.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.78 – 2.02 92.78 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.78-2.02) 99.9 (92.78-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.02Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.183 , 0.223 0.189 , 0.231	Depositor DCC
R_{free} test set	5135 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10744	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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, CA, DWG

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	1/3378 (0.0%)	1.28	3/4556 (0.1%)
1	B	0.84	0/3378	1.28	6/4555 (0.1%)
1	C	0.88	0/3365	1.23	7/4540 (0.2%)
All	All	0.86	1/10121 (0.0%)	1.26	16/13651 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	-6.40	1.63	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	VAL	N-CA-C	-6.92	105.02	111.45
1	C	335	ALA	N-CA-C	-6.19	104.45	111.07
1	B	393	ASN	CA-CB-CG	6.15	118.75	112.60
1	C	393	ASN	CA-CB-CG	5.99	118.59	112.60
1	C	122	SER	N-CA-C	5.71	117.96	111.11
1	A	77	THR	CB-CA-C	5.68	115.55	110.44
1	C	169	VAL	N-CA-C	-5.32	105.66	110.82
1	C	120	LEU	N-CA-C	-5.27	106.69	113.23
1	C	307	ALA	N-CA-C	-5.15	100.11	108.41
1	A	123	GLY	N-CA-C	5.13	120.37	114.16
1	B	318	MET	CA-C-N	5.08	127.09	120.28
1	B	318	MET	C-N-CA	5.08	127.09	120.28
1	A	335	ALA	N-CA-C	-5.06	105.66	111.07
1	B	299	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	192	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	16	ASP	N-CA-C	5.01	117.77	109.85

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	3303	0	3269	8	0
1	B	3303	0	3274	13	0
1	C	3293	0	3250	12	0
2	B	26	0	8	0	0
2	C	13	0	4	0	0
3	A	31	0	0	1	0
3	B	31	0	0	0	0
3	C	31	0	0	1	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	204	0	0	0	0
5	B	193	0	0	0	0
5	C	313	0	0	1	0
All	All	10744	0	9805	31	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 (31) 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:A:315:HIS:NE2	3:A:501:DWG:C8	2.36	0.88
1:C:315:HIS:NE2	3:C:503:DWG:C8	2.46	0.78
1:C:101[B]:ASN:ND2	1:C:140:ARG:HD2	2.03	0.73
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.78	0.66
1:B:142:THR:HG21	1:A:167:TYR:HB3	1.84	0.60
1:B:180:MET:HE2	1:B:182:MET:HE2	1.84	0.59
1:A:180:MET:HE2	1:A:182:MET:HE2	1.86	0.57
1:C:293:SER:HB2	1:C:308:ALA:HB2	1.90	0.54
1:B:101[B]:ASN:ND2	1:B:140:ARG:HD2	2.24	0.53
1:A:363:SER:HA	1:A:401:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLN:HE22	1:A:277:GLN:HE22	1.63	0.47
1:C:362:VAL:HG21	1:C:405:LEU:HA	1.96	0.47
1:B:55:GLN:HA	1:B:58:LYS:HE3	1.97	0.46
1:C:310:GLY:HA3	5:C:761:HOH:O	2.15	0.46
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.97	0.46
1:B:362:VAL:HG21	1:B:405:LEU:HA	1.99	0.45
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.96	0.45
1:B:132:ARG:HG3	1:B:274:GLY:HA3	1.98	0.45
1:C:22:ILE:HD11	1:C:327:THR:HB	1.99	0.45
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.99	0.45
1:C:180:MET:HE2	1:C:182:MET:HE2	2.00	0.44
1:A:330:ILE:HD12	1:A:363:SER:HB3	2.01	0.42
1:B:164[B]:LYS:H	1:B:164[B]:LYS:HG2	1.64	0.42
1:B:330:ILE:HD12	1:B:363:SER:HB3	2.02	0.42
1:C:211:THR:HB	1:C:220:ASP:HB3	2.01	0.41
1:C:197:PHE:CZ	1:C:231:TYR:HB2	2.56	0.41
1:B:20:ARG:HH21	1:B:45:GLY:HA3	1.86	0.41
1:B:359:LEU:HD13	1:B:405:LEU:HD22	2.03	0.41
1:B:107:VAL:HG23	1:B:134:ALA:HB2	2.03	0.41
1:A:359:LEU:HD13	1:A:405:LEU:HD22	2.03	0.41
1:C:123:GLY:O	1:C:262:GLU:HA	2.22	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	416/425 (98%)	402 (97%)	14 (3%)	0	100	100
1	B	416/425 (98%)	397 (95%)	19 (5%)	0	100	100
1	C	415/425 (98%)	403 (97%)	12 (3%)	0	100	100
All	All	1247/1275 (98%)	1202 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/361 (98%)	345 (98%)	7 (2%)	48	48
1	B	352/361 (98%)	339 (96%)	13 (4%)	30	24
1	C	350/361 (97%)	343 (98%)	7 (2%)	48	48
All	All	1054/1083 (97%)	1027 (97%)	27 (3%)	42	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	GLU
1	B	22	ILE
1	B	69	VAL
1	B	84	GLU
1	B	140	ARG
1	B	160	ASP
1	B	163	GLN
1	B	164[A]	LYS
1	B	164[B]	LYS
1	B	243	LYS
1	B	323	GLN
1	B	327	THR
1	B	417	GLU
1	C	12	GLU
1	C	69	VAL
1	C	84	GLU
1	C	140	ARG
1	C	243	LYS
1	C	312	VAL
1	C	348	ASN
1	A	3	LYS
1	A	12	GLU
1	A	22	ILE

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Mol	Chain	Res	Type
1	A	69	VAL
1	A	84	GLU
1	A	243	LYS
1	A	312	VAL

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

Mol	Chain	Res	Type
1	B	14	GLN
1	B	55	GLN
1	B	67	HIS
1	B	68	ASN
1	B	213	ASN
1	B	228	GLN
1	B	277	GLN
1	B	323	GLN
1	B	404	ASN
1	C	14	GLN
1	C	53	ASN
1	C	198	GLN
1	A	14	GLN
1	A	67	HIS
1	A	185	GLN
1	A	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	DWG	A	501	-	33,35,35	0.80	3 (9%)	39,51,51	1.83	9 (23%)
2	ICT	C	502	4	12,12,12	1.19	0	13,16,16	2.25	6 (46%)
3	DWG	C	503	-	33,35,35	0.89	3 (9%)	39,51,51	2.00	8 (20%)
2	ICT	B	501	4	12,12,12	1.14	0	13,16,16	1.87	4 (30%)
3	DWG	B	502	1	33,35,35	0.66	1 (3%)	39,51,51	1.84	8 (20%)
2	ICT	B	505	4	12,12,12	1.10	0	13,16,16	1.98	7 (53%)

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	DWG	A	501	-	-	0/10/46/46	0/5/5/5
2	ICT	C	502	4	-	2/16/16/16	-
3	DWG	C	503	-	-	1/10/46/46	0/5/5/5
2	ICT	B	501	4	-	5/16/16/16	-
3	DWG	B	502	1	-	0/10/46/46	0/5/5/5
2	ICT	B	505	4	-	0/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	DWG	C23-N24	2.73	1.42	1.36
3	C	503	DWG	C8-C9	-2.66	1.53	1.55
3	B	502	DWG	C23-N24	2.58	1.41	1.36
3	A	501	DWG	C23-N24	2.27	1.41	1.36
3	C	503	DWG	C5-C4	-2.20	1.50	1.53
3	A	501	DWG	C5-C4	-2.04	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	DWG	C8-C9	-2.02	1.53	1.55

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	DWG	O33-C4-C5	-7.02	116.18	123.07
3	A	501	DWG	O33-C4-C5	-5.38	117.79	123.07
3	B	502	DWG	O33-C4-C5	-4.85	118.30	123.07
3	A	501	DWG	C9-C8-C5	4.44	120.30	111.68
3	C	503	DWG	C2-C4-C5	4.34	122.20	113.67
3	B	502	DWG	C2-C4-C5	4.08	121.68	113.67
3	C	503	DWG	C9-C8-C5	4.03	119.52	111.68
3	B	502	DWG	C6-C5-C4	3.68	113.50	109.04
3	A	501	DWG	C2-C4-C5	3.59	120.71	113.67
2	B	501	ICT	O5-C6-C3	-3.58	114.57	123.01
3	A	501	DWG	C19-C20-C21	3.56	124.52	121.64
3	A	501	DWG	C6-C5-C4	3.55	113.34	109.04
2	C	502	ICT	C3-C4-C5	-3.49	107.41	113.95
3	B	502	DWG	N31-C23-N22	-3.41	123.12	126.42
3	B	502	DWG	C19-C20-C21	3.40	124.39	121.64
3	C	503	DWG	N31-C23-N22	-3.38	123.15	126.42
2	C	502	ICT	C4-C3-C6	-3.36	105.91	111.25
2	C	502	ICT	O3-C5-C4	-3.26	112.83	122.84
3	C	503	DWG	C19-C20-C21	3.10	124.15	121.64
2	B	505	ICT	O3-C5-C4	-2.89	113.97	122.84
2	B	505	ICT	O1-C1-C2	-2.76	114.26	121.62
3	C	503	DWG	C6-C5-C4	2.67	112.28	109.04
3	C	503	DWG	C10-C9-C21	-2.63	106.38	110.88
2	B	505	ICT	C4-C3-C6	-2.63	107.07	111.25
3	A	501	DWG	N31-C23-N22	-2.62	123.88	126.42
2	C	502	ICT	O1-C1-C2	-2.60	114.68	121.62
3	B	502	DWG	C1-C2-C16	-2.55	109.99	113.94
3	B	502	DWG	C8-C9-C21	-2.52	108.39	114.77
2	C	502	ICT	O4-C5-O3	2.49	129.74	123.33
2	B	505	ICT	O5-C6-C3	-2.46	117.20	123.01
3	C	503	DWG	C8-C9-C21	-2.44	108.61	114.77
2	B	505	ICT	C3-C4-C5	-2.42	109.43	113.95
3	A	501	DWG	C8-C9-C10	-2.38	106.54	111.01
2	B	501	ICT	O1-C1-C2	-2.35	115.37	121.62
2	C	502	ICT	O5-C6-C3	-2.32	117.53	123.01
3	A	501	DWG	C19-C20-C32	-2.24	118.38	121.97
2	B	501	ICT	C3-C4-C5	-2.22	109.80	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	DWG	C12-C11-C10	2.20	122.99	120.75
2	B	505	ICT	O2-C1-O1	2.17	129.00	124.08
3	B	502	DWG	C10-C9-C21	-2.12	107.26	110.88
2	B	505	ICT	O4-C5-O3	2.07	128.66	123.33
2	B	501	ICT	O4-C5-O3	2.01	128.51	123.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

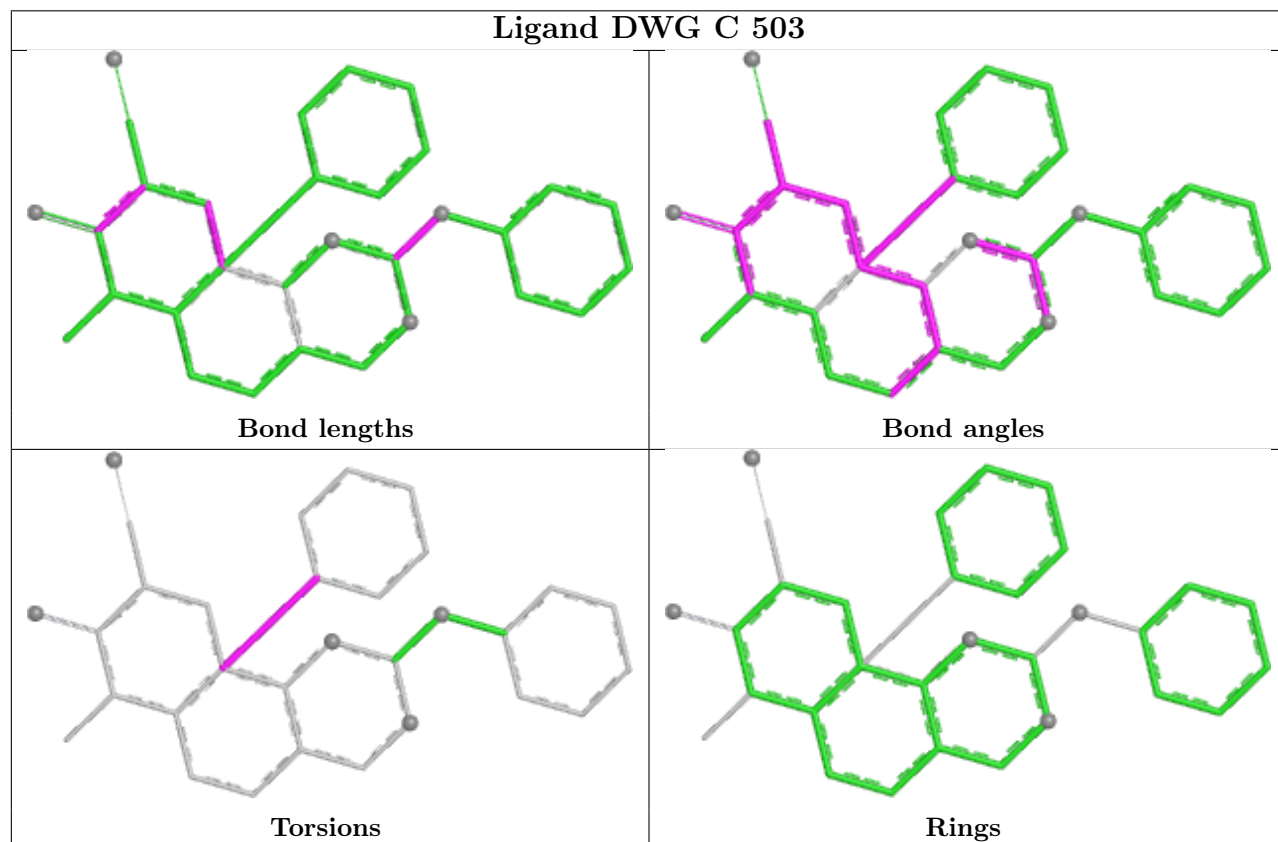
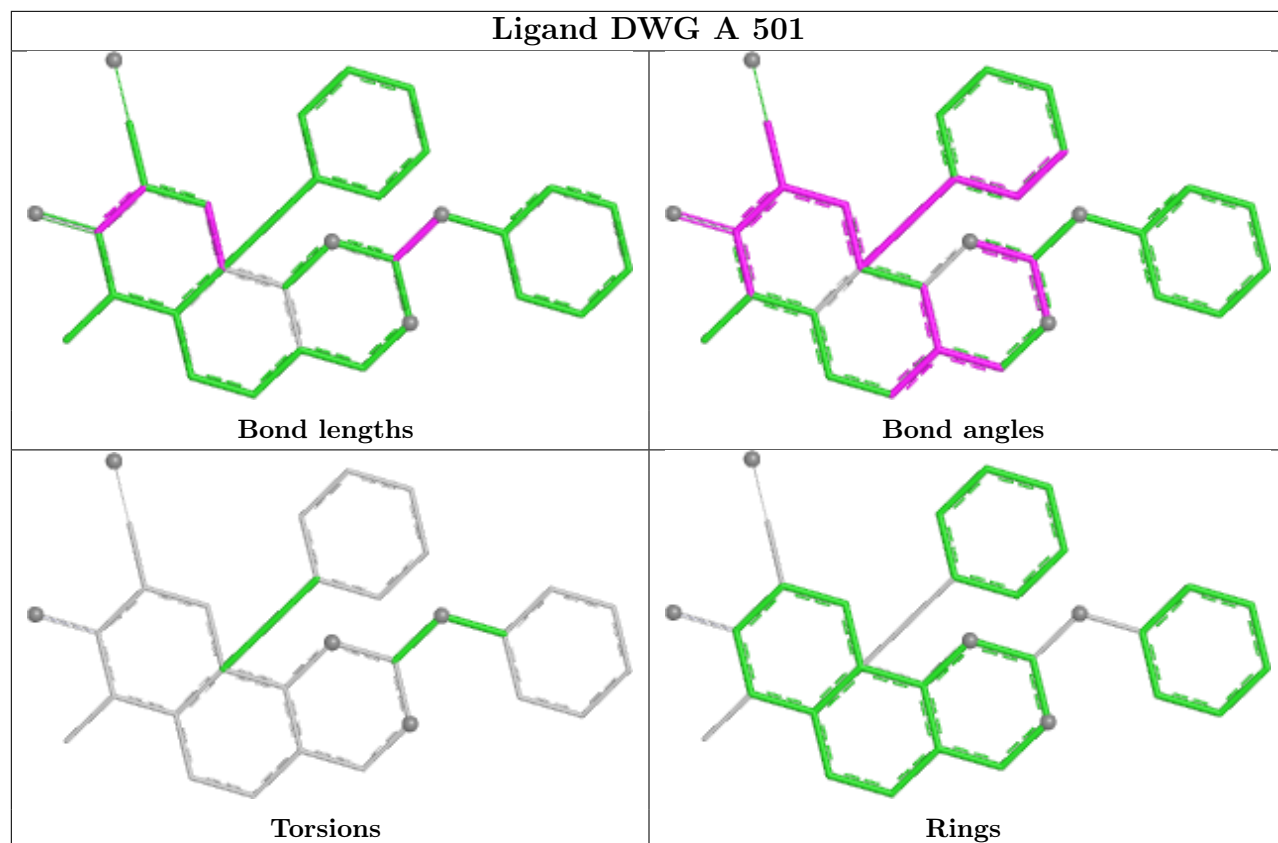
Mol	Chain	Res	Type	Atoms
2	B	501	ICT	C4-C3-C6-O5
2	B	501	ICT	C4-C3-C6-O6
2	C	502	ICT	C1-C2-C3-C6
3	C	503	DWG	C15-C10-C9-C21
2	B	501	ICT	O1-C1-C2-C3
2	B	501	ICT	O2-C1-C2-C3
2	B	501	ICT	C1-C2-C3-C6
2	C	502	ICT	C3-C4-C5-O4

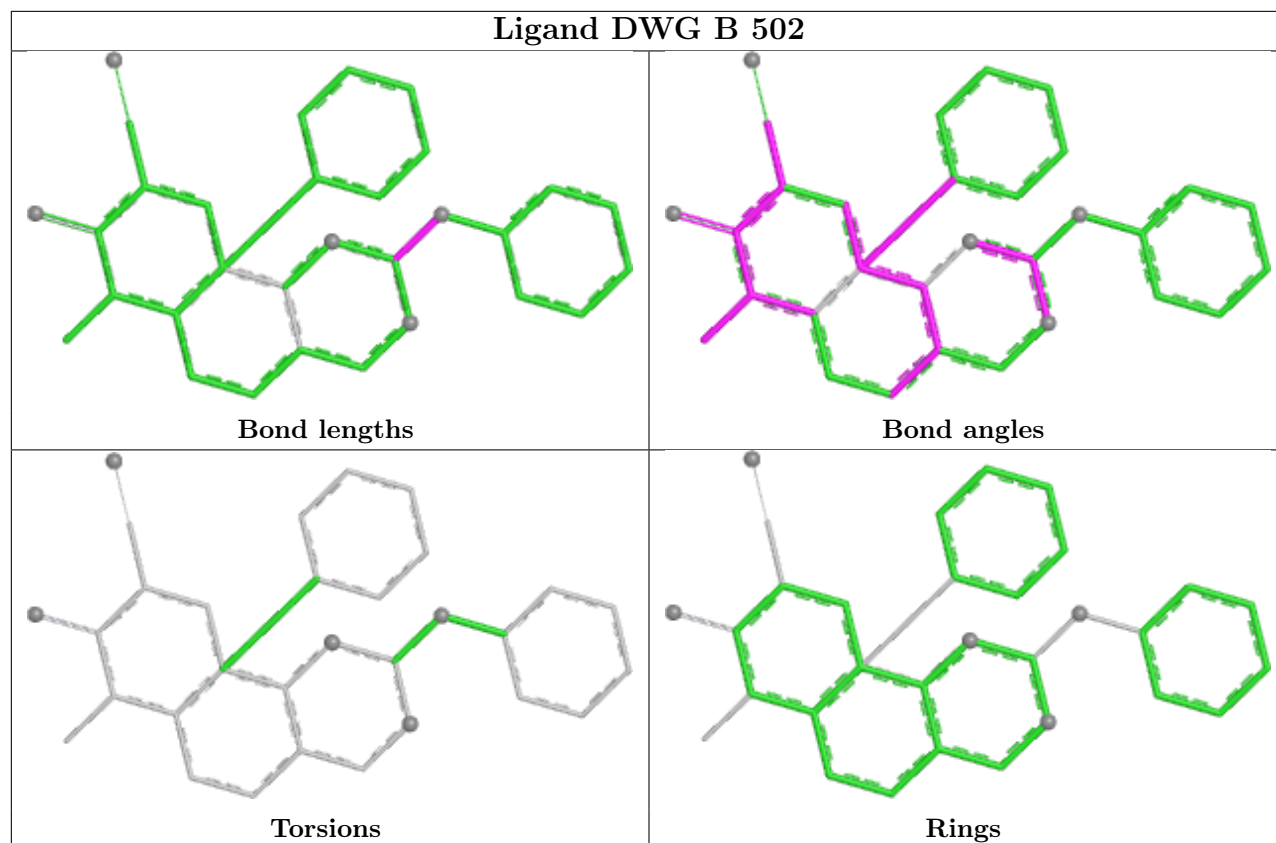
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	DWG	1	0
3	C	503	DWG	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.





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%)	0.36	9 (2%) 62 62	18, 40, 64, 110	2 (0%)
1	B	416/425 (97%)	0.52	36 (8%) 16 15	21, 39, 72, 147	2 (0%)
1	C	416/425 (97%)	-0.14	5 (1%) 76 76	16, 29, 53, 91	1 (0%)
All	All	1248/1275 (97%)	0.25	50 (4%) 42 41	16, 36, 64, 147	5 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	THR	5.4
1	B	416	LEU	5.2
1	B	164[A]	LYS	4.9
1	C	418	HIS	4.6
1	B	386	VAL	4.1
1	B	383	LEU	4.1
1	B	414	LEU	3.9
1	B	377	ALA	3.8
1	B	376	LEU	3.6
1	B	384	PRO	3.6
1	A	418	HIS	3.6
1	B	380	ILE	3.6
1	B	288	LEU	3.5
1	B	160	ASP	3.3
1	B	378	ALA	3.3
1	B	382	GLY	3.2
1	B	118	PRO	3.2
1	A	395	PHE	3.2
1	B	315	HIS	3.1
1	A	253	ASP	3.0
1	B	117	ILE	2.9
1	C	83	VAL	2.9
1	B	163	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	2.8
1	B	379	CYS	2.8
1	B	375	ASP	2.8
1	B	381	LYS	2.8
1	B	312	VAL	2.7
1	B	385	ASN	2.7
1	B	418	HIS	2.7
1	B	308	ALA	2.6
1	B	316	TYR	2.6
1	A	414	LEU	2.6
1	B	114	CYS	2.5
1	B	307	ALA	2.5
1	B	205	TRP	2.5
1	C	28	GLU	2.4
1	C	160	ASP	2.4
1	B	395	PHE	2.4
1	A	257[A]	GLN	2.4
1	B	389	SER	2.4
1	A	413	LYS	2.4
1	B	320	GLN	2.3
1	B	161	GLY	2.3
1	A	415	SER	2.2
1	B	291	MET	2.2
1	B	319	TYR	2.1
1	C	416	LEU	2.1
1	A	288	LEU	2.1
1	B	201	LEU	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.

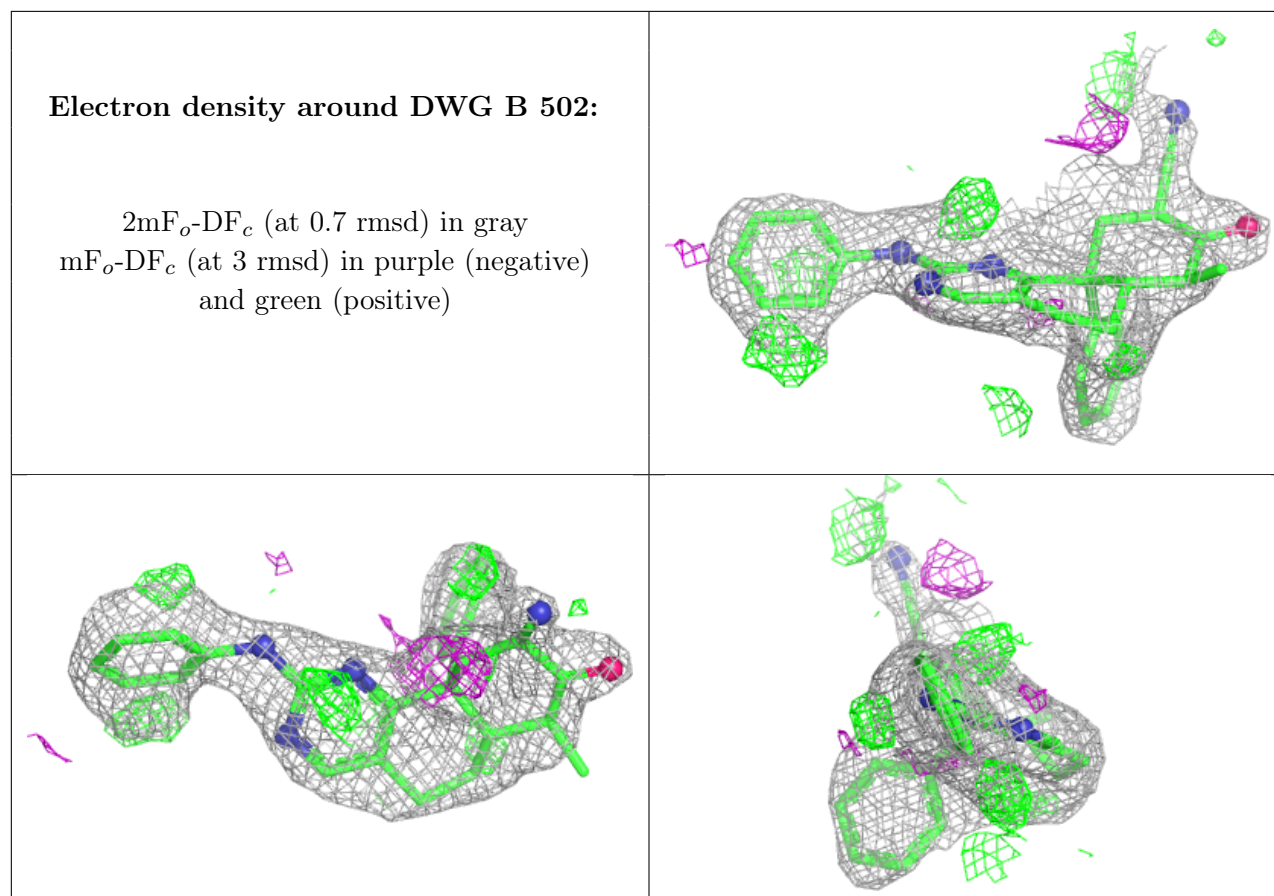
6.4 Ligands [i](#)

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.

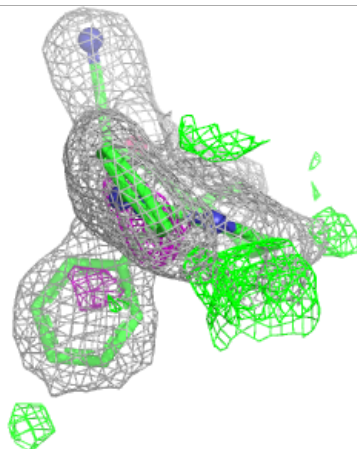
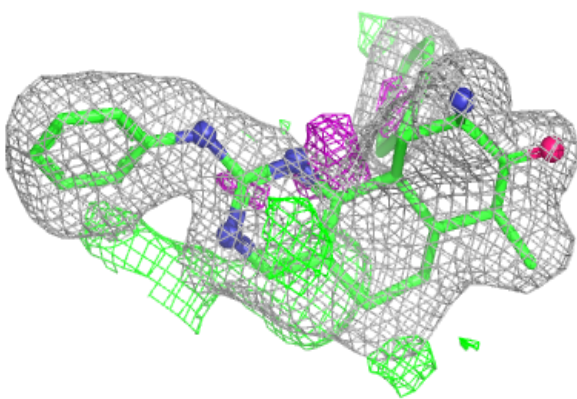
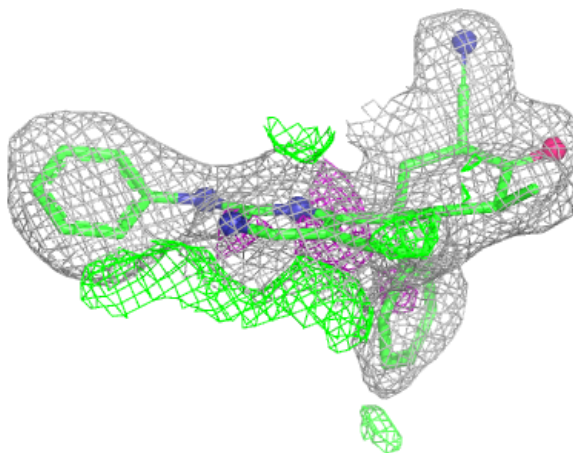
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DWG	B	502	31/31	0.80	0.16	62,65,68,69	0
3	DWG	C	503	31/31	0.83	0.14	32,45,49,50	0
3	DWG	A	501	31/31	0.88	0.13	46,50,54,56	0
2	ICT	C	502	13/13	0.90	0.11	34,40,50,52	0
2	ICT	B	505	13/13	0.90	0.11	44,48,55,56	0
2	ICT	B	501	13/13	0.91	0.10	41,45,46,47	0
4	CA	C	501	1/1	0.97	0.08	37,37,37,37	0
4	CA	B	504	1/1	0.99	0.04	51,51,51,51	0
4	CA	B	503	1/1	0.99	0.15	45,45,45,45	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.



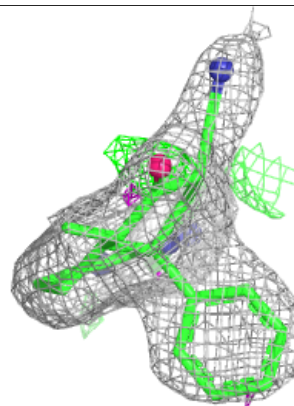
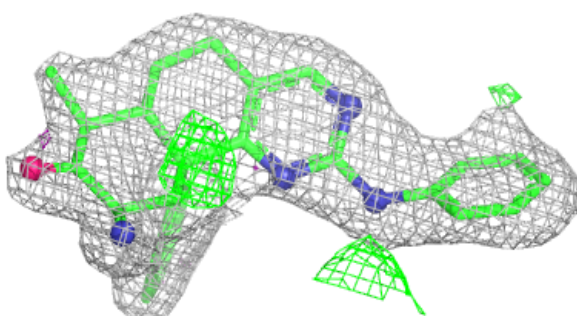
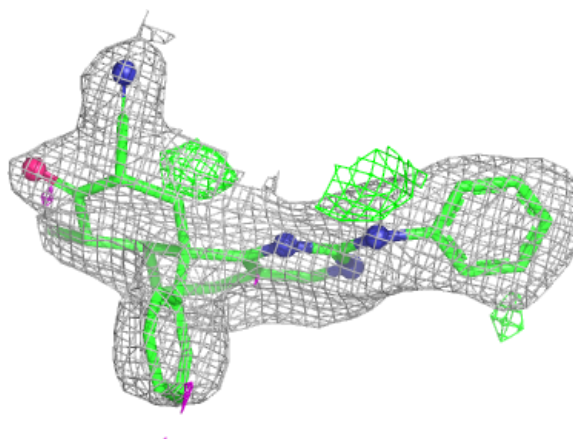
Electron density around DWG C 503:

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



Electron density around DWG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.