



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:52 PM BST

PDB ID : 6CG2  
Title : Crystal Structure of KDM4A with Compound 8  
Authors : Hosfield, D.J.; Nie, Z.  
Deposited on : 2018-02-19  
Resolution : 2.34 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

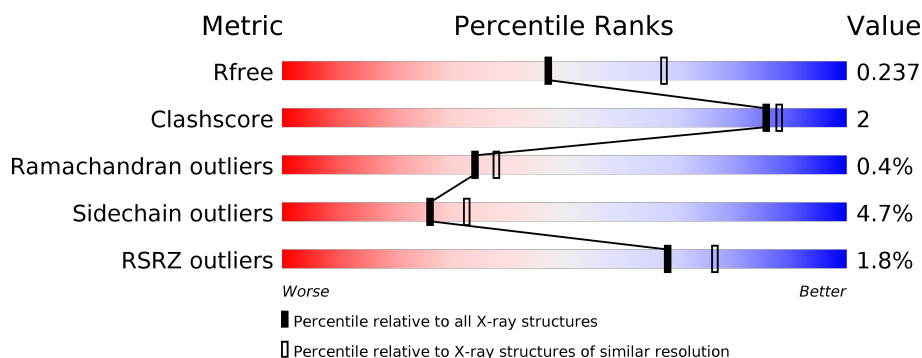
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	350	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	350	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	350	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	350	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11860 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2835	1835	477	509	14			
1	B	347	Total	C	N	O	S	0	1	0
			2858	1847	481	516	14			
1	C	335	Total	C	N	O	S	0	0	0
			2761	1792	465	490	14			
1	D	341	Total	C	N	O	S	0	0	0
			2806	1814	473	505	14			

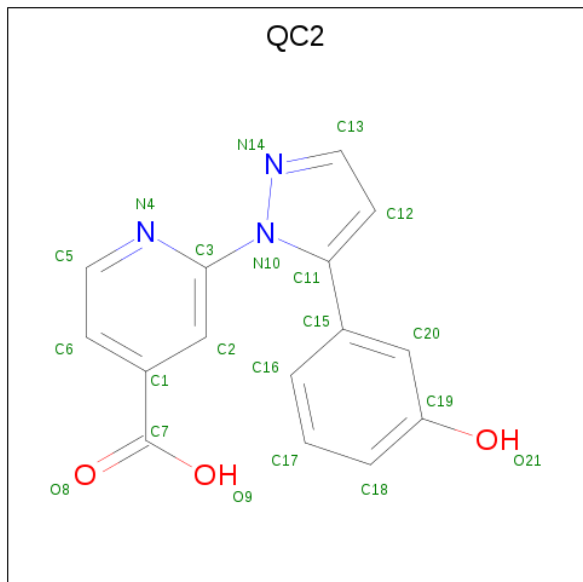
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	D	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-[5-(3-hydroxyphenyl)-1H-pyrazol-1-yl]pyridine-4-carboxylic acid (three-letter code: QC2) (formula: C<sub>15</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	15	3	3		
4	B	1	Total	C	N	O	0	0
			21	15	3	3		
4	C	1	Total	C	N	O	0	0
			21	15	3	3		
4	D	1	Total	C	N	O	0	0
			21	15	3	3		

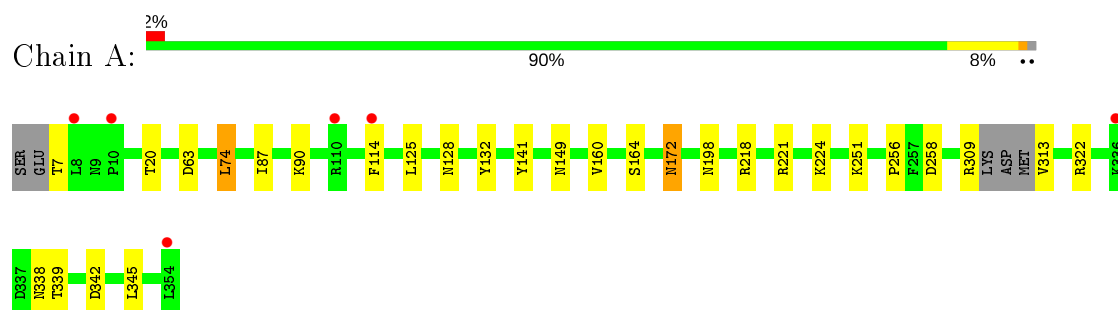
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	120	Total	O	0	0
			120	120		
5	C	124	Total	O	0	0
			124	124		
5	D	145	Total	O	0	0
			145	145		

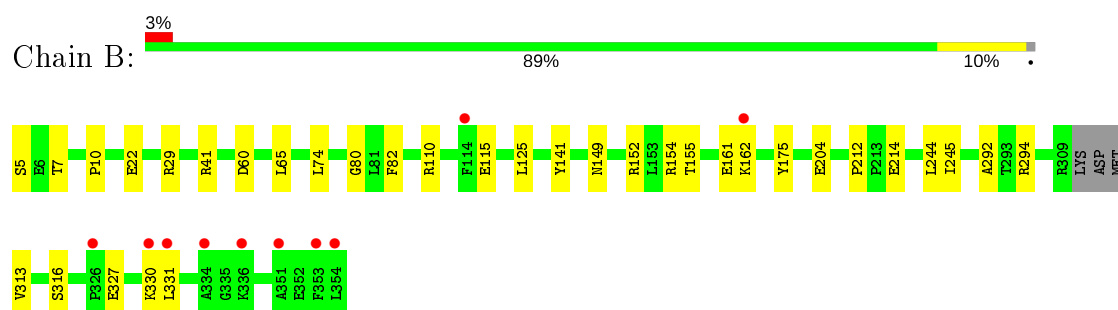
### 3 Residue-property plots [i](#)

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.

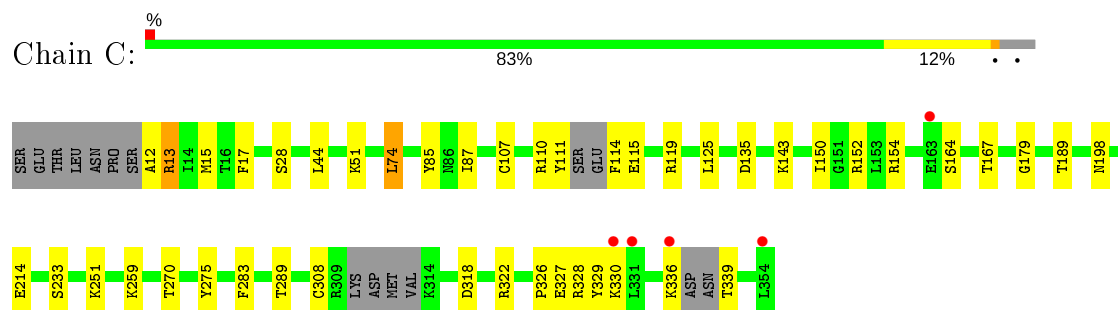
#### • Molecule 1: Lysine-specific demethylase 4A



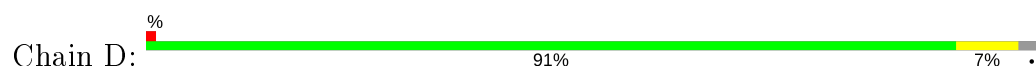
#### • Molecule 1: Lysine-specific demethylase 4A

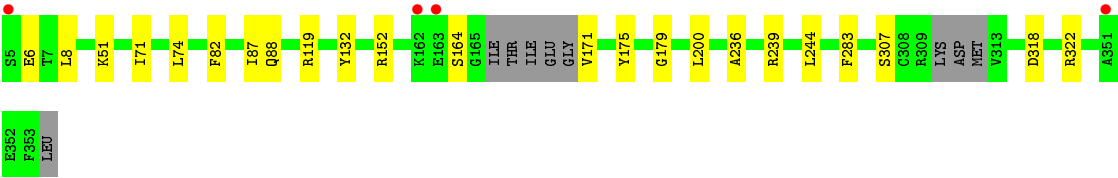


#### • Molecule 1: Lysine-specific demethylase 4A



#### • Molecule 1: Lysine-specific demethylase 4A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.46 Å 101.74 Å 142.29 Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	140.30 – 2.34 48.96 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.7 (140.30-2.34) 98.7 (48.96-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.174 , 0.234 0.178 , 0.237	Depositor DCC
$R_{free}$ test set	3442 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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 21.18 % 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 7.4095e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: QC2, ZN, NI

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	0.76	0/2921	0.88	3/3955 (0.1%)
1	B	0.76	0/2944	0.85	0/3986
1	C	0.81	2/2844 (0.1%)	0.90	4/3845 (0.1%)
1	D	0.79	0/2891	0.87	1/3912 (0.0%)
All	All	0.78	2/11600 (0.0%)	0.88	8/15698 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	TYR	CZ-OH	5.35	1.47	1.37
1	C	214	GLU	CD-OE2	5.34	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	119	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	342	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	135	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	13	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	C	152	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	258	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	221	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	2835	0	2762	14	0
1	B	2858	0	2778	9	0
1	C	2761	0	2694	19	0
1	D	2806	0	2723	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
4	C	21	0	0	0	0
4	D	21	0	0	0	0
5	A	119	0	0	8	0
5	B	120	0	0	2	0
5	C	124	0	0	7	0
5	D	145	0	0	3	0
All	All	11860	0	10957	50	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 (50) 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:313:VAL:N	5:A:601:HOH:O	1.99	0.96
1:C:114:PHE:N	5:C:601:HOH:O	2.16	0.78
1:D:322:ARG:HD2	5:D:607:HOH:O	1.96	0.66
1:A:114:PHE:HB3	5:A:715:HOH:O	1.96	0.65
1:C:198:ASN:HB2	5:C:694:HOH:O	1.98	0.63
1:C:12:ALA:N	5:C:603:HOH:O	2.33	0.60
1:B:313:VAL:N	5:B:603:HOH:O	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD23	1:A:87:ILE:HD11	1.84	0.59
1:C:87:ILE:HD11	1:D:87:ILE:HG12	1.85	0.58
1:A:198:ASN:HB2	5:A:659:HOH:O	2.03	0.57
1:C:328:ARG:NH2	1:C:336:LYS:O	2.38	0.55
1:C:328:ARG:HD2	5:C:702:HOH:O	2.09	0.53
1:C:13:ARG:NH1	5:C:607:HOH:O	2.42	0.52
1:C:87:ILE:HD11	1:D:87:ILE:CG1	2.39	0.52
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.46	0.51
1:D:82:PHE:HB2	1:D:244:LEU:HB2	1.93	0.51
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.92	0.50
1:A:198:ASN:ND2	5:A:603:HOH:O	2.42	0.50
1:C:107:CYS:HB2	5:C:703:HOH:O	2.12	0.49
1:A:251:LYS:NZ	5:A:607:HOH:O	2.44	0.49
1:C:179:GLY:O	1:C:283:PHE:HA	2.13	0.48
1:D:179:GLY:O	1:D:283:PHE:HA	2.13	0.48
1:C:15:MET:HE3	1:C:17:PHE:HZ	1.78	0.48
1:D:318:ASP:OD1	1:D:322:ARG:HD3	2.14	0.47
1:A:74:LEU:HD23	1:A:87:ILE:CD1	2.45	0.47
1:C:44:LEU:HD13	1:C:270:THR:HG22	1.96	0.47
1:C:15:MET:CE	1:C:17:PHE:HZ	2.27	0.47
1:C:322:ARG:HG3	1:C:329:TYR:CD2	2.50	0.47
1:D:236:ALA:HB1	1:D:239:ARG:HG3	1.97	0.47
1:B:204:GLU:OE2	5:B:601:HOH:O	2.21	0.46
1:A:7:THR:HA	1:A:256:PRO:HB3	1.97	0.46
1:C:150:ILE:HG23	1:C:289:THR:HG22	1.98	0.46
1:D:322:ARG:CD	5:D:607:HOH:O	2.60	0.45
1:C:74:LEU:CD2	1:C:87:ILE:HD12	2.46	0.45
1:B:41:ARG:O	1:B:212:PRO:HB3	2.17	0.45
1:D:322:ARG:NE	5:D:607:HOH:O	2.50	0.45
1:A:141:TYR:CE2	1:A:149:ASN:HA	2.53	0.43
1:B:212:PRO:HB2	1:B:214:GLU:HG2	2.01	0.43
1:A:7:THR:HG21	5:A:699:HOH:O	2.19	0.43
1:A:172:ASN:HA	1:A:172:ASN:HD22	1.58	0.42
1:B:7:THR:O	1:B:10:PRO:HD3	2.19	0.42
1:D:200:LEU:HA	1:D:200:LEU:HD12	1.94	0.41
1:A:160:VAL:O	1:A:164:SER:HB2	2.20	0.41
1:A:7:THR:HG23	5:A:709:HOH:O	2.20	0.41
1:A:20:THR:HA	5:A:667:HOH:O	2.20	0.41
1:C:189:THR:HG23	1:C:275:TYR:CE1	2.56	0.41
1:B:80:GLY:O	1:B:245:ILE:HA	2.21	0.41
1:C:85:TYR:CD1	1:D:74:LEU:HD11	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:THR:N	5:C:616:HOH:O	2.54	0.40
1:B:155:THR:HB	1:B:292:ALA:O	2.21	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	341/350 (97%)	326 (96%)	15 (4%)	0	100	100
1	B	344/350 (98%)	332 (96%)	10 (3%)	2 (1%)	25	26
1	C	327/350 (93%)	313 (96%)	12 (4%)	2 (1%)	25	26
1	D	335/350 (96%)	328 (98%)	5 (2%)	2 (1%)	25	26
All	All	1347/1400 (96%)	1299 (96%)	42 (3%)	6 (0%)	34	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	ARG
1	B	152	ARG
1	C	154	ARG
1	D	152	ARG
1	D	164	SER
1	C	326	PRO

### 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	302/307 (98%)	288 (95%)	14 (5%)	27	33
1	B	305/307 (99%)	288 (94%)	17 (6%)	21	24
1	C	292/307 (95%)	276 (94%)	16 (6%)	21	25
1	D	299/307 (97%)	290 (97%)	9 (3%)	41	50
All	All	1198/1228 (98%)	1142 (95%)	56 (5%)	26	33

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	74	LEU
1	A	90	LYS
1	A	125	LEU
1	A	128	ASN
1	A	132	TYR
1	A	172	ASN
1	A	218	ARG
1	A	224	LYS
1	A	309	ARG
1	A	322	ARG
1	A	338	ASN
1	A	339	THR
1	A	345	LEU
1	B	5	SER
1	B	22	GLU
1	B	29	ARG
1	B	60	ASP
1	B	65	LEU
1	B	74	LEU
1	B	110	ARG
1	B	115	GLU
1	B	125	LEU
1	B	161	GLU
1	B	162	LYS
1	B	175	TYR
1	B	294	ARG
1	B	316	SER
1	B	327	GLU
1	B	330	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	331	LEU
1	C	28	SER
1	C	51	LYS
1	C	74	LEU
1	C	110	ARG
1	C	115	GLU
1	C	125	LEU
1	C	143	LYS
1	C	164	SER
1	C	167	THR
1	C	233	SER
1	C	251	LYS
1	C	259	LYS
1	C	308	CYS
1	C	318	ASP
1	C	327	GLU
1	C	330	LYS
1	D	6	GLU
1	D	8	LEU
1	D	51	LYS
1	D	71	ILE
1	D	88	GLN
1	D	132	TYR
1	D	171	VAL
1	D	175	TYR
1	D	307	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	172	ASN
1	B	215	HIS
1	D	172	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
4	QC2	C	503	2	20,23,23	3.05	7 (35%)	22,32,32	2.68	9 (40%)
4	QC2	D	503	2	20,23,23	3.19	8 (40%)	22,32,32	3.13	8 (36%)
4	QC2	A	503	2	20,23,23	3.12	6 (30%)	22,32,32	2.29	7 (31%)
4	QC2	B	503	2	20,23,23	2.96	8 (40%)	22,32,32	2.86	8 (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
4	QC2	C	503	2	-	0/4/12/12	0/3/3/3
4	QC2	D	503	2	-	0/4/12/12	0/3/3/3
4	QC2	A	503	2	-	1/4/12/12	0/3/3/3
4	QC2	B	503	2	-	1/4/12/12	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	QC2	C1-C7	-7.84	1.39	1.47
4	D	503	QC2	C1-C7	-7.69	1.40	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	QC2	C3-N10	-7.00	1.32	1.44
4	D	503	QC2	C15-C11	-6.93	1.36	1.48
4	B	503	QC2	C15-C11	-6.90	1.36	1.48
4	A	503	QC2	C1-C7	-6.87	1.40	1.47
4	A	503	QC2	C3-N10	-6.71	1.33	1.44
4	A	503	QC2	C15-C11	-6.66	1.36	1.48
4	B	503	QC2	C1-C7	-6.57	1.41	1.47
4	C	503	QC2	C3-N10	-6.36	1.33	1.44
4	C	503	QC2	C15-C11	-6.18	1.37	1.48
4	B	503	QC2	C3-N10	-5.11	1.35	1.44
4	A	503	QC2	C3-N4	5.01	1.42	1.32
4	B	503	QC2	C12-C11	-4.43	1.33	1.39
4	C	503	QC2	C12-C11	-4.13	1.33	1.39
4	A	503	QC2	C12-C11	-4.06	1.33	1.39
4	D	503	QC2	C12-C11	-3.76	1.34	1.39
4	B	503	QC2	C3-N4	3.61	1.39	1.32
4	C	503	QC2	C3-N4	3.21	1.38	1.32
4	B	503	QC2	C12-C13	-2.90	1.34	1.38
4	A	503	QC2	C5-N4	-2.65	1.29	1.34
4	D	503	QC2	N14-N10	-2.56	1.34	1.39
4	D	503	QC2	C17-C16	2.54	1.44	1.38
4	B	503	QC2	C5-N4	-2.33	1.29	1.34
4	C	503	QC2	C12-C13	-2.33	1.34	1.38
4	D	503	QC2	C12-C13	-2.26	1.34	1.38
4	D	503	QC2	C5-N4	-2.07	1.30	1.34
4	B	503	QC2	C20-C19	2.06	1.42	1.39
4	C	503	QC2	C5-N4	-2.01	1.30	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	QC2	C5-N4-C3	9.09	123.50	115.56
4	D	503	QC2	C5-N4-C3	8.90	123.33	115.56
4	C	503	QC2	C5-N4-C3	8.40	122.89	115.56
4	D	503	QC2	C13-N14-N10	7.14	108.90	103.70
4	A	503	QC2	C5-N4-C3	5.42	120.29	115.56
4	C	503	QC2	C13-C12-C11	4.99	108.82	104.80
4	B	503	QC2	C13-N14-N10	4.98	107.33	103.70
4	A	503	QC2	C13-C12-C11	4.76	108.64	104.80
4	B	503	QC2	C13-C12-C11	4.33	108.29	104.80
4	A	503	QC2	C13-N14-N10	4.01	106.62	103.70
4	D	503	QC2	C18-C19-C20	3.94	124.50	120.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	QC2	C13-C12-C11	3.94	107.98	104.80
4	C	503	QC2	C1-C2-C3	3.57	120.73	118.12
4	B	503	QC2	C18-C19-C20	3.48	123.99	120.17
4	D	503	QC2	C12-C11-C15	-3.25	121.72	127.54
4	A	503	QC2	C1-C2-C3	3.17	120.44	118.12
4	A	503	QC2	C18-C19-C20	3.09	123.56	120.17
4	D	503	QC2	C16-C15-C11	2.99	126.09	120.74
4	C	503	QC2	C17-C16-C15	2.80	124.08	120.56
4	B	503	QC2	C17-C18-C19	-2.73	115.45	119.31
4	C	503	QC2	C6-C5-N4	-2.69	120.61	123.96
4	C	503	QC2	C12-C11-C15	-2.59	122.89	127.54
4	B	503	QC2	C12-C11-C15	-2.51	123.04	127.54
4	B	503	QC2	C1-C2-C3	2.41	119.89	118.12
4	D	503	QC2	C17-C16-C15	2.35	123.52	120.56
4	A	503	QC2	C17-C16-C15	2.35	123.52	120.56
4	C	503	QC2	C2-C3-N10	2.34	124.86	120.58
4	B	503	QC2	C6-C5-N4	-2.32	121.07	123.96
4	C	503	QC2	C13-N14-N10	2.32	105.39	103.70
4	C	503	QC2	C18-C19-C20	2.27	122.66	120.17
4	D	503	QC2	C6-C1-C7	-2.12	117.52	120.37
4	A	503	QC2	C2-C1-C7	2.09	123.11	120.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	QC2	C12-C11-C15-C16
4	A	503	QC2	N10-C11-C15-C16

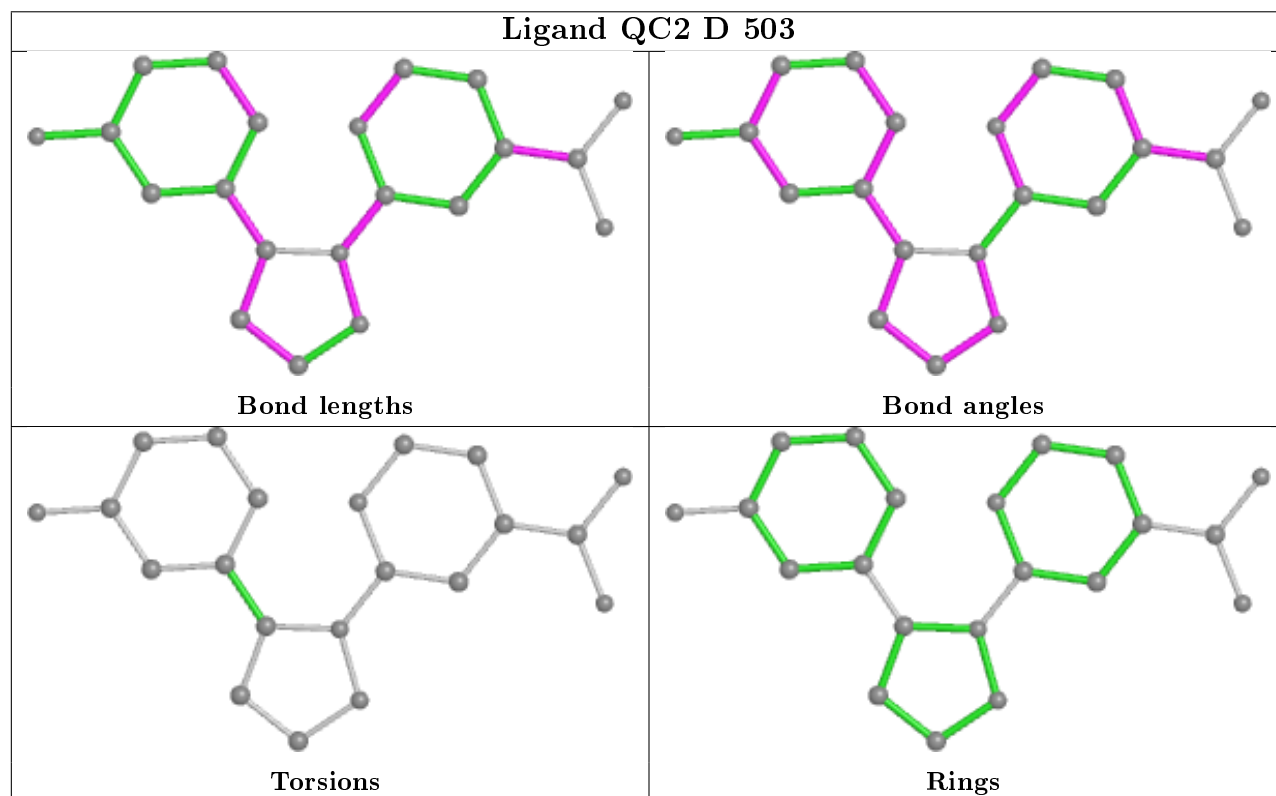
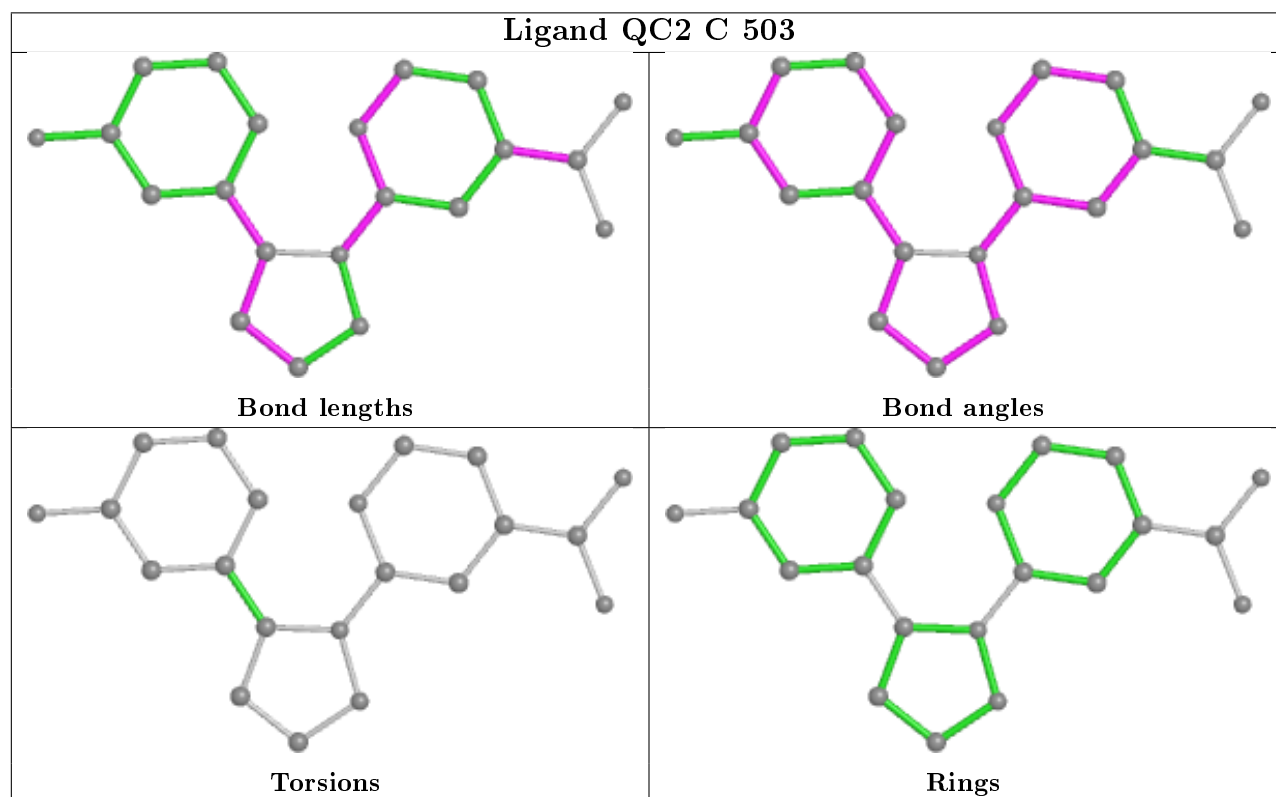
There are no ring outliers.

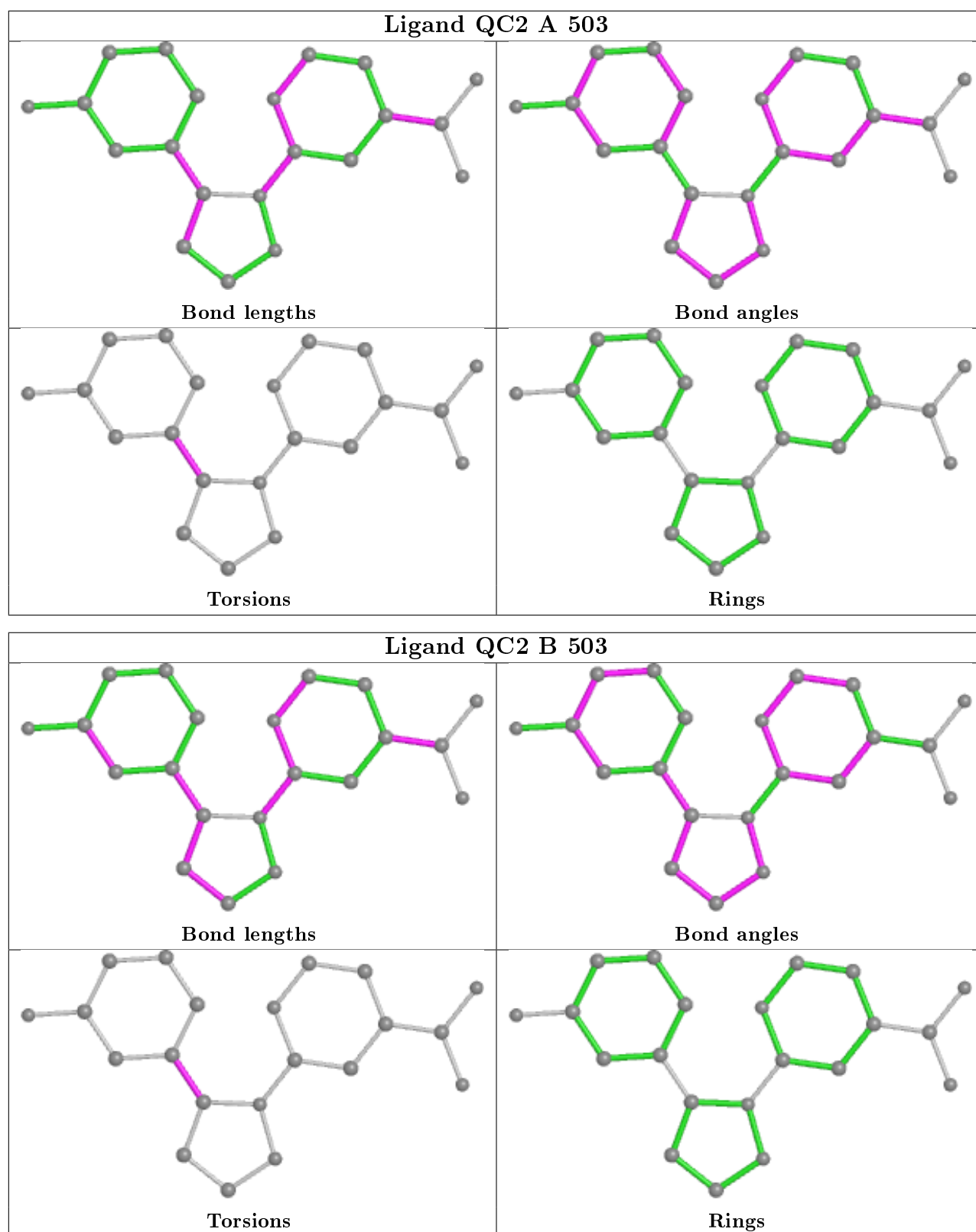
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	345/350 (98%)	0.01	6 (1%) 70 78	23, 42, 76, 97	1 (0%)
1	B	347/350 (99%)	-0.03	10 (2%) 51 61	20, 41, 79, 102	0
1	C	335/350 (95%)	-0.09	5 (1%) 73 81	19, 40, 80, 101	0
1	D	341/350 (97%)	-0.12	4 (1%) 79 85	19, 35, 68, 121	0
All	All	1368/1400 (97%)	-0.06	25 (1%) 68 76	19, 39, 77, 121	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	3.3
1	D	351	ALA	3.3
1	A	114	PHE	3.2
1	A	354	LEU	3.2
1	D	162	LYS	3.2
1	C	331	LEU	3.1
1	C	336	LYS	3.1
1	B	162	LYS	3.0
1	D	163	GLU	3.0
1	B	336	LYS	2.9
1	A	336	LYS	2.9
1	B	330	LYS	2.9
1	B	351	ALA	2.8
1	D	5	SER	2.8
1	B	331	LEU	2.5
1	A	10	PRO	2.3
1	A	8	LEU	2.2
1	B	353	PHE	2.2
1	C	163	GLU	2.2
1	B	354	LEU	2.2
1	C	330	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	326	PRO	2.1
1	B	114	PHE	2.1
1	A	110	ARG	2.0
1	B	334	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

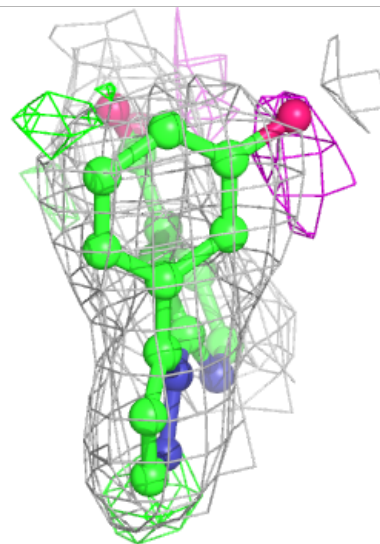
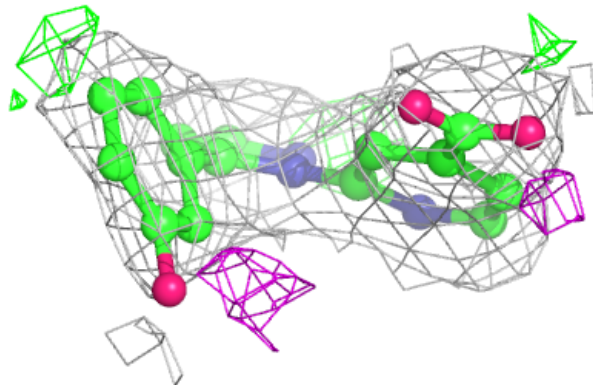
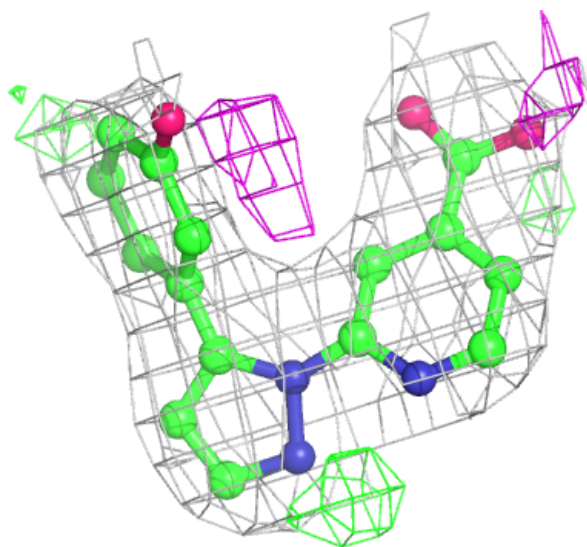
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	QC2	C	503	21/21	0.95	0.16	34,39,47,59	0
4	QC2	D	503	21/21	0.96	0.13	25,29,36,48	0
4	QC2	A	503	21/21	0.96	0.15	31,34,45,54	0
4	QC2	B	503	21/21	0.97	0.13	31,34,41,54	0
3	ZN	B	502	1/1	0.99	0.10	42,42,42,42	0
3	ZN	C	502	1/1	0.99	0.09	53,53,53,53	0
2	NI	C	501	1/1	0.99	0.14	30,30,30,30	0
3	ZN	D	502	1/1	0.99	0.11	34,34,34,34	0
2	NI	B	501	1/1	1.00	0.13	28,28,28,28	0
3	ZN	A	502	1/1	1.00	0.10	39,39,39,39	0
2	NI	D	501	1/1	1.00	0.14	25,25,25,25	0
2	NI	A	501	1/1	1.00	0.14	26,26,26,26	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.

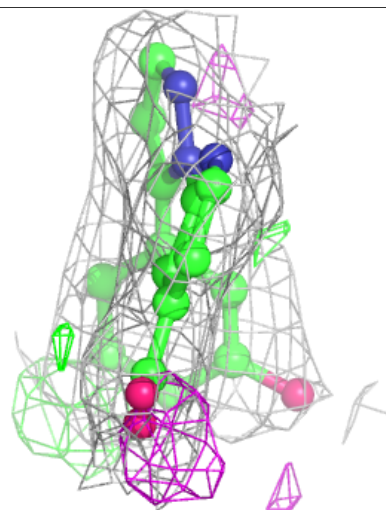
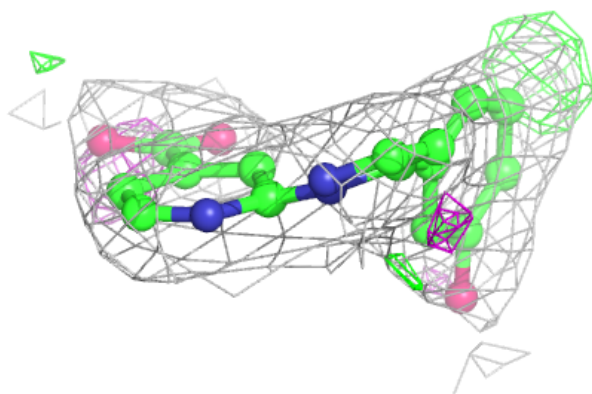
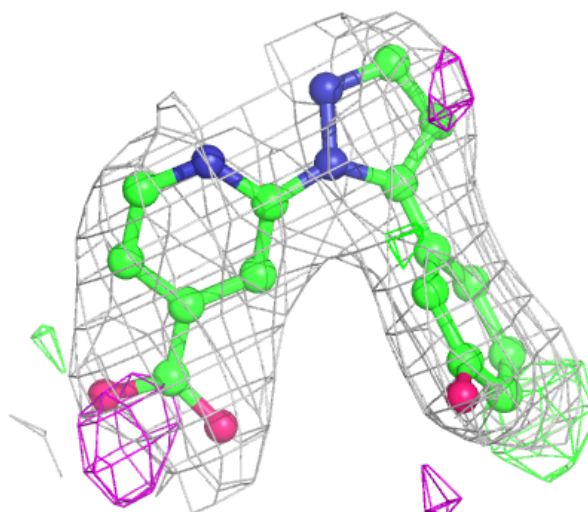
**Electron density around QC2 C 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



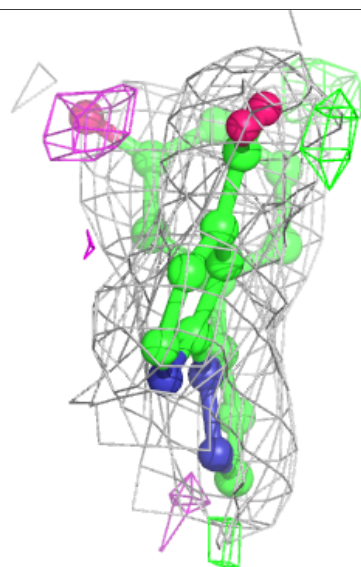
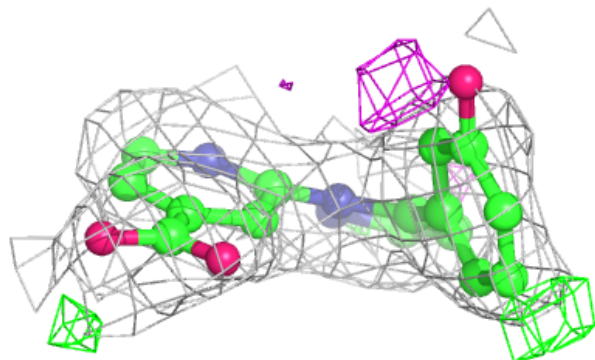
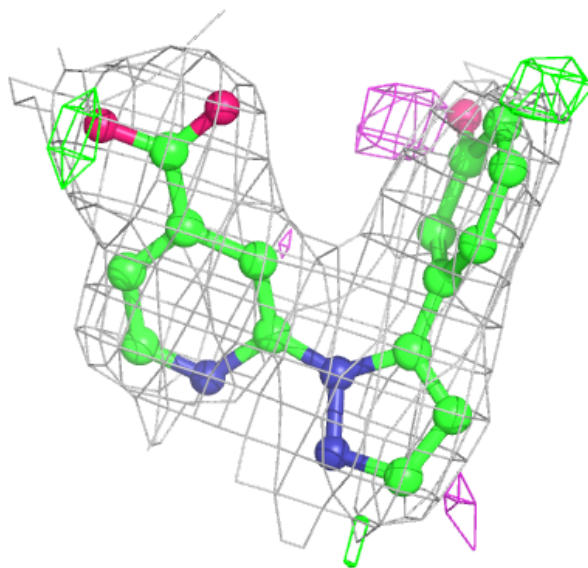
**Electron density around QC2 D 503:**

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



**Electron density around QC2 A 503:**

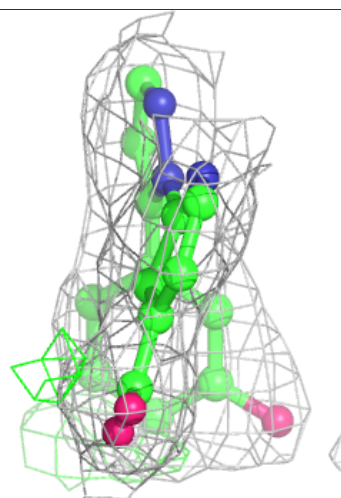
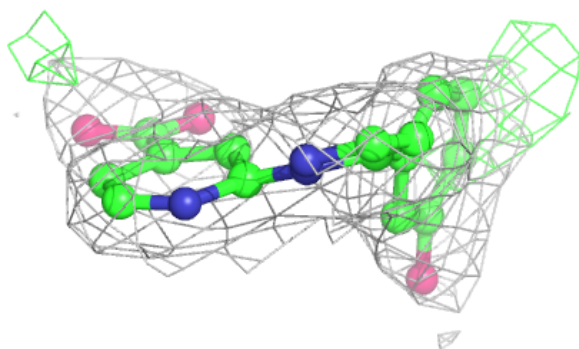
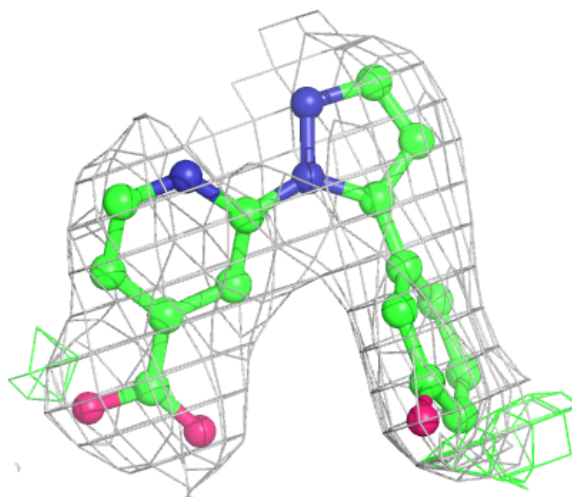
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QC2 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.