



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:37 am BST

PDB ID : 6SZM
Title : Crystal structure of the ACVR1 (ALK2) kinase in complex with the compound M4K2009
Authors : Adamson, R.J.; Williams, E.P.; Smil, D.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.N.
Deposited on : 2019-10-02
Resolution : 1.42 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 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 : 2.11
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) : 2.11

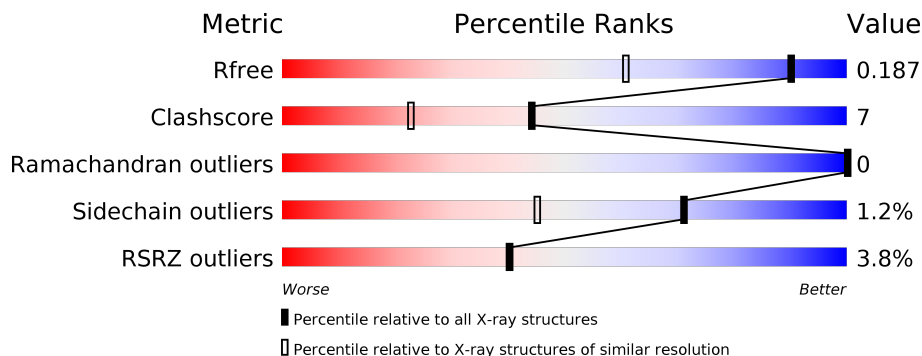
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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 ≥ 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	301	 4% 88% 7%
1	B	301	 3% 89% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMS	B	503	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10371 atoms, of which 4717 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.

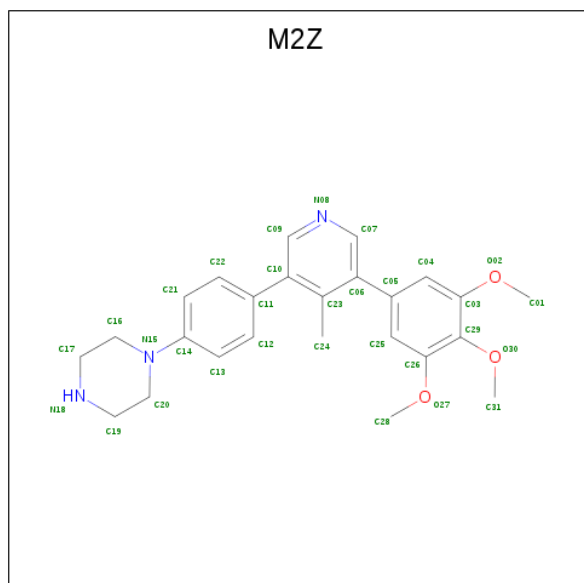
- Molecule 1 is a protein called Activin receptor type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	288	4687	1509	2312	415	436	15	0	11	0
1	B	295	4640	1523	2237	421	444	15	0	7	0

There are 6 discrepancies between the modelled and reference sequences:

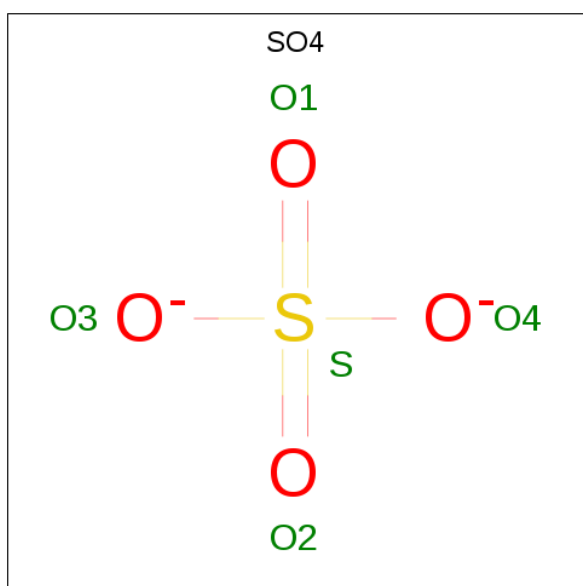
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	conflict	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	conflict	UNP Q04771

- Molecule 2 is 1-[4-[4-methyl-5-(3,4,5-trimethoxyphenyl)pyridin-3-yl]phenyl]piperazine (three-letter code: M2Z) (formula: C₂₅H₂₉N₃O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	0	0
			60	25	29	3	3		
2	A	1	Total	C	H	N	O	0	0
			60	25	29	3	3		
2	A	1	Total	C	H	N	O	0	0
			60	25	29	3	3		
2	B	1	Total	C	H	N	O	0	0
			60	25	29	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



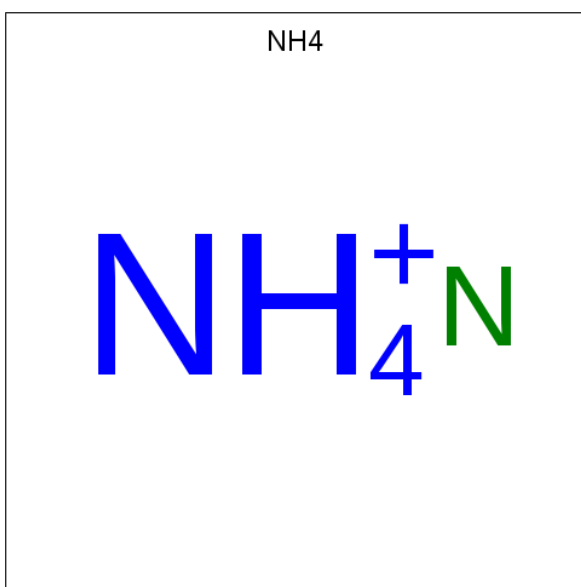
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



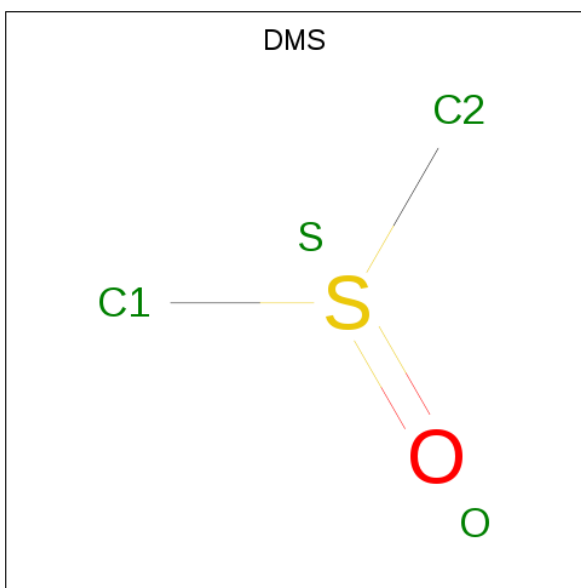
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	N		
5	A	1	5	4	1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
6	B	1	10	2	6	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	350	Total 350	O 350	0	0
7	B	344	Total 344	O 344	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.34Å 84.43Å 88.14Å 90.00° 131.16° 90.00°	Depositor
Resolution (Å)	63.36 – 1.42 63.36 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.36-1.42) 99.9 (63.36-1.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.152 , 0.188 0.151 , 0.187	Depositor DCC
R_{free} test set	6591 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10371	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: NH4, DMS, EDO, M2Z, SO4

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	0.44	0/2450	0.65	0/3321
1	B	0.43	0/2476	0.64	0/3357
All	All	0.43	0/4926	0.65	0/6678

There are no bond length outliers.

There are no bond angle outliers.

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	2375	2312	2335	23	0
1	B	2403	2237	2367	35	0
2	A	93	87	0	1	0
2	B	31	29	0	1	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
4	A	20	30	30	0	0
4	B	8	12	12	5	0
5	A	1	4	0	0	0
6	B	4	6	6	7	0
7	A	350	0	0	10	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	344	0	0	15	0
All	All	5654	4717	4750	64	2

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 7.

All (64) 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:373:ASN:HB3	1:A:374:PRO:HD3	1.43	0.97
1:B:258:ARG:NH1	7:B:601:HOH:O	1.99	0.93
1:A:293[A]:ASP:OD1	7:A:603:HOH:O	1.88	0.91
1:B:218:ARG:NH2	7:B:602:HOH:O	2.04	0.90
1:A:230:GLU:OE2	7:A:604:HOH:O	1.97	0.82
1:B:216:LYS:HD2	1:B:221:GLU:HG2	1.66	0.79
1:A:230:GLU:HB2	7:A:604:HOH:O	1.87	0.74
1:B:379:LYS:H	6:B:503:DMS:H11	1.54	0.73
1:A:373:ASN:HB3	1:A:374:PRO:CD	2.20	0.69
6:B:503:DMS:H23	7:B:781:HOH:O	1.92	0.68
1:A:230:GLU:HB3	7:A:701:HOH:O	1.94	0.67
1:B:361:HIS:HE1	1:B:363:GLN:HG3	1.60	0.67
1:B:380:ARG:HE	4:B:504:EDO:H11	1.60	0.66
1:A:373:ASN:CB	1:A:374:PRO:HD3	2.20	0.66
6:B:503:DMS:C2	7:B:781:HOH:O	2.45	0.65
1:B:258:ARG:HD2	7:B:889:HOH:O	1.98	0.64
1:B:217:GLY:HA3	7:B:602:HOH:O	1.98	0.63
1:B:361:HIS:CE1	1:B:363:GLN:HG3	2.35	0.61
1:B:258:ARG:HD3	7:B:657:HOH:O	2.01	0.60
1:B:258:ARG:NH1	7:B:604:HOH:O	2.26	0.59
1:B:218:ARG:CZ	7:B:602:HOH:O	2.47	0.56
1:B:216:LYS:HD2	1:B:221:GLU:CG	2.35	0.54
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.42	0.54
1:A:476[A]:GLU:HB3	1:A:486:LEU:HG	1.93	0.50
6:B:503:DMS:C1	7:B:684:HOH:O	2.60	0.50
1:A:218:ARG:NH2	7:A:601:HOH:O	1.60	0.49
1:A:336:ASP:OD2	7:A:605:HOH:O	2.19	0.49
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.49	0.48
1:A:492:LYS:O	1:A:496:THR:HG23	2.12	0.48
1:B:498:ILE:O	1:B:499:ASP:HB2	2.13	0.48
1:B:480:GLN:H	4:B:505:EDO:C2	2.28	0.47
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:GLN:HG3	7:B:664:HOH:O	2.13	0.47
1:B:218:ARG:NH1	7:B:602:HOH:O	2.48	0.46
1:B:248:GLU:OE1	7:B:603:HOH:O	2.20	0.46
1:A:400[B]:LYS:NZ	7:A:602:HOH:O	1.82	0.46
1:A:476[B]:GLU:HB3	1:A:486:LEU:HG	1.98	0.45
2:A:503:M2Z:C24	2:A:503:M2Z:C12	2.95	0.44
1:A:427:TYR:CD2	1:A:427:TYR:C	2.91	0.44
1:B:247:ARG:HH21	1:B:359:VAL:HA	1.81	0.44
1:A:396:PHE:HE2	1:A:400[B]:LYS:HE3	1.83	0.44
1:A:373:ASN:CB	1:A:374:PRO:CD	2.88	0.43
1:B:262[B]:ILE:HD12	1:B:318:HIS:HD2	1.83	0.43
6:B:503:DMS:H12	7:B:684:HOH:O	2.17	0.43
1:B:380:ARG:HE	4:B:504:EDO:C1	2.29	0.43
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.54	0.43
1:B:252:TYR:CE1	1:B:265:PHE:HB2	2.54	0.43
1:B:258:ARG:HH22	1:B:265:PHE:HB3	1.84	0.43
1:B:379:LYS:N	6:B:503:DMS:H11	2.27	0.43
1:B:252:TYR:CE1	7:B:601:HOH:O	2.70	0.43
1:A:270:MET:HG3	1:A:277:THR:CG2	2.49	0.43
1:A:396:PHE:CE2	1:A:400[B]:LYS:HE3	2.54	0.42
1:A:346:LYS:HE3	7:A:853:HOH:O	2.19	0.42
1:B:479:TYR:HA	4:B:505:EDO:H21	2.02	0.42
1:A:241:ASP:OD2	7:A:606:HOH:O	2.22	0.41
1:A:284:HIS:CD2	7:A:856:HOH:O	2.73	0.41
1:B:258:ARG:NH1	1:B:265:PHE:H	2.18	0.41
2:B:501:M2Z:C12	2:B:501:M2Z:C24	2.99	0.41
1:B:378:THR:HA	6:B:503:DMS:C1	2.52	0.40
1:B:258:ARG:HD3	1:B:258:ARG:HA	1.89	0.40
1:B:480:GLN:H	4:B:505:EDO:H21	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:787:HOH:O	7:A:831:HOH:O[4_445]	2.02	0.18
7:A:656:HOH:O	7:A:833:HOH:O[4_445]	2.09	0.11

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	295/301 (98%)	290 (98%)	5 (2%)	0	100	100
1	B	300/301 (100%)	297 (99%)	3 (1%)	0	100	100
All	All	595/602 (99%)	587 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	265/270 (98%)	262 (99%)	3 (1%)	73	48
1	B	270/270 (100%)	267 (99%)	3 (1%)	73	48
All	All	535/540 (99%)	529 (99%)	6 (1%)	71	48

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	362	SER
1	A	499	ASP
1	B	218	ARG
1	B	240	ARG
1	B	241	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	GLN
1	B	318	HIS
1	B	327	GLN
1	B	361	HIS
1	B	366	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is modelled with single atom - leaving 17 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	EDO	A	508	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	A	510	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	B	505	-	3,3,3	0.54	0	2,2,2	0.28	0
4	EDO	A	506	-	3,3,3	0.60	0	2,2,2	0.53	0
6	DMS	B	503	-	3,3,3	0.40	0	3,3,3	1.18	0
2	M2Z	B	501	-	34,34,34	1.39	6 (17%)	44,47,47	1.56	7 (15%)
4	EDO	A	505	-	3,3,3	0.52	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.21	0
2	M2Z	A	501	-	34,34,34	1.40	4 (11%)	44,47,47	1.57	7 (15%)
3	SO4	B	506	-	4,4,4	0.18	0	6,6,6	0.34	0
3	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.27	0
2	M2Z	A	502	-	34,34,34	1.29	4 (11%)	44,47,47	1.08	3 (6%)
4	EDO	A	507	-	3,3,3	0.60	0	2,2,2	0.27	0
2	M2Z	A	503	-	34,34,34	1.33	6 (17%)	44,47,47	1.10	1 (2%)
4	EDO	B	504	-	3,3,3	0.56	0	2,2,2	0.28	0
3	SO4	B	507	-	4,4,4	0.24	0	6,6,6	0.46	0
3	SO4	A	511	-	4,4,4	0.17	0	6,6,6	0.45	0

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	EDO	A	508	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
2	M2Z	B	501	-	-	0/18/26/26	0/4/4/4
4	EDO	B	505	-	-	1/1/1/1	-
2	M2Z	A	501	-	-	0/18/26/26	0/4/4/4
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	A	507	-	-	0/1/1/1	-
2	M2Z	A	503	-	-	0/18/26/26	0/4/4/4
4	EDO	B	504	-	-	1/1/1/1	-
2	M2Z	A	502	-	-	4/18/26/26	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	M2Z	C14-N15	3.97	1.49	1.38
2	B	501	M2Z	C14-N15	3.91	1.49	1.38
2	A	501	M2Z	C14-N15	3.83	1.49	1.38
2	A	501	M2Z	C10-C11	-3.60	1.42	1.49
2	A	502	M2Z	C14-N15	3.19	1.47	1.38
2	A	502	M2Z	C10-C11	-2.97	1.44	1.49
2	B	501	M2Z	C22-C21	2.59	1.43	1.38
2	A	501	M2Z	O02-C03	2.57	1.41	1.37
2	B	501	M2Z	C16-N15	2.49	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	M2Z	C06-C05	-2.44	1.45	1.49
2	B	501	M2Z	C10-C23	2.42	1.44	1.40
2	B	501	M2Z	C10-C11	-2.36	1.45	1.49
2	A	503	M2Z	C20-N15	2.36	1.50	1.46
2	A	501	M2Z	C06-C05	-2.24	1.45	1.49
2	B	501	M2Z	O27-C26	2.23	1.40	1.37
2	A	503	M2Z	C10-C11	-2.23	1.45	1.49
2	A	503	M2Z	C16-N15	2.21	1.50	1.46
2	A	502	M2Z	C20-N15	2.10	1.50	1.46
2	A	503	M2Z	C22-C21	2.08	1.42	1.38
2	A	503	M2Z	C06-C05	-2.06	1.45	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	M2Z	C17-C16-N15	4.84	120.96	110.48
2	A	501	M2Z	C12-C11-C10	-4.00	114.43	120.91
2	B	501	M2Z	C13-C14-N15	-3.87	116.04	121.38
2	A	501	M2Z	C22-C11-C10	3.82	127.10	120.91
2	A	501	M2Z	C04-C05-C06	-3.48	114.86	120.61
2	A	502	M2Z	C07-C06-C05	3.12	124.19	119.52
2	A	501	M2Z	C25-C05-C06	3.07	125.69	120.61
2	B	501	M2Z	C16-C17-N18	3.04	119.00	111.12
2	A	501	M2Z	C07-C06-C05	-2.77	115.37	119.52
2	A	502	M2Z	C05-C06-C23	-2.67	117.61	122.42
2	A	501	M2Z	C16-N15-C20	-2.58	105.83	111.52
2	B	501	M2Z	C19-N18-C17	2.50	117.51	110.34
2	A	503	M2Z	C16-N15-C20	-2.49	106.02	111.52
2	B	501	M2Z	C09-N08-C07	2.25	120.55	117.48
2	A	501	M2Z	C09-N08-C07	2.24	120.53	117.48
2	B	501	M2Z	C06-C07-N08	-2.18	120.86	124.16
2	A	502	M2Z	C09-N08-C07	2.08	120.31	117.48
2	B	501	M2Z	C03-C29-C26	2.07	121.69	119.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	EDO	O1-C1-C2-O2
2	A	502	M2Z	C25-C05-C06-C07
4	B	505	EDO	O1-C1-C2-O2
2	A	502	M2Z	C25-C05-C06-C23

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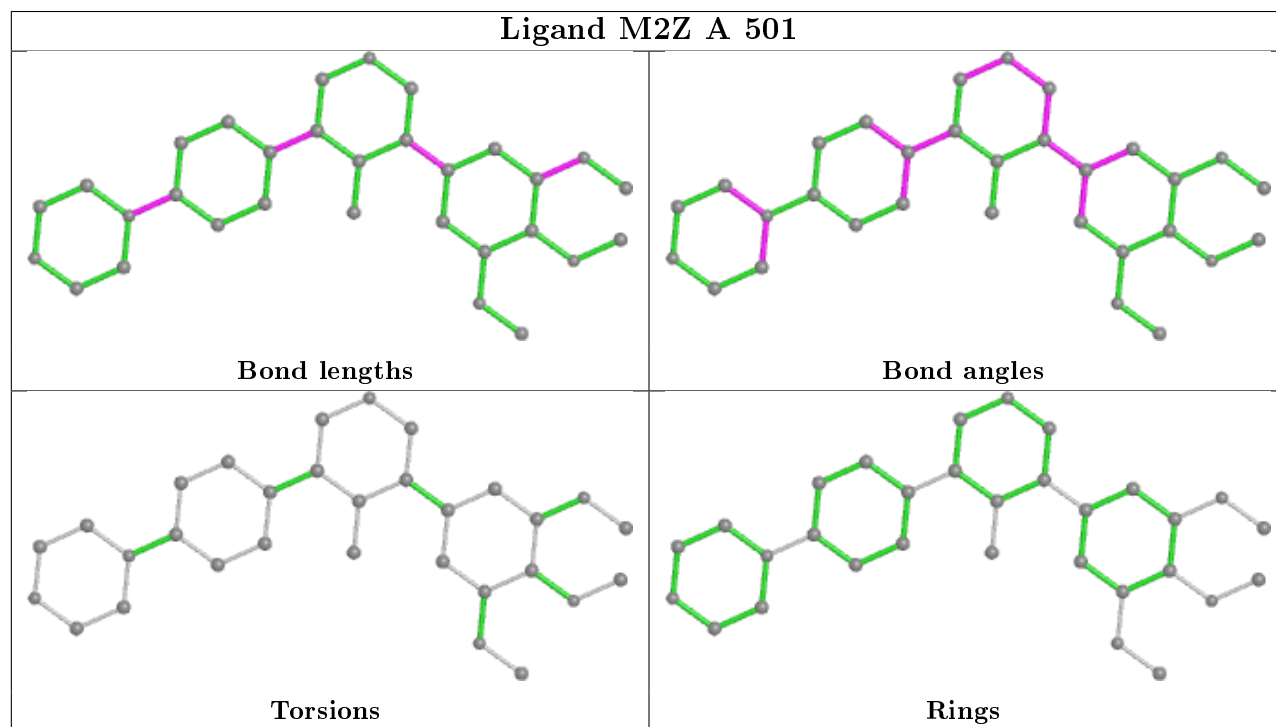
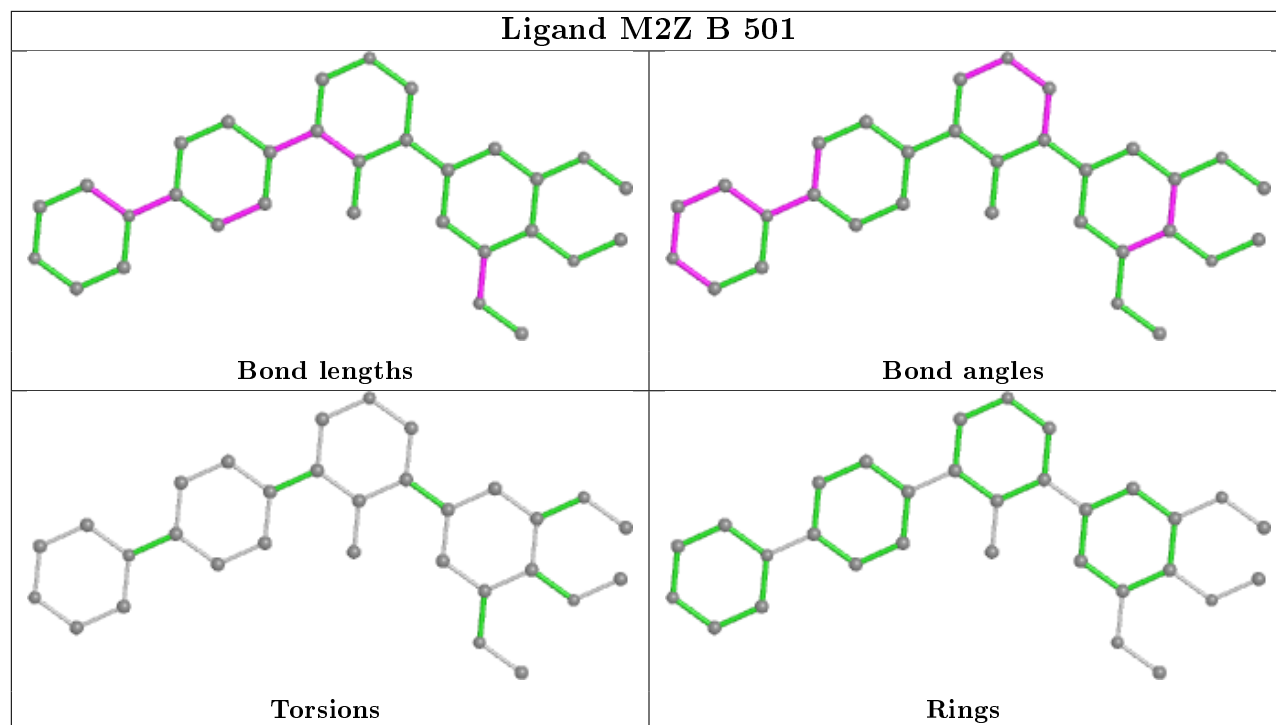
Mol	Chain	Res	Type	Atoms
2	A	502	M2Z	C04-C05-C06-C07
2	A	502	M2Z	C04-C05-C06-C23

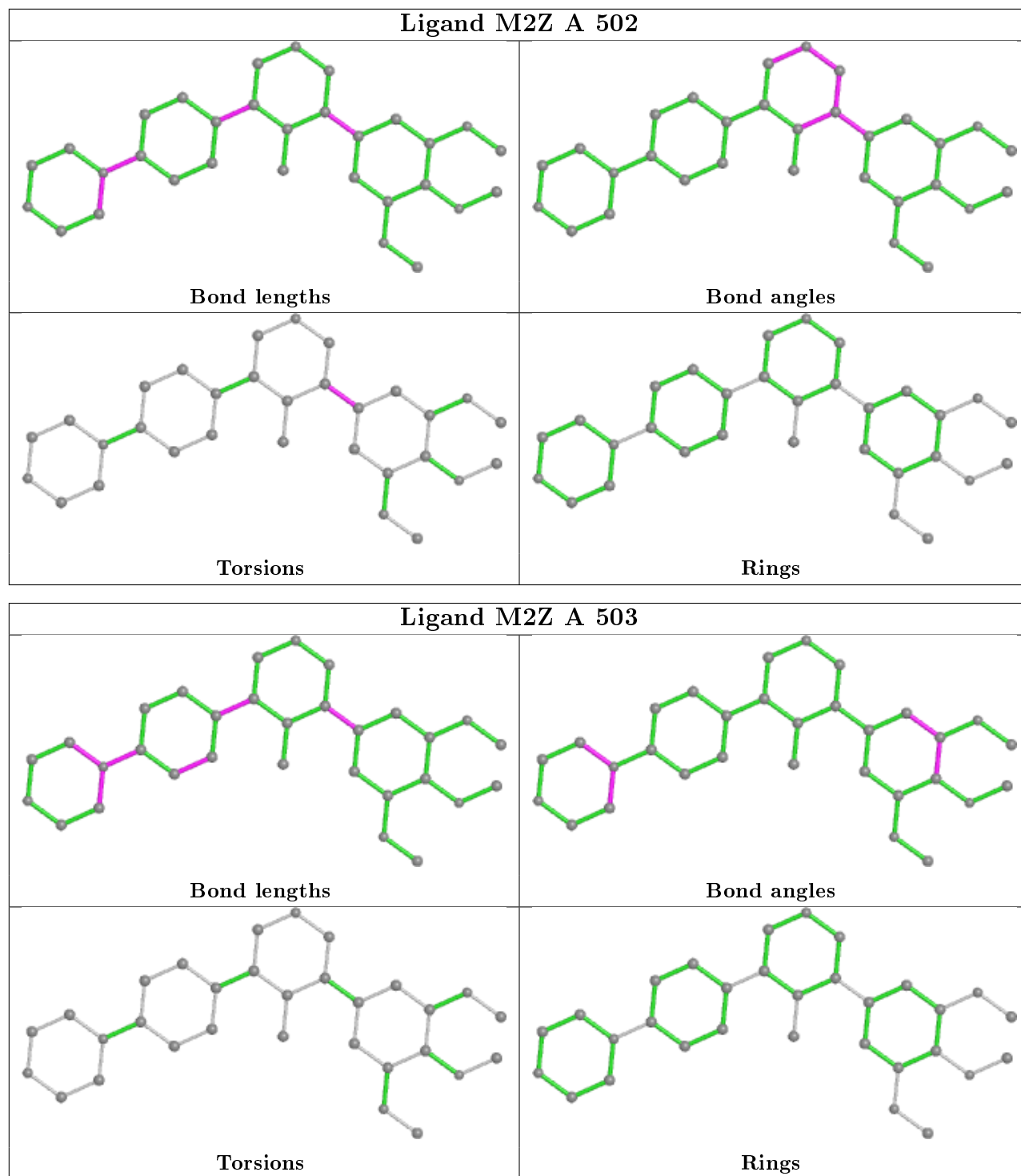
There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	EDO	3	0
6	B	503	DMS	7	0
2	B	501	M2Z	1	0
2	A	503	M2Z	1	0
4	B	504	EDO	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

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	288/301 (95%)	-0.20	12 (4%) 36 36	12, 18, 44, 79	0
1	B	295/301 (98%)	-0.22	10 (3%) 45 44	13, 19, 43, 94	0
All	All	583/602 (96%)	-0.21	22 (3%) 40 40	12, 18, 44, 94	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	THR	9.2
1	B	326	THR	6.1
1	A	325	GLY	5.9
1	A	373	ASN	5.5
1	B	325	GLY	5.3
1	B	327	GLN	4.3
1	A	324	PHE	4.0
1	A	327	GLN	3.6
1	B	324	PHE	3.3
1	B	328	GLY	3.1
1	A	297	LEU	3.0
1	A	274	HIS	2.6
1	A	499	ASP	2.6
1	B	370	VAL	2.3
1	B	394	ASP	2.3
1	B	258	ARG	2.2
1	B	255	VAL	2.2
1	B	372	ASN	2.1
1	A	275	SER	2.1
1	A	374	PRO	2.1
1	A	362	SER	2.0
1	A	394	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

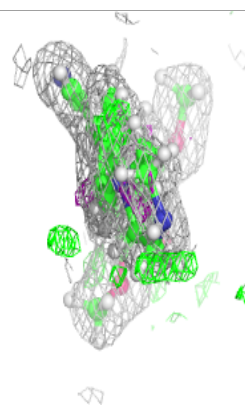
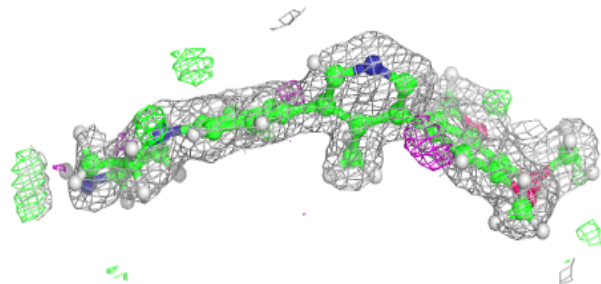
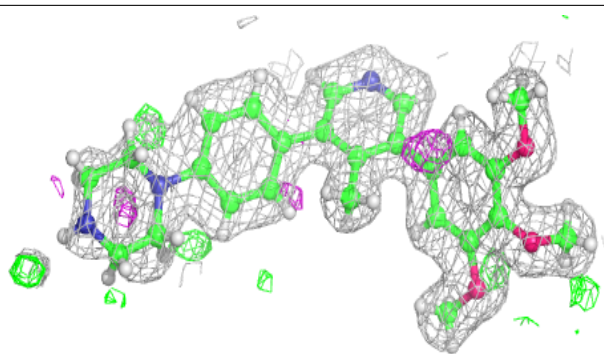
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	507	5/5	0.78	0.34	33,60,77,82	0
4	EDO	B	505	4/4	0.83	0.13	32,40,49,50	0
4	EDO	A	510	4/4	0.86	0.11	35,46,55,58	0
4	EDO	A	508	4/4	0.89	0.20	29,35,41,41	0
4	EDO	B	504	4/4	0.91	0.11	19,24,30,33	0
5	NH4	A	509	1/1	0.93	0.23	16,20,20,20	0
6	DMS	B	503	4/4	0.95	0.15	35,47,51,60	0
4	EDO	A	505	4/4	0.95	0.09	16,21,25,27	0
2	M2Z	B	501	31/31	0.96	0.09	13,20,64,77	0
4	EDO	A	506	4/4	0.96	0.11	14,25,30,36	0
2	M2Z	A	503	31/31	0.97	0.07	13,18,78,86	0
2	M2Z	A	502	31/31	0.97	0.06	14,19,34,36	0
2	M2Z	A	501	31/31	0.97	0.08	14,21,67,67	0
4	EDO	A	507	4/4	0.99	0.08	14,23,38,38	0
3	SO4	B	502	5/5	0.99	0.05	22,22,24,28	0
3	SO4	B	506	5/5	0.99	0.05	16,16,17,20	0
3	SO4	A	504	5/5	0.99	0.06	18,18,22,23	0
3	SO4	A	511	5/5	0.99	0.07	15,19,37,40	0

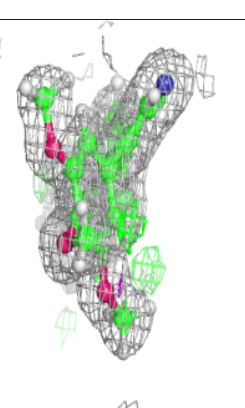
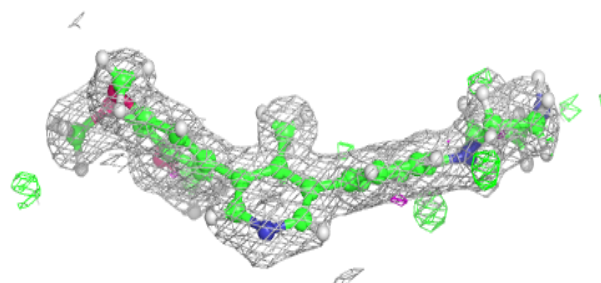
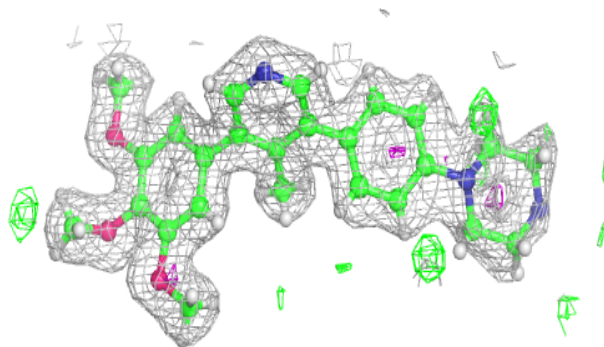
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M2Z 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)

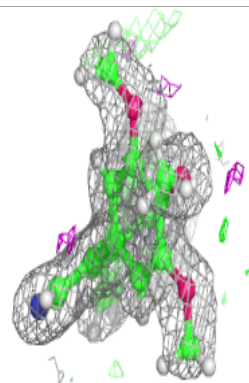
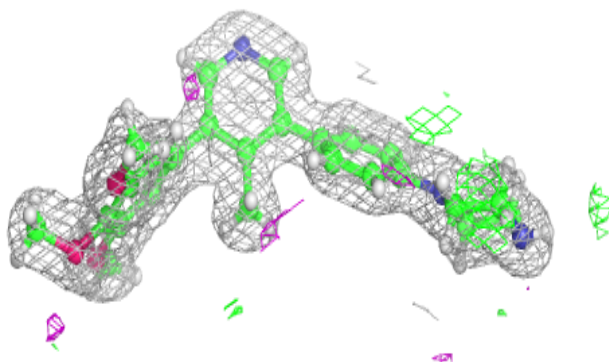
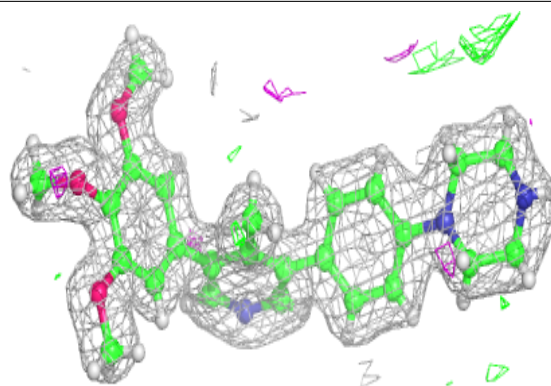
**Electron density around M2Z A 503:**

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

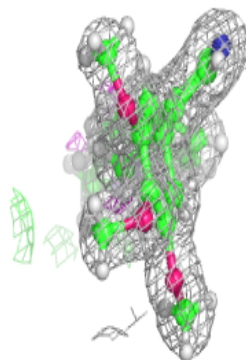
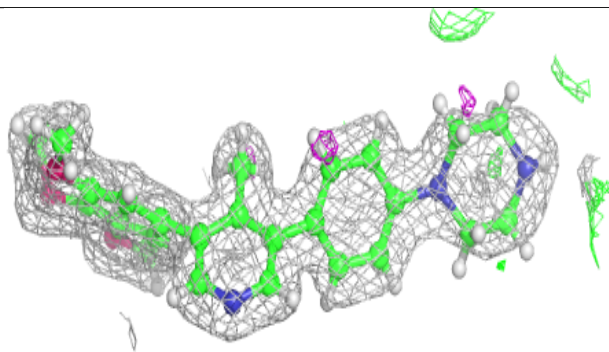
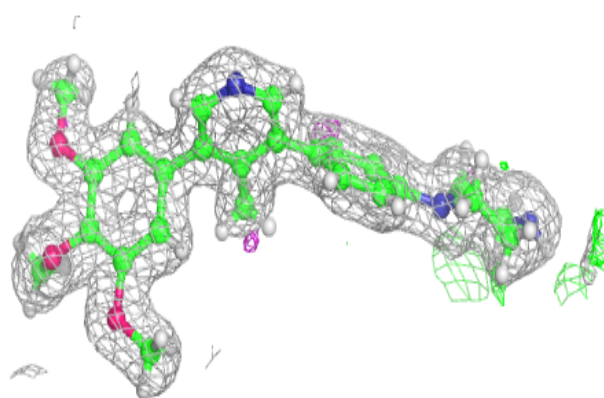


Electron density around M2Z A 502:

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

**Electron density around M2Z 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.