



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:20 PM UTC

PDB ID : 9BOX / pdb_00009box
Title : Room-temperature X-ray structure of human mitochondrial serine hydroxymethyltransferase (hSHMT2) with PLP-glycine external aldimine and 5-formyl tetrahydrofolate (folinic acid)
Authors : Drago, V.N.; Kovalevsky, A.
Deposited on : 2024-05-06
Resolution : 2.10 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

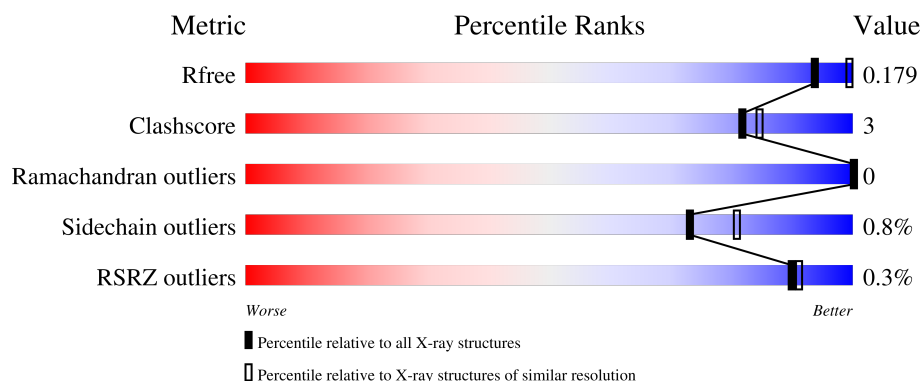
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	462	92% 8%
1	B	462	93% 7%
1	C	462	88% 9% .
1	D	462	90% 8% .

2 Entry composition [i](#)

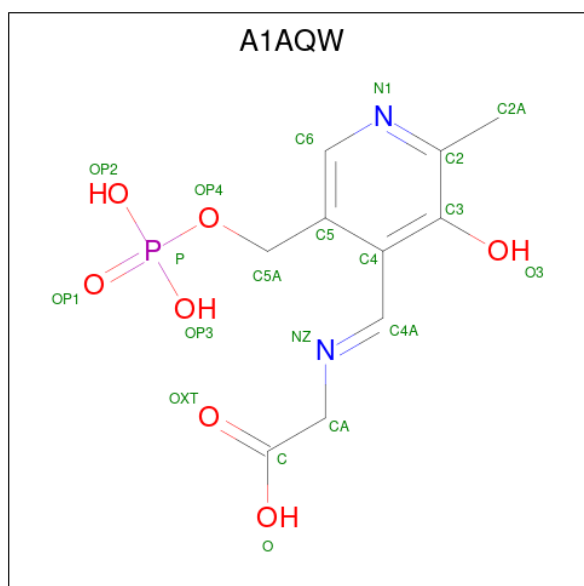
There are 4 unique types of molecules in this entry. The entry contains 15295 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3608	2273	648	671	16			
1	B	462	Total	C	N	O	S	0	1	0
			3619	2279	652	672	16			
1	C	453	Total	C	N	O	S	0	0	0
			3538	2230	635	657	16			
1	D	453	Total	C	N	O	S	0	1	0
			3549	2236	639	658	16			

- Molecule 2 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)glycine (CCD ID: A1AQW) (formula: C₁₀H₁₃N₂O₇P) (labeled as "Ligand of Interest" by depositor).



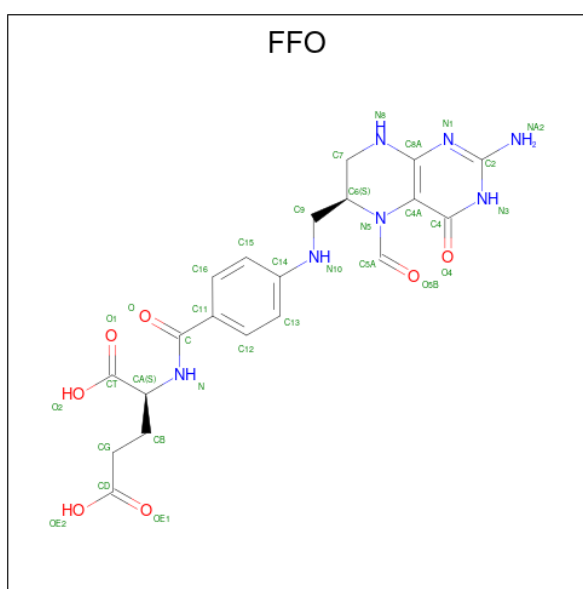
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (CCD ID: FFO) (formula: C₂₀H₂₃N₇O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	20	7	7		
3	B	1	Total	C	N	O	0	0
			34	20	7	7		
3	C	1	Total	C	N	O	0	0
			34	20	7	7		
3	D	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		

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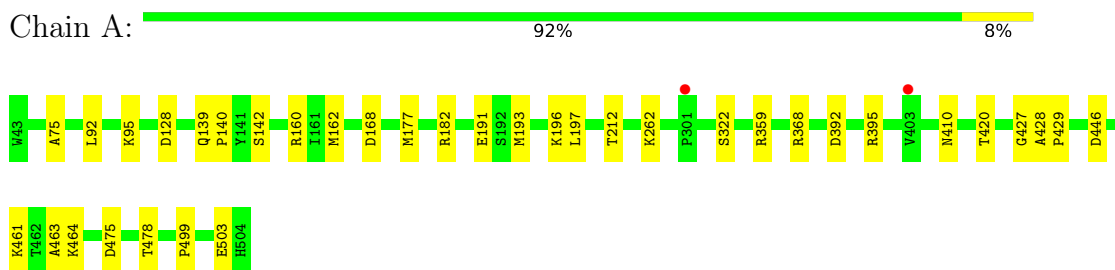
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	169	Total 169	O 169	0	0
4	C	207	Total 207	O 207	0	0
4	D	180	Total 180	O 180	0	0

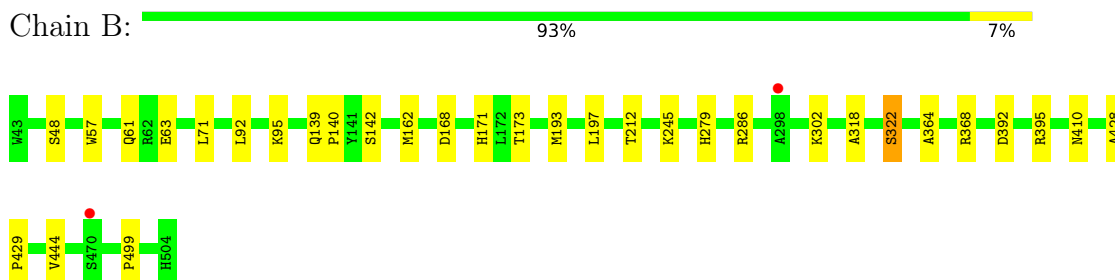
3 Residue-property plots

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.

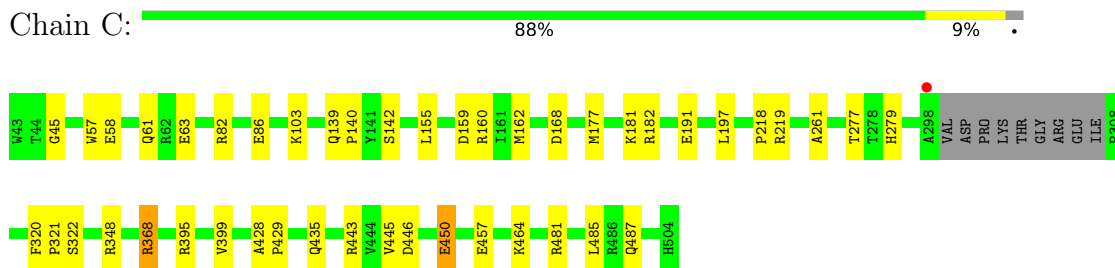
- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



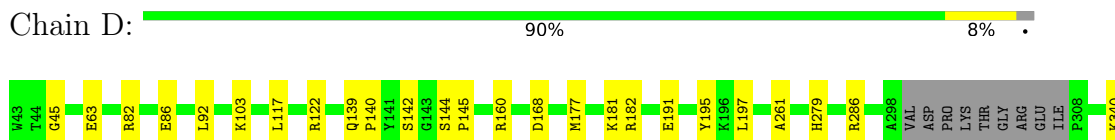
- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	142.98Å 119.30Å 134.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.82 – 2.10 42.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.6 (42.82-2.10) 90.7 (42.82-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.162 , 0.189 0.157 , 0.179	Depositor DCC
R_{free} test set	6068 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15295	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.61% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FFO, A1AQW

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	0.47	0/3681	0.58	3/4978 (0.1%)
1	B	0.40	0/3692	0.52	2/4992 (0.0%)
1	C	0.44	1/3609 (0.0%)	0.55	5/4878 (0.1%)
1	D	0.46	4/3620 (0.1%)	0.51	1/4892 (0.0%)
All	All	0.44	5/14602 (0.0%)	0.54	11/19740 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	456	LEU	C-N	-7.60	1.23	1.33
1	D	195	TYR	C-N	7.11	1.42	1.33
1	D	377	THR	C-N	6.24	1.43	1.33
1	D	457	GLU	C-N	-6.20	1.26	1.33
1	C	450	GLU	C-N	-5.54	1.27	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LYS	N-CA-C	7.21	121.00	109.24
1	A	196	LYS	N-CA-C	7.11	119.73	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	GLU	O-C-N	6.87	129.40	122.12
1	A	95	LYS	N-CA-C	6.76	120.25	109.24
1	A	322	SER	N-CA-C	6.21	117.85	111.14
1	C	181	LYS	N-CA-C	6.14	117.73	108.46
1	C	322	SER	N-CA-C	6.13	117.77	111.14
1	B	322	SER	N-CA-C	6.04	117.66	111.14
1	D	181	LYS	N-CA-C	5.66	117.01	108.46
1	C	57	TRP	CA-C-N	5.06	127.06	120.28
1	C	57	TRP	C-N-CA	5.06	127.06	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ARG	Sidechain
1	C	368	ARG	Sidechain

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	3608	0	3605	18	0
1	B	3619	0	3617	19	0
1	C	3538	0	3532	23	0
1	D	3549	0	3544	19	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	34	0	21	0	0
3	B	34	0	21	0	0
3	C	34	0	21	0	0
3	D	34	0	21	1	0
4	A	209	0	0	0	0
4	B	169	0	0	0	0
4	C	207	0	0	2	0
4	D	180	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15295	0	14382	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:HE1	1:B:212:THR:HB	1.77	0.67
1:A:162:MET:HE3	1:A:193:MET:HE2	1.82	0.62
1:A:463:ALA:HB1	1:A:464:LYS:HE3	1.89	0.55
1:A:193:MET:HE1	1:A:212:THR:HB	1.91	0.53
1:B:48:SER:HA	1:D:82:ARG:HE	1.74	0.52
1:C:368:ARG:NH2	1:C:446:ASP:OD1	2.42	0.52
1:C:168:ASP:HB3	1:C:197:LEU:HG	1.92	0.52
1:C:450:GLU:HG2	1:C:485:LEU:HD22	1.93	0.50
1:D:168:ASP:HB3	1:D:197:LEU:HG	1.93	0.50
1:B:364:ALA:O	1:B:368:ARG:HG2	2.13	0.49
1:C:82:ARG:NE	1:C:86:GLU:OE2	2.37	0.49
1:C:435:GLN:HA	4:C:814:HOH:O	2.13	0.49
1:A:177:MET:HB2	1:A:182:ARG:HA	1.95	0.48
1:A:193:MET:CE	1:A:212:THR:HB	2.43	0.48
1:C:103:LYS:HA	1:C:103:LYS:HD2	1.53	0.48
1:A:168:ASP:HB3	1:A:197:LEU:HG	1.95	0.48
1:D:419:ILE:HD12	3:D:602:FFO:CD	2.44	0.47
1:A:420:THR:HG22	1:A:420:THR:O	2.14	0.47
1:D:177:MET:HB2	1:D:182:ARG:HA	1.95	0.47
1:C:428:ALA:N	1:C:429:PRO:CD	2.78	0.47
1:B:162:MET:HE3	1:B:193:MET:HE2	1.96	0.46
1:A:128:ASP:OD2	1:A:262:LYS:NZ	2.49	0.46
1:A:461:LYS:HA	1:A:461:LYS:HD2	1.71	0.46
1:C:443:ARG:HA	1:C:446:ASP:OD2	2.15	0.46
1:B:171:HIS:HD1	1:B:173:THR:H	1.64	0.46
1:B:499:PRO:HB3	1:D:45:GLY:HA3	1.99	0.45
1:C:177:MET:HB3	1:C:182:ARG:HA	1.98	0.45
1:C:464:LYS:HA	1:C:464:LYS:HD2	1.55	0.44
1:D:261:ALA:HB1	1:D:348[B]:ARG:HA	1.99	0.44
1:D:279:HIS:ND1	1:D:286:ARG:HA	2.32	0.44
1:A:475:ASP:HB3	1:A:478:THR:HB	1.99	0.44
1:A:392:ASP:OD2	1:A:395:ARG:HD2	2.18	0.43
1:A:499:PRO:HB3	1:C:45:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.71	0.43
1:A:75:ALA:HA	1:A:427:GLY:HA3	2.00	0.43
1:B:168:ASP:HB3	1:B:197:LEU:HG	2.01	0.43
1:C:155:LEU:HB3	1:C:159:ASP:HB2	2.00	0.43
1:D:82:ARG:NE	1:D:86:GLU:OE2	2.51	0.43
1:D:416:ARG:O	1:D:416:ARG:HG3	2.18	0.43
1:C:261:ALA:HB1	1:C:348:ARG:HA	2.00	0.43
1:C:277:THR:HB	1:C:279:HIS:CE1	2.53	0.43
1:D:428:ALA:N	1:D:429:PRO:CD	2.82	0.43
1:B:63:GLU:HG2	1:D:92:LEU:HD23	2.01	0.43
1:C:162:MET:HG3	1:C:218:PRO:HB3	2.01	0.43
1:C:160:ARG:HA	1:C:191:GLU:O	2.19	0.43
1:D:359:ARG:HE	1:D:359:ARG:HB2	1.72	0.43
1:C:320:PHE:CD2	1:C:321:PRO:HA	2.53	0.42
1:A:160:ARG:HA	1:A:191:GLU:O	2.19	0.42
1:A:92:LEU:HD23	1:C:63:GLU:HG2	2.01	0.42
1:B:428:ALA:N	1:B:429:PRO:HD3	2.35	0.42
1:D:261:ALA:HB1	1:D:348[A]:ARG:HA	2.01	0.42
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.35	0.41
1:B:392:ASP:OD2	1:B:395:ARG:HD2	2.20	0.41
1:A:139:GLN:N	1:A:140:PRO:CD	2.83	0.41
1:A:428:ALA:N	1:A:429:PRO:CD	2.83	0.41
1:B:318:ALA:HA	1:B:322:SER:HB2	2.02	0.41
1:B:71:LEU:HD13	1:B:444:VAL:HG22	2.01	0.41
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.91	0.41
1:C:219:ARG:HD2	4:C:785:HOH:O	2.20	0.41
1:B:57:TRP:O	1:B:61:GLN:HG3	2.21	0.41
1:C:139:GLN:N	1:C:140:PRO:CD	2.83	0.41
1:D:144:SER:HB2	1:D:145:PRO:HD3	2.03	0.41
1:B:428:ALA:N	1:B:429:PRO:CD	2.83	0.41
1:D:160:ARG:HA	1:D:191:GLU:O	2.21	0.41
1:A:368:ARG:NH2	1:A:446:ASP:OD1	2.54	0.40
1:C:395:ARG:O	1:C:399:VAL:HG23	2.21	0.40
1:D:139:GLN:N	1:D:140:PRO:CD	2.84	0.40
1:B:92:LEU:HD23	1:D:63:GLU:HG2	2.03	0.40
1:B:139:GLN:N	1:B:140:PRO:CD	2.84	0.40
1:B:245:LYS:HB3	1:B:245:LYS:HE3	1.75	0.40
1:C:445:VAL:O	1:C:446:ASP:C	2.64	0.40
1:D:122:ARG:CZ	1:D:340:LYS:HD3	2.52	0.40
1:C:457:GLU:OE1	1:C:481:ARG:NH1	2.40	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	460/462 (100%)	448 (97%)	12 (3%)	0	100	100
1	B	461/462 (100%)	448 (97%)	13 (3%)	0	100	100
1	C	449/462 (97%)	436 (97%)	13 (3%)	0	100	100
1	D	450/462 (97%)	439 (98%)	11 (2%)	0	100	100
All	All	1820/1848 (98%)	1771 (97%)	49 (3%)	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	381/381 (100%)	378 (99%)	3 (1%)	73	81
1	B	382/381 (100%)	380 (100%)	2 (0%)	81	88
1	C	373/381 (98%)	370 (99%)	3 (1%)	73	81
1	D	374/381 (98%)	370 (99%)	4 (1%)	65	74
All	All	1510/1524 (99%)	1498 (99%)	12 (1%)	73	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	410	ASN

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Mol	Chain	Res	Type
1	A	503	GLU
1	B	142	SER
1	B	410	ASN
1	C	61	GLN
1	C	142	SER
1	C	487	GLN
1	D	103	LYS
1	D	142	SER
1	D	410	ASN
1	D	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	329	ASN
1	A	480	GLN
1	B	156	GLN
1	B	270	HIS
1	C	353	GLN
1	C	357	ASN
1	D	156	GLN
1	D	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FFO	C	602	-	33,36,36	1.13	3 (9%)	35,50,50	1.38	3 (8%)
2	A1AQW	A	601	-	20,20,20	1.86	4 (20%)	26,28,28	2.21	9 (34%)
3	FFO	B	602	-	33,36,36	1.11	2 (6%)	35,50,50	1.38	3 (8%)
3	FFO	D	602	-	33,36,36	1.11	3 (9%)	35,50,50	1.39	3 (8%)
2	A1AQW	D	601	-	20,20,20	1.84	4 (20%)	26,28,28	2.23	8 (30%)
2	A1AQW	B	601	-	20,20,20	1.83	4 (20%)	26,28,28	2.26	8 (30%)
2	A1AQW	C	601	-	20,20,20	1.86	4 (20%)	26,28,28	2.23	9 (34%)
3	FFO	A	602	-	33,36,36	1.13	3 (9%)	35,50,50	1.39	4 (11%)

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	FFO	C	602	-	-	7/24/37/37	0/3/3/3
2	A1AQW	A	601	-	-	0/12/12/12	0/1/1/1
3	FFO	B	602	-	-	13/24/37/37	0/3/3/3
3	FFO	D	602	-	-	7/24/37/37	0/3/3/3
2	A1AQW	D	601	-	-	1/12/12/12	0/1/1/1
2	A1AQW	B	601	-	-	0/12/12/12	0/1/1/1
2	A1AQW	C	601	-	-	0/12/12/12	0/1/1/1
3	FFO	A	602	-	-	7/24/37/37	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1AQW	O3-C3	-4.48	1.26	1.36
2	D	601	A1AQW	O3-C3	-4.43	1.26	1.36
2	C	601	A1AQW	O3-C3	-4.40	1.26	1.36
2	B	601	A1AQW	O3-C3	-4.36	1.26	1.36
2	C	601	A1AQW	C3-C2	3.98	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1AQW	C3-C2	3.94	1.45	1.41
2	D	601	A1AQW	C3-C2	3.77	1.44	1.41
2	B	601	A1AQW	C3-C2	3.77	1.44	1.41
2	D	601	A1AQW	P-OP4	3.73	1.72	1.60
2	C	601	A1AQW	P-OP4	3.71	1.72	1.60
2	B	601	A1AQW	P-OP4	3.68	1.71	1.60
2	A	601	A1AQW	P-OP4	3.65	1.71	1.60
3	B	602	FFO	C2-N3	-3.14	1.30	1.37
3	C	602	FFO	C2-N3	-3.02	1.30	1.37
3	A	602	FFO	C2-N3	-3.02	1.30	1.37
3	D	602	FFO	C2-N3	-3.01	1.30	1.37
3	A	602	FFO	C4A-N5	2.78	1.42	1.38
3	C	602	FFO	C4A-N5	2.72	1.42	1.38
3	B	602	FFO	C4A-N5	2.71	1.42	1.38
3	D	602	FFO	C4A-N5	2.70	1.42	1.38
2	C	601	A1AQW	C4-C3	2.27	1.44	1.41
2	D	601	A1AQW	C4-C3	2.13	1.44	1.41
2	A	601	A1AQW	C4-C3	2.13	1.44	1.41
3	A	602	FFO	CG-CD	2.11	1.55	1.50
3	C	602	FFO	CG-CD	2.10	1.55	1.50
2	B	601	A1AQW	C4-C3	2.10	1.44	1.41
3	D	602	FFO	CG-CD	2.09	1.55	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	A1AQW	C4-C3-C2	-6.37	116.56	120.14
2	C	601	A1AQW	C4-C3-C2	-6.31	116.59	120.14
2	D	601	A1AQW	C4-C3-C2	-6.24	116.63	120.14
2	A	601	A1AQW	C4-C3-C2	-6.19	116.66	120.14
2	B	601	A1AQW	CA-NZ-C4A	4.22	125.84	118.42
2	D	601	A1AQW	CA-NZ-C4A	4.13	125.68	118.42
2	C	601	A1AQW	CA-NZ-C4A	4.05	125.53	118.42
2	A	601	A1AQW	CA-NZ-C4A	3.99	125.44	118.42
2	B	601	A1AQW	C6-N1-C2	3.97	126.39	119.20
3	B	602	FFO	C2-N1-C8A	3.96	120.34	113.36
3	A	602	FFO	C2-N1-C8A	3.94	120.31	113.36
3	C	602	FFO	C2-N1-C8A	3.93	120.30	113.36
2	C	601	A1AQW	C6-N1-C2	3.93	126.32	119.20
3	D	602	FFO	C2-N1-C8A	3.92	120.27	113.36
2	A	601	A1AQW	C6-N1-C2	3.87	126.22	119.20
2	D	601	A1AQW	C6-N1-C2	3.85	126.19	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	FFO	C4A-C4-N3	3.79	117.62	110.94
3	C	602	FFO	C4A-C4-N3	3.79	117.61	110.94
3	D	602	FFO	C4A-C4-N3	3.77	117.57	110.94
3	B	602	FFO	C4A-C4-N3	3.72	117.49	110.94
2	B	601	A1AQW	C3-C4-C5	3.38	120.99	118.28
2	D	601	A1AQW	C3-C4-C5	3.27	120.90	118.28
2	A	601	A1AQW	C3-C4-C5	3.14	120.80	118.28
2	C	601	A1AQW	C3-C4-C5	3.10	120.77	118.28
2	B	601	A1AQW	C5-C6-N1	-2.68	119.47	123.83
2	D	601	A1AQW	OXT-C-CA	-2.64	115.19	122.77
2	A	601	A1AQW	C5-C6-N1	-2.62	119.58	123.83
2	C	601	A1AQW	C5-C6-N1	-2.61	119.58	123.83
2	C	601	A1AQW	OXT-C-CA	-2.61	115.29	122.77
2	D	601	A1AQW	C5-C6-N1	-2.58	119.64	123.83
2	A	601	A1AQW	OXT-C-CA	-2.57	115.39	122.77
2	B	601	A1AQW	OXT-C-CA	-2.55	115.46	122.77
3	C	602	FFO	C2-N3-C4	-2.47	120.64	125.11
3	A	602	FFO	C2-N3-C4	-2.46	120.65	125.11
3	D	602	FFO	C2-N3-C4	-2.45	120.67	125.11
2	D	601	A1AQW	OP2-P-OP4	-2.36	100.52	106.67
2	A	601	A1AQW	OP2-P-OP4	-2.30	100.67	106.67
3	B	602	FFO	C2-N3-C4	-2.30	120.95	125.11
2	C	601	A1AQW	OP2-P-OP4	-2.25	100.80	106.67
2	B	601	A1AQW	OP2-P-OP4	-2.20	100.92	106.67
2	B	601	A1AQW	C3-C2-N1	-2.16	118.24	120.96
2	C	601	A1AQW	C3-C2-N1	-2.13	118.28	120.96
2	A	601	A1AQW	C3-C2-N1	-2.11	118.30	120.96
2	D	601	A1AQW	C3-C2-N1	-2.10	118.31	120.96
2	C	601	A1AQW	OP3-P-OP2	2.06	115.54	107.80
2	A	601	A1AQW	OP3-P-OP2	2.06	115.53	107.80
3	A	602	FFO	O1-CT-CA	-2.03	115.70	122.26

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	FFO	O5B-C5A-N5-C4A
3	A	602	FFO	O5B-C5A-N5-C6
3	B	602	FFO	O5B-C5A-N5-C4A
3	B	602	FFO	O5B-C5A-N5-C6
3	C	602	FFO	O5B-C5A-N5-C4A
3	C	602	FFO	O5B-C5A-N5-C6

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Mol	Chain	Res	Type	Atoms
3	D	602	FFO	O5B-C5A-N5-C4A
3	D	602	FFO	O5B-C5A-N5-C6
3	C	602	FFO	C15-C14-N10-C9
3	C	602	FFO	C13-C14-N10-C9
3	B	602	FFO	C11-C-N-CA
3	A	602	FFO	C13-C14-N10-C9
3	B	602	FFO	O-C-N-CA
3	B	602	FFO	C15-C14-N10-C9
3	A	602	FFO	C15-C14-N10-C9
3	B	602	FFO	CT-CA-N-C
3	D	602	FFO	C15-C14-N10-C9
3	B	602	FFO	C13-C14-N10-C9
3	D	602	FFO	C13-C14-N10-C9
3	B	602	FFO	CT-CA-CB-CG
3	A	602	FFO	C6-C9-N10-C14
2	D	601	A1AQW	C5A-OP4-P-OP1
3	B	602	FFO	N-CA-CB-CG
3	A	602	FFO	OE2-CD-CG-CB
3	B	602	FFO	CB-CA-N-C
3	C	602	FFO	OE1-CD-CG-CB
3	D	602	FFO	OE1-CD-CG-CB
3	A	602	FFO	OE1-CD-CG-CB
3	C	602	FFO	OE2-CD-CG-CB
3	D	602	FFO	OE2-CD-CG-CB
3	B	602	FFO	C6-C9-N10-C14
3	C	602	FFO	C6-C9-N10-C14
3	D	602	FFO	C6-C9-N10-C14
3	B	602	FFO	OE2-CD-CG-CB
3	B	602	FFO	OE1-CD-CG-CB

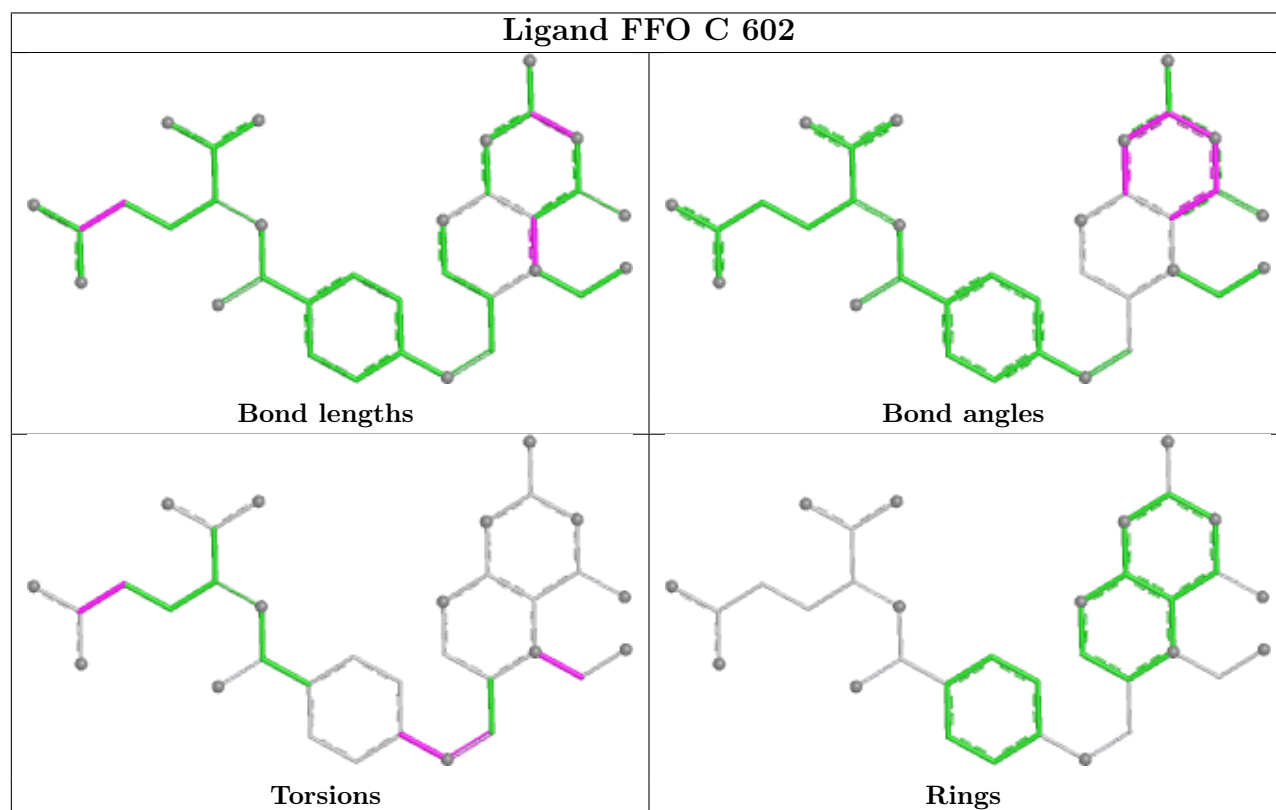
There are no ring outliers.

1 monomer is involved in 1 short contact:

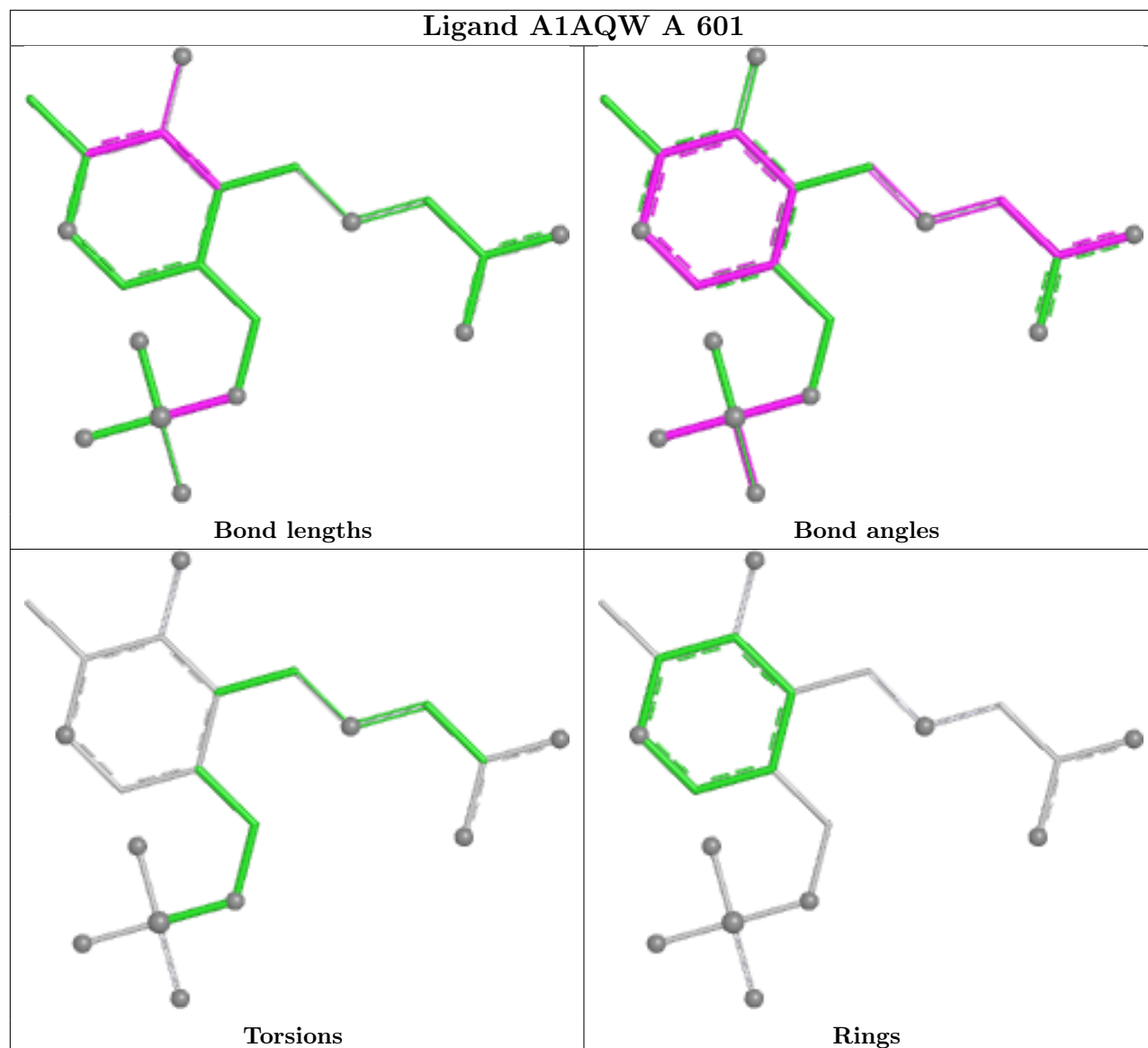
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	FFO	1	0

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

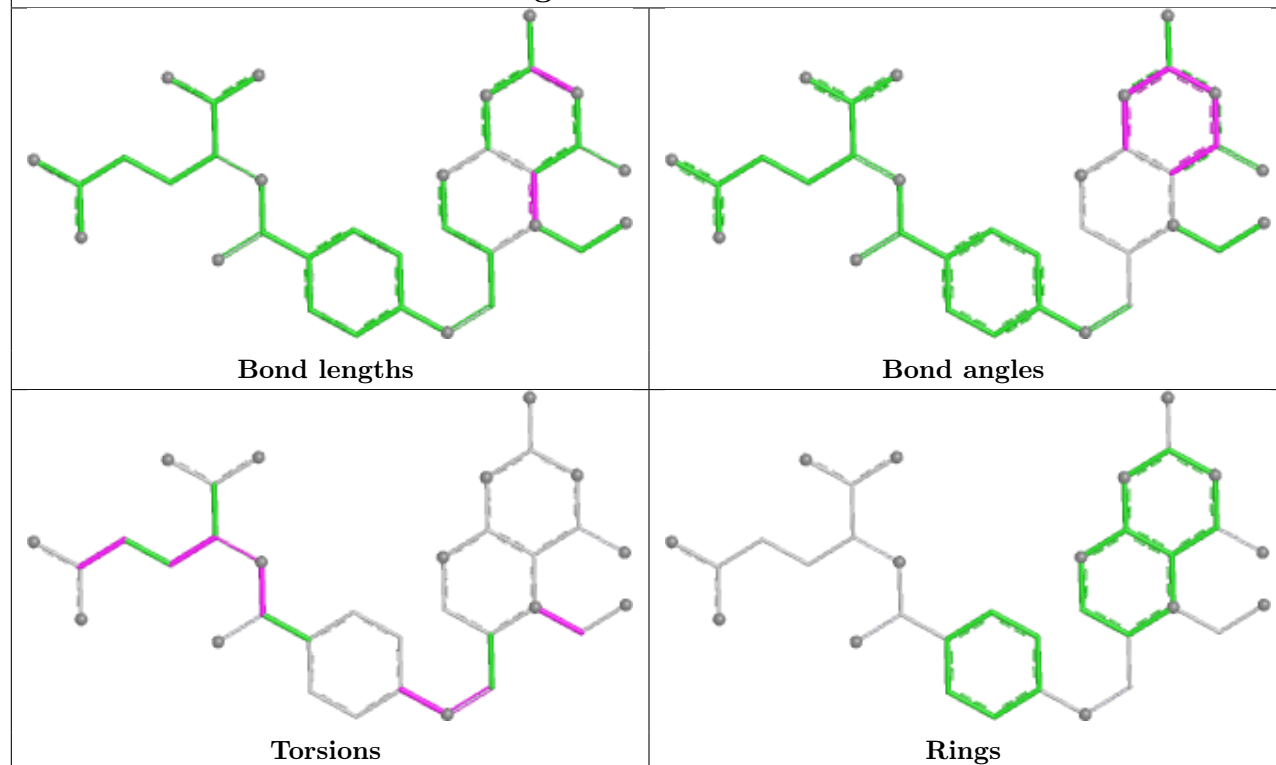
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



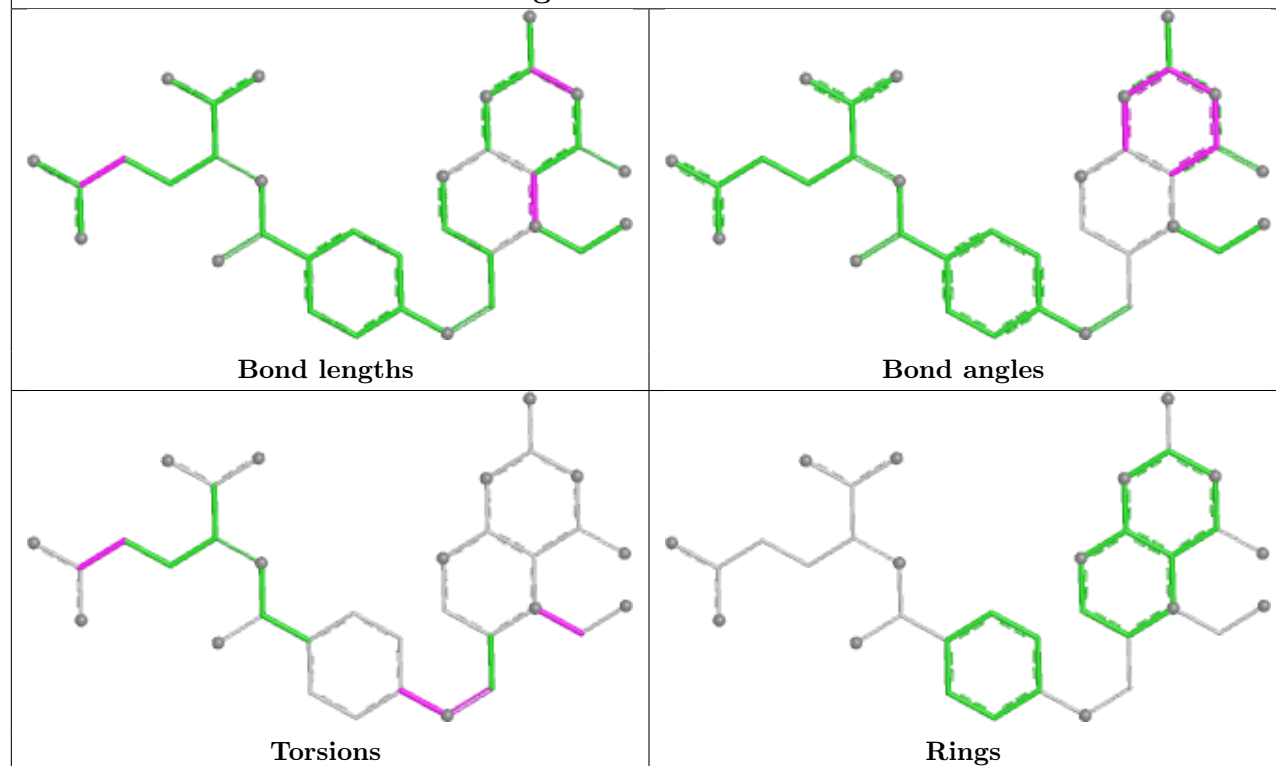
Ligand A1AQW A 601



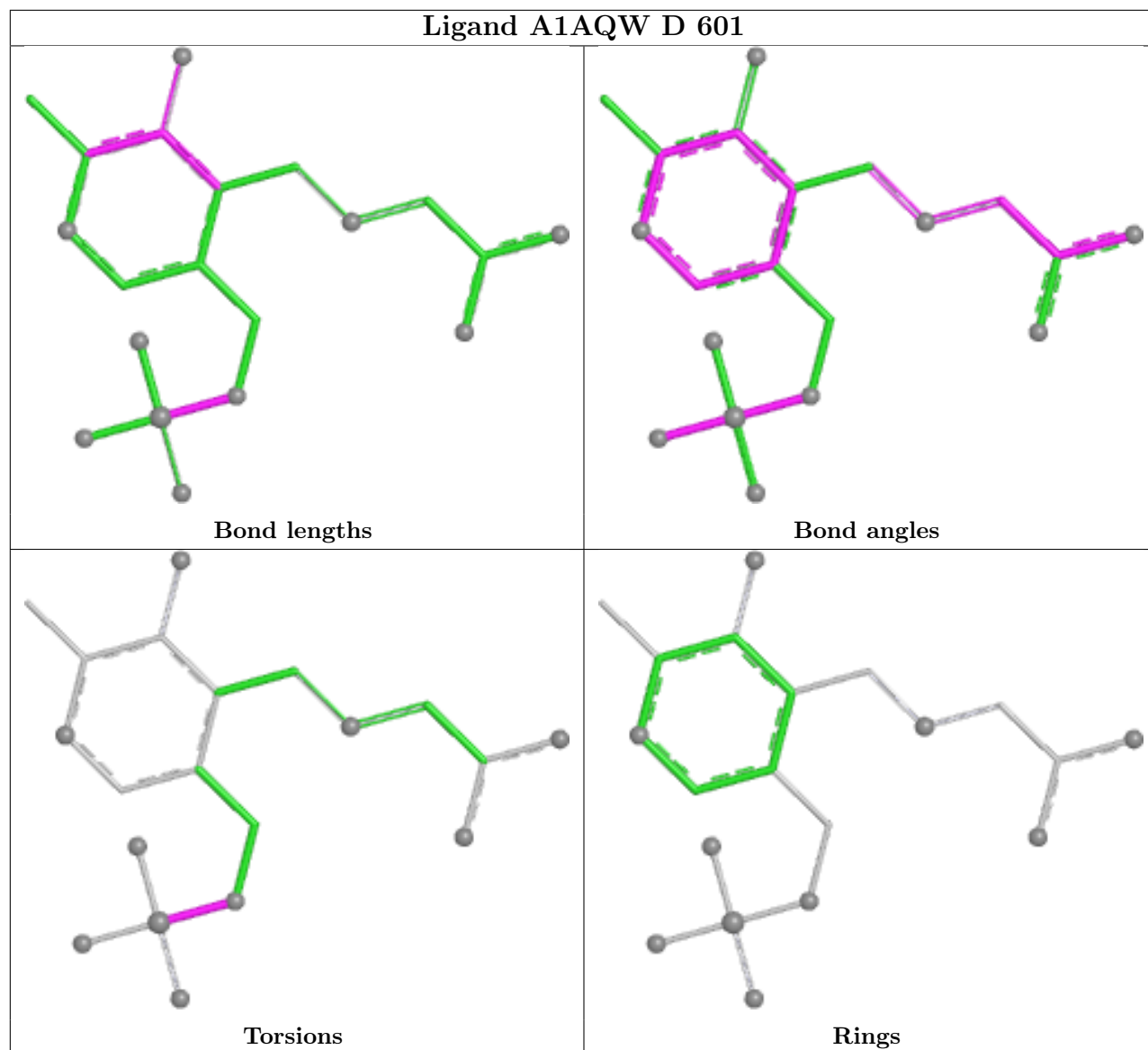
Ligand FFO B 602



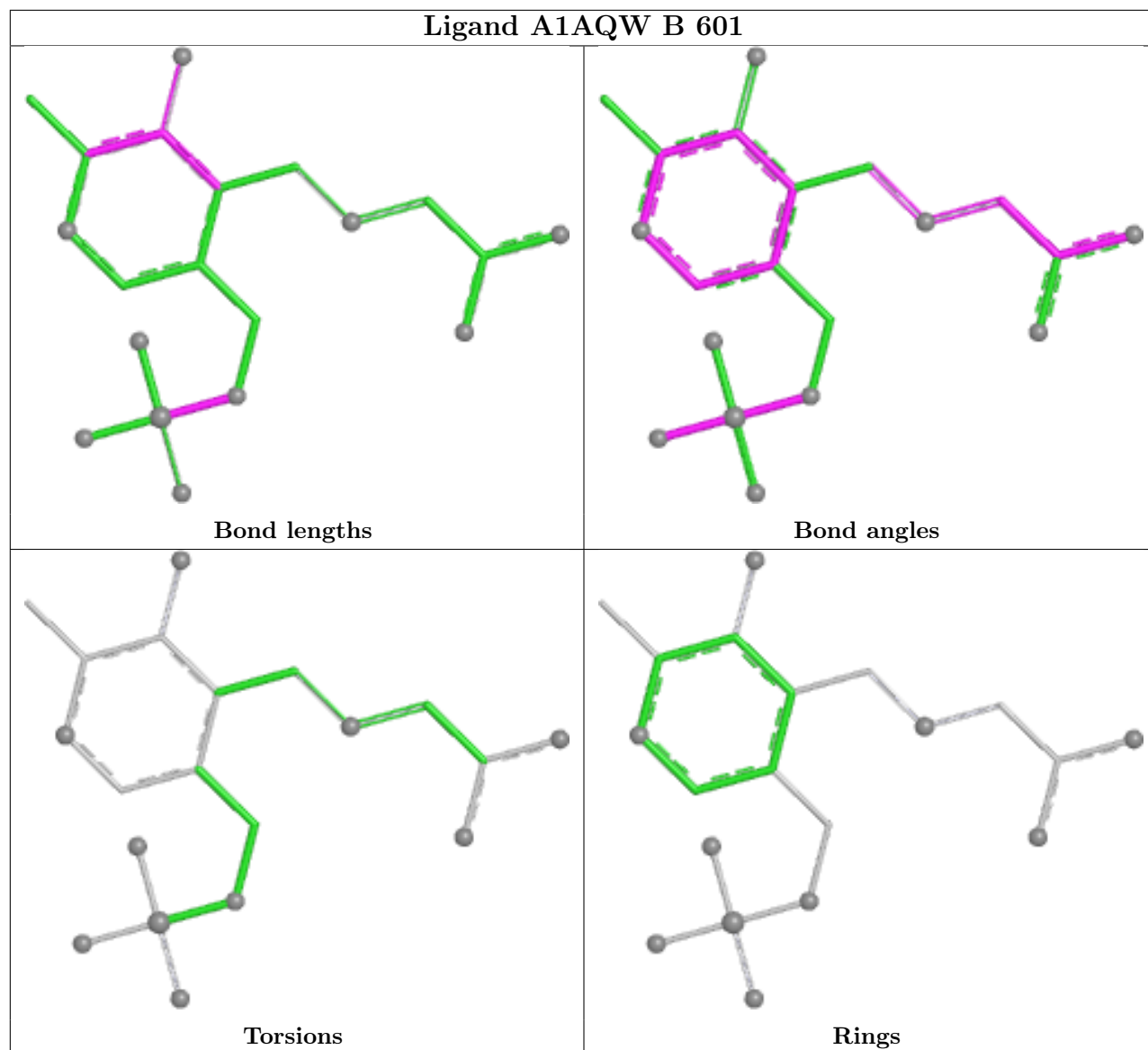
Ligand FFO D 602



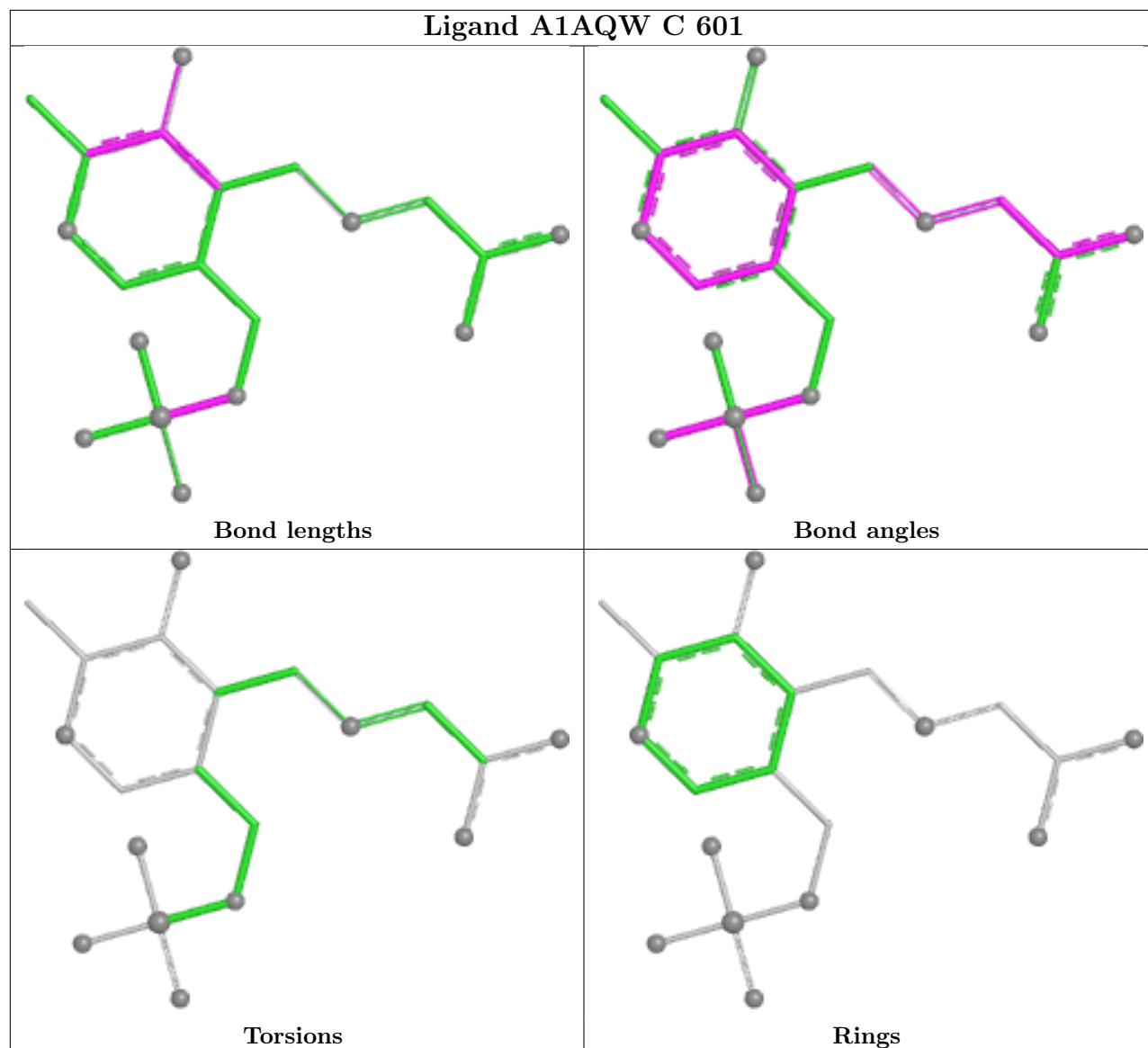
Ligand A1AQW D 601

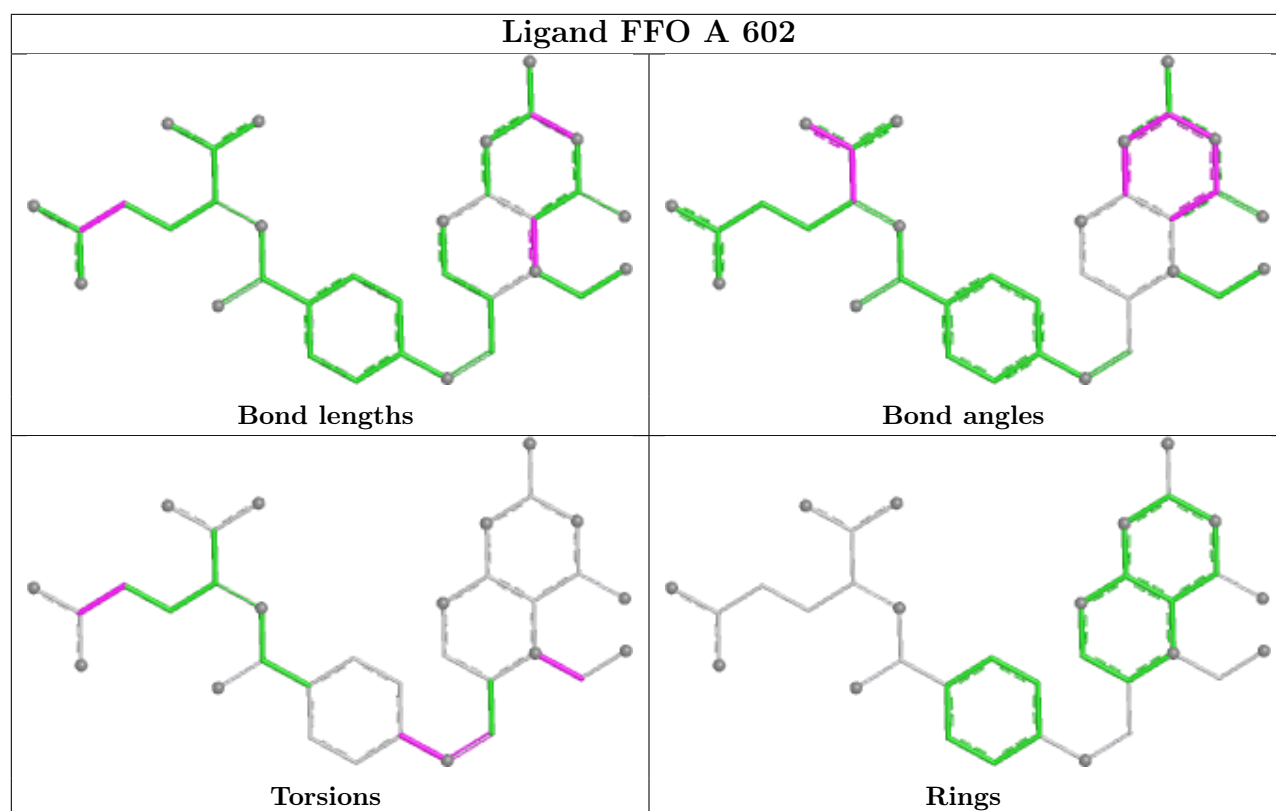


Ligand A1AQW B 601



Ligand A1AQW C 601





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	462/462 (100%)	-0.44	2 (0%) 88 90	11, 22, 47, 68	0
1	B	462/462 (100%)	-0.30	2 (0%) 88 90	13, 25, 54, 73	1 (0%)
1	C	453/462 (98%)	-0.49	1 (0%) 91 92	11, 20, 41, 64	0
1	D	453/462 (98%)	-0.28	0 100 100	14, 25, 46, 70	1 (0%)
All	All	1830/1848 (99%)	-0.38	5 (0%) 90 91	11, 23, 47, 73	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	298	ALA	2.9
1	A	301	PRO	2.5
1	B	470	SER	2.2
1	B	298	ALA	2.2
1	A	403	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

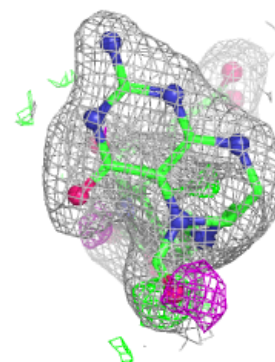
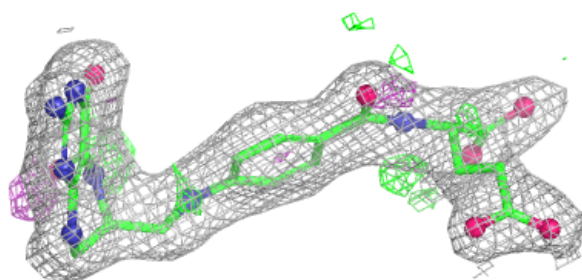
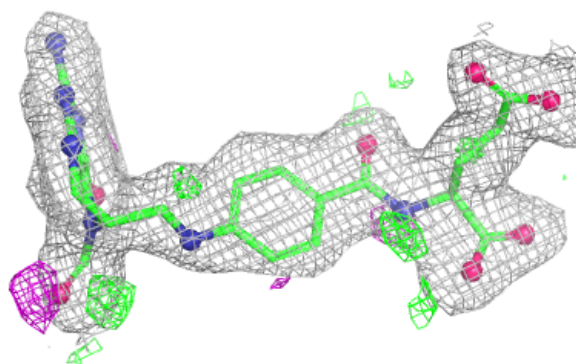
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FFO	B	602	34/34	0.94	0.07	18,24,45,57	0
3	FFO	D	602	34/34	0.94	0.07	14,20,36,39	0
3	FFO	C	602	34/34	0.95	0.07	12,16,34,37	0
3	FFO	A	602	34/34	0.95	0.07	15,21,38,43	0
2	A1AQW	D	601	20/20	0.97	0.06	13,16,19,19	0
2	A1AQW	C	601	20/20	0.98	0.05	8,12,16,16	0
2	A1AQW	A	601	20/20	0.98	0.05	11,14,17,18	0
2	A1AQW	B	601	20/20	0.98	0.06	13,17,24,25	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.

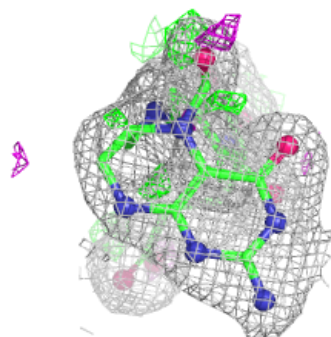
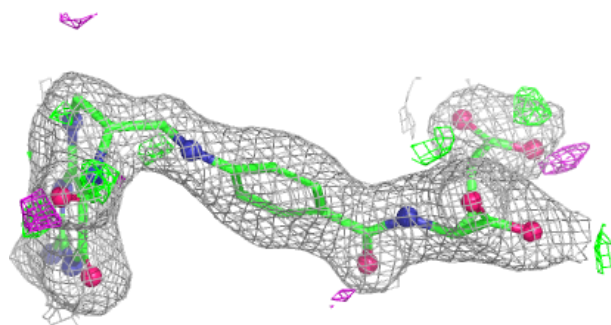
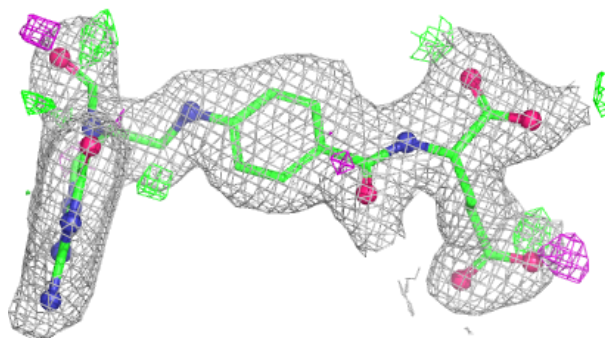
Electron density around FFO B 602:

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

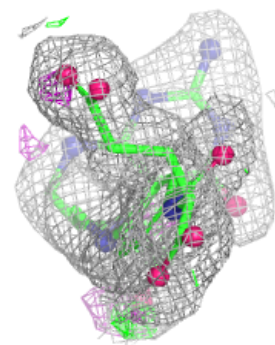
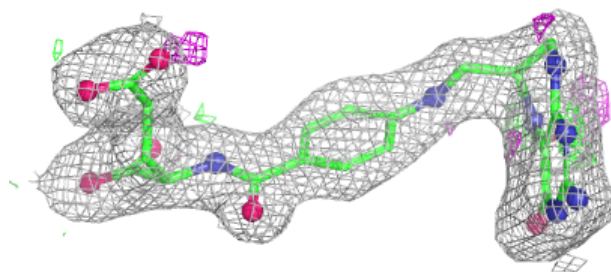
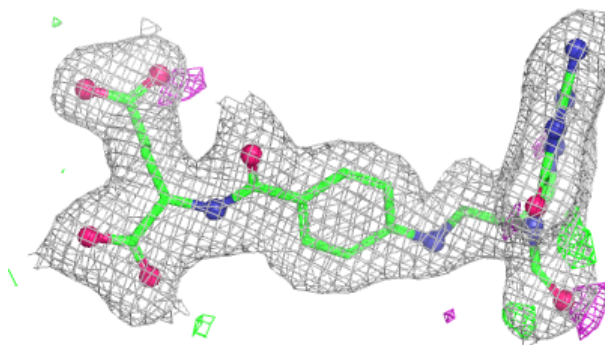


Electron density around FFO D 602:

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

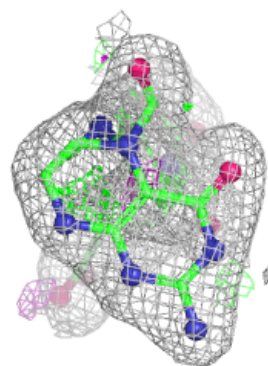
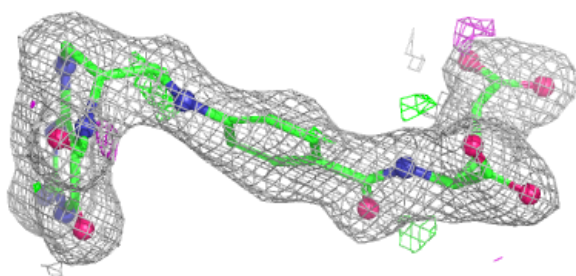
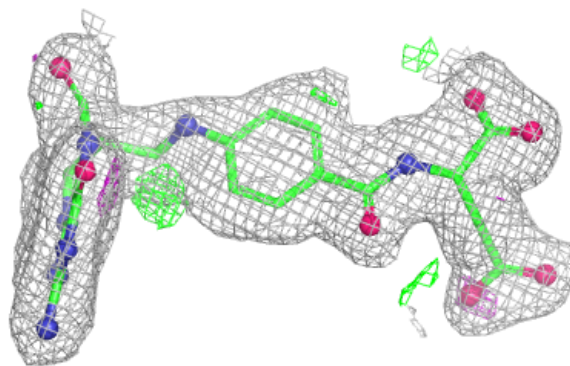
**Electron density around FFO C 602:**

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



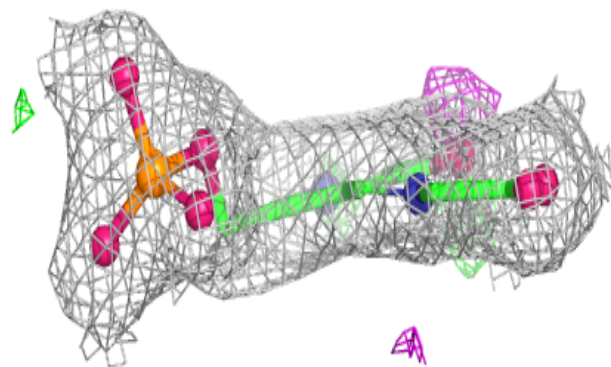
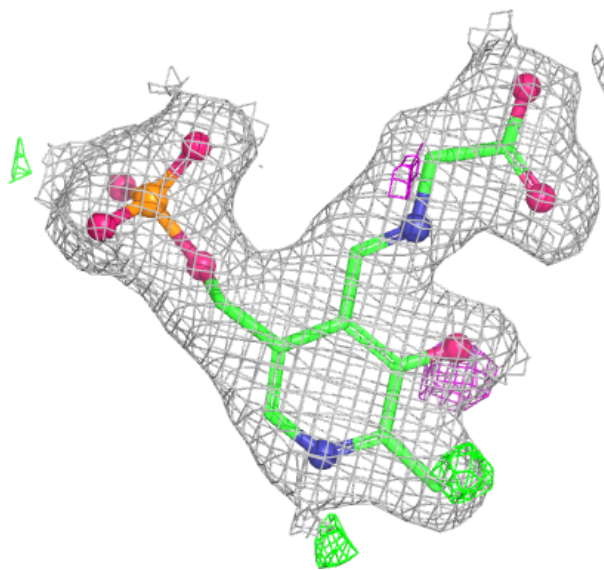
Electron density around FFO A 602:

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



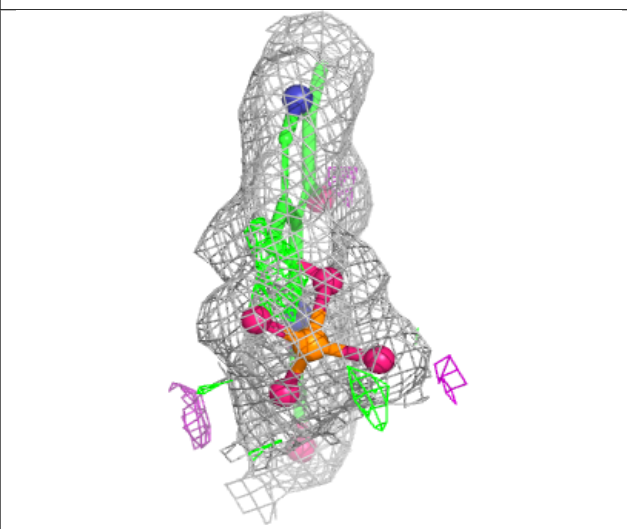
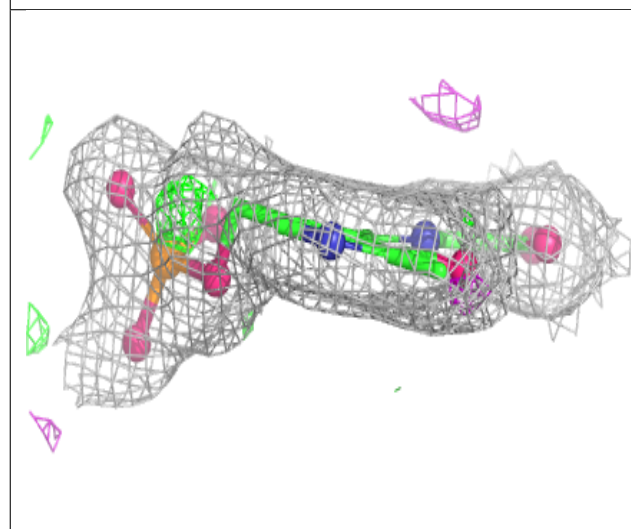
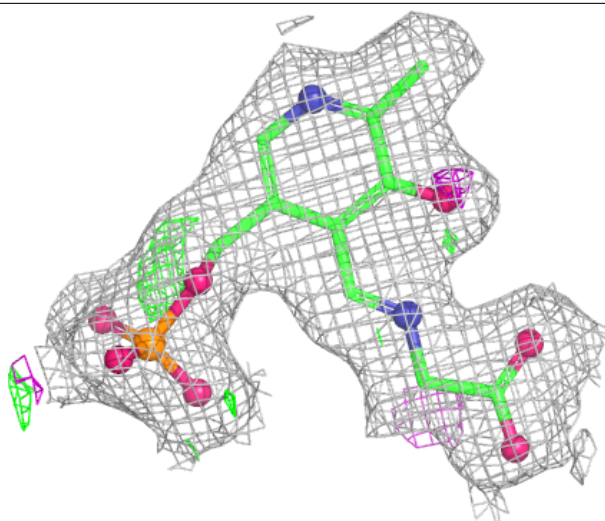
Electron density around A1AQW D 601:

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



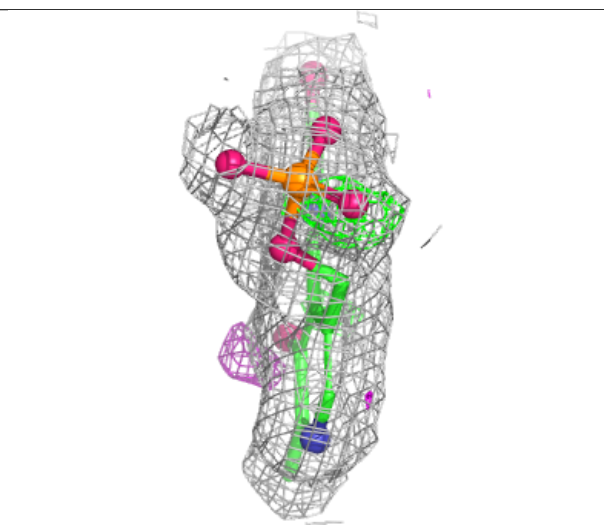
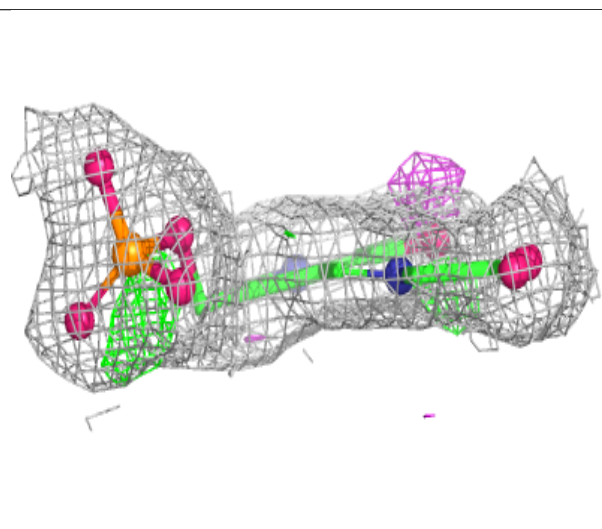
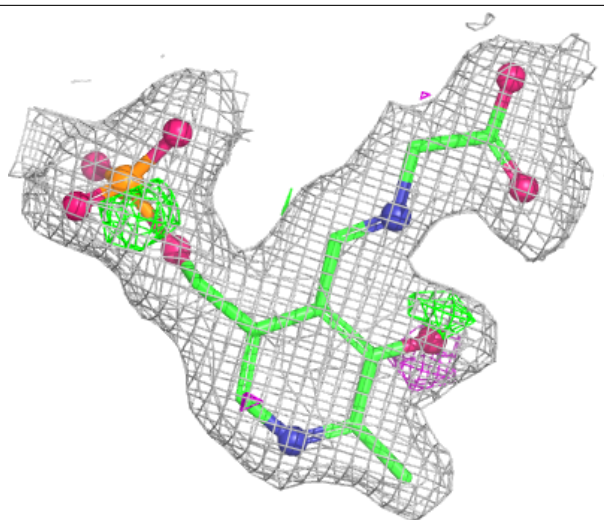
Electron density around A1AQW C 601:

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



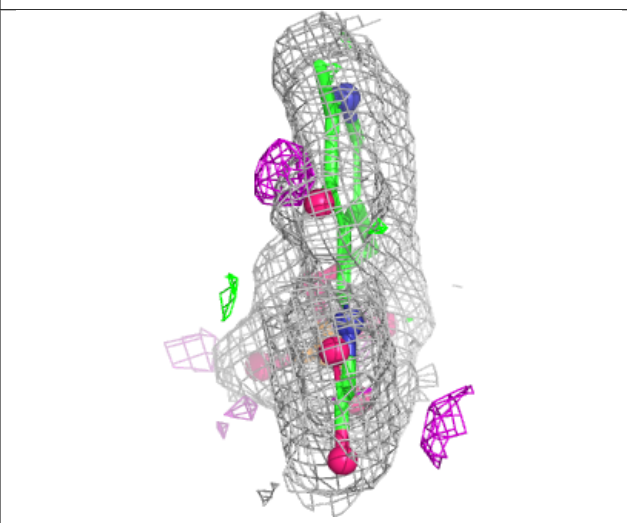
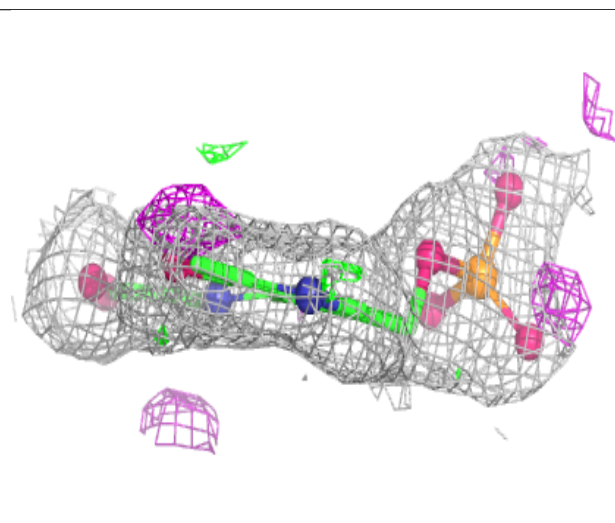
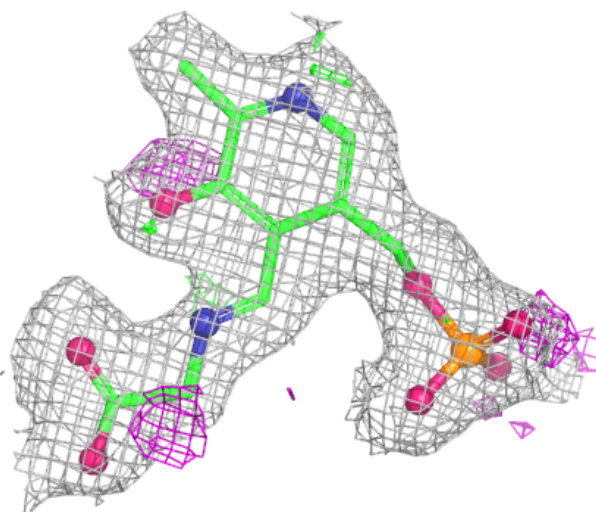
Electron density around A1AQW A 601:

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



Electron density around A1AQW B 601:

$2mF_o-DF_c$ (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.