Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 12:54 PM EDT

PDB ID	:	8EH0
Title	:	Engineered tyrosine synthase (TmTyrS1) derived from T. maritima TrpB with Ser bound as the amino-acrylate intermediate and complexed with quinoline N-oxide
Authors	:	Porter, N.J.; Almhjell, P.J.; Arnold, F.H.
Deposited on	:	2022-09-13
Resolution	:	1.70 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
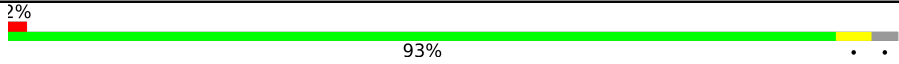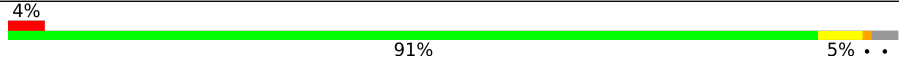*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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.
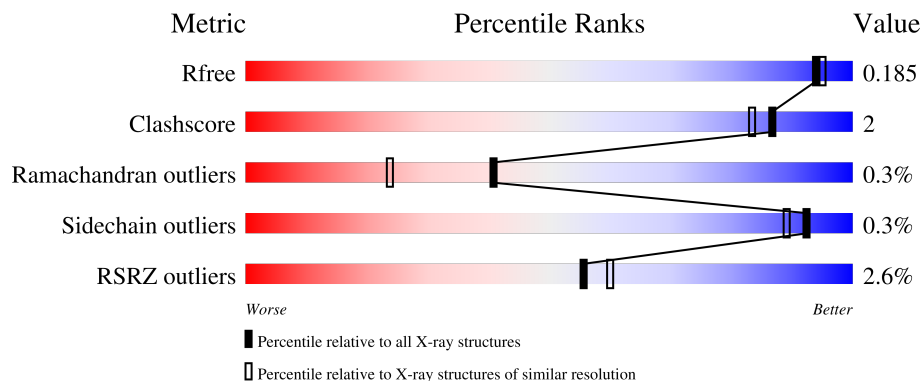
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	397	2% 93% · ·
1	B	397	4% 91% 5% · ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6419 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total 3026	C 1926	N 527	O 565	S 8	0	9	0
1	B	386	Total 2990	C 1905	N 518	O 559	S 8	0	4	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ASN	TYR	engineered mutation	UNP P50909
A	12	ASN	TYR	engineered mutation	UNP P50909
A	19	GLY	PRO	engineered mutation	UNP P50909
A	30	GLY	GLU	engineered mutation	UNP P50909
A	41	TYR	PHE	engineered mutation	UNP P50909
A	69	VAL	ILE	engineered mutation	UNP P50909
A	96	LEU	LYS	engineered mutation	UNP P50909
A	103	THR	ILE	engineered mutation	UNP P50909
A	105	GLY	GLU	engineered mutation	UNP P50909
A	140	LEU	PRO	engineered mutation	UNP P50909
A	167	ASP	ASN	engineered mutation	UNP P50909
A	184	PRO	ILE	engineered mutation	UNP P50909
A	213	PRO	LEU	engineered mutation	UNP P50909
A	228	SER	GLY	engineered mutation	UNP P50909
A	291	ALA	VAL	engineered mutation	UNP P50909
A	292	SER	THR	engineered mutation	UNP P50909
A	302	PRO	SER	engineered mutation	UNP P50909
A	389	HIS	ARG	engineered mutation	UNP P50909
A	390	LEU	-	expression tag	UNP P50909
A	391	GLU	-	expression tag	UNP P50909
A	392	HIS	-	expression tag	UNP P50909
A	393	HIS	-	expression tag	UNP P50909
A	394	HIS	-	expression tag	UNP P50909
A	395	HIS	-	expression tag	UNP P50909
A	396	HIS	-	expression tag	UNP P50909

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Chain	Residue	Modelled	Actual	Comment	Reference
A	397	HIS	-	expression tag	UNP P50909
B	4	ASN	TYR	engineered mutation	UNP P50909
B	12	ASN	TYR	engineered mutation	UNP P50909
B	19	GLY	PRO	engineered mutation	UNP P50909
B	30	GLY	GLU	engineered mutation	UNP P50909
B	41	TYR	PHE	engineered mutation	UNP P50909
B	69	VAL	ILE	engineered mutation	UNP P50909
B	96	LEU	LYS	engineered mutation	UNP P50909
B	103	THR	ILE	engineered mutation	UNP P50909
B	105	GLY	GLU	engineered mutation	UNP P50909
B	140	LEU	PRO	engineered mutation	UNP P50909
B	167	ASP	ASN	engineered mutation	UNP P50909
B	184	PRO	ILE	engineered mutation	UNP P50909
B	213	PRO	LEU	engineered mutation	UNP P50909
B	228	SER	GLY	engineered mutation	UNP P50909
B	291	ALA	VAL	engineered mutation	UNP P50909
B	292	SER	THR	engineered mutation	UNP P50909
B	302	PRO	SER	engineered mutation	UNP P50909
B	389	HIS	ARG	engineered mutation	UNP P50909
B	390	LEU	-	expression tag	UNP P50909
B	391	GLU	-	expression tag	UNP P50909
B	392	HIS	-	expression tag	UNP P50909
B	393	HIS	-	expression tag	UNP P50909
B	394	HIS	-	expression tag	UNP P50909
B	395	HIS	-	expression tag	UNP P50909
B	396	HIS	-	expression tag	UNP P50909
B	397	HIS	-	expression tag	UNP P50909

- Molecule 2 is 2-{[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyli dene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula: $C_{11}H_{13}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).
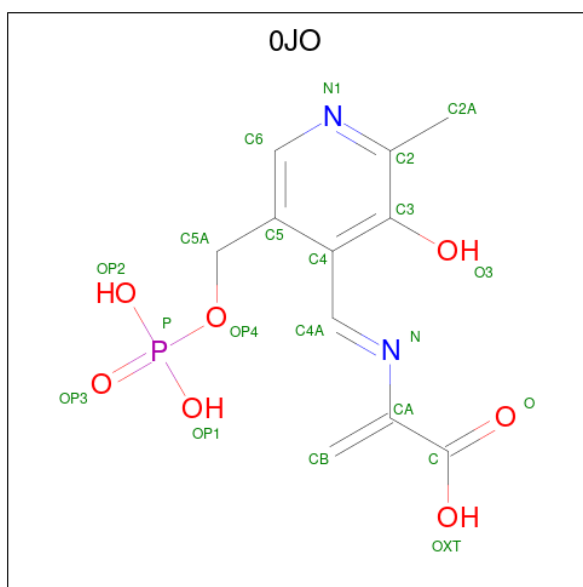
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

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WORLDWIDE
PDB
PROTEIN DATA BANK

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

- Molecule 4 is 1-oxo-1lambda 5 -quinoline (three-letter code: QOX) (formula: C_9H_7NO) (labeled as "Ligand of Interest" by depositor).
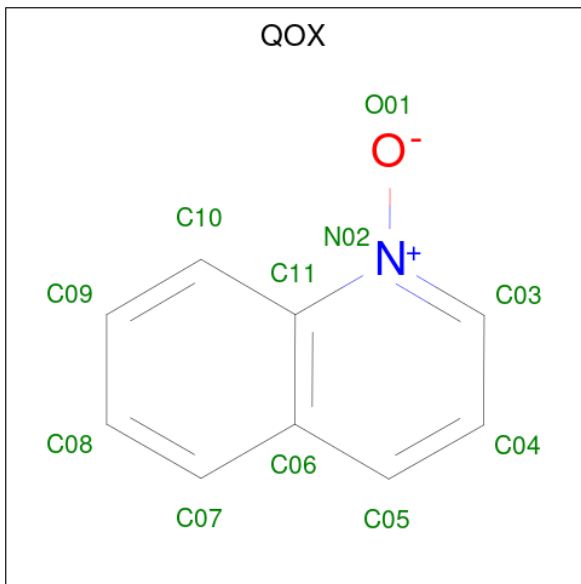
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total C N O 11 9 1 1				0	0
4	B	1	Total C N O 11 9 1 1				0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total K 1 1		0	0
5	B	1	Total K 1 1		0	0

- Molecule 6 is water.

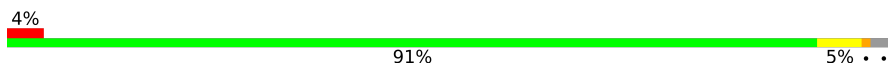| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total 176	O 176	0	0
6	B	145	Total 145	O 145	0	0

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: Tryptophan synthase beta chain 1

Chain A:

• Molecule 1: Tryptophan synthase beta chain 1

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	164.37Å 164.37Å 84.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.74 – 1.70 38.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.74-1.70) 100.0 (38.74-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.186 0.166 , 0.185	Depositor DCC
R_{free} test set	6325 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6419	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: K, 0JO, QOX, EDO

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	0.87	0/3103	0.88	0/4197
1	B	0.80	0/3064	0.86	0/4145
All	All	0.84	0/6167	0.87	0/8342

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	3026	0	3029	11	0
1	B	2990	0	2995	15	0
2	A	21	0	10	0	0
2	B	21	0	9	0	0
3	A	8	0	12	1	0
3	B	8	0	12	0	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	176	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	145	0	0	0	0
All	All	6419	0	6067	26	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 (26) 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:198:ARG:HH12	3:A:405:EDO:H12	1.40	0.87
1:B:60:ARG:HB3	1:B:60:ARG:HH11	1.50	0.77
1:A:65:TYR:OH	1:A:354:LYS:NZ	2.24	0.69
1:B:60:ARG:HD3	1:B:337:LEU:O	1.94	0.67
1:A:271:ILE:HD11	1:A:278:LYS:HE2	1.75	0.67
1:B:25:GLU:O	1:B:29:GLU:HG2	1.95	0.66
1:A:32:MET:HE2	1:A:38:TRP:HZ2	1.70	0.57
1:A:385:ARG:HH11	1:A:385:ARG:HG3	1.71	0.55
1:B:357:ASN:OD1	1:B:359:LYS:HG2	2.12	0.49
1:B:60:ARG:HH11	1:B:60:ARG:CB	2.22	0.49
1:B:31:ILE:HD13	1:B:93:LEU:HD13	1.94	0.48
1:B:62:SER:HB3	1:B:67:ALA:O	2.15	0.47
1:B:2:LYS:HD3	1:B:4:ASN:H	1.78	0.47
1:B:270:LYS:HE2	1:B:285:ASP:OD1	2.16	0.46
1:B:386:GLU:O	1:B:387:ARG:HG2	2.17	0.45
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.76	0.45
1:A:212:ILE:HG21	1:A:220:PRO:HD3	1.99	0.45
1:A:59[A]:ARG:HG2	6:A:570:HOH:O	2.17	0.44
1:A:162:LEU:HD23	1:A:301:TYR:HB2	1.98	0.44
1:A:385:ARG:HG3	1:A:385:ARG:NH1	2.33	0.43
1:A:59[A]:ARG:HG3	1:A:60:ARG:N	2.34	0.43
1:B:223:ILE:HG13	1:B:245:VAL:HG11	2.01	0.42
1:A:238:TYR:HB3	1:A:239:PRO:HD3	2.00	0.42
1:B:384:VAL:O	1:B:387:ARG:HB2	2.19	0.42
1:B:28:TYR:O	1:B:31:ILE:HG12	2.20	0.42
1:B:258:GLU:OE1	1:B:258:GLU:HA	2.21	0.41

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	392/397 (99%)	384 (98%)	7 (2%)	1 (0%)	41	24
1	B	388/397 (98%)	379 (98%)	8 (2%)	1 (0%)	41	24
All	All	780/794 (98%)	763 (98%)	15 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	VAL
1	A	187	VAL

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	313/319 (98%)	313 (100%)	0	100	100
1	B	309/319 (97%)	307 (99%)	2 (1%)	86	80
All	All	622/638 (98%)	620 (100%)	2 (0%)	92	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
1	B	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	EDO	A	405	-	3,3,3	0.73	0	2,2,2	0.03	0
2	0JO	A	401	-	20,21,21	2.00	6 (30%)	23,30,30	1.43	6 (26%)
3	EDO	B	405	-	3,3,3	0.96	0	2,2,2	0.58	0
2	0JO	B	401	-	20,21,21	2.08	6 (30%)	23,30,30	1.41	5 (21%)
3	EDO	B	404	-	3,3,3	0.58	0	2,2,2	0.88	0
4	QOX	B	402	-	10,12,12	2.43	3 (30%)	13,16,16	1.08	1 (7%)
4	QOX	A	403	-	10,12,12	2.05	4 (40%)	13,16,16	1.07	1 (7%)
3	EDO	A	402	-	3,3,3	0.79	0	2,2,2	0.20	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
3	EDO	A	405	-	-	1/1/1/1	-
2	0JO	A	401	-	-	0/10/15/15	0/1/1/1
3	EDO	B	405	-	-	0/1/1/1	-
2	0JO	B	401	-	-	0/10/15/15	0/1/1/1
3	EDO	B	404	-	-	0/1/1/1	-
4	QOX	B	402	-	-	-	0/2/2/2
4	QOX	A	403	-	-	-	0/2/2/2
3	EDO	A	402	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	QOX	O01-N02	-5.22	1.26	1.37
4	A	403	QOX	O01-N02	-4.54	1.27	1.37
2	B	401	0JO	C2A-C2	4.49	1.58	1.50
2	A	401	0JO	C2A-C2	4.25	1.57	1.50
2	B	401	0JO	C4-C4A	4.25	1.54	1.46
2	A	401	0JO	C4A-N	4.24	1.33	1.28
2	A	401	0JO	C4-C3	3.55	1.46	1.40
2	B	401	0JO	C5A-C5	3.46	1.60	1.50
2	B	401	0JO	OXT-C	-3.21	1.21	1.30
2	B	401	0JO	C4-C3	3.03	1.45	1.40
4	B	402	QOX	C09-C08	2.93	1.45	1.38
4	B	402	QOX	C03-C04	2.71	1.44	1.38
2	A	401	0JO	CA-N	2.63	1.47	1.36
4	A	403	QOX	C06-C11	2.60	1.46	1.42
4	A	403	QOX	C03-C04	2.57	1.44	1.38
2	A	401	0JO	C6-C5	2.32	1.42	1.37
2	A	401	0JO	C4-C4A	2.23	1.50	1.46
2	B	401	0JO	C6-C5	2.11	1.42	1.37
4	A	403	QOX	C09-C08	2.05	1.43	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	0JO	C2A-C2-C3	-2.88	117.34	120.89
2	A	401	0JO	C4-C3-C2	-2.74	118.49	120.19
2	A	401	0JO	C3-C2-N1	2.66	124.20	120.77
4	A	403	QOX	C03-C04-C05	2.61	123.07	119.39
2	A	401	0JO	CB-CA-C	2.60	127.35	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	0JO	C4-C4A-N	-2.28	117.64	123.19
2	B	401	0JO	CB-CA-C	2.28	126.57	121.06
2	B	401	0JO	C3-C2-N1	2.27	123.70	120.77
2	A	401	0JO	C4-C4A-N	-2.22	117.79	123.19
2	A	401	0JO	C2A-C2-C3	-2.08	118.32	120.89
2	A	401	0JO	C3-C4-C5	-2.07	116.67	118.26
4	B	402	QOX	C10-C11-C06	2.06	122.01	119.25
2	B	401	0JO	C4-C3-C2	-2.04	118.92	120.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

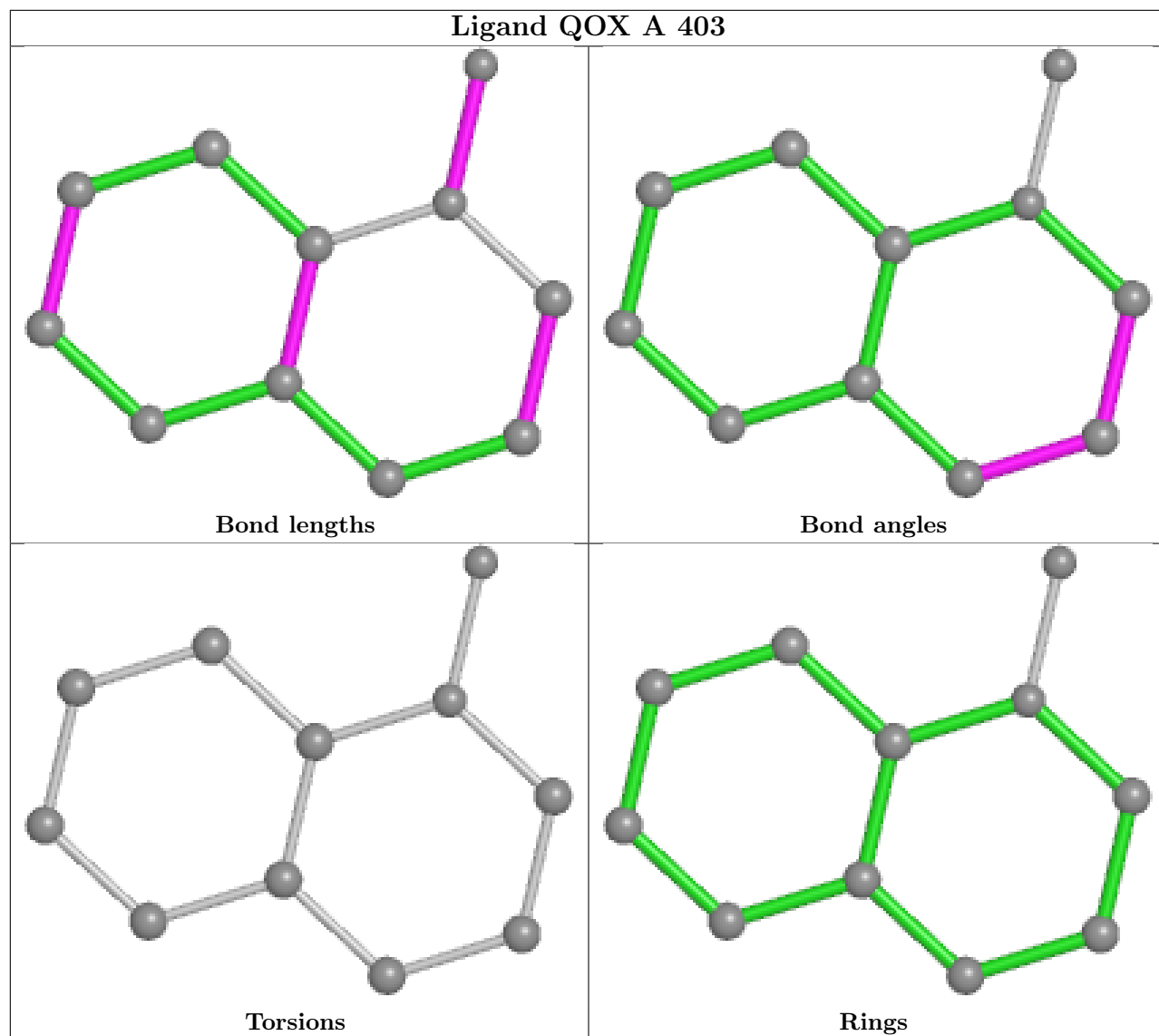| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	EDO	1	0

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 then 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 0JO A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 0JO B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand QOX B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand QOX A 403

Bond lengths

Bond angles

Torsions

Rings
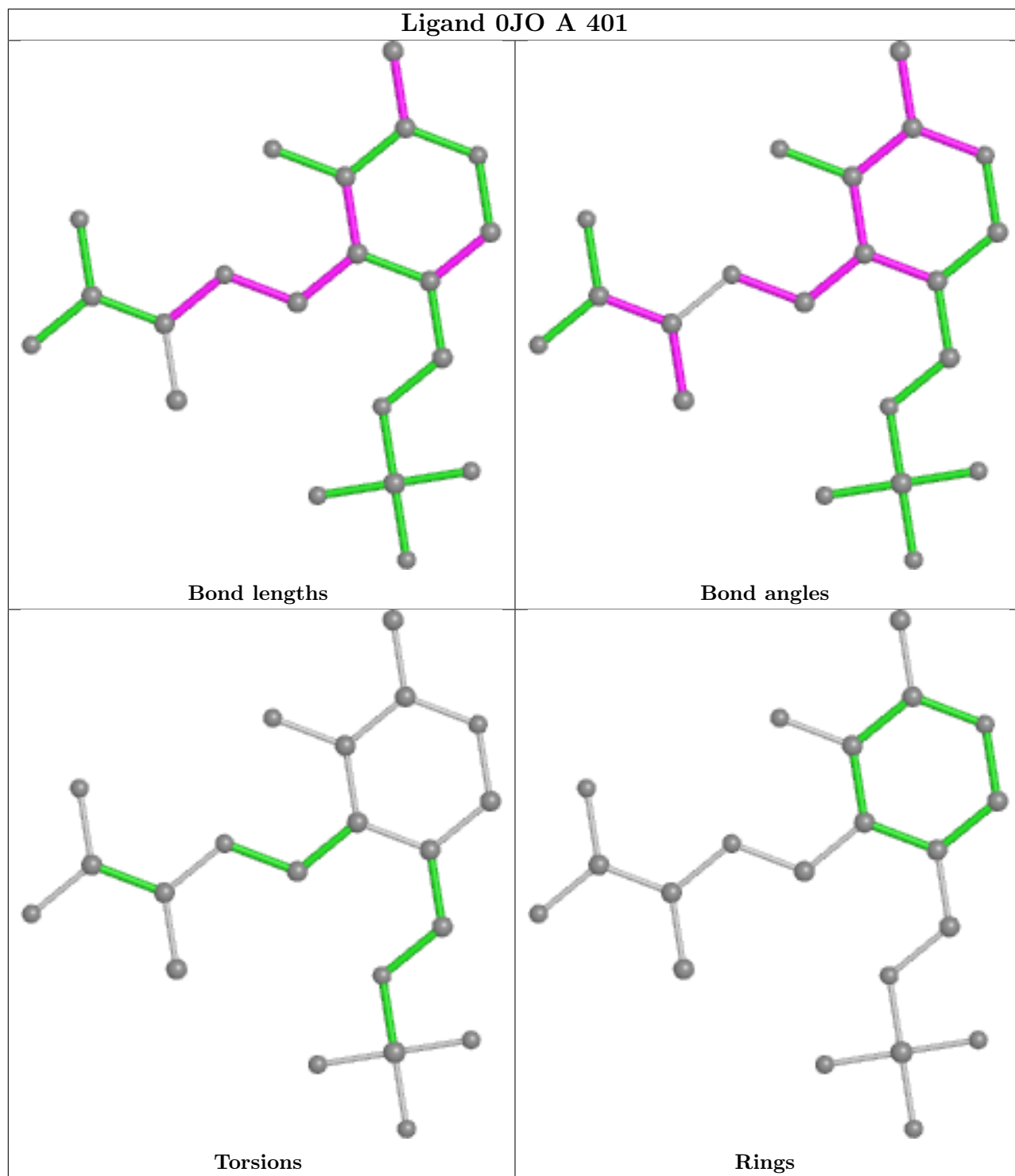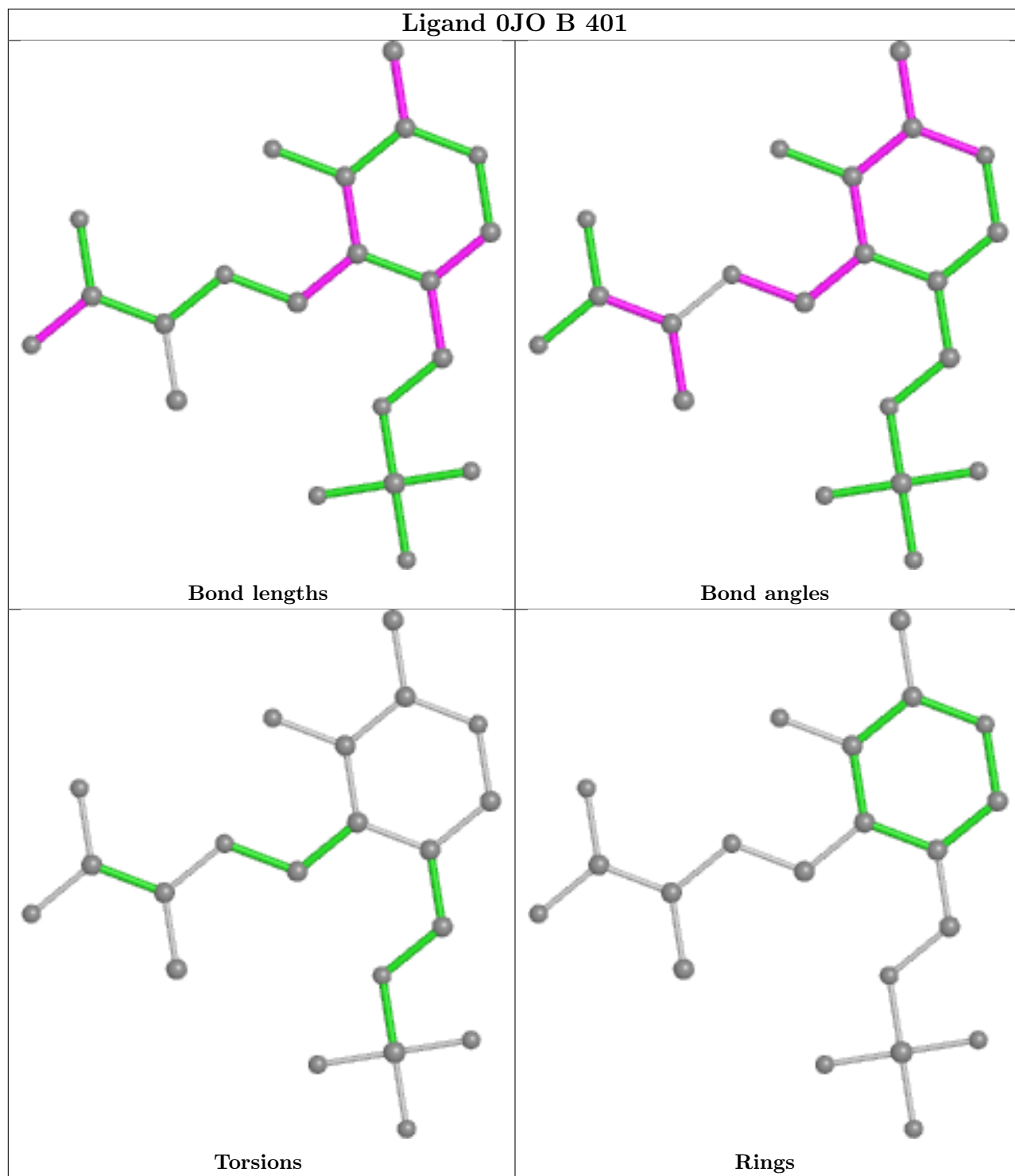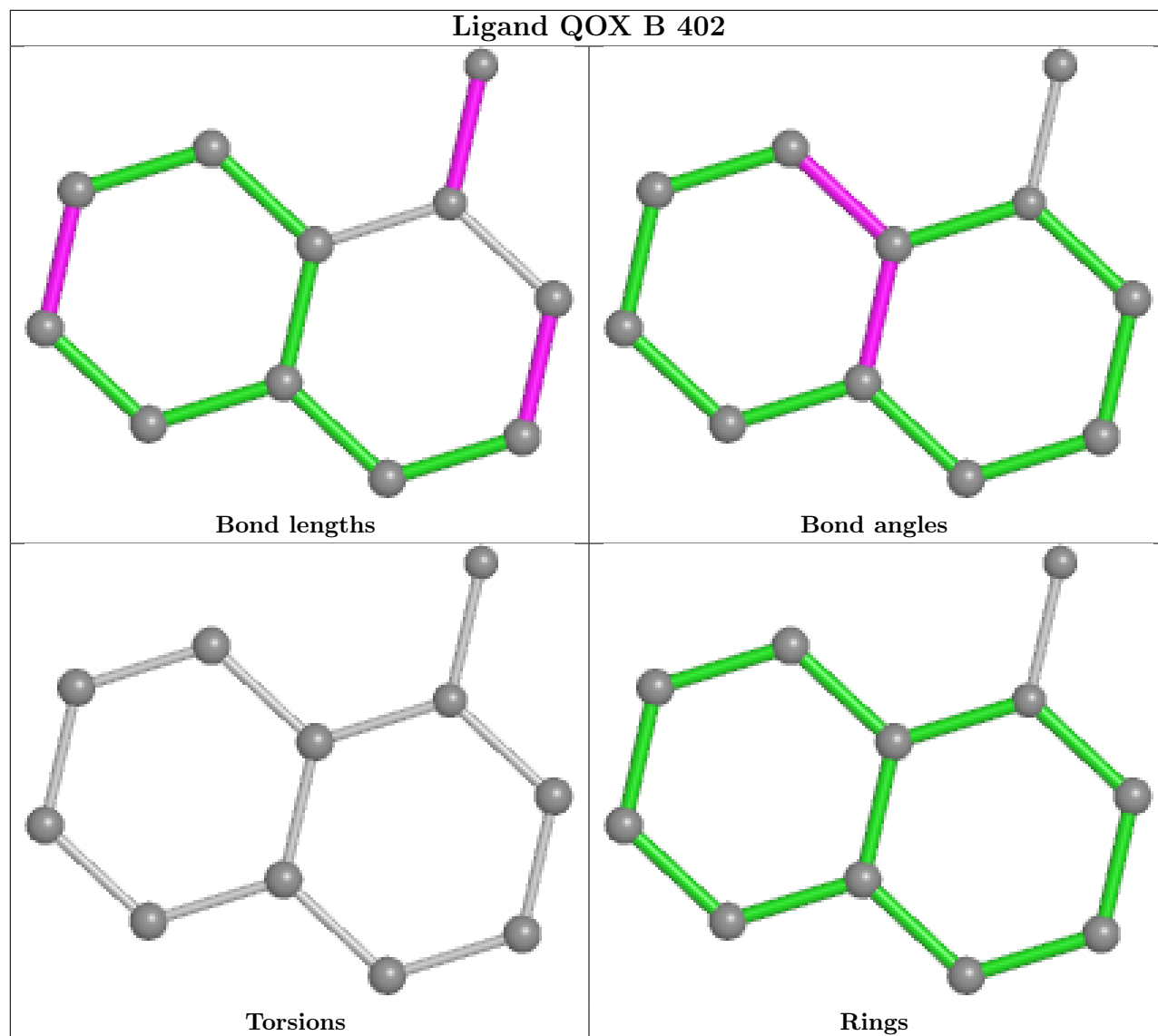
5.7 Other polymers ⓘ

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, 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	385/397 (96%)	-0.27	6 (1%) 72	76	20, 26, 39, 69	0
1	B	386/397 (97%)	-0.07	14 (3%) 42	47	22, 28, 46, 74	0
All	All	771/794 (97%)	-0.17	20 (2%) 56	60	20, 27, 44, 74	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	GLU	4.3
1	A	385	ARG	3.5
1	B	387	ARG	3.3
1	B	385	ARG	3.3
1	A	387	ARG	3.1
1	B	357	ASN	2.9
1	B	35	GLU	2.9
1	A	386	GLU	2.7
1	B	2	LYS	2.6
1	B	38	TRP	2.3
1	B	84	ILE	2.3
1	B	32	MET	2.3
1	B	358	ILE	2.3
1	A	226	CYS	2.3
1	B	80	GLY	2.2
1	A	80	GLY	2.1
1	B	372[A]	ASP	2.1
1	B	382	PRO	2.1
1	A	81	ALA	2.0
1	B	217	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

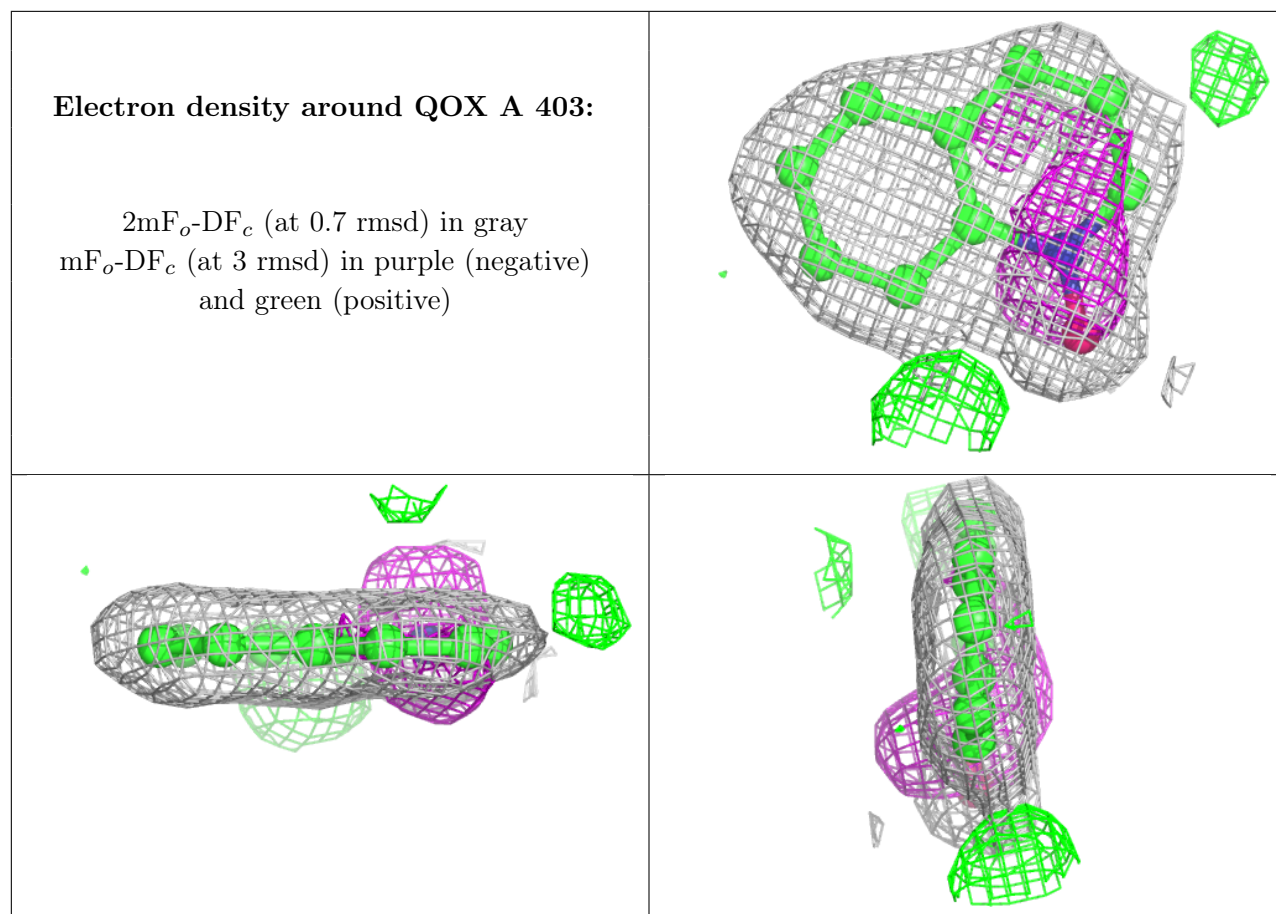There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, $95^{th}$ 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	EDO	A	405	4/4	0.70	0.23	42,44,48,52	0
3	EDO	B	405	4/4	0.80	0.25	36,44,45,46	0
3	EDO	A	402	4/4	0.86	0.20	29,43,44,44	0
4	QOX	A	403	11/11	0.88	0.13	33,35,37,37	0
4	QOX	B	402	11/11	0.88	0.14	33,37,41,41	0
3	EDO	B	404	4/4	0.92	0.10	33,37,38,40	0
2	0JO	A	401	21/21	0.99	0.12	20,24,26,29	0
2	0JO	B	401	21/21	0.99	0.11	20,24,27,28	0
5	K	A	404	1/1	1.00	0.07	26,26,26,26	0
5	K	B	403	1/1	1.00	0.05	28,28,28,28	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.
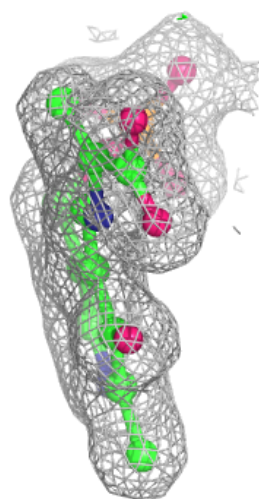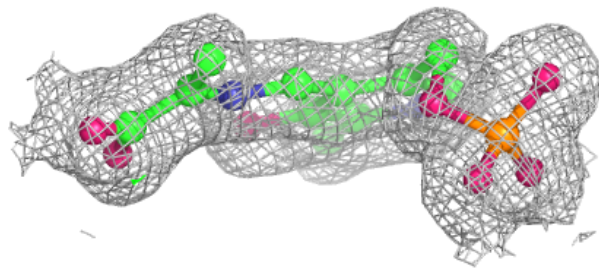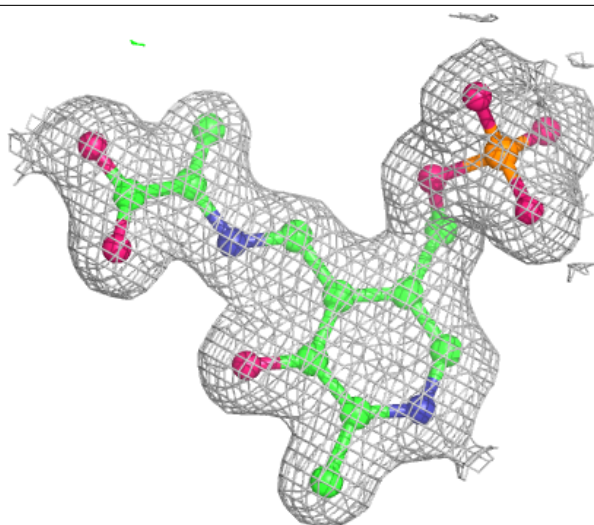
Electron density around QOX A 403:

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

Electron density around QOX B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
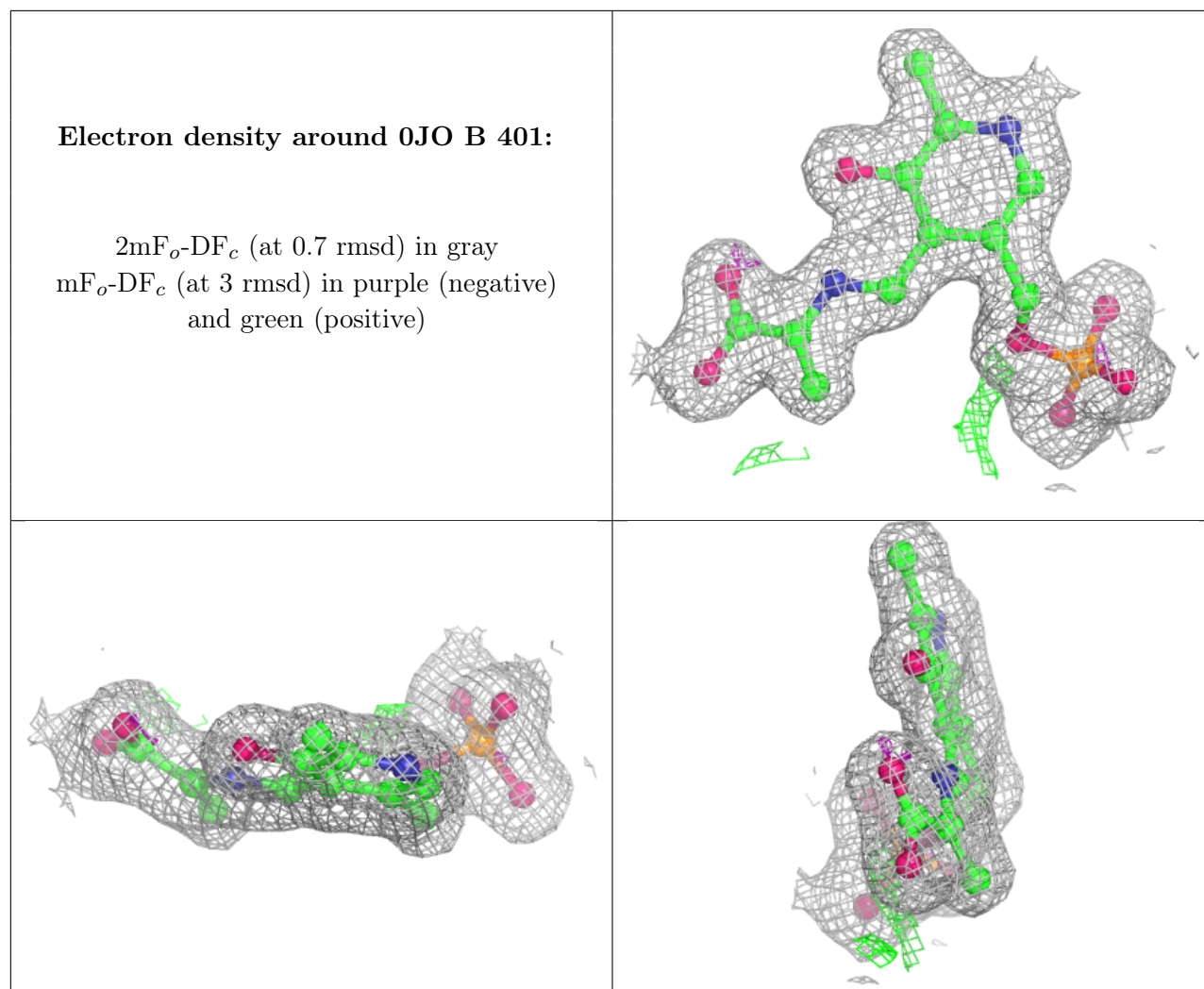mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
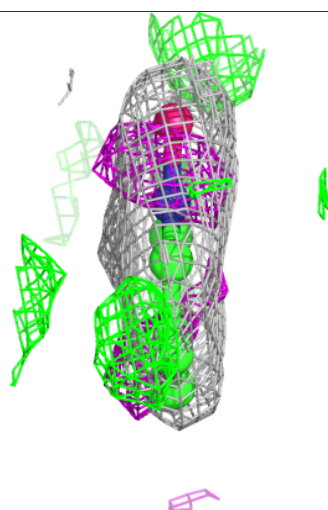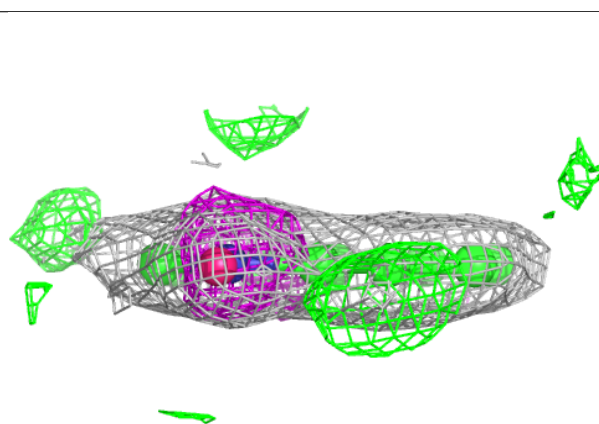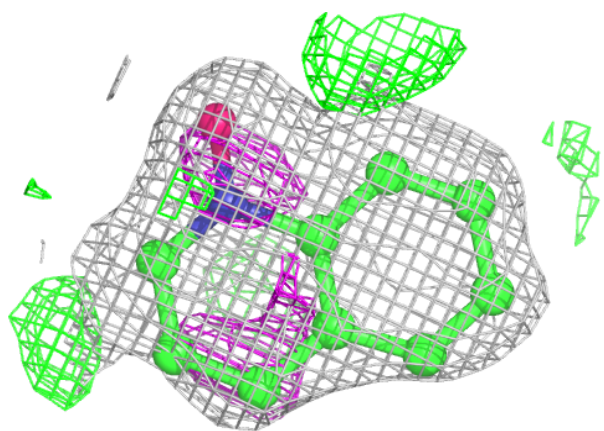
Electron density around 0JO A 401:

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

Electron density around 0JO B 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.