WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2022 – 04:19 pm BST

PDB ID	:	7POL
Title	:	Crystal structure of profragilysin-3 (proBFT-3) from Bacteroides fragilis in complex with flumequine
Authors	:	Eckhard, U.; Guevara, T.; Gomis-Ruth, F.X.
Deposited on	:	2021-09-09
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

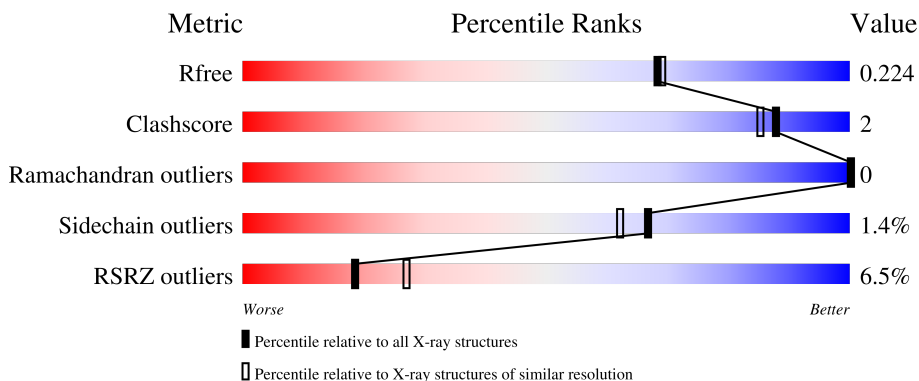|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 1.95 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.4%
RSRZ outliers		6.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	402	4% — 79% — 5% — 16%
1	B	402	6% — 78% — 5% — 16%

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	407	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6137 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 BFT-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total 2706	C 1715	N 448	O 529	S 14	0	3	0
1	B	336	Total 2672	C 1695	N 440	O 523	S 14	0	2	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP O86049
A	-3	GLY	-	expression tag	UNP O86049
A	-2	SER	-	expression tag	UNP O86049
A	-1	SER	-	expression tag	UNP O86049
A	0	HIS	-	expression tag	UNP O86049
A	1	HIS	-	expression tag	UNP O86049
A	2	HIS	-	expression tag	UNP O86049
A	3	HIS	-	expression tag	UNP O86049
A	4	HIS	-	expression tag	UNP O86049
A	5	HIS	-	expression tag	UNP O86049
A	6	SER	-	expression tag	UNP O86049
A	7	SER	-	expression tag	UNP O86049
A	8	GLY	-	expression tag	UNP O86049
A	9	GLU	-	expression tag	UNP O86049
A	10	ASN	-	expression tag	UNP O86049
A	11	LEU	-	expression tag	UNP O86049
A	12	TYR	-	expression tag	UNP O86049
A	13	PHE	-	expression tag	UNP O86049
A	14	GLN	-	expression tag	UNP O86049
A	15	GLY	-	expression tag	UNP O86049
A	16	ALA	-	expression tag	UNP O86049
A	17	MET	-	expression tag	UNP O86049
B	-4	MET	-	initiating methionine	UNP O86049
B	-3	GLY	-	expression tag	UNP O86049
B	-2	SER	-	expression tag	UNP O86049

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP O86049
B	0	HIS	-	expression tag	UNP O86049
B	1	HIS	-	expression tag	UNP O86049
B	2	HIS	-	expression tag	UNP O86049
B	3	HIS	-	expression tag	UNP O86049
B	4	HIS	-	expression tag	UNP O86049
B	5	HIS	-	expression tag	UNP O86049
B	6	SER	-	expression tag	UNP O86049
B	7	SER	-	expression tag	UNP O86049
B	8	GLY	-	expression tag	UNP O86049
B	9	GLU	-	expression tag	UNP O86049
B	10	ASN	-	expression tag	UNP O86049
B	11	LEU	-	expression tag	UNP O86049
B	12	TYR	-	expression tag	UNP O86049
B	13	PHE	-	expression tag	UNP O86049
B	14	GLN	-	expression tag	UNP O86049
B	15	GLY	-	expression tag	UNP O86049
B	16	ALA	-	expression tag	UNP O86049
B	17	MET	-	expression tag	UNP O86049

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total Zn		0	0
			1	1		

- Molecule 3 is (12 {R})-7-fluoranyl-12-methyl-4-oxidanylidene-1-azatricyclo[7.3.1.0^{5,13}]trideca-2,5(13),6,8-tetraene-3-carboxylic acid (three-letter code: 7X9) (formula: $C_{14}H_{12}FNO_3$) (labeled as "Ligand of Interest" by depositor).
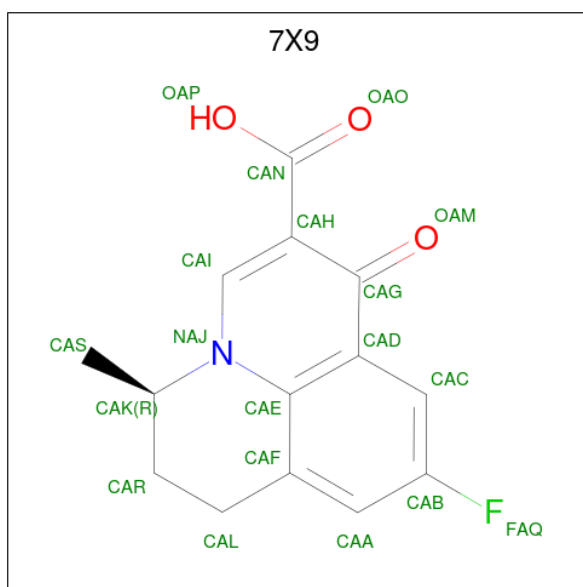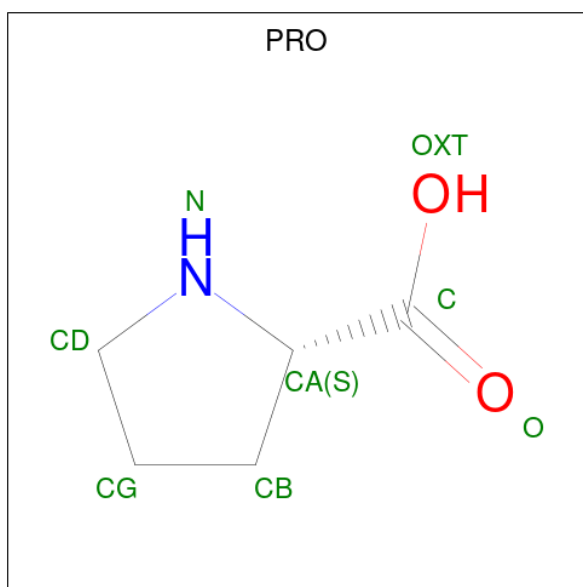
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			19	14	1	1	3		
3	A	1	Total	C	F	N	O	0	0
			19	14	1	1	3		
3	B	1	Total	C	F	N	O	0	0
			19	14	1	1	3		
3	B	1	Total	C	F	N	O	0	0
			19	14	1	1	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).

PRO

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	5	1	2		
5	A	1	Total	C	N	O	0	0
			8	5	1	2		
5	A	1	Total	C	N	O	0	0
			8	5	1	2		
5	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

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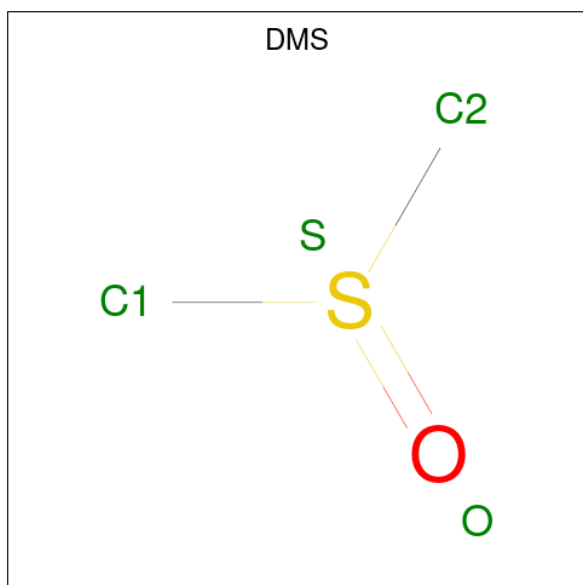
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	300	Total 313	O 313	0	14
7	B	291	Total 311	O 311	0	20

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: BFT-3

Chain A:

• Molecule 1: BFT-3

Chain B:
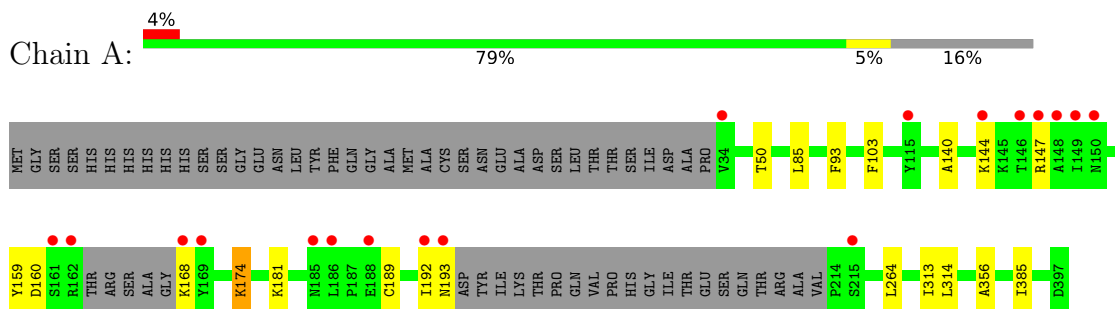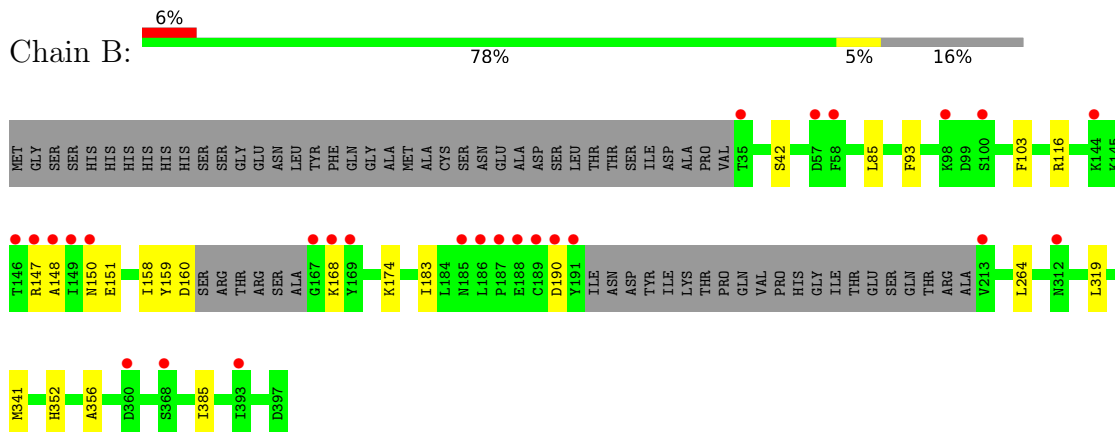
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.02Å 84.02Å 267.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.15 – 1.95 80.15 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.15-1.95) 100.0 (80.15-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.43 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.201 , 0.215 0.200 , 0.224	Depositor DCC
R_{free} test set	716 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning [2]	$<|L|> = 0.51$, $<L^2> = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6137	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: ZN, CL, DMS, 7X9

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	0.42	0/2771	0.53	0/3747
1	B	0.41	0/2734	0.55	0/3698
All	All	0.42	0/5505	0.54	0/7445

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	2706	0	2617	9	0
1	B	2672	0	2578	11	0
2	A	1	0	0	0	0
3	A	38	0	0	0	0
3	B	38	0	0	1	0
4	A	2	0	0	0	0
5	A	24	0	21	1	0
5	B	8	0	7	0	0
6	A	8	0	12	0	0
6	B	16	0	24	1	0
7	A	313	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	311	0	0	1	0
All	All	6137	0	5259	21	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 (21) 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:140:ALA:HB1	1:A:144:LYS:HE3	1.77	0.66
1:B:116:ARG:NH1	6:B:407:DMS:O	2.28	0.66
1:A:192:ILE:HG12	1:A:313:ILE:HD13	1.90	0.54
5:A:407:PRO:N	5:A:408:PRO:O	2.42	0.53
1:B:319:LEU:HD13	1:B:352:HIS:CD2	2.44	0.52
1:B:158:ILE:HD11	1:B:174:LYS:HB2	1.92	0.52
1:B:148:ALA:HB3	1:B:151:GLU:HG3	1.93	0.51
1:B:93:PHE:HB2	1:B:103:PHE:HB2	1.94	0.49
1:B:42:SER:HB2	1:B:160:ASP:HB2	1.95	0.48
1:A:159:TYR:HB3	1:A:168:LYS:HD3	1.96	0.46
1:B:150:ASN:ND2	1:B:183:ILE:HD11	2.30	0.46
1:B:356:ALA:HB2	1:B:385:ILE:HD11	1.97	0.46
1:B:85:LEU:HA	1:B:264:LEU:HB3	1.98	0.46
1:A:356:ALA:HB2	1:A:385:ILE:HD11	1.99	0.45
1:A:85:LEU:HA	1:A:264:LEU:HB3	1.99	0.45
1:A:93:PHE:HB2	1:A:103:PHE:HB2	1.98	0.45
1:A:50:THR:HB	3:B:402:7X9:CAL	2.47	0.44
1:A:189:CYS:HB3	1:A:314:LEU:HD21	2.00	0.43
1:A:174:LYS:HB3	1:A:174:LYS:HE2	1.92	0.42
1:B:341:MET:HG2	7:B:659:HOH:O	2.20	0.41
1:B:159:TYR:O	1:B:160:ASP:HB2	2.21	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	336/402 (84%)	332 (99%)	4 (1%)	0	100	100
1	B	332/402 (83%)	329 (99%)	3 (1%)	0	100	100
All	All	668/804 (83%)	661 (99%)	7 (1%)	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	294/344 (86%)	289 (98%)	5 (2%)	60	55
1	B	289/344 (84%)	286 (99%)	3 (1%)	76	74
All	All	583/688 (85%)	575 (99%)	8 (1%)	67	62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	160	ASP
1	A	174	LYS
1	A	181	LYS
1	A	193	ASN
1	B	147	ARG
1	B	168	LYS
1	B	190	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	B	74	HIS

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 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
5	PRO	B	403	-	8,8,8	0.89	0	10,10,10	1.25	1 (10%)
6	DMS	B	406	-	3,3,3	0.30	0	3,3,3	0.41	0
3	7X9	A	403	-	21,21,21	2.55	6 (28%)	32,32,32	1.36	4 (12%)
3	7X9	B	402	-	21,21,21	2.55	7 (33%)	32,32,32	1.37	4 (12%)
3	7X9	A	402	-	21,21,21	2.46	5 (23%)	32,32,32	1.36	6 (18%)
6	DMS	B	404	-	3,3,3	0.36	0	3,3,3	0.48	0
5	PRO	A	406	-	8,8,8	0.81	0	10,10,10	1.15	0
5	PRO	A	408	-	8,8,8	0.87	0	10,10,10	1.09	0
3	7X9	B	401	-	21,21,21	2.50	6 (28%)	32,32,32	1.47	7 (21%)
6	DMS	A	409	-	3,3,3	0.29	0	3,3,3	0.17	0
6	DMS	A	410	-	3,3,3	0.28	0	3,3,3	0.38	0
5	PRO	A	407	-	8,8,8	0.86	0	10,10,10	1.03	0
6	DMS	B	407	-	3,3,3	0.36	0	3,3,3	0.36	0
6	DMS	B	405	-	3,3,3	0.25	0	3,3,3	0.43	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
5	PRO	B	403	-	-	0/4/11/11	0/1/1/1
3	7X9	A	403	-	-	4/4/13/13	0/3/3/3
3	7X9	B	402	-	-	4/4/13/13	0/3/3/3
3	7X9	A	402	-	-	0/4/13/13	0/3/3/3
5	PRO	A	406	-	-	1/4/11/11	0/1/1/1
5	PRO	A	408	-	-	0/4/11/11	0/1/1/1
3	7X9	B	401	-	-	0/4/13/13	0/3/3/3
5	PRO	A	407	-	-	0/4/11/11	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	7X9	CAL-CAF	-6.53	1.40	1.51
3	B	402	7X9	CAL-CAF	-6.44	1.40	1.51
3	A	402	7X9	CAL-CAF	-6.43	1.40	1.51
3	B	401	7X9	CAL-CAF	-6.28	1.40	1.51
3	A	403	7X9	CAH-CAN	-5.17	1.40	1.48
3	B	402	7X9	CAH-CAN	-5.08	1.40	1.48
3	B	401	7X9	CAH-CAN	-5.07	1.40	1.48
3	A	402	7X9	CAH-CAN	-5.02	1.40	1.48
3	B	401	7X9	CAE-NAJ	-4.59	1.34	1.40
3	B	402	7X9	CAD-CAG	-4.58	1.39	1.48
3	B	401	7X9	CAD-CAG	-4.43	1.39	1.48
3	A	403	7X9	CAD-CAG	-4.30	1.40	1.48
3	A	403	7X9	CAI-NAJ	4.21	1.41	1.34
3	A	402	7X9	CAD-CAG	-4.19	1.40	1.48
3	A	403	7X9	CAE-NAJ	-4.08	1.34	1.40
3	B	402	7X9	CAI-NAJ	4.03	1.40	1.34
3	B	402	7X9	CAE-NAJ	-3.87	1.35	1.40
3	A	402	7X9	CAE-NAJ	-3.87	1.35	1.40
3	A	402	7X9	CAI-NAJ	3.79	1.40	1.34
3	B	401	7X9	CAI-NAJ	3.48	1.40	1.34
3	B	402	7X9	FAQ-CAB	-2.39	1.30	1.36
3	B	402	7X9	CAH-CAG	-2.17	1.39	1.44
3	A	403	7X9	CAH-CAG	-2.06	1.39	1.44
3	B	401	7X9	CAH-CAG	-2.00	1.39	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	7X9	CAH-CAI-NAJ	-3.35	120.74	124.49
3	B	402	7X9	CAH-CAI-NAJ	-3.31	120.78	124.49
3	A	402	7X9	CAH-CAI-NAJ	-3.12	121.00	124.49
3	B	401	7X9	CAH-CAI-NAJ	-2.84	121.30	124.49
3	B	402	7X9	CAD-CAG-CAH	2.73	119.06	115.59
3	B	401	7X9	CAA-CAB-CAC	-2.60	120.23	123.52
3	B	401	7X9	CAD-CAG-CAH	2.58	118.87	115.59
3	A	403	7X9	CAA-CAB-CAC	-2.54	120.31	123.52
3	A	402	7X9	CAR-CAK-NAJ	2.52	113.06	108.07
3	B	401	7X9	OAP-CAN-CAH	2.50	122.06	115.83
3	A	403	7X9	CAD-CAG-CAH	2.49	118.75	115.59
3	A	402	7X9	CAD-CAG-CAH	2.47	118.73	115.59
3	B	401	7X9	CAR-CAK-NAJ	2.46	112.96	108.07
3	A	402	7X9	CAA-CAB-CAC	-2.45	120.42	123.52
3	B	402	7X9	CAA-CAB-CAC	-2.42	120.46	123.52
3	A	402	7X9	CAL-CAF-CAE	2.29	123.22	119.47
3	A	403	7X9	CAR-CAK-NAJ	2.22	112.47	108.07
3	B	401	7X9	CAL-CAF-CAE	2.21	123.09	119.47
3	B	402	7X9	CAR-CAK-NAJ	2.18	112.40	108.07
3	B	401	7X9	OAP-CAN-OAO	-2.03	118.95	123.61
5	B	403	PRO	OXT-C-CA	2.03	120.15	113.40
3	A	402	7X9	OAP-CAN-OAO	-2.00	119.03	123.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	7X9	CAG-CAH-CAN-OAP
3	A	403	7X9	CAG-CAH-CAN-OAO
3	B	402	7X9	CAG-CAH-CAN-OAP
3	B	402	7X9	CAG-CAH-CAN-OAO
3	B	402	7X9	CAI-CAH-CAN-OAP
3	B	402	7X9	CAI-CAH-CAN-OAO
3	A	403	7X9	CAI-CAH-CAN-OAP
3	A	403	7X9	CAI-CAH-CAN-OAO
5	A	406	PRO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 3 short contacts:

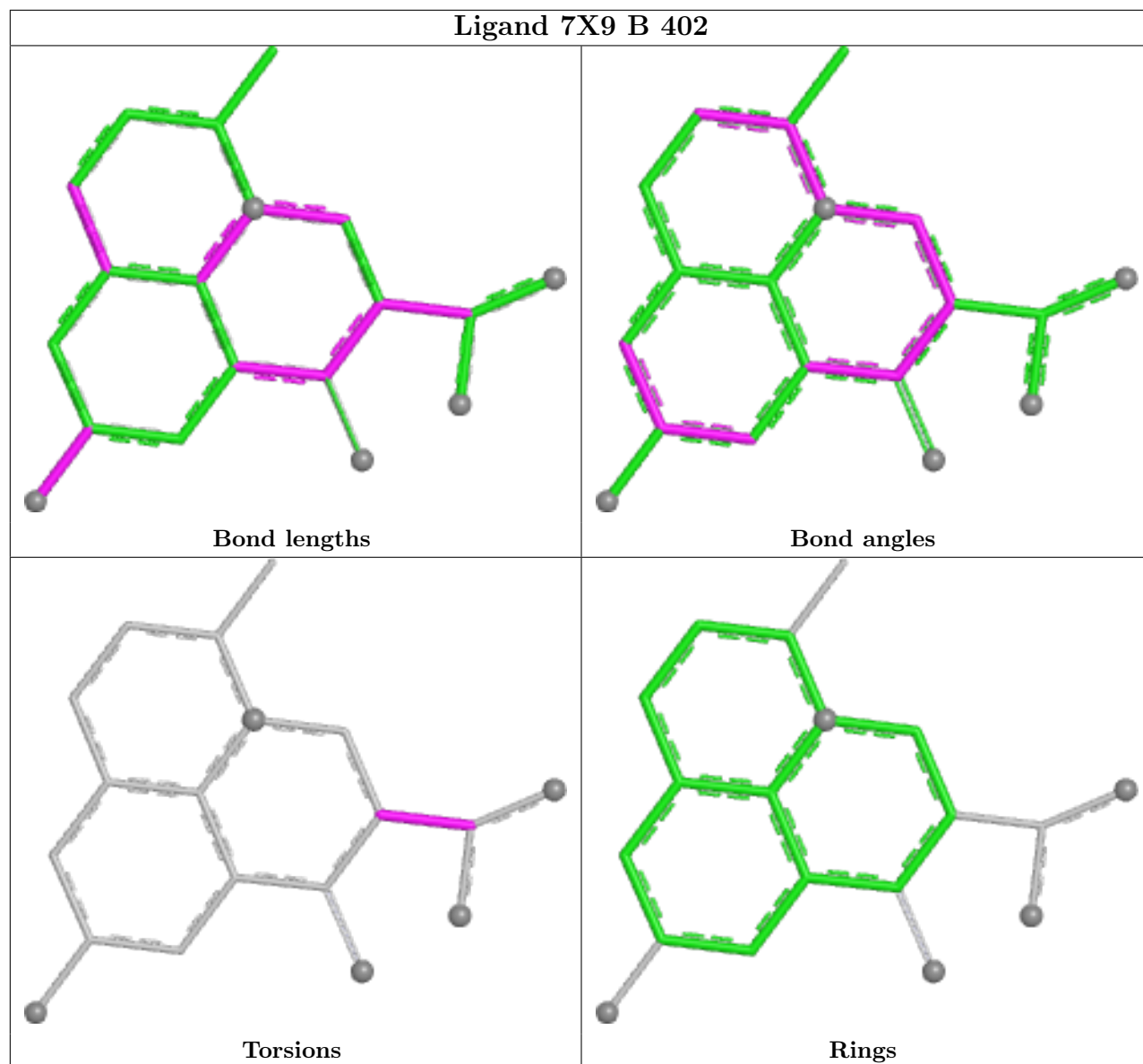| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	7X9	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	PRO	1	0
5	A	407	PRO	1	0
6	B	407	DMS	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 7X9 A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand 7X9 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 7X9 A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 7X9 B 401
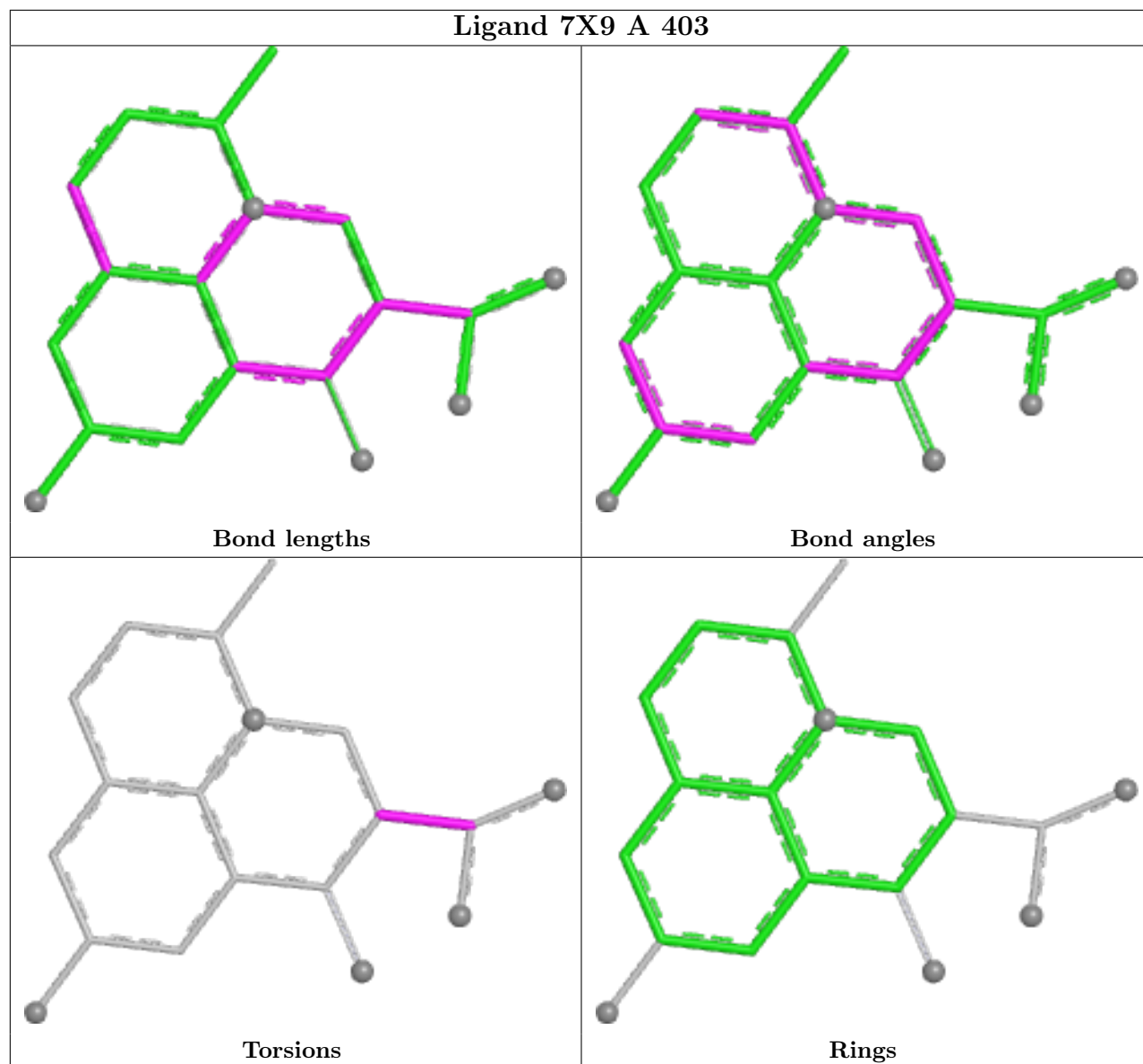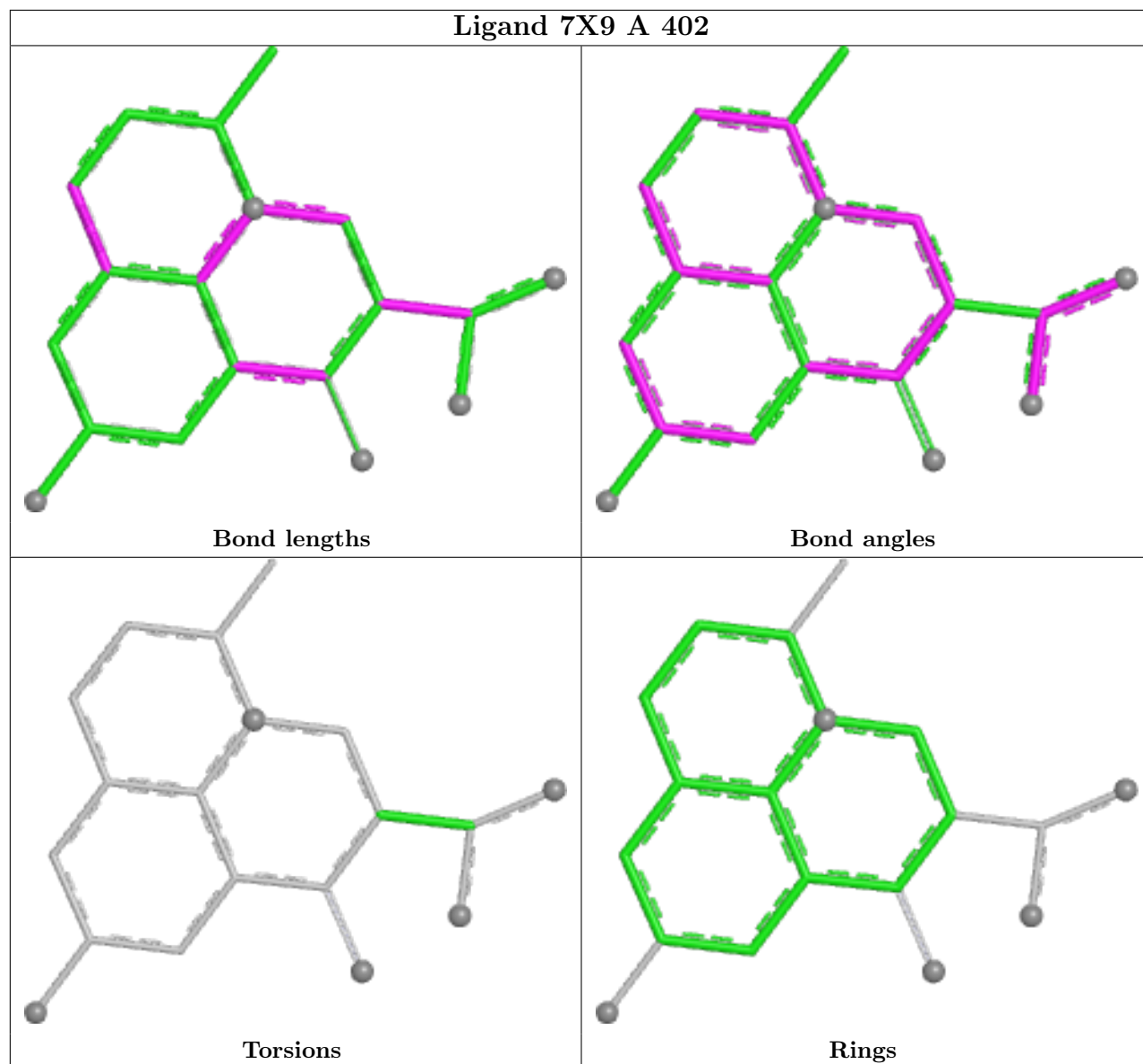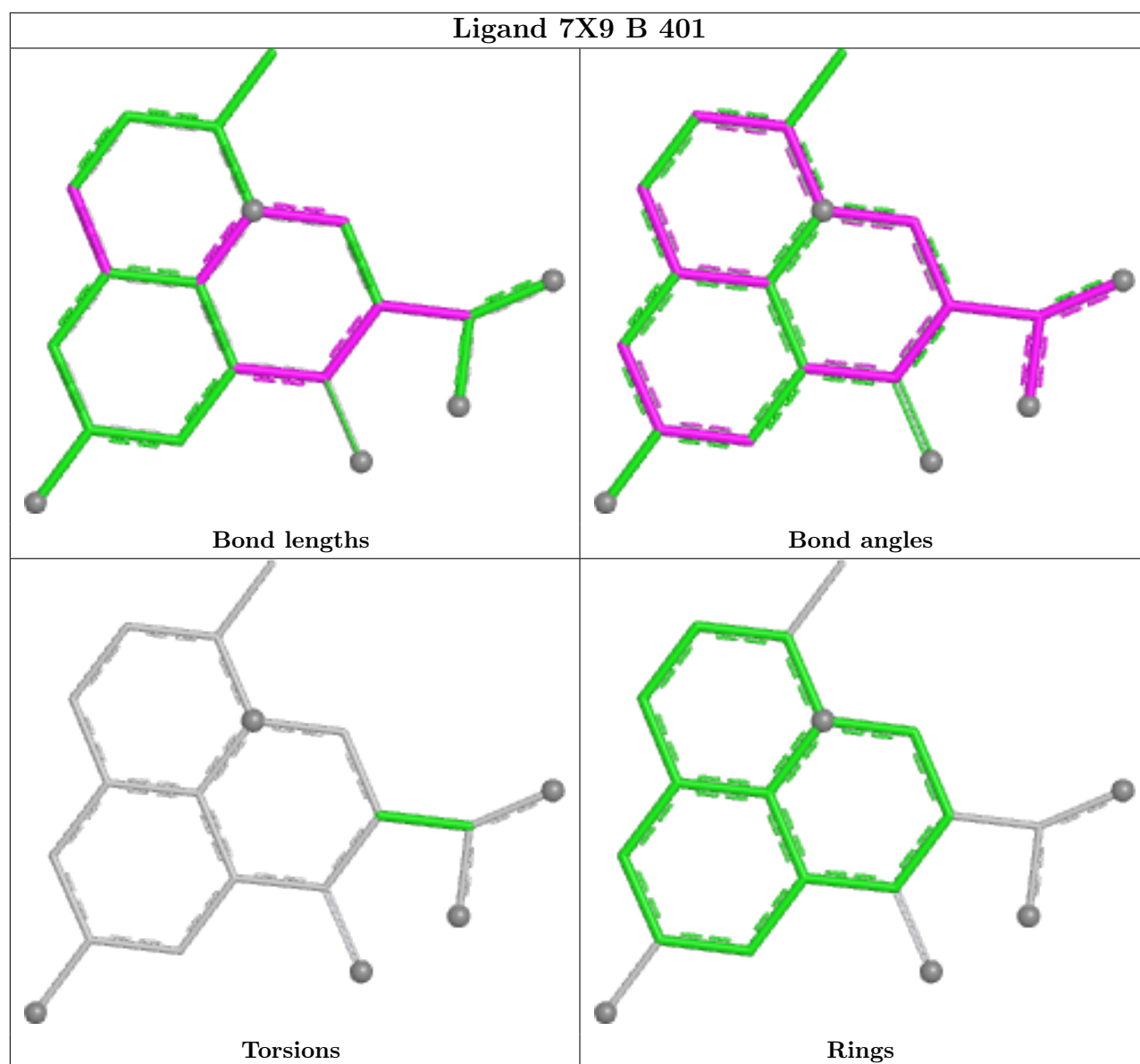
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	339/402 (84%)	0.50	18 (5%)	26	35	24, 37, 65, 87	0
1	B	336/402 (83%)	0.61	26 (7%)	13	21	23, 36, 68, 89	0
All	All	675/804 (83%)	0.56	44 (6%)	18	27	23, 36, 66, 89	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	GLY	8.5
1	A	148	ALA	7.7
1	B	150	ASN	6.7
1	B	187	PRO	6.2
1	B	149	ILE	5.7
1	A	193	ASN	5.7
1	A	147	ARG	5.4
1	B	147	ARG	5.4
1	B	188	GLU	5.2
1	B	186	LEU	5.1
1	B	148	ALA	4.7
1	A	161	SER	4.5
1	A	188	GLU	4.5
1	A	34	VAL	4.4
1	A	149	ILE	4.3
1	B	169	TYR	4.1
1	A	169	TYR	4.0
1	B	189	CYS	4.0
1	A	192	ILE	3.9
1	A	186	LEU	3.8
1	B	213	VAL	3.7
1	A	144	LYS	3.7
1	B	368	SER	3.2
1	A	162	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	190	ASP	3.0
1	B	393	ILE	3.0
1	A	146	THR	3.0
1	B	58	PHE	2.8
1	B	35	THR	2.8
1	A	115	TYR	2.7
1	B	191	TYR	2.5
1	B	144	LYS	2.5
1	B	185	ASN	2.5
1	B	360	ASP	2.4
1	B	146	THR	2.4
1	A	150	ASN	2.4
1	B	100	SER	2.3
1	B	57	ASP	2.3
1	A	168	LYS	2.3
1	B	98	LYS	2.2
1	A	215	SER	2.2
1	B	312	ASN	2.2
1	A	185	ASN	2.0
1	B	168	LYS	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, 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
6	DMS	B	407	4/4	0.22	0.55	81,81,81,81	4
3	7X9	B	402	19/19	0.63	0.27	74,74,75,75	19
3	7X9	A	403	19/19	0.72	0.29	74,75,76,76	19

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	B	404	4/4	0.77	0.18	91,91,91,91	0
6	DMS	A	410	4/4	0.80	0.22	109,109,109,109	0
5	PRO	A	408	8/8	0.85	0.17	55,56,57,57	7
5	PRO	A	407	8/8	0.86	0.17	44,45,46,46	7
6	DMS	B	406	4/4	0.87	0.35	105,105,105,105	4
4	CL	A	405	1/1	0.87	0.24	77,77,77,77	0
5	PRO	A	406	8/8	0.89	0.20	49,50,51,54	0
5	PRO	B	403	8/8	0.89	0.22	50,50,51,53	0
4	CL	A	404	1/1	0.92	0.16	77,77,77,77	0
3	7X9	B	401	19/19	0.93	0.12	41,42,44,45	0
3	7X9	A	402	19/19	0.93	0.12	38,39,41,42	19
6	DMS	A	409	4/4	0.94	0.15	43,44,45,45	4
2	ZN	A	401	1/1	0.95	0.13	53,53,53,53	1
6	DMS	B	405	4/4	0.95	0.16	39,39,40,40	4

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 7X9 B 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
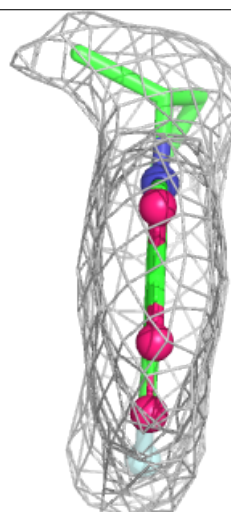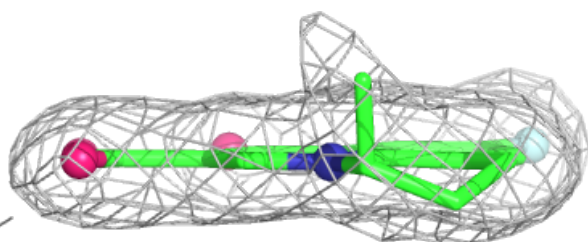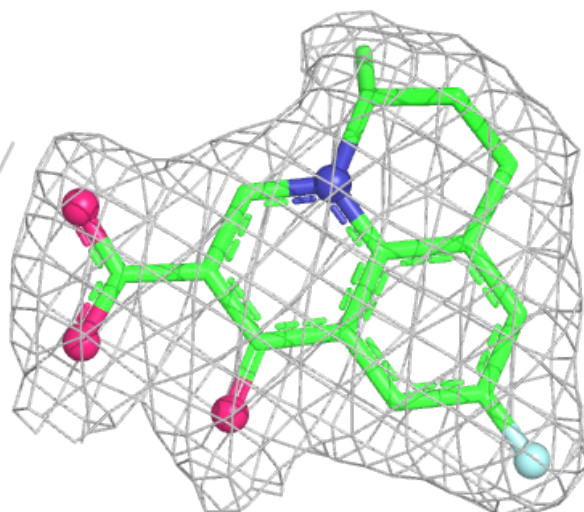and green (positive)
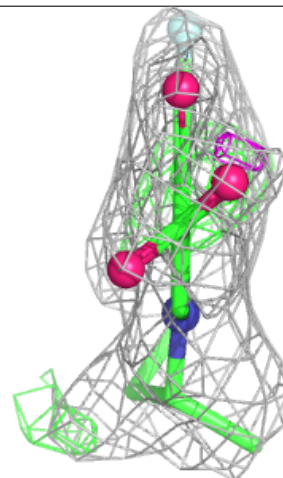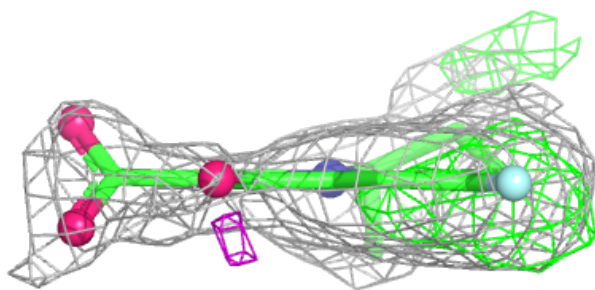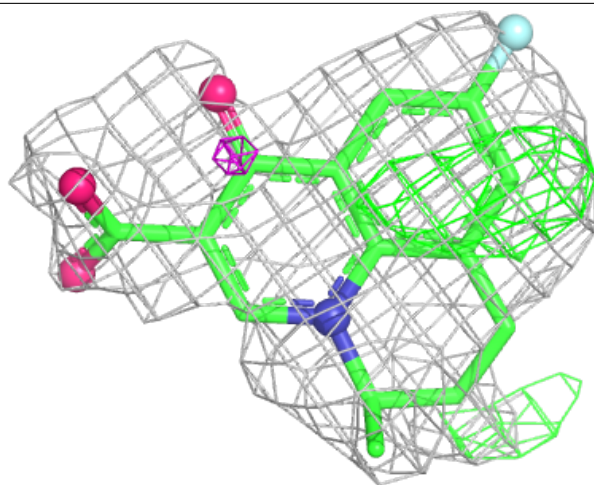
Electron density around 7X9 A 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
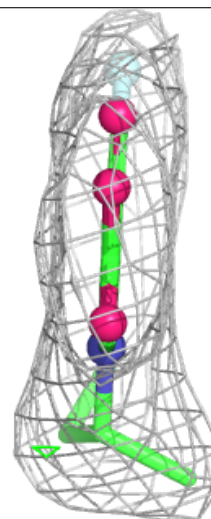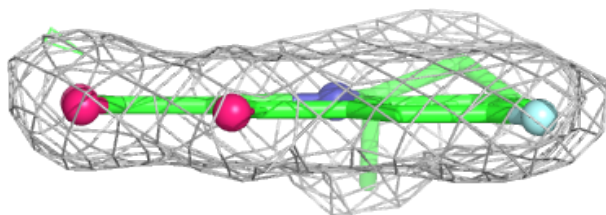mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
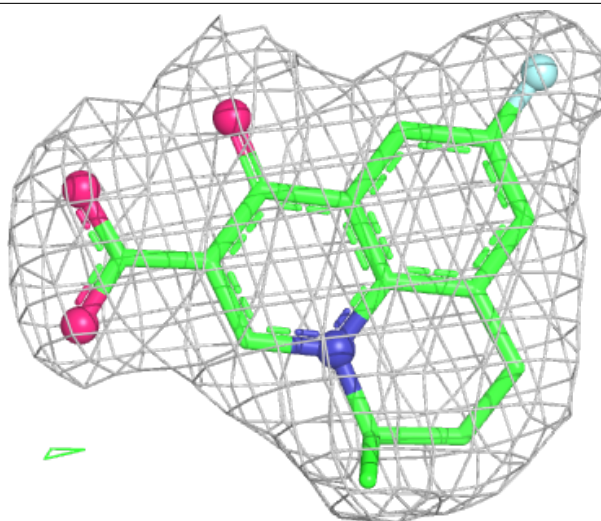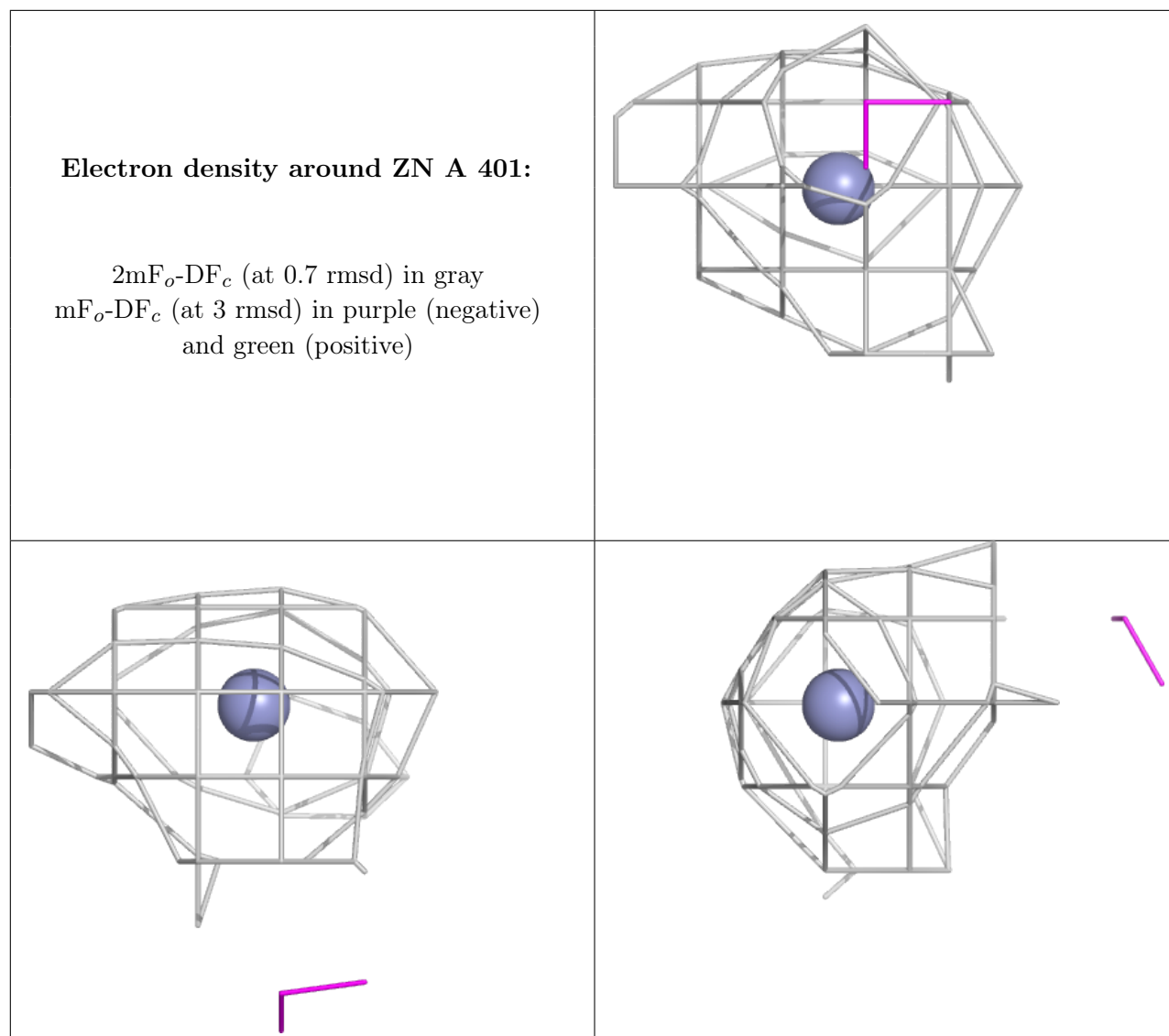and green (positive)
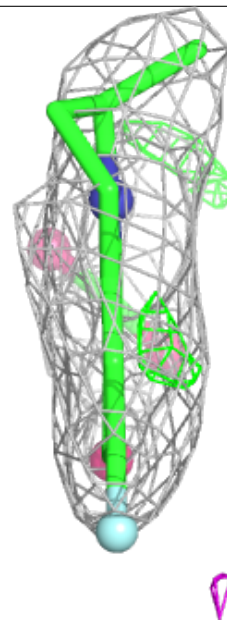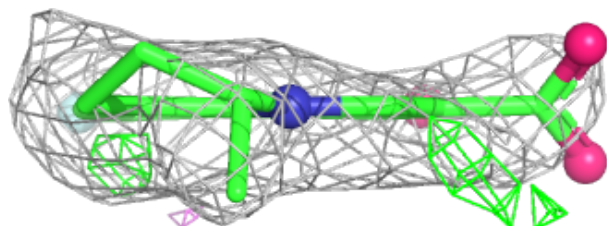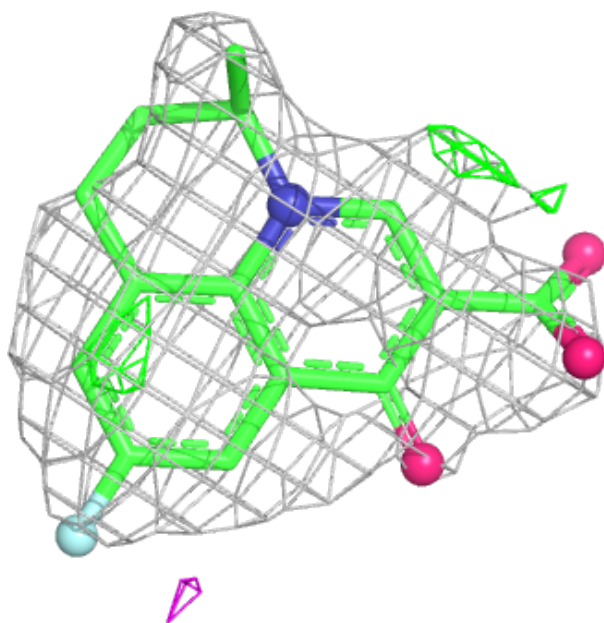
Electron density around 7X9 B 401:

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 7X9 A 402:

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

Electron density around ZN A 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.