WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 12:07 AM EDT

PDB ID	:	3GAN
Title	:	Crystal structure of gene product from Arabidopsis thaliana At3g22680 with bound suramin
Authors	:	Burgie, E.S.; Bingman, C.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2009-02-17
Resolution	:	2.00 Å(reported)

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

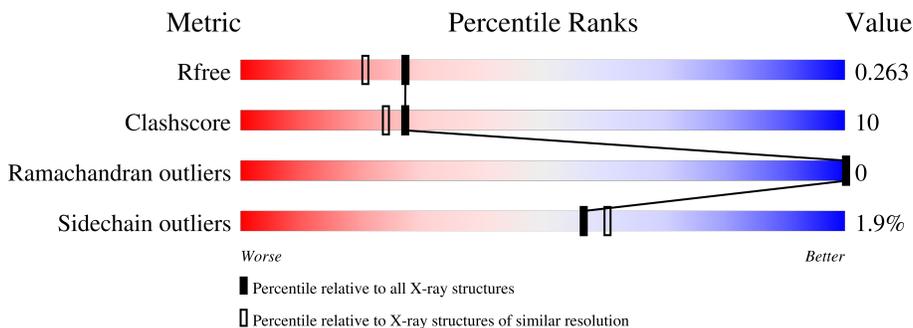|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.00 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		0.263
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		1.9%

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Mol	Chain	Length	Quality of chain
1	A	157	58%　　　　13%　·　28%

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1186 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 Uncharacterized protein At3g22680.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total 956	C 621	N 167	O 163	Se 5	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9LUJ3

- Molecule 2 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFON IC ACID (three-letter code: SVR) (formula: $C_{51}H_{40}N_6O_{23}S_6$).
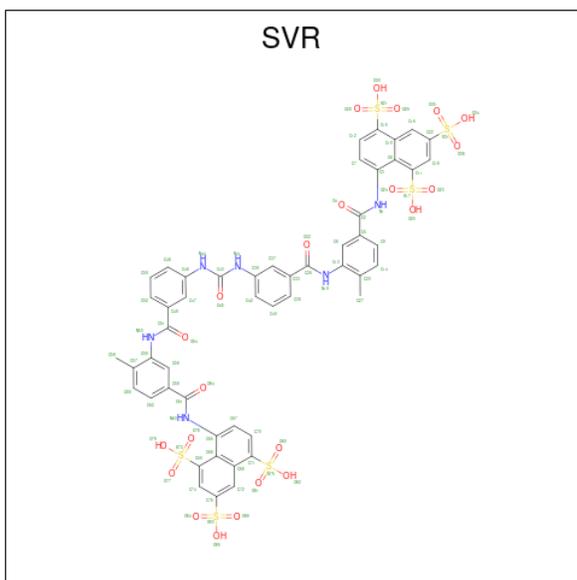
SVR

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 86	C 51	N 6	O 23	S 6	24	0
2	A	1	Total 86	C 51	N 6	O 23	S 6	35	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Uncharacterized protein At3g22680

Chain A:
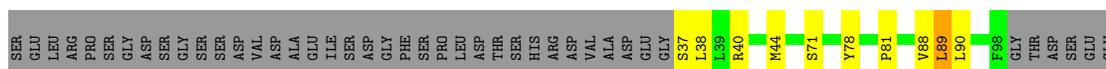
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	58.38Å 58.38Å 90.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 44.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.00) 99.5 (44.11-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.190 , 0.241 0.236 , 0.263	Depositor DCC
R_{free} test set	598 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.3	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	1186	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: SVR, CL

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	1.05	2/981 (0.2%)	0.95	2/1326 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	TYR	CD2-CE2	5.77	1.48	1.39
1	A	88	VAL	CB-CG2	5.02	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	LEU	CB-CG-CD1	-6.43	100.06	111.00
1	A	38	LEU	CA-CB-CG	-5.37	102.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	956	0	952	15	0
2	A	172	0	73	7	0
3	A	1	0	0	0	0
4	A	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1186	0	1025	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 10.

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)
2:A:159:SVR:S73	2:A:159:SVR:N63	2.55	0.78
1:A:138:LEU:HD23	1:A:141:ARG:NH1	2.11	0.66
2:A:158:SVR:N63	2:A:158:SVR:S73	2.69	0.64
2:A:158:SVR:H72	2:A:158:SVR:O80	1.96	0.64
2:A:159:SVR:N63	2:A:159:SVR:O77	2.31	0.63
1:A:145:MSE:HE2	1:A:145:MSE:HA	1.81	0.61
1:A:71:SER:HB3	1:A:90:LEU:HD13	1.83	0.61
1:A:138:LEU:CD2	1:A:141:ARG:NH1	2.68	0.56
1:A:130:THR:H	1:A:131:PRO:HD3	1.77	0.49
2:A:158:SVR:O80	2:A:158:SVR:C72	2.61	0.48
1:A:130:THR:N	1:A:131:PRO:CD	2.78	0.46
1:A:138:LEU:CD2	1:A:141:ARG:HH11	2.29	0.45
2:A:158:SVR:O45	2:A:158:SVR:H42	2.18	0.44
1:A:150:ILE:CD1	2:A:158:SVR:H273	2.47	0.44
1:A:40:ARG:O	1:A:44:MSE:HG3	2.17	0.44
1:A:147:HIS:CD2	1:A:148:SER:N	2.88	0.42
1:A:89:LEU:HD23	1:A:123:VAL:HG11	2.00	0.42
1:A:81:PRO:HA	1:A:151:ASP:OD2	2.19	0.41
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.87	0.41
1:A:138:LEU:HD23	1:A:141:ARG:HH11	1.82	0.41
1:A:147:HIS:HD2	1:A:148:SER:N	2.20	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	110/157 (70%)	107 (97%)	3 (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	107/138 (78%)	105 (98%)	2 (2%)	57 61

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

Mol	Chain	Res	Type
1	A	37	SER
1	A	113	PRO

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	147	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	#$|Z| > 2$
2	SVR	A	158	-	89,93,93	1.77	12 (13%)	129,145,145	1.69	25 (19%)
2	SVR	A	159	-	89,93,93	1.86	8 (8%)	129,145,145	2.38	34 (26%)

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
2	SVR	A	158	-	-	11/76/76/76	0/8/8/8
2	SVR	A	159	-	-	14/76/76/76	0/8/8/8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	159	SVR	C22-S31	-10.54	1.54	1.77
2	A	158	SVR	C22-S31	-7.76	1.60	1.77
2	A	159	SVR	C76-S83	-6.95	1.62	1.77
2	A	158	SVR	C76-S83	-6.64	1.63	1.77
2	A	158	SVR	C11-C6	-4.77	1.37	1.43
2	A	158	SVR	C2-N1	4.56	1.47	1.35
2	A	159	SVR	O64-C61	4.27	1.32	1.23
2	A	158	SVR	O64-C61	3.95	1.31	1.23
2	A	159	SVR	C3-C6	-3.85	1.37	1.42
2	A	158	SVR	C71-C68	-3.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	159	SVR	C70-C71	3.22	1.41	1.37
2	A	159	SVR	C33-C26	-3.08	1.43	1.50
2	A	158	SVR	C70-C71	3.04	1.41	1.37
2	A	159	SVR	C11-C6	-2.56	1.40	1.43
2	A	158	SVR	C56-C55	2.38	1.43	1.39
2	A	158	SVR	C65-N63	-2.30	1.35	1.41
2	A	158	SVR	C15-C10	-2.28	1.39	1.43
2	A	158	SVR	C70-C67	2.15	1.42	1.38
2	A	158	SVR	C69-C66	-2.14	1.41	1.43
2	A	159	SVR	C59-C57	2.06	1.55	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	159	SVR	C46-N44-C43	10.67	148.45	126.61
2	A	159	SVR	C20-C13-N19	7.84	131.02	118.81
2	A	159	SVR	C3-N1-C2	-7.59	106.15	128.64
2	A	158	SVR	O4-C2-N1	-7.15	107.37	123.71
2	A	159	SVR	C11-C6-C10	7.09	123.01	116.34
2	A	159	SVR	C39-N41-C43	6.21	139.31	126.61
2	A	159	SVR	C69-C66-C68	5.20	121.23	116.34
2	A	159	SVR	O64-C61-N63	-5.16	111.92	123.71
2	A	159	SVR	O32-C26-C33	5.16	130.13	120.94
2	A	159	SVR	C6-C3-N1	-4.93	113.23	120.58
2	A	158	SVR	C5-C2-N1	4.59	126.03	115.92
2	A	158	SVR	C70-C71-C68	-4.55	116.44	121.00
2	A	159	SVR	C8-C13-N19	-4.46	110.11	121.90
2	A	158	SVR	C60-C57-C55	4.21	121.41	117.44
2	A	159	SVR	C58-C61-N63	4.01	124.75	115.92
2	A	159	SVR	C49-C47-C46	3.80	125.57	120.44
2	A	159	SVR	C48-C46-C47	-3.66	115.31	119.65
2	A	159	SVR	C18-C22-S31	-3.56	113.75	119.89
2	A	158	SVR	C6-C3-N1	3.24	125.40	120.58
2	A	159	SVR	C50-C52-C49	-3.19	116.57	120.34
2	A	158	SVR	C62-C58-C56	3.15	122.96	119.24
2	A	159	SVR	C48-C46-N44	3.14	130.97	120.40
2	A	158	SVR	C7-C3-C6	-3.13	116.99	120.27
2	A	158	SVR	C57-C55-N53	3.10	123.63	118.81
2	A	158	SVR	C69-C66-C68	3.09	119.25	116.34
2	A	158	SVR	C3-N1-C2	-3.07	119.55	128.64
2	A	158	SVR	C59-C57-C60	-3.07	114.33	120.31
2	A	158	SVR	C71-C68-C66	2.98	122.78	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	158	SVR	C13-N19-C26	-2.95	118.84	126.93
2	A	159	SVR	C16-C22-C18	2.94	124.14	120.97
2	A	159	SVR	C70-C71-C68	-2.84	118.15	121.00
2	A	159	SVR	C27-C20-C13	2.77	124.38	121.25
2	A	159	SVR	C66-C65-N63	-2.71	116.54	120.58
2	A	158	SVR	C59-C57-C55	2.66	124.27	121.25
2	A	159	SVR	O45-C43-N44	2.59	128.01	123.62
2	A	159	SVR	C52-C50-C48	2.58	123.91	120.25
2	A	159	SVR	C33-C26-N19	-2.51	110.39	115.92
2	A	158	SVR	O84-S83-O86	2.48	125.72	112.86
2	A	158	SVR	O86-S83-C76	2.47	112.34	106.65
2	A	159	SVR	C7-C3-C6	2.46	122.85	120.27
2	A	159	SVR	O54-C51-N53	-2.44	118.14	123.71
2	A	159	SVR	C33-C37-C39	2.40	123.67	120.44
2	A	158	SVR	C56-C55-N53	-2.37	115.64	121.90
2	A	159	SVR	C14-C9-C5	-2.35	118.05	120.78
2	A	158	SVR	C8-C13-C20	2.34	122.50	119.77
2	A	159	SVR	C18-C11-C6	-2.31	118.40	121.25
2	A	158	SVR	C38-C33-C37	2.29	121.94	119.24
2	A	159	SVR	C74-C69-C66	-2.24	118.49	121.25
2	A	158	SVR	C55-N53-C51	-2.21	120.88	126.93
2	A	159	SVR	C71-C68-C66	2.18	121.50	118.01
2	A	158	SVR	C16-C22-C18	-2.18	118.61	120.97
2	A	159	SVR	C42-C39-C37	-2.17	117.08	119.65
2	A	158	SVR	C62-C60-C57	-2.16	118.69	121.97
2	A	159	SVR	N44-C43-N41	-2.13	108.76	112.49
2	A	158	SVR	O85-S83-O84	-2.07	101.63	111.54
2	A	159	SVR	C27-C20-C14	-2.06	116.30	120.31
2	A	158	SVR	C7-C3-N1	-2.05	117.61	123.29
2	A	158	SVR	C3-C6-C10	2.02	121.05	117.40
2	A	159	SVR	O29-S21-C15	2.02	112.45	106.43

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	158	SVR	C10-C15-S21-O28
2	A	158	SVR	C10-C15-S21-O29
2	A	158	SVR	C12-C15-S21-O28
2	A	158	SVR	C12-C15-S21-O29
2	A	159	SVR	C10-C15-S21-O28
2	A	159	SVR	C20-C13-N19-C26

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Mol	Chain	Res	Type	Atoms
2	A	159	SVR	O64-C61-N63-C65
2	A	159	SVR	C8-C13-N19-C26
2	A	158	SVR	C7-C3-N1-C2
2	A	159	SVR	C10-C15-S21-O29
2	A	159	SVR	O54-C51-N53-C55
2	A	159	SVR	C12-C15-S21-O28
2	A	159	SVR	C7-C3-N1-C2
2	A	158	SVR	C10-C15-S21-O30
2	A	158	SVR	C12-C15-S21-O30
2	A	159	SVR	C56-C58-C61-N63
2	A	159	SVR	C12-C15-S21-O29
2	A	158	SVR	C68-C71-S75-O80
2	A	158	SVR	N1-C2-C5-C8
2	A	159	SVR	C62-C58-C61-N63
2	A	158	SVR	C6-C3-N1-C2
2	A	158	SVR	C57-C55-N53-C51
2	A	159	SVR	C66-C69-S73-O78
2	A	159	SVR	C6-C3-N1-C2
2	A	159	SVR	C16-C22-S31-O34

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	158	SVR	5	0
2	A	159	SVR	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 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 SVR A 158

Bond lengths

Bond angles

Torsions

Rings

Ligand SVR A 159

Bond lengths

Bond angles

Torsions

Rings
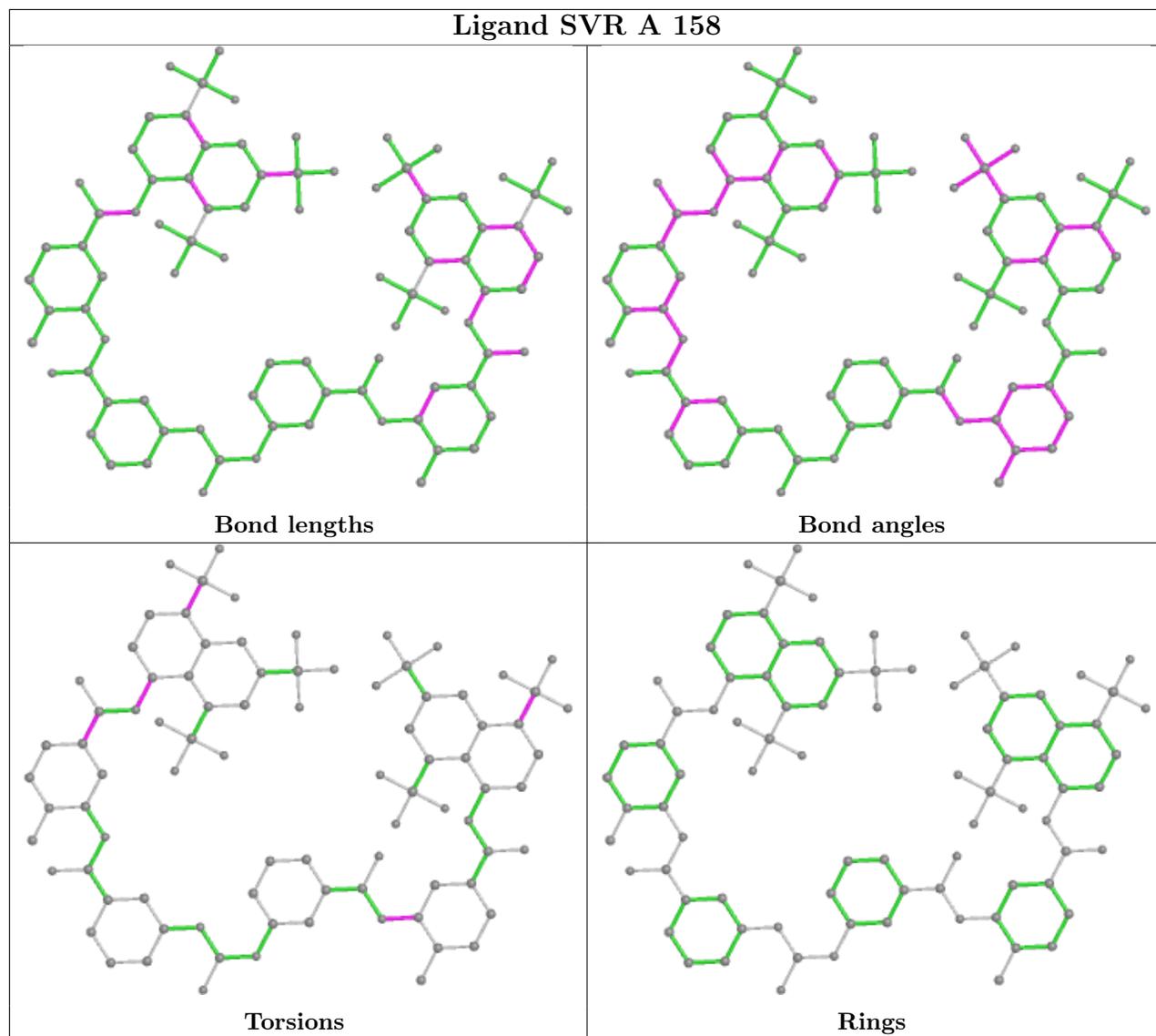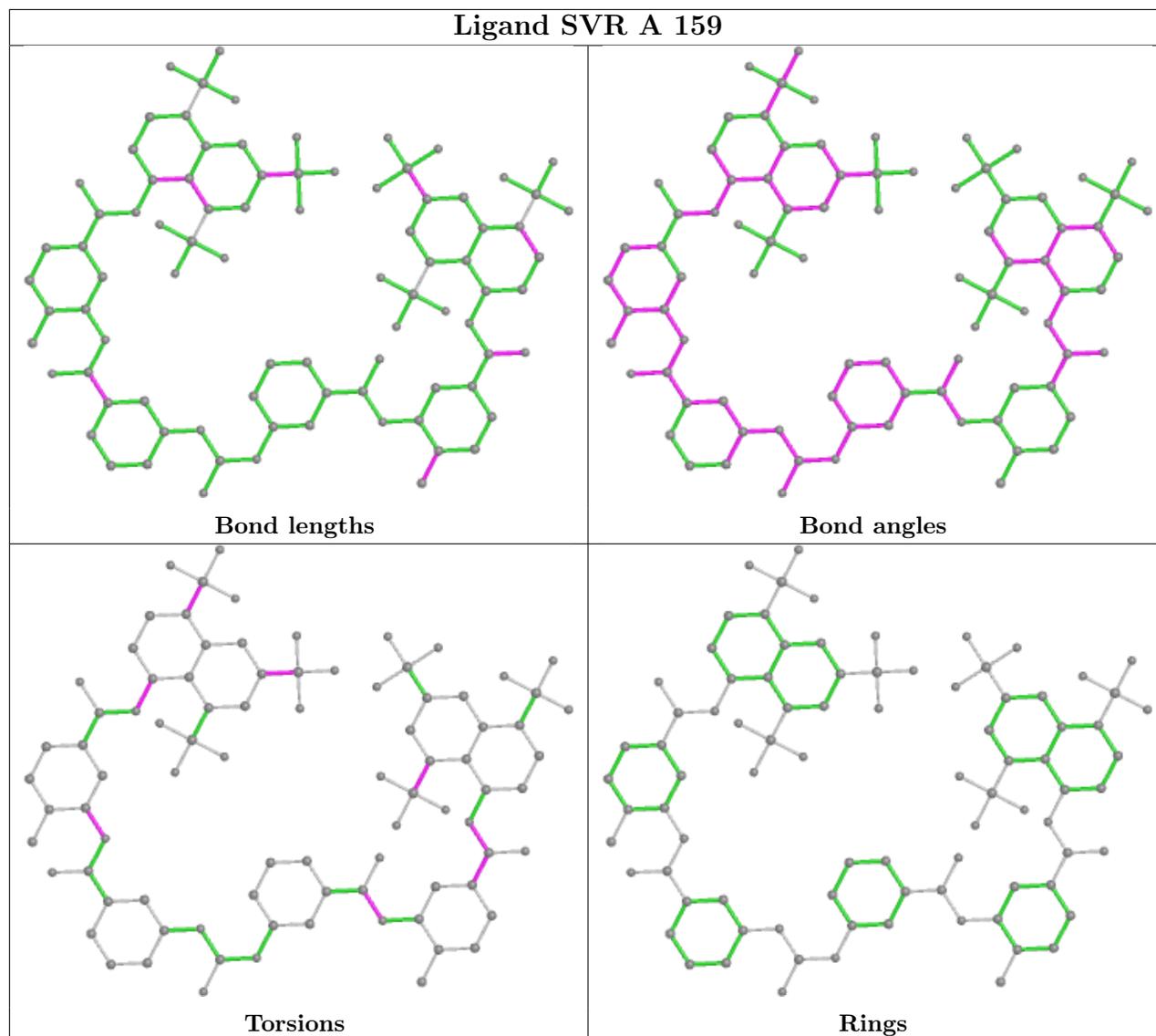
5.7 Other polymers ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

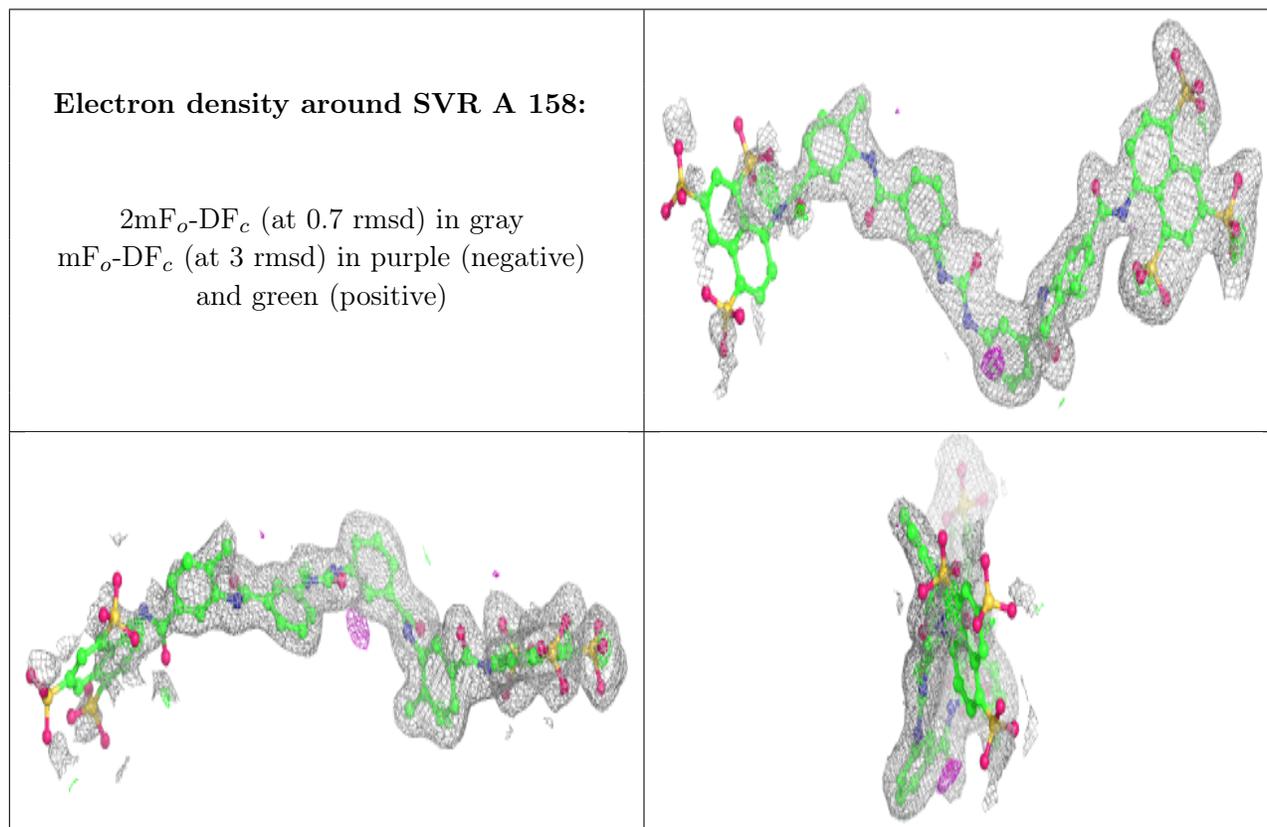Unable to reproduce the depositors R factor - this section is therefore empty.
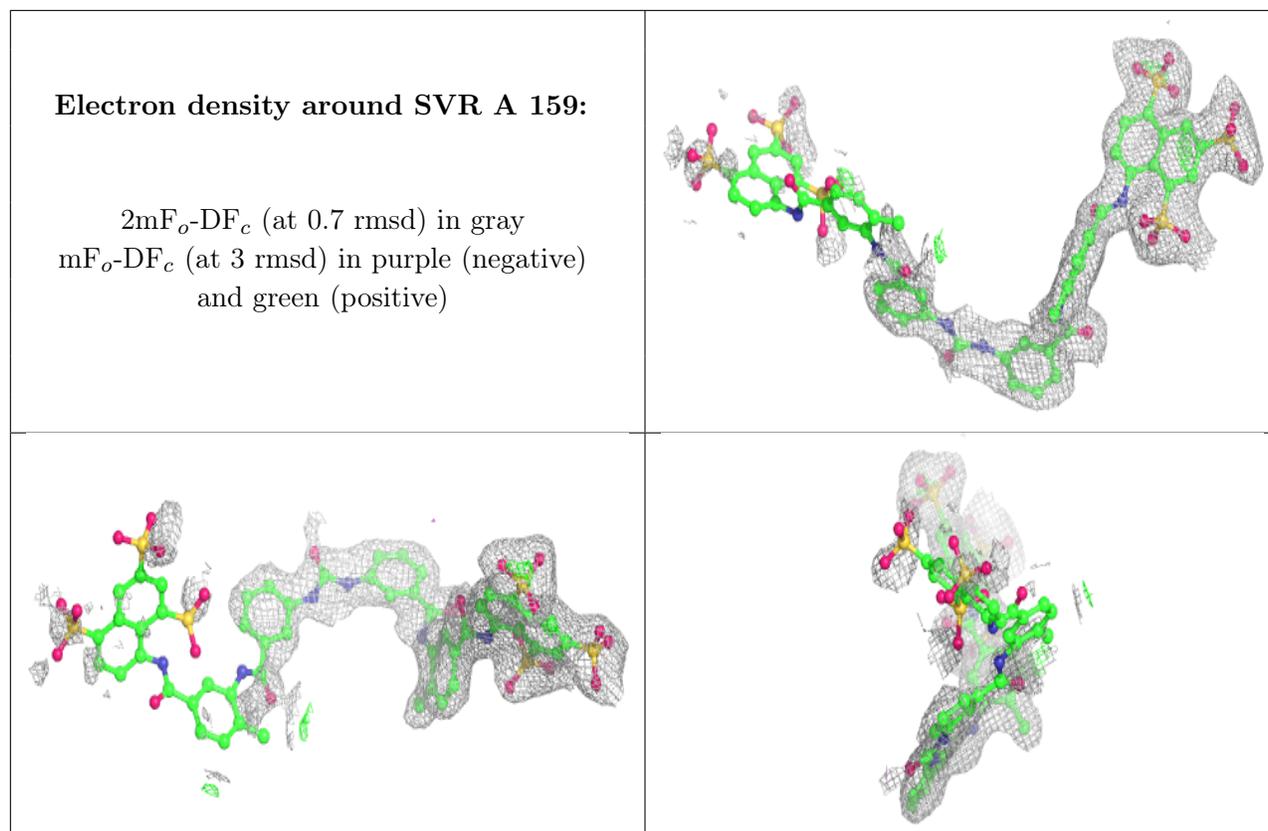
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 SVR A 158:

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

Electron density around SVR A 159:

$2mF_o$-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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.