



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:30 pm BST

PDB ID : 2AOB  
Title : Crystal structures of a high-affinity macrocyclic peptide mimetic in complex with the Grb2 SH2 domain  
Authors : Phan, J.; Shi, Z.D.; Burke, T.R.; Waugh, D.S.  
Deposited on : 2005-08-12  
Resolution : 1.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

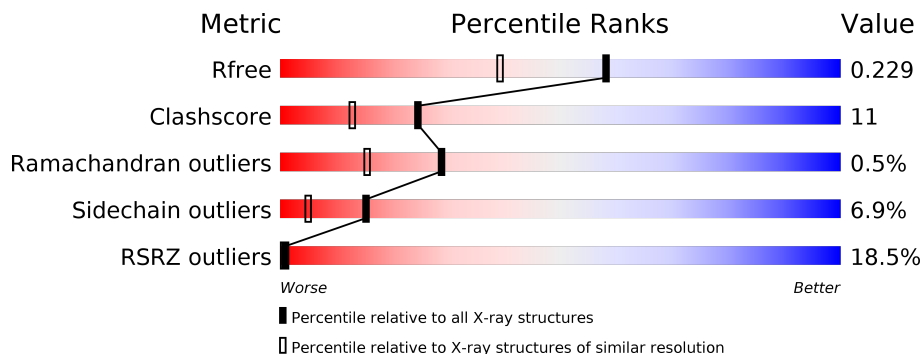
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	99	
1	B	99	
1	C	99	
1	D	99	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	S1S	A	1201	X	-	-	-
2	S1S	A	1401	X	-	-	-
2	S1S	A	1501	X	-	-	-
2	S1S	A	1601	X	-	-	-
2	S1S	A	1701	X	-	-	-
2	S1S	B	1301	X	-	-	-
2	S1S	C	2201	X	-	-	-
2	S1S	C	2501	X	-	-	-
2	S1S	C	2601	X	-	-	-
2	S1S	D	2301	X	-	-	-
2	S1S	D	2701	X	-	-	-

## 2 Entry composition i

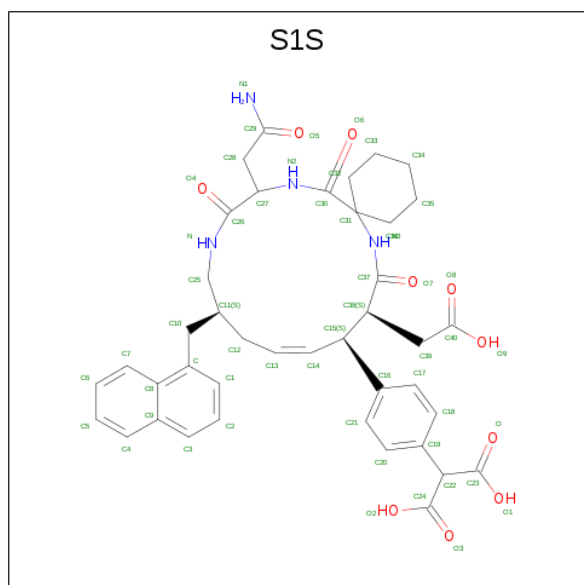
There are 3 unique types of molecules in this entry. The entry contains 4036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Growth factor receptor-bound protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	96	Total 765	C 495	N 134	O 135	S 1	0	0	0
1	B	93	Total 741	C 477	N 134	O 130		0	0	0
1	C	96	Total 775	C 501	N 138	O 135	S 1	0	0	0
1	D	93	Total 722	C 464	N 129	O 129		0	0	0

- Molecule 2 is 2-(4-((9S,10S,14S,Z)-18-(2-AMINO-2-OXOETHYL)-9-(CARBOXYMETHYL)-14-(NAPHTHALEN-1-YLMETHYL)-8,17,20-TRIOXO-7,16,19-TRIAZASPIRO [5.14]ICOS-11-EN-10-YL)PHENYL)MALONIC ACID (three-letter code: S1S) (formula: C<sub>41</sub>H<sub>46</sub>N<sub>4</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 55	C 41	N 4	O 10	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	B	1	Total	C	N	O	0	0
			55	41	4	10		
2	C	1	Total	C	N	O	0	0
			55	41	4	10		
2	C	1	Total	C	N	O	0	0
			55	41	4	10		
2	C	1	Total	C	N	O	0	0
			55	41	4	10		
2	C	1	Total	C	N	O	0	0
			55	41	4	10		
2	D	1	Total	C	N	O	0	0
			55	41	4	10		
2	D	1	Total	C	N	O	0	0
			55	41	4	10		

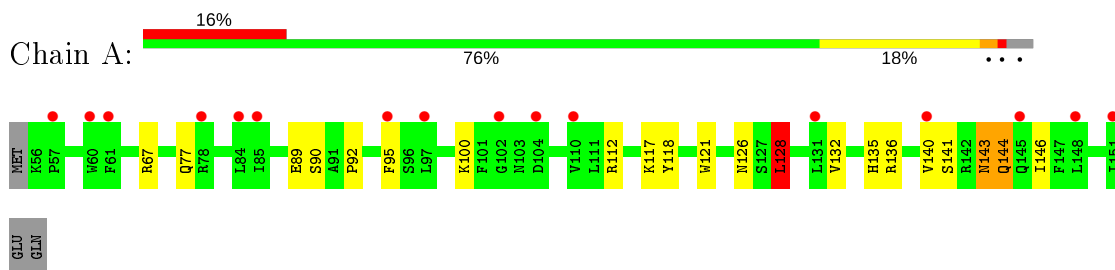
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	84	Total	O	0	0
			84	84		
3	C	106	Total	O	0	0
			106	106		
3	D	68	Total	O	0	0
			68	68		

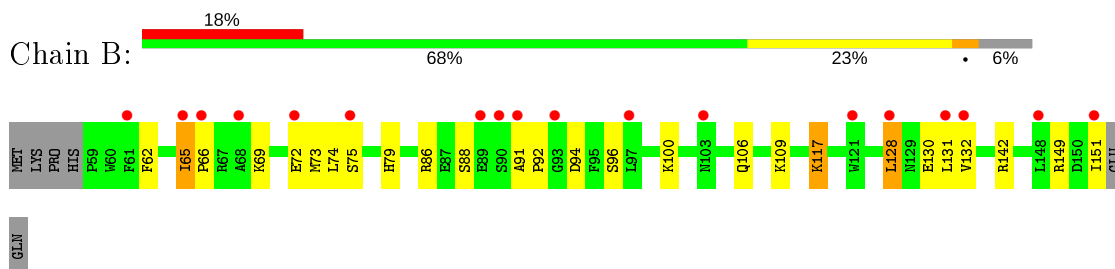
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

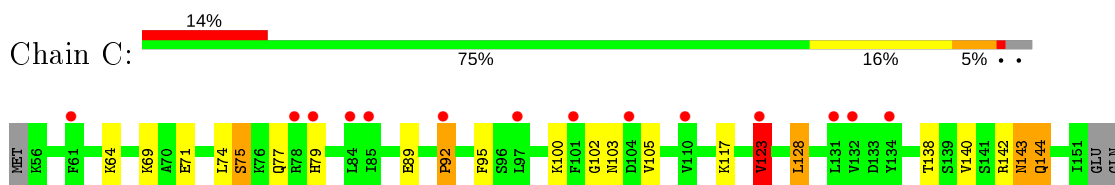
- Molecule 1: Growth factor receptor-bound protein 2



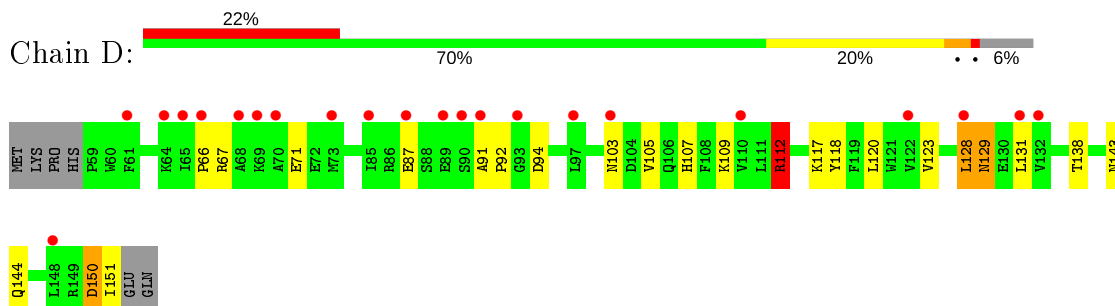
- Molecule 1: Growth factor receptor-bound protein 2



- Molecule 1: Growth factor receptor-bound protein 2



- Molecule 1: Growth factor receptor-bound protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.82Å 106.19Å 102.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 24.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-1.80) 99.7 (24.70-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.232 , 0.293 0.234 , 0.229	Depositor DCC
$R_{free}$ test set	2212 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0181e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: S1S

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	1.09	1/787 (0.1%)	1.04	4/1063 (0.4%)
1	B	1.02	1/760 (0.1%)	1.01	3/1025 (0.3%)
1	C	1.07	1/797 (0.1%)	1.03	3/1074 (0.3%)
1	D	0.99	0/740	1.09	4/1000 (0.4%)
All	All	1.04	3/3084 (0.1%)	1.04	14/4162 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	TRP	CB-CG	6.69	1.62	1.50
1	B	132	VAL	CB-CG2	5.27	1.64	1.52
1	C	140	VAL	CB-CG2	5.12	1.63	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	112	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	66	PRO	N-CA-CB	6.67	111.31	103.30
1	C	123	VAL	CG1-CB-CG2	6.09	120.64	110.90
1	C	142	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	128	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	66	PRO	N-CA-CB	5.70	110.14	103.30
1	B	142	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	120	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	D	112	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	128	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	136	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	112	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	92	PRO	N-CA-CB	5.16	109.49	103.30



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	765	0	726	15	0
1	B	741	0	697	20	0
1	C	775	0	748	14	0
1	D	722	0	654	17	0
2	A	275	0	208	16	0
2	B	55	0	42	3	0
2	C	220	0	166	12	0
2	D	110	0	82	2	0
3	A	115	0	0	1	0
3	B	84	0	0	4	0
3	C	106	0	0	4	0
3	D	68	0	0	1	0
All	All	4036	0	3323	76	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 11.

All (76) 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:95:PHE:CE2	2:A:1601:S1S:O	2.36	0.78
1:B:62:PHE:HB3	1:B:65:ILE:HD11	1.65	0.78
1:C:95:PHE:CE2	2:C:2601:S1S:O1	2.38	0.76
1:C:103:ASN:O	3:C:2657:HOH:O	2.05	0.72
1:D:94:ASP:OD2	1:D:109:LYS:NZ	2.24	0.71
1:B:74:LEU:O	1:B:100:LYS:HD3	1.93	0.69
2:A:1601:S1S:C23	1:B:128:LEU:HD22	2.22	0.69
1:B:73:MET:O	3:B:1357:HOH:O	2.12	0.67
2:C:2601:S1S:O	1:D:128:LEU:HD13	1.95	0.66
3:C:2632:HOH:O	1:D:144:GLN:CB	2.44	0.65
1:D:67:ARG:HG3	1:D:107:HIS:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASP:OD2	1:B:109:LYS:NZ	2.25	0.64
1:C:143:ASN:HD22	1:C:144:GLN:HG2	1.62	0.64
1:B:88:SER:HB3	1:B:91:ALA:O	2.01	0.61
2:C:2401:S1S:H122	2:C:2501:S1S:H20	1.82	0.60
1:B:130:GLU:OE1	3:B:1341:HOH:O	2.17	0.59
1:C:123:VAL:HG13	1:D:123:VAL:HB	1.87	0.57
3:C:2653:HOH:O	1:D:151:ILE:HG12	2.03	0.57
2:A:1501:S1S:N1	3:A:1764:HOH:O	2.32	0.57
1:B:96:SER:OG	2:B:1301:S1S:O3	2.23	0.57
2:C:2601:S1S:C23	1:D:128:LEU:HD22	2.35	0.57
1:C:100:LYS:NZ	1:C:102:GLY:O	2.40	0.54
1:A:143:ASN:HD22	1:A:144:GLN:HG2	1.73	0.54
1:C:79:HIS:O	1:C:100:LYS:HG2	2.09	0.53
1:C:89:GLU:HG2	2:C:2201:S1S:C23	2.39	0.52
1:C:74:LEU:O	1:C:77:GLN:HB2	2.10	0.52
1:C:105:VAL:O	3:C:2646:HOH:O	2.19	0.51
2:A:1401:S1S:HC5	2:A:1501:S1S:C40	2.41	0.51
1:A:95:PHE:HE2	2:A:1601:S1S:O	1.92	0.50
1:D:131:LEU:C	1:D:131:LEU:HD23	2.32	0.50
1:A:141:SER:HB2	1:A:146:ILE:HD12	1.93	0.50
1:C:71:GLU:O	1:C:75:SER:HB3	2.12	0.49
1:D:129:ASN:OD1	3:D:2722:HOH:O	2.20	0.49
1:B:92:PRO:HB3	3:B:1378:HOH:O	2.13	0.49
1:B:65:ILE:CG2	1:B:69:LYS:CB	2.90	0.49
2:A:1401:S1S:H122	2:A:1501:S1S:H20	1.95	0.48
1:C:117:LYS:HE3	2:C:2501:S1S:O3	2.14	0.47
1:A:118:TYR:CZ	2:A:1601:S1S:O1	2.67	0.47
1:B:106:GLN:HB3	2:B:1301:S1S:H331	1.95	0.47
2:C:2501:S1S:HC7	2:C:2501:S1S:H102	1.55	0.47
1:C:64:LYS:HE2	1:C:64:LYS:HB2	1.83	0.47
1:A:77:GLN:NE2	1:B:151:ILE:HG23	2.30	0.47
1:B:79:HIS:HD2	1:D:143:ASN:HA	1.81	0.46
2:C:2501:S1S:N	2:C:2501:S1S:C13	2.79	0.46
2:C:2601:S1S:H14	2:C:2601:S1S:H17	1.80	0.46
1:D:71:GLU:HA	1:D:105:VAL:HG21	1.97	0.46
1:D:150:ASP:N	1:D:150:ASP:OD1	2.46	0.45
1:B:131:LEU:HD23	1:B:131:LEU:C	2.36	0.45
1:C:89:GLU:HG2	2:C:2201:S1S:O1	2.15	0.45
2:A:1601:S1S:O1	1:B:128:LEU:HD13	2.17	0.45
1:A:128:LEU:O	1:A:132:VAL:HG23	2.16	0.45
2:A:1401:S1S:H102	2:A:1401:S1S:HC7	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2501:S1S:C37	2:C:2501:S1S:H27	2.47	0.44
1:A:77:GLN:CD	1:B:151:ILE:HG23	2.38	0.44
1:A:135:HIS:HB3	1:A:140:VAL:HG13	1.99	0.43
2:D:2301:S1S:O7	2:D:2301:S1S:C30	2.65	0.43
1:A:117:LYS:HE3	2:A:1401:S1S:O2	2.19	0.43
1:B:65:ILE:HG22	1:B:69:LYS:CB	2.48	0.43
1:B:86:ARG:NH1	3:B:1325:HOH:O	2.46	0.43
2:D:2301:S1S:O7	2:D:2301:S1S:H361	2.13	0.43
2:B:1301:S1S:O7	2:B:1301:S1S:C30	2.67	0.43
1:C:138:THR:OG1	1:D:138:THR:HG23	2.19	0.42
2:A:1501:S1S:H102	2:A:1501:S1S:HC7	1.83	0.42
1:A:77:GLN:O	1:A:100:LYS:HE3	2.19	0.42
1:A:67:ARG:HD2	2:A:1201:S1S:O	2.20	0.42
1:A:90:SER:O	1:A:92:PRO:HD3	2.20	0.42
2:C:2601:S1S:O	1:D:128:LEU:HB2	2.20	0.41
1:A:126:ASN:OD1	1:B:117:LYS:NZ	2.43	0.41
2:A:1401:S1S:C30	2:A:1401:S1S:O7	2.68	0.41
1:B:72:GLU:O	1:B:75:SER:HB2	2.20	0.41
1:D:94:ASP:CG	1:D:109:LYS:HZ1	2.20	0.41
1:A:118:TYR:CZ	2:A:1601:S1S:C23	3.03	0.41
1:D:94:ASP:CG	1:D:109:LYS:NZ	2.73	0.41
1:D:112:ARG:NE	1:D:118:TYR:CE1	2.87	0.41
2:A:1201:S1S:H102	2:A:1201:S1S:HC7	1.82	0.40
2:A:1501:S1S:H27	2:A:1501:S1S:N3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	94/99 (95%)	93 (99%)	1 (1%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
1	C	94/99 (95%)	91 (97%)	2 (2%)	1 (1%)	14	4
1	D	91/99 (92%)	86 (94%)	4 (4%)	1 (1%)	14	4
All	All	370/396 (93%)	355 (96%)	13 (4%)	2 (0%)	29	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	91	ALA
1	C	92	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/88 (90%)	75 (95%)	4 (5%)	24	10
1	B	74/88 (84%)	71 (96%)	3 (4%)	30	16
1	C	81/88 (92%)	74 (91%)	7 (9%)	10	3
1	D	69/88 (78%)	62 (90%)	7 (10%)	7	2
All	All	303/352 (86%)	282 (93%)	21 (7%)	15	5

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	128	LEU
1	A	143	ASN
1	A	144	GLN
1	B	65	ILE
1	B	117	LYS
1	B	128	LEU
1	C	69	LYS
1	C	75	SER

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Mol	Chain	Res	Type
1	C	92	PRO
1	C	123	VAL
1	C	128	LEU
1	C	143	ASN
1	C	144	GLN
1	D	87	GLU
1	D	103	ASN
1	D	112	ARG
1	D	117	LYS
1	D	128	LEU
1	D	129	ASN
1	D	150	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	143	ASN
1	A	144	GLN
1	B	79	HIS
1	B	144	GLN
1	C	106	GLN
1	C	143	ASN
1	C	144	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

12 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
2	S1S	A	1601	-	48,59,59	1.19	3 (6%)	63,83,83	3.08	16 (25%)
2	S1S	A	1401	-	48,59,59	1.39	7 (14%)	63,83,83	3.55	25 (39%)
2	S1S	A	1201	-	48,59,59	1.31	5 (10%)	63,83,83	2.97	17 (26%)
2	S1S	C	2201	-	48,59,59	1.24	3 (6%)	63,83,83	3.64	23 (36%)
2	S1S	A	1701	-	48,59,59	1.62	11 (22%)	63,83,83	4.45	27 (42%)
2	S1S	A	1501	-	48,59,59	1.32	6 (12%)	63,83,83	2.09	16 (25%)
2	S1S	D	2301	-	48,59,59	1.58	7 (14%)	63,83,83	4.23	25 (39%)
2	S1S	C	2601	-	48,59,59	1.30	6 (12%)	63,83,83	2.20	16 (25%)
2	S1S	B	1301	-	48,59,59	1.76	12 (25%)	63,83,83	4.02	24 (38%)
2	S1S	C	2501	-	48,59,59	1.48	6 (12%)	63,83,83	2.53	24 (38%)
2	S1S	D	2701	-	48,59,59	1.68	12 (25%)	63,83,83	4.16	20 (31%)
2	S1S	C	2401	-	48,59,59	1.30	4 (8%)	63,83,83	3.81	22 (34%)

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	S1S	A	1601	-	1/1/13/18	14/56/76/76	0/4/5/5
2	S1S	A	1401	-	2/2/13/18	14/56/76/76	0/4/5/5
2	S1S	A	1201	-	2/2/13/18	12/56/76/76	0/4/5/5
2	S1S	C	2201	-	2/2/13/18	10/56/76/76	0/4/5/5
2	S1S	A	1701	-	1/1/13/18	17/56/76/76	0/4/5/5
2	S1S	A	1501	-	1/1/13/18	15/56/76/76	0/4/5/5
2	S1S	D	2301	-	2/2/13/18	13/56/76/76	0/4/5/5
2	S1S	C	2601	-	1/1/13/18	13/56/76/76	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S1S	B	1301	-	2/2/13/18	9/56/76/76	0/4/5/5
2	S1S	C	2501	-	1/1/13/18	12/56/76/76	0/4/5/5
2	S1S	D	2701	-	1/1/13/18	17/56/76/76	0/4/5/5
2	S1S	C	2401	-	-	16/56/76/76	0/4/5/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2301	S1S	C16-C15	-4.35	1.47	1.52
2	B	1301	S1S	C36-C31	4.33	1.59	1.54
2	A	1701	S1S	C16-C15	-4.24	1.47	1.52
2	D	2701	S1S	C36-C31	4.21	1.59	1.54
2	C	2501	S1S	C32-C31	4.05	1.59	1.54
2	A	1501	S1S	C32-C31	3.78	1.59	1.54
2	D	2301	S1S	C-C8	3.74	1.51	1.42
2	B	1301	S1S	C-C8	3.73	1.51	1.42
2	A	1701	S1S	C-C8	3.68	1.51	1.42
2	A	1701	S1S	C31-N3	3.52	1.53	1.46
2	C	2501	S1S	C36-C31	3.47	1.58	1.54
2	D	2701	S1S	C-C8	3.44	1.50	1.42
2	D	2301	S1S	C37-N3	3.31	1.41	1.34
2	C	2501	S1S	C16-C15	-3.30	1.48	1.52
2	D	2701	S1S	C31-N3	3.26	1.52	1.46
2	C	2601	S1S	C21-C16	3.23	1.44	1.39
2	B	1301	S1S	C38-C37	-3.15	1.46	1.51
2	C	2601	S1S	C32-C31	3.13	1.58	1.54
2	D	2301	S1S	C19-C22	-3.06	1.48	1.53
2	A	1701	S1S	C19-C22	-3.01	1.48	1.53
2	A	1501	S1S	C36-C31	3.00	1.58	1.54
2	A	1601	S1S	C32-C31	2.98	1.58	1.54
2	A	1401	S1S	C21-C20	2.94	1.44	1.38
2	D	2701	S1S	C25-C11	2.93	1.57	1.51
2	C	2401	S1S	C21-C20	2.90	1.44	1.38
2	B	1301	S1S	C17-C16	2.90	1.43	1.39
2	C	2401	S1S	C31-N3	2.86	1.51	1.46
2	D	2701	S1S	C16-C15	-2.85	1.49	1.52
2	A	1201	S1S	C-C8	2.83	1.49	1.42
2	A	1401	S1S	C31-N3	2.79	1.51	1.46
2	A	1701	S1S	C37-N3	2.77	1.40	1.34
2	A	1701	S1S	C25-C11	2.76	1.57	1.51
2	D	2701	S1S	C31-C30	2.73	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2201	S1S	C-C8	2.71	1.48	1.42
2	A	1201	S1S	C27-C26	-2.70	1.45	1.52
2	C	2601	S1S	C8-C9	-2.66	1.38	1.43
2	D	2701	S1S	C18-C19	2.63	1.43	1.39
2	B	1301	S1S	C16-C15	-2.62	1.49	1.52
2	D	2701	S1S	C2-C3	2.62	1.42	1.36
2	A	1401	S1S	C1-C	2.61	1.42	1.37
2	A	1401	S1S	C36-C35	2.59	1.59	1.52
2	A	1701	S1S	C32-C31	2.55	1.57	1.54
2	A	1201	S1S	C1-C	2.54	1.42	1.37
2	B	1301	S1S	O6-C30	2.53	1.27	1.22
2	D	2301	S1S	C2-C3	2.52	1.42	1.36
2	C	2601	S1S	C36-C31	2.50	1.57	1.54
2	B	1301	S1S	C37-N3	2.48	1.39	1.34
2	B	1301	S1S	C36-C35	2.47	1.58	1.52
2	B	1301	S1S	C6-C7	2.46	1.42	1.36
2	B	1301	S1S	C31-C30	-2.45	1.48	1.53
2	D	2701	S1S	C37-N3	2.45	1.39	1.34
2	A	1701	S1S	C2-C3	2.41	1.42	1.36
2	C	2601	S1S	C-C8	2.40	1.48	1.42
2	A	1201	S1S	C21-C16	2.40	1.42	1.39
2	D	2301	S1S	C1-C	2.39	1.42	1.37
2	C	2501	S1S	C31-C30	2.39	1.58	1.53
2	C	2501	S1S	C36-C35	2.38	1.58	1.52
2	C	2401	S1S	O6-C30	2.38	1.27	1.22
2	C	2501	S1S	C32-C33	2.37	1.58	1.52
2	B	1301	S1S	C39-C38	2.36	1.57	1.54
2	A	1501	S1S	C32-C33	2.35	1.58	1.52
2	B	1301	S1S	C2-C1	2.34	1.43	1.38
2	A	1501	S1S	C36-C35	2.31	1.58	1.52
2	A	1401	S1S	C32-C33	2.31	1.58	1.52
2	C	2401	S1S	C38-C37	-2.30	1.48	1.51
2	C	2601	S1S	C19-C22	-2.29	1.49	1.53
2	C	2201	S1S	C19-C22	-2.29	1.49	1.53
2	D	2701	S1S	C1-C	2.26	1.41	1.37
2	D	2701	S1S	C36-C35	2.25	1.58	1.52
2	A	1401	S1S	C19-C22	-2.23	1.49	1.53
2	A	1701	S1S	C32-C33	2.21	1.58	1.52
2	A	1701	S1S	C8-C9	-2.18	1.39	1.43
2	A	1201	S1S	C32-C31	2.18	1.56	1.54
2	C	2201	S1S	O6-C30	2.17	1.26	1.22
2	A	1501	S1S	C16-C15	-2.15	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2301	S1S	C31-N3	2.10	1.50	1.46
2	A	1601	S1S	C19-C22	-2.09	1.49	1.53
2	A	1701	S1S	C36-C35	2.05	1.57	1.52
2	D	2701	S1S	C32-C33	2.04	1.57	1.52
2	A	1401	S1S	C35-C34	2.04	1.59	1.51
2	A	1601	S1S	C-C8	2.01	1.47	1.42
2	A	1501	S1S	C-C8	2.01	1.47	1.42

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2201	S1S	C39-C38-C15	16.21	136.18	110.15
2	D	2301	S1S	C38-C37-N3	14.76	136.44	116.25
2	B	1301	S1S	O7-C37-C38	-14.70	104.02	121.73
2	D	2701	S1S	C36-C31-N3	-14.35	82.20	109.59
2	C	2401	S1S	O7-C37-C38	-14.18	104.64	121.73
2	B	1301	S1S	C38-C37-N3	13.88	135.23	116.25
2	D	2301	S1S	C36-C31-C32	13.79	126.79	109.30
2	A	1701	S1S	C38-C37-N3	13.68	134.96	116.25
2	C	2201	S1S	O7-C37-C38	-13.16	105.87	121.73
2	A	1701	S1S	O7-C37-C38	-13.13	105.91	121.73
2	A	1601	S1S	C38-C37-N3	13.06	134.11	116.25
2	A	1701	S1S	C36-C31-N3	-12.71	85.33	109.59
2	A	1601	S1S	O7-C37-C38	-12.66	106.48	121.73
2	D	2701	S1S	C36-C31-C32	12.62	125.31	109.30
2	A	1401	S1S	O7-C37-C38	-12.42	106.77	121.73
2	D	2301	S1S	O7-C37-C38	-12.30	106.91	121.73
2	B	1301	S1S	C36-C31-C32	12.30	124.90	109.30
2	D	2701	S1S	C32-C31-N3	-12.17	86.37	109.59
2	D	2701	S1S	C38-C37-N3	11.87	132.49	116.25
2	A	1201	S1S	C39-C38-C15	11.84	129.16	110.15
2	A	1701	S1S	C36-C31-C32	11.72	124.17	109.30
2	D	2301	S1S	C39-C38-C15	11.24	128.21	110.15
2	A	1701	S1S	C32-C31-N3	-11.21	88.20	109.59
2	A	1201	S1S	O7-C37-C38	-11.04	108.42	121.73
2	D	2301	S1S	C32-C31-N3	-10.85	88.89	109.59
2	D	2701	S1S	O7-C37-C38	-10.74	108.78	121.73
2	A	1401	S1S	C38-C37-N3	10.53	130.65	116.25
2	A	1201	S1S	C38-C37-N3	10.00	129.93	116.25
2	C	2401	S1S	C38-C37-N3	9.57	129.34	116.25
2	C	2401	S1S	C36-C31-N3	-9.37	91.70	109.59
2	A	1401	S1S	C36-C31-N3	-9.08	92.27	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2501	S1S	C39-C38-C15	8.77	124.23	110.15
2	C	2401	S1S	C32-C31-N3	-8.36	93.63	109.59
2	C	2401	S1S	C33-C32-C31	-8.24	100.15	112.41
2	B	1301	S1S	C32-C31-N3	-8.23	93.87	109.59
2	C	2201	S1S	C27-C28-C29	-8.19	95.95	112.24
2	A	1401	S1S	C32-C31-N3	-8.17	94.01	109.59
2	A	1701	S1S	C28-C27-N2	8.09	126.44	110.60
2	C	2601	S1S	C39-C38-C15	8.07	123.10	110.15
2	D	2701	S1S	C11-C25-N	-7.97	97.72	112.73
2	C	2501	S1S	C11-C25-N	-7.89	97.88	112.73
2	A	1701	S1S	C11-C25-N	-7.82	98.00	112.73
2	C	2201	S1S	C38-C37-N3	7.72	126.81	116.25
2	C	2401	S1S	C35-C36-C31	-7.42	101.38	112.41
2	C	2401	S1S	C28-C27-N2	7.20	124.70	110.60
2	B	1301	S1S	O6-C30-C31	-7.16	110.19	121.00
2	C	2401	S1S	C27-N2-C30	7.12	135.10	121.50
2	D	2301	S1S	C36-C31-N3	-6.81	96.59	109.59
2	A	1601	S1S	C39-C38-C15	6.71	120.93	110.15
2	A	1701	S1S	C30-C31-N3	-6.56	98.45	110.06
2	A	1401	S1S	C28-C27-N2	6.54	123.41	110.60
2	A	1401	S1S	C35-C36-C31	-6.52	102.72	112.41
2	B	1301	S1S	C39-C38-C15	6.46	120.53	110.15
2	C	2201	S1S	C27-N2-C30	6.45	133.84	121.50
2	D	2701	S1S	C30-C31-N3	-5.95	99.53	110.06
2	A	1201	S1S	C27-C28-C29	-5.94	100.43	112.24
2	C	2401	S1S	C32-C31-C30	5.93	124.82	108.96
2	D	2301	S1S	C27-C28-C29	-5.81	100.69	112.24
2	A	1701	S1S	C21-C16-C15	-5.78	112.40	120.93
2	A	1601	S1S	C27-N2-C30	5.77	132.52	121.50
2	A	1501	S1S	C11-C25-N	-5.75	101.89	112.73
2	C	2201	S1S	C26-C27-N2	5.59	126.38	111.16
2	A	1401	S1S	C33-C32-C31	-5.56	104.13	112.41
2	A	1401	S1S	C27-N2-C30	5.56	132.12	121.50
2	C	2501	S1S	O7-C37-C38	-5.50	115.10	121.73
2	C	2601	S1S	C27-N2-C30	5.44	131.90	121.50
2	B	1301	S1S	C30-C31-N3	-5.24	100.77	110.06
2	D	2301	S1S	C28-C27-N2	5.23	120.85	110.60
2	A	1501	S1S	O7-C37-C38	-5.19	115.47	121.73
2	C	2401	S1S	C39-C38-C15	5.15	118.43	110.15
2	A	1401	S1S	C36-C31-C30	5.14	122.71	108.96
2	A	1201	S1S	C26-C27-N2	5.10	125.05	111.16
2	D	2301	S1S	C30-C31-N3	-5.08	101.06	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	S1S	C21-C20-C19	-5.08	116.09	121.20
2	A	1701	S1S	C27-N2-C30	5.06	131.17	121.50
2	A	1501	S1S	C33-C32-C31	5.05	119.93	112.41
2	B	1301	S1S	C28-C27-N2	5.03	120.45	110.60
2	C	2601	S1S	C20-C21-C16	-5.00	116.17	121.20
2	D	2301	S1S	C26-C27-N2	4.99	124.75	111.16
2	A	1601	S1S	C18-C17-C16	-4.94	116.23	121.20
2	B	1301	S1S	C35-C36-C31	-4.92	105.09	112.41
2	D	2701	S1S	C28-C27-N2	4.92	120.23	110.60
2	C	2601	S1S	C17-C18-C19	-4.92	116.25	121.20
2	B	1301	S1S	C27-C28-C29	-4.92	102.47	112.24
2	C	2501	S1S	C25-N-C26	4.91	132.04	122.67
2	A	1501	S1S	C27-N2-C30	4.85	130.77	121.50
2	A	1601	S1S	C25-N-C26	4.80	131.83	122.67
2	A	1701	S1S	C36-C31-C30	4.79	121.75	108.96
2	B	1301	S1S	O6-C30-N2	4.72	132.34	122.74
2	C	2501	S1S	C10-C-C1	4.66	127.80	119.86
2	A	1701	S1S	C17-C18-C19	-4.64	116.53	121.20
2	A	1401	S1S	C36-C31-C32	4.62	115.16	109.30
2	C	2401	S1S	C11-C25-N	-4.61	104.05	112.73
2	D	2701	S1S	C26-C27-N2	4.59	123.64	111.16
2	D	2701	S1S	C36-C31-C30	4.58	121.20	108.96
2	A	1701	S1S	C20-C19-C22	-4.52	111.11	120.98
2	D	2701	S1S	C21-C16-C15	-4.48	114.32	120.93
2	A	1401	S1S	C39-C38-C15	4.47	117.33	110.15
2	D	2701	S1S	C17-C16-C15	4.41	127.44	120.93
2	A	1701	S1S	C17-C16-C15	4.36	127.36	120.93
2	C	2201	S1S	C25-N-C26	4.31	130.91	122.67
2	C	2601	S1S	C18-C17-C16	4.30	125.53	121.20
2	C	2401	S1S	C7-C8-C9	4.30	123.45	117.89
2	A	1401	S1S	C11-C25-N	-4.22	104.79	112.73
2	A	1501	S1S	C31-C30-N2	4.15	123.89	116.58
2	D	2701	S1S	C27-N2-C30	4.13	129.39	121.50
2	C	2601	S1S	O7-C37-C38	-4.10	116.79	121.73
2	A	1701	S1S	C12-C11-C10	-4.05	105.42	110.75
2	A	1601	S1S	C27-C28-C29	-4.03	104.22	112.24
2	A	1701	S1S	C25-N-C26	3.99	130.28	122.67
2	D	2301	S1S	O6-C30-C31	-3.88	115.13	121.00
2	A	1201	S1S	C33-C32-C31	-3.88	106.64	112.41
2	A	1501	S1S	C39-C38-C15	3.78	116.22	110.15
2	B	1301	S1S	C32-C33-C34	-3.75	105.57	111.37
2	C	2201	S1S	C28-C27-C26	3.75	119.24	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	S1S	C7-C8-C9	3.72	122.70	117.89
2	B	1301	S1S	C26-C27-N2	3.71	121.26	111.16
2	A	1501	S1S	C31-N3-C37	3.63	128.26	122.13
2	C	2501	S1S	C7-C8-C	-3.62	116.56	122.55
2	C	2201	S1S	C33-C32-C31	-3.53	107.17	112.41
2	D	2701	S1S	C27-C26-N	-3.52	109.45	116.54
2	D	2301	S1S	O6-C30-N2	3.52	129.89	122.74
2	C	2401	S1S	C21-C20-C19	-3.51	117.66	121.20
2	C	2501	S1S	C31-C30-N2	3.48	122.71	116.58
2	A	1501	S1S	C10-C-C1	3.46	125.76	119.86
2	C	2201	S1S	C36-C31-C32	3.44	113.66	109.30
2	A	1501	S1S	C26-C27-N2	3.44	120.52	111.16
2	C	2401	S1S	C36-C31-C30	3.41	118.08	108.96
2	A	1601	S1S	C20-C21-C16	3.40	124.62	121.20
2	D	2301	S1S	C28-C29-N1	3.40	124.39	116.21
2	A	1501	S1S	C28-C27-C26	-3.39	102.44	110.42
2	A	1501	S1S	O6-C30-C31	-3.32	115.98	121.00
2	B	1301	S1S	C12-C11-C10	-3.30	106.41	110.75
2	B	1301	S1S	C11-C25-N	-3.28	106.55	112.73
2	D	2701	S1S	C17-C18-C19	-3.26	117.92	121.20
2	A	1701	S1S	C26-C27-N2	3.20	119.88	111.16
2	A	1401	S1S	O6-C30-C31	-3.19	116.17	121.00
2	A	1401	S1S	C26-C27-N2	3.18	119.83	111.16
2	C	2501	S1S	C10-C-C8	-3.18	115.74	120.76
2	C	2201	S1S	C31-C30-N2	-3.17	111.00	116.58
2	A	1201	S1S	C28-C27-C26	3.16	117.87	110.42
2	A	1701	S1S	C39-C38-C15	3.16	115.23	110.15
2	C	2401	S1S	C7-C8-C	-3.12	117.39	122.55
2	C	2601	S1S	C18-C19-C22	-3.10	114.19	120.98
2	D	2701	S1S	C20-C19-C22	-3.09	114.22	120.98
2	A	1701	S1S	C18-C19-C22	3.09	127.73	120.98
2	D	2301	S1S	O7-C37-N3	-3.08	116.56	123.14
2	C	2601	S1S	C26-C27-N2	3.08	119.54	111.16
2	A	1201	S1S	C36-C35-C34	-3.07	106.61	111.37
2	C	2501	S1S	C27-C26-N	-3.07	110.36	116.54
2	C	2201	S1S	C21-C16-C17	3.06	122.11	118.29
2	C	2501	S1S	C7-C8-C9	3.06	121.85	117.89
2	A	1201	S1S	C7-C8-C9	3.05	121.84	117.89
2	B	1301	S1S	C18-C17-C16	-3.03	118.14	121.20
2	A	1601	S1S	C30-C31-N3	3.03	115.42	110.06
2	C	2401	S1S	C26-C27-N2	3.03	119.40	111.16
2	A	1401	S1S	C32-C31-C30	3.03	117.05	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2501	S1S	O4-C26-C27	3.02	126.81	120.45
2	C	2601	S1S	C21-C20-C19	3.01	124.22	121.20
2	B	1301	S1S	C21-C20-C19	-2.97	118.20	121.20
2	D	2301	S1S	C2-C1-C	-2.97	116.22	121.48
2	B	1301	S1S	C36-C35-C34	2.94	115.92	111.37
2	D	2301	S1S	C36-C31-C30	2.94	116.81	108.96
2	C	2601	S1S	C36-C31-C32	2.92	113.00	109.30
2	B	1301	S1S	C32-C31-C30	2.91	116.75	108.96
2	A	1701	S1S	C15-C14-C13	-2.90	119.50	126.01
2	C	2201	S1S	C20-C19-C18	2.87	121.87	118.29
2	B	1301	S1S	O4-C26-C27	2.86	126.47	120.45
2	C	2501	S1S	C20-C19-C22	-2.84	114.78	120.98
2	C	2201	S1S	C20-C21-C16	-2.83	118.35	121.20
2	D	2301	S1S	C18-C17-C16	-2.82	118.36	121.20
2	C	2401	S1S	C3-C9-C8	2.81	122.82	119.12
2	C	2501	S1S	C31-N3-C37	2.78	126.82	122.13
2	C	2201	S1S	C17-C18-C19	-2.77	118.41	121.20
2	C	2401	S1S	O6-C30-C31	-2.77	116.81	121.00
2	C	2601	S1S	C27-C28-C29	-2.77	106.73	112.24
2	C	2201	S1S	C12-C11-C10	2.76	114.40	110.75
2	A	1701	S1S	O6-C30-C31	-2.76	116.82	121.00
2	A	1601	S1S	C36-C35-C34	2.74	115.61	111.37
2	A	1401	S1S	C7-C8-C	-2.74	118.02	122.55
2	D	2301	S1S	C11-C25-N	-2.74	107.58	112.73
2	A	1201	S1S	C27-N2-C30	2.72	126.70	121.50
2	A	1401	S1S	C28-C27-C26	2.69	116.76	110.42
2	A	1201	S1S	C18-C17-C16	-2.68	118.50	121.20
2	A	1201	S1S	C10-C-C1	2.67	124.41	119.86
2	C	2501	S1S	C26-C27-N2	2.67	118.42	111.16
2	A	1401	S1S	C27-C26-N	-2.63	111.23	116.54
2	B	1301	S1S	C21-C16-C15	-2.63	117.04	120.93
2	C	2201	S1S	C30-C31-N3	2.63	114.71	110.06
2	A	1501	S1S	C7-C8-C	-2.63	118.20	122.55
2	C	2501	S1S	C36-C31-C32	2.62	112.62	109.30
2	A	1501	S1S	C7-C8-C9	2.62	121.27	117.89
2	C	2601	S1S	C11-C25-N	-2.61	107.82	112.73
2	C	2401	S1S	C6-C7-C8	-2.60	117.29	120.89
2	A	1701	S1S	C27-C26-N	-2.59	111.31	116.54
2	C	2501	S1S	C2-C3-C9	-2.58	116.41	120.44
2	C	2601	S1S	C31-C30-N2	-2.56	112.07	116.58
2	A	1401	S1S	C27-C28-C29	2.54	117.29	112.24
2	C	2601	S1S	C25-N-C26	2.54	127.52	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	S1S	C-C10-C11	-2.51	108.53	114.34
2	C	2201	S1S	C10-C-C1	2.50	124.12	119.86
2	C	2201	S1S	C21-C16-C15	-2.50	117.24	120.93
2	A	1501	S1S	C-C10-C11	2.48	120.09	114.34
2	A	1701	S1S	C31-N3-C37	2.48	126.32	122.13
2	A	1701	S1S	O5-C29-C28	-2.47	115.66	120.87
2	C	2401	S1S	C10-C-C1	2.43	123.99	119.86
2	D	2301	S1S	C21-C16-C17	2.41	121.30	118.29
2	A	1401	S1S	C30-C31-N3	-2.38	105.85	110.06
2	A	1501	S1S	C12-C11-C10	2.38	113.89	110.75
2	C	2601	S1S	C28-C27-C26	2.37	116.01	110.42
2	D	2301	S1S	C10-C-C1	-2.37	115.82	119.86
2	C	2201	S1S	C20-C19-C22	-2.37	115.81	120.98
2	C	2201	S1S	C36-C31-N3	-2.36	105.09	109.59
2	D	2301	S1S	C21-C16-C15	-2.36	117.45	120.93
2	C	2601	S1S	C20-C19-C22	2.31	126.03	120.98
2	C	2501	S1S	C33-C32-C31	2.30	115.84	112.41
2	C	2201	S1S	C7-C8-C9	2.30	120.87	117.89
2	D	2701	S1S	C15-C14-C13	-2.30	120.84	126.01
2	A	1201	S1S	C6-C7-C8	-2.29	117.72	120.89
2	D	2701	S1S	C12-C11-C10	-2.28	107.75	110.75
2	A	1701	S1S	C20-C19-C18	2.27	121.13	118.29
2	A	1201	S1S	C17-C16-C15	-2.27	117.58	120.93
2	B	1301	S1S	C20-C21-C16	2.27	123.48	121.20
2	A	1701	S1S	O4-C26-C27	2.26	125.21	120.45
2	C	2501	S1S	C15-C14-C13	2.26	131.09	126.01
2	A	1401	S1S	C3-C9-C8	2.25	122.09	119.12
2	A	1501	S1S	C10-C-C8	-2.24	117.22	120.76
2	D	2301	S1S	C32-C33-C34	2.23	114.82	111.37
2	A	1401	S1S	C21-C16-C15	-2.22	117.64	120.93
2	A	1201	S1S	C12-C13-C14	-2.22	114.61	125.81
2	C	2501	S1S	C21-C16-C15	-2.22	117.66	120.93
2	A	1401	S1S	O4-C26-C27	2.21	125.11	120.45
2	A	1701	S1S	C32-C33-C34	2.20	114.77	111.37
2	A	1201	S1S	C12-C11-C10	2.18	113.62	110.75
2	C	2501	S1S	C30-C31-N3	2.17	113.90	110.06
2	A	1601	S1S	C17-C18-C19	2.17	123.38	121.20
2	D	2701	S1S	C18-C19-C22	2.16	125.71	120.98
2	D	2701	S1S	O7-C37-N3	-2.16	118.53	123.14
2	A	1601	S1S	C36-C31-C30	-2.14	103.24	108.96
2	C	2501	S1S	O6-C30-C31	-2.14	117.77	121.00
2	A	1601	S1S	C28-C27-C26	2.13	115.45	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	S1S	C27-C26-N	-2.10	112.32	116.54
2	D	2301	S1S	C3-C2-C1	2.08	124.31	120.99
2	C	2501	S1S	C18-C19-C22	2.08	125.53	120.98
2	C	2501	S1S	C38-C37-N3	2.06	119.07	116.25
2	A	1601	S1S	C26-C27-N2	2.06	116.76	111.16
2	A	1201	S1S	C-C10-C11	-2.05	109.58	114.34
2	C	2401	S1S	C31-N3-C37	2.05	125.59	122.13
2	C	2501	S1S	C-C8-C9	2.05	121.52	118.98
2	B	1301	S1S	C4-C9-C3	-2.04	118.42	123.19
2	A	1601	S1S	C7-C8-C9	2.02	120.51	117.89
2	D	2301	S1S	C27-N2-C30	2.02	125.36	121.50
2	C	2201	S1S	C15-C14-C13	2.02	130.55	126.01
2	D	2301	S1S	C36-C35-C34	2.01	114.49	111.37
2	C	2401	S1S	C-C10-C11	-2.00	109.70	114.34

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1601	S1S	C38
2	A	1401	S1S	C38
2	A	1401	S1S	C27
2	A	1201	S1S	C27
2	A	1201	S1S	C38
2	C	2201	S1S	C27
2	C	2201	S1S	C38
2	D	2301	S1S	C38
2	D	2301	S1S	C27
2	A	1701	S1S	C38
2	A	1501	S1S	C38
2	C	2601	S1S	C38
2	B	1301	S1S	C38
2	B	1301	S1S	C27
2	C	2501	S1S	C38
2	D	2701	S1S	C38

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	S1S	C37-C38-C39-C40
2	A	1601	S1S	C16-C15-C38-C39
2	A	1601	S1S	C14-C15-C38-C39
2	A	1601	S1S	C14-C15-C38-C37

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Mol	Chain	Res	Type	Atoms
2	A	1601	S1S	O7-C37-C38-C39
2	A	1401	S1S	C37-C38-C39-C40
2	A	1401	S1S	C14-C15-C38-C37
2	A	1401	S1S	N2-C30-C31-C32
2	A	1401	S1S	N2-C27-C28-C29
2	A	1201	S1S	C15-C38-C39-C40
2	A	1201	S1S	C37-C38-C39-C40
2	A	1201	S1S	C14-C15-C38-C39
2	A	1201	S1S	C14-C15-C38-C37
2	A	1201	S1S	O7-C37-C38-C15
2	A	1201	S1S	N3-C37-C38-C15
2	C	2201	S1S	C15-C38-C39-C40
2	C	2201	S1S	C37-C38-C39-C40
2	C	2201	S1S	C14-C15-C38-C39
2	C	2201	S1S	O7-C37-C38-C39
2	C	2201	S1S	N3-C37-C38-C39
2	D	2301	S1S	C15-C38-C39-C40
2	D	2301	S1S	C16-C15-C38-C39
2	D	2301	S1S	C14-C15-C38-C39
2	D	2301	S1S	C14-C15-C38-C37
2	A	1701	S1S	C37-C38-C39-C40
2	A	1701	S1S	C14-C15-C38-C39
2	A	1701	S1S	C14-C15-C38-C37
2	A	1701	S1S	O7-C37-C38-C39
2	A	1701	S1S	N3-C37-C38-C39
2	A	1701	S1S	O6-C30-C31-C32
2	A	1701	S1S	N2-C30-C31-C32
2	A	1701	S1S	N2-C27-C28-C29
2	A	1501	S1S	O7-C37-C38-C15
2	A	1501	S1S	N3-C37-C38-C15
2	A	1501	S1S	C31-C30-N2-C27
2	A	1501	S1S	O6-C30-N2-C27
2	A	1501	S1S	C27-C28-C29-O5
2	C	2401	S1S	C14-C15-C38-C37
2	C	2401	S1S	N2-C27-C28-C29
2	C	2601	S1S	C15-C38-C39-C40
2	C	2601	S1S	C37-C38-C39-C40
2	C	2601	S1S	C16-C15-C38-C39
2	C	2601	S1S	C14-C15-C38-C39
2	C	2601	S1S	N2-C27-C28-C29
2	B	1301	S1S	C15-C38-C39-C40
2	B	1301	S1S	C16-C15-C38-C39

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Mol	Chain	Res	Type	Atoms
2	B	1301	S1S	C14-C15-C38-C39
2	B	1301	S1S	C14-C15-C38-C37
2	C	2501	S1S	C16-C15-C38-C39
2	C	2501	S1S	C14-C15-C38-C39
2	C	2501	S1S	C31-C30-N2-C27
2	C	2501	S1S	O6-C30-N2-C27
2	C	2501	S1S	N2-C27-C28-C29
2	D	2701	S1S	C37-C38-C39-C40
2	D	2701	S1S	C14-C15-C38-C39
2	D	2701	S1S	C14-C15-C38-C37
2	D	2701	S1S	O7-C37-C38-C39
2	D	2701	S1S	N3-C37-C38-C39
2	D	2701	S1S	O6-C30-C31-C32
2	D	2701	S1S	N2-C30-C31-C32
2	D	2701	S1S	C26-C27-N2-C30
2	D	2701	S1S	N2-C27-C28-C29
2	A	1501	S1S	O7-C37-N3-C31
2	A	1501	S1S	C38-C37-N3-C31
2	A	1501	S1S	C27-C28-C29-N1
2	C	2401	S1S	N2-C30-C31-C32
2	D	2701	S1S	O6-C30-N2-C27
2	A	1501	S1S	C32-C31-N3-C37
2	A	1601	S1S	C27-C28-C29-O5
2	A	1701	S1S	C26-C27-N2-C30
2	A	1401	S1S	O6-C30-C31-C32
2	C	2401	S1S	O6-C30-C31-C32
2	A	1601	S1S	C27-C28-C29-N1
2	D	2301	S1S	N2-C30-C31-C32
2	D	2701	S1S	C14-C15-C16-C17
2	C	2601	S1S	C27-C28-C29-N1
2	A	1601	S1S	C16-C15-C38-C37
2	A	1401	S1S	C16-C15-C38-C37
2	A	1701	S1S	C16-C15-C38-C37
2	C	2401	S1S	C16-C15-C38-C37
2	D	2701	S1S	C16-C15-C38-C37
2	A	1501	S1S	C13-C14-C15-C38
2	A	1601	S1S	C14-C15-C16-C21
2	D	2701	S1S	C14-C15-C16-C21
2	A	1601	S1S	C10-C11-C25-N
2	A	1401	S1S	C10-C11-C25-N
2	C	2401	S1S	C10-C11-C25-N
2	D	2701	S1S	C10-C11-C25-N

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Mol	Chain	Res	Type	Atoms
2	A	1601	S1S	N3-C37-C38-C15
2	C	2201	S1S	O7-C37-C38-C15
2	C	2201	S1S	N3-C37-C38-C15
2	D	2301	S1S	O7-C37-C38-C15
2	D	2301	S1S	N3-C37-C38-C15
2	A	1701	S1S	O7-C37-C38-C15
2	A	1701	S1S	N3-C37-C38-C15
2	C	2401	S1S	O7-C37-C38-C15
2	C	2601	S1S	O7-C37-C38-C15
2	B	1301	S1S	O7-C37-C38-C15
2	D	2701	S1S	O7-C37-C38-C15
2	D	2701	S1S	N3-C37-C38-C15
2	A	1201	S1S	C10-C11-C12-C13
2	A	1401	S1S	C26-C27-C28-C29
2	D	2301	S1S	C26-C27-C28-C29
2	A	1601	S1S	C14-C15-C16-C17
2	C	2501	S1S	C14-C15-C16-C21
2	A	1201	S1S	C25-C11-C12-C13
2	A	1201	S1S	C-C10-C11-C12
2	A	1201	S1S	C-C10-C11-C25
2	A	1501	S1S	C25-C11-C12-C13
2	C	2401	S1S	C-C10-C11-C25
2	A	1501	S1S	O4-C26-C27-N2
2	A	1701	S1S	C14-C15-C16-C17
2	C	2601	S1S	C14-C15-C16-C17
2	C	2501	S1S	C14-C15-C16-C17
2	A	1601	S1S	N3-C37-C38-C39
2	A	1501	S1S	C11-C12-C13-C14
2	C	2601	S1S	C27-C28-C29-O5
2	C	2501	S1S	C15-C38-C39-C40
2	A	1201	S1S	O4-C26-C27-C28
2	C	2601	S1S	C14-C15-C16-C21
2	C	2401	S1S	O4-C26-C27-C28
2	D	2301	S1S	C14-C15-C16-C21
2	A	1501	S1S	C30-C31-N3-C37
2	A	1501	S1S	N-C26-C27-N2
2	A	1601	S1S	O7-C37-C38-C15
2	A	1401	S1S	O7-C37-C38-C15
2	A	1401	S1S	C14-C15-C16-C21
2	C	2401	S1S	N3-C37-C38-C15
2	C	2401	S1S	C14-C15-C16-C17
2	B	1301	S1S	N3-C37-C38-C15

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Mol	Chain	Res	Type	Atoms
2	C	2501	S1S	O7-C37-C38-C15
2	C	2501	S1S	N3-C37-C38-C15
2	C	2401	S1S	C26-C27-C28-C29
2	C	2501	S1S	C26-C27-C28-C29
2	C	2201	S1S	O4-C26-C27-C28
2	D	2301	S1S	O6-C30-C31-C36
2	D	2301	S1S	C14-C15-C16-C17
2	A	1701	S1S	C14-C15-C16-C21
2	B	1301	S1S	C14-C15-C16-C21
2	A	1401	S1S	C36-C31-N3-C37
2	C	2401	S1S	C30-C31-N3-C37
2	D	2301	S1S	C16-C15-C38-C37
2	A	1401	S1S	C14-C15-C16-C17
2	C	2401	S1S	C14-C15-C16-C21
2	B	1301	S1S	C14-C15-C16-C17
2	C	2601	S1S	O4-C26-C27-C28
2	C	2201	S1S	C14-C15-C38-C37
2	A	1701	S1S	C16-C15-C38-C39
2	C	2401	S1S	C37-C38-C39-C40
2	C	2601	S1S	C14-C15-C38-C37
2	B	1301	S1S	C37-C38-C39-C40
2	C	2501	S1S	C14-C15-C38-C37
2	A	1401	S1S	O4-C26-C27-C28
2	A	1701	S1S	O6-C30-C31-C36
2	A	1701	S1S	C10-C11-C25-N
2	A	1401	S1S	N3-C37-C38-C15
2	D	2301	S1S	O4-C26-C27-C28
2	D	2701	S1S	O4-C26-C27-C28
2	A	1201	S1S	N-C26-C27-C28
2	C	2601	S1S	N-C26-C27-C28
2	C	2401	S1S	N-C26-C27-C28
2	C	2201	S1S	N-C26-C27-C28

There are no ring outliers.

10 monomers are involved in 33 short contacts:

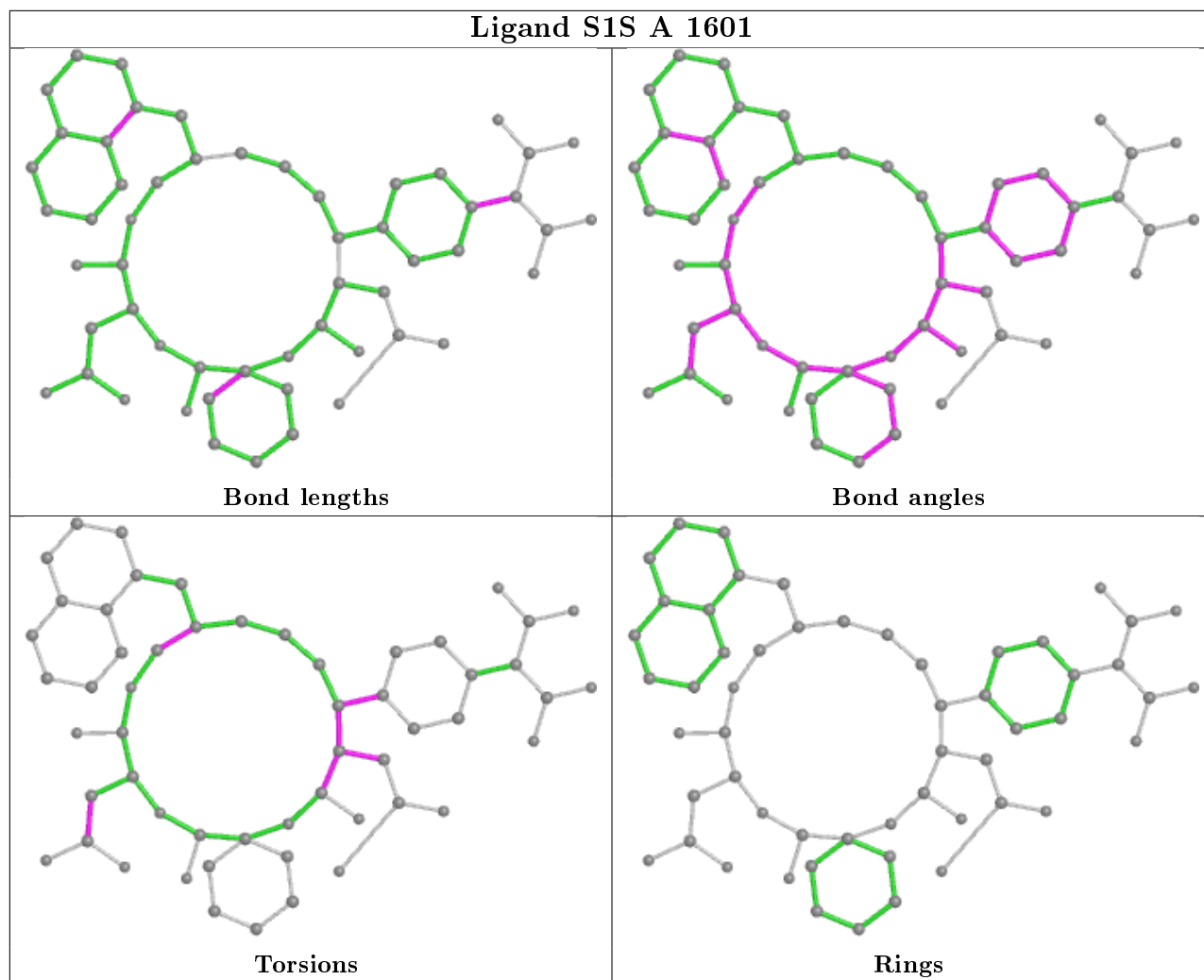
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	S1S	6	0
2	A	1401	S1S	5	0
2	A	1201	S1S	2	0
2	C	2201	S1S	2	0
2	A	1501	S1S	5	0

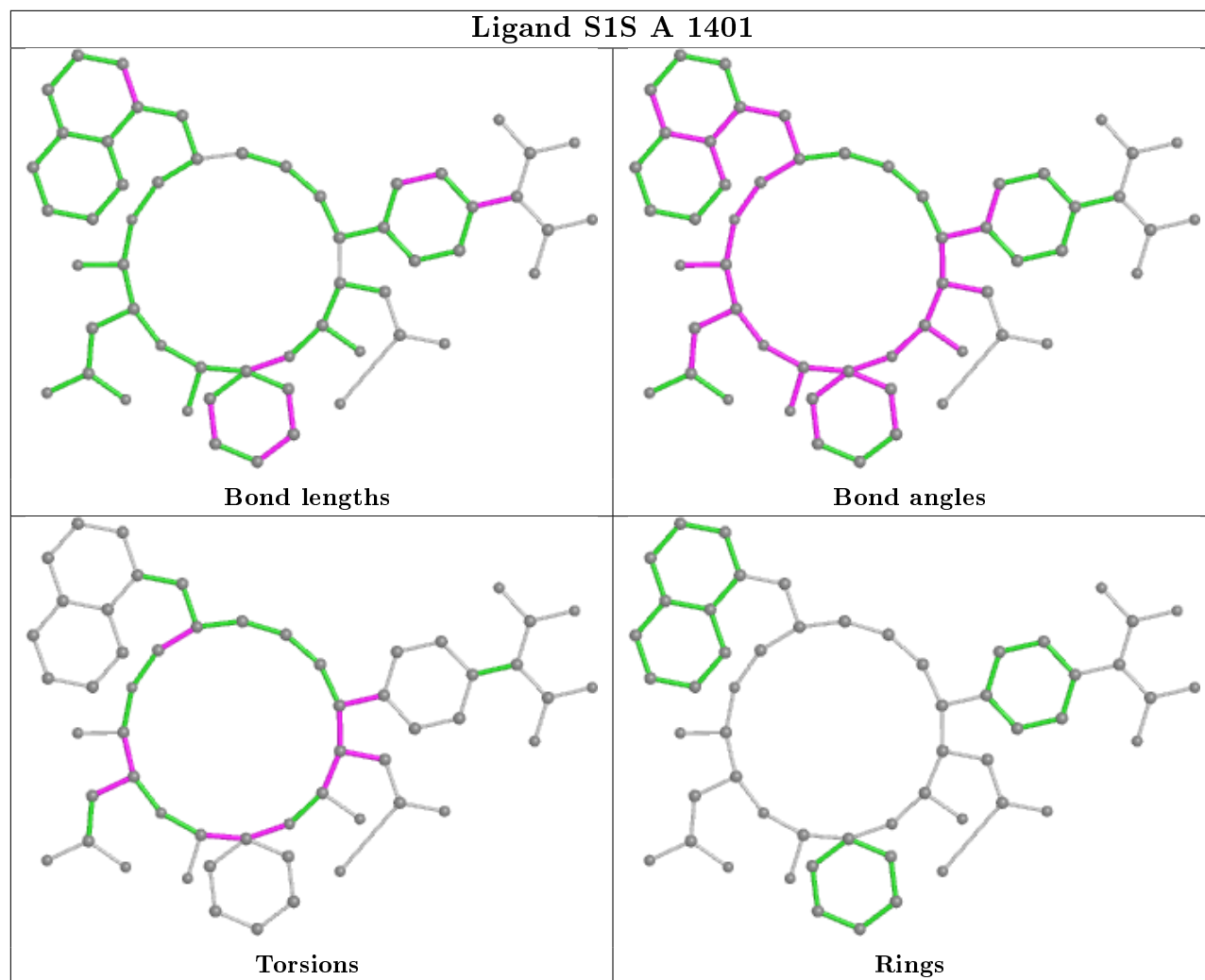
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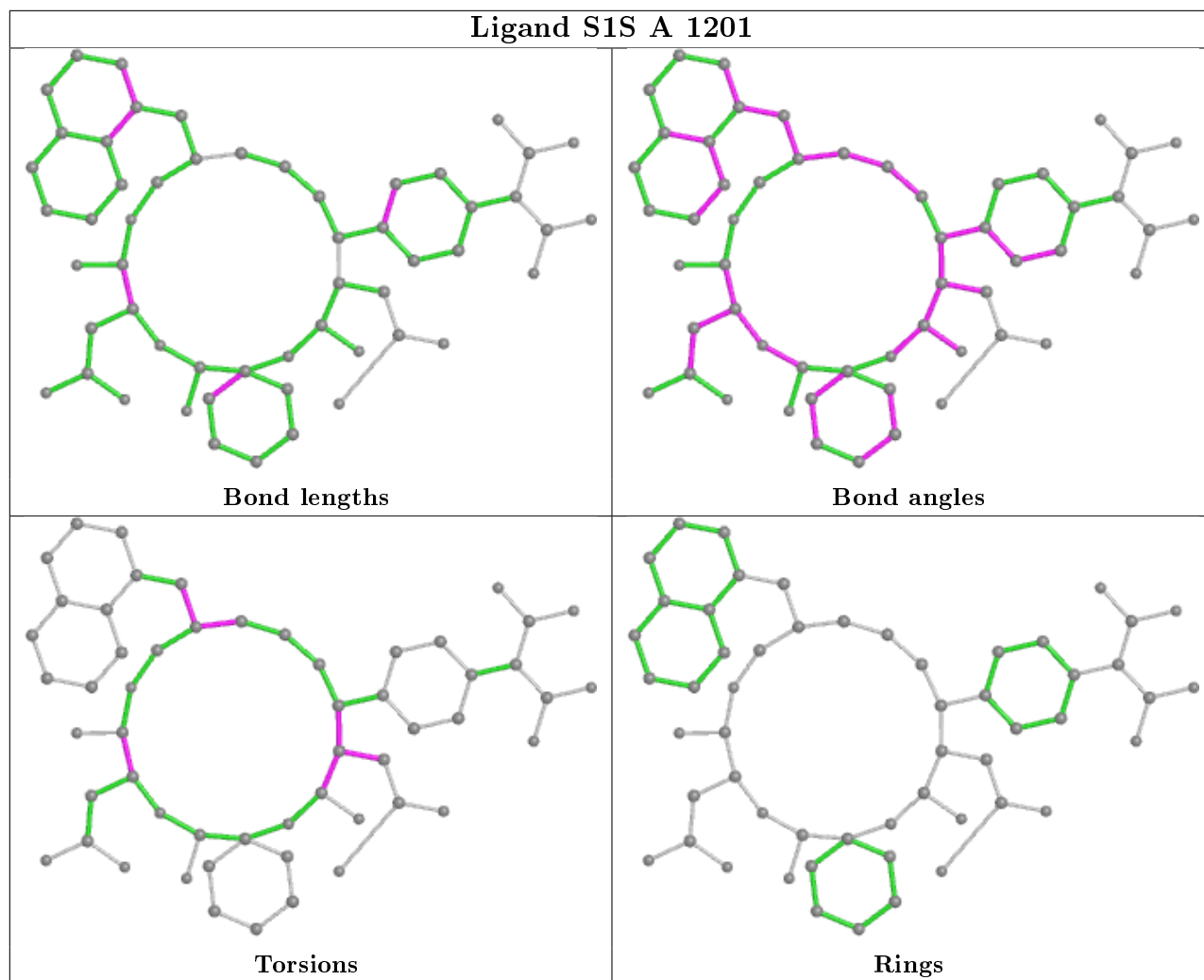
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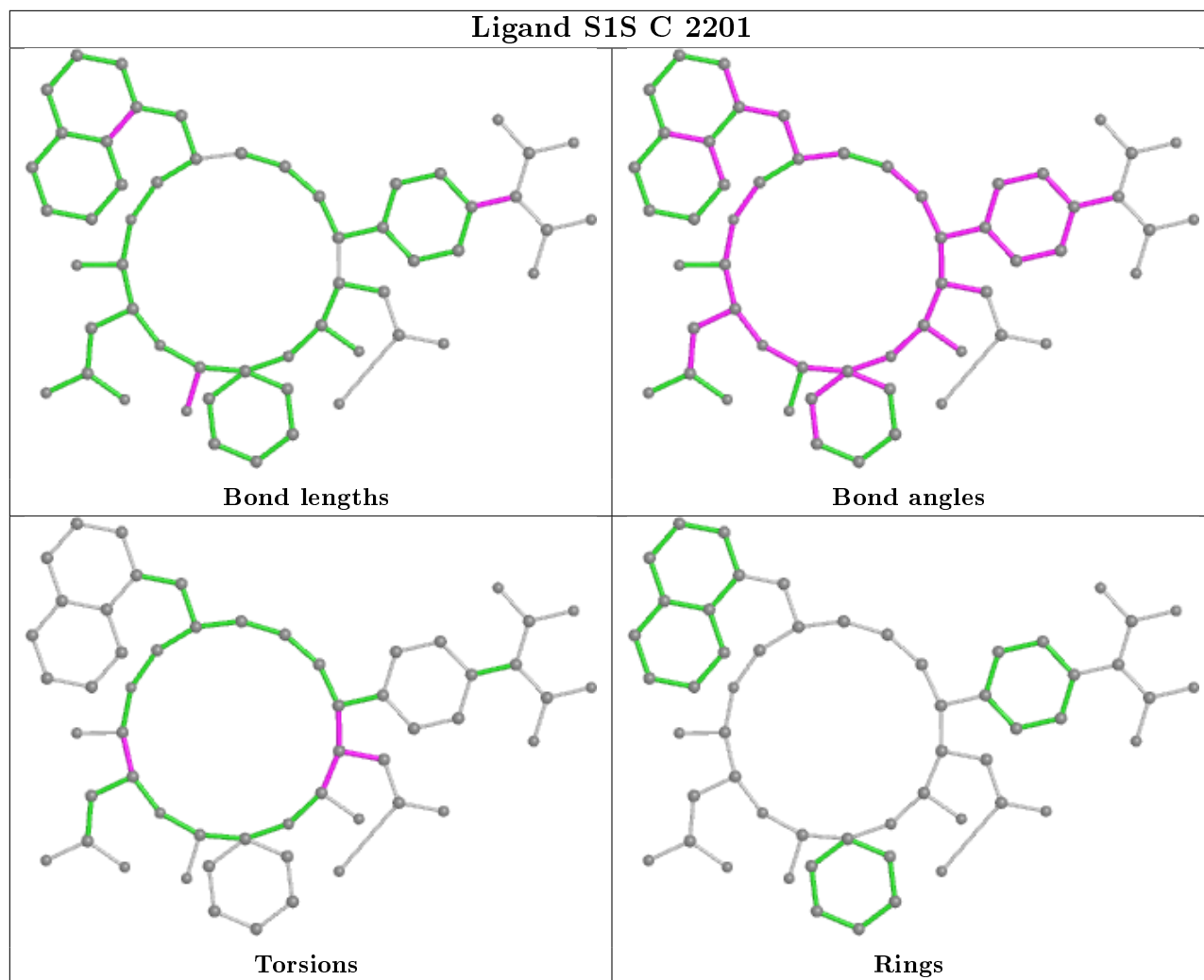
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2301	S1S	2	0
2	C	2601	S1S	5	0
2	B	1301	S1S	3	0
2	C	2501	S1S	5	0
2	C	2401	S1S	1	0

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.

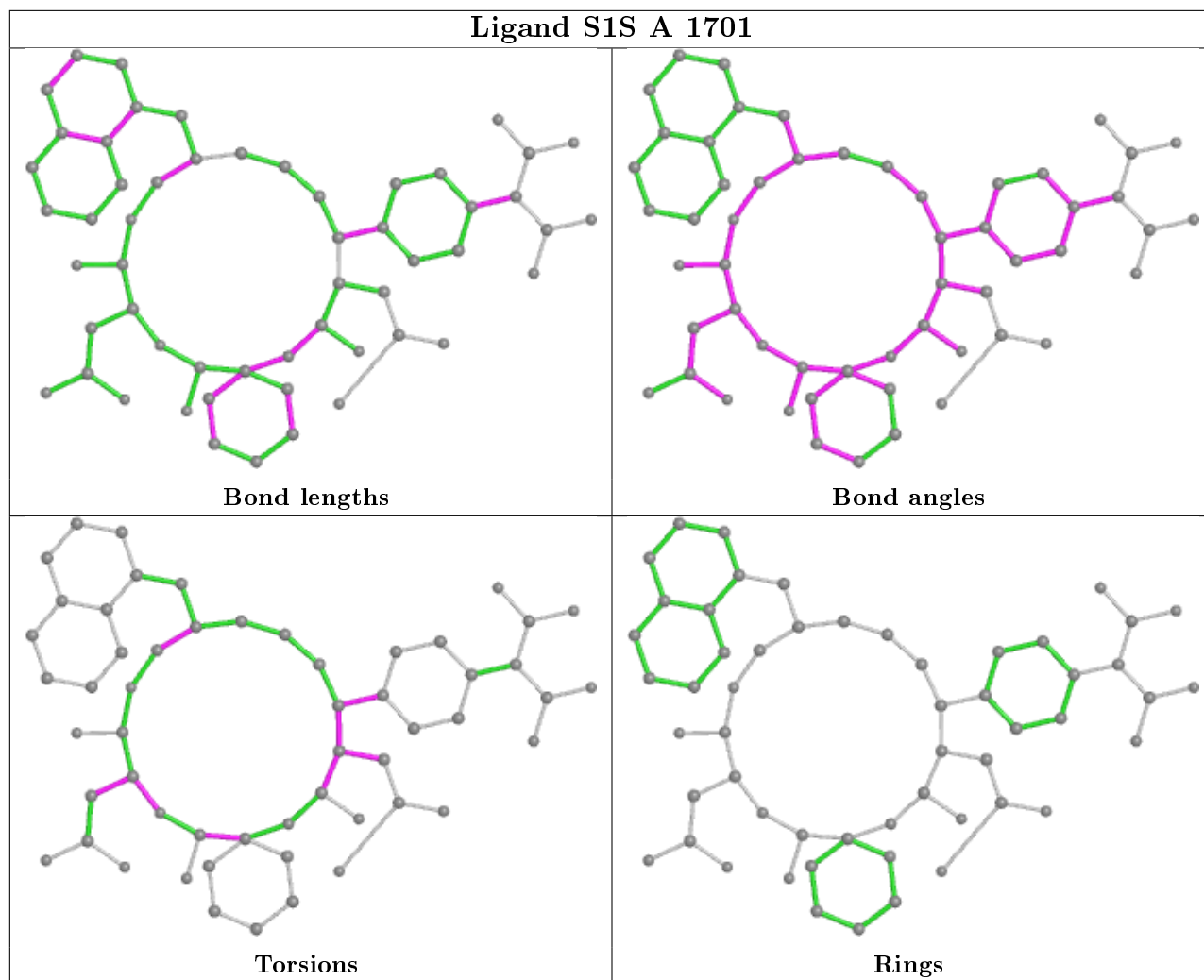


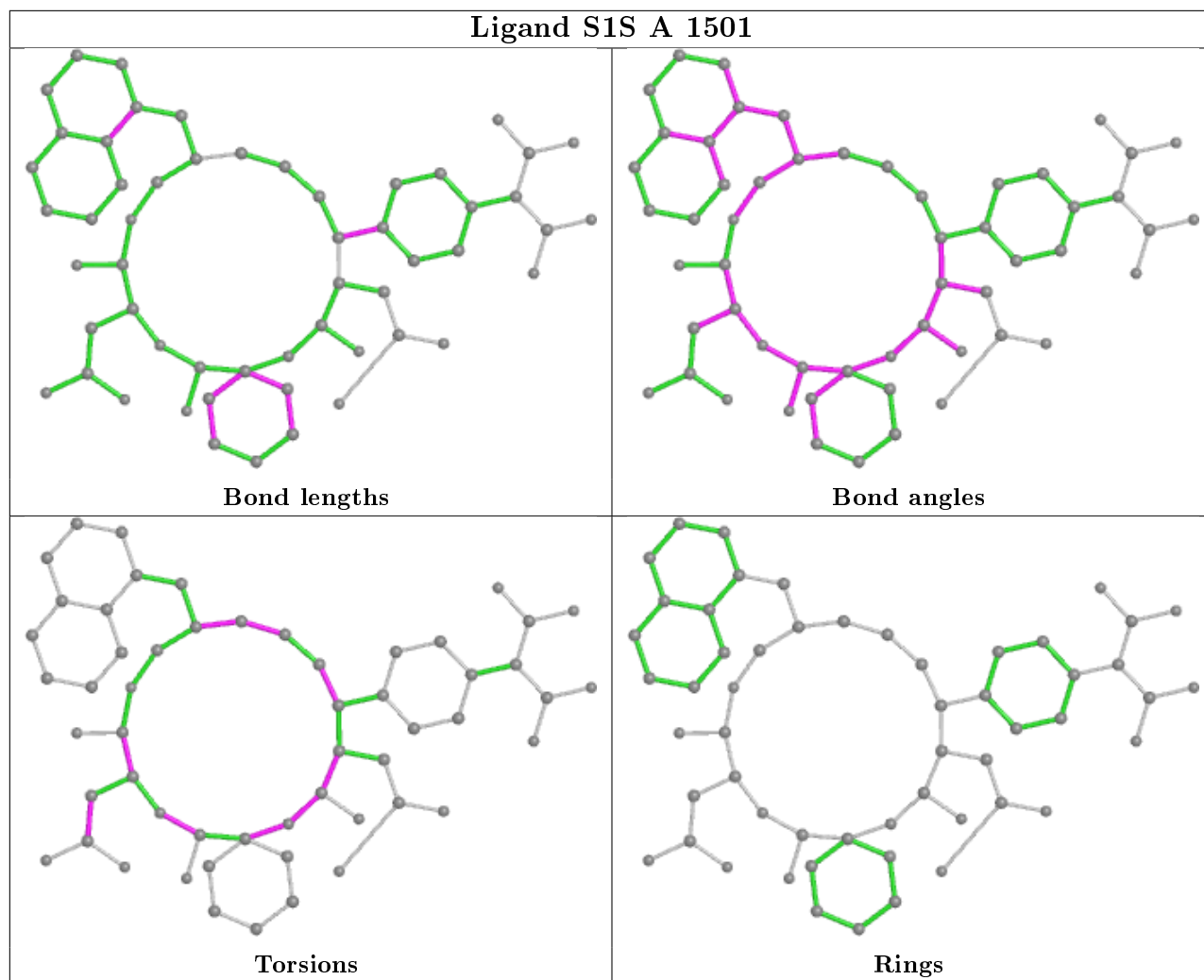


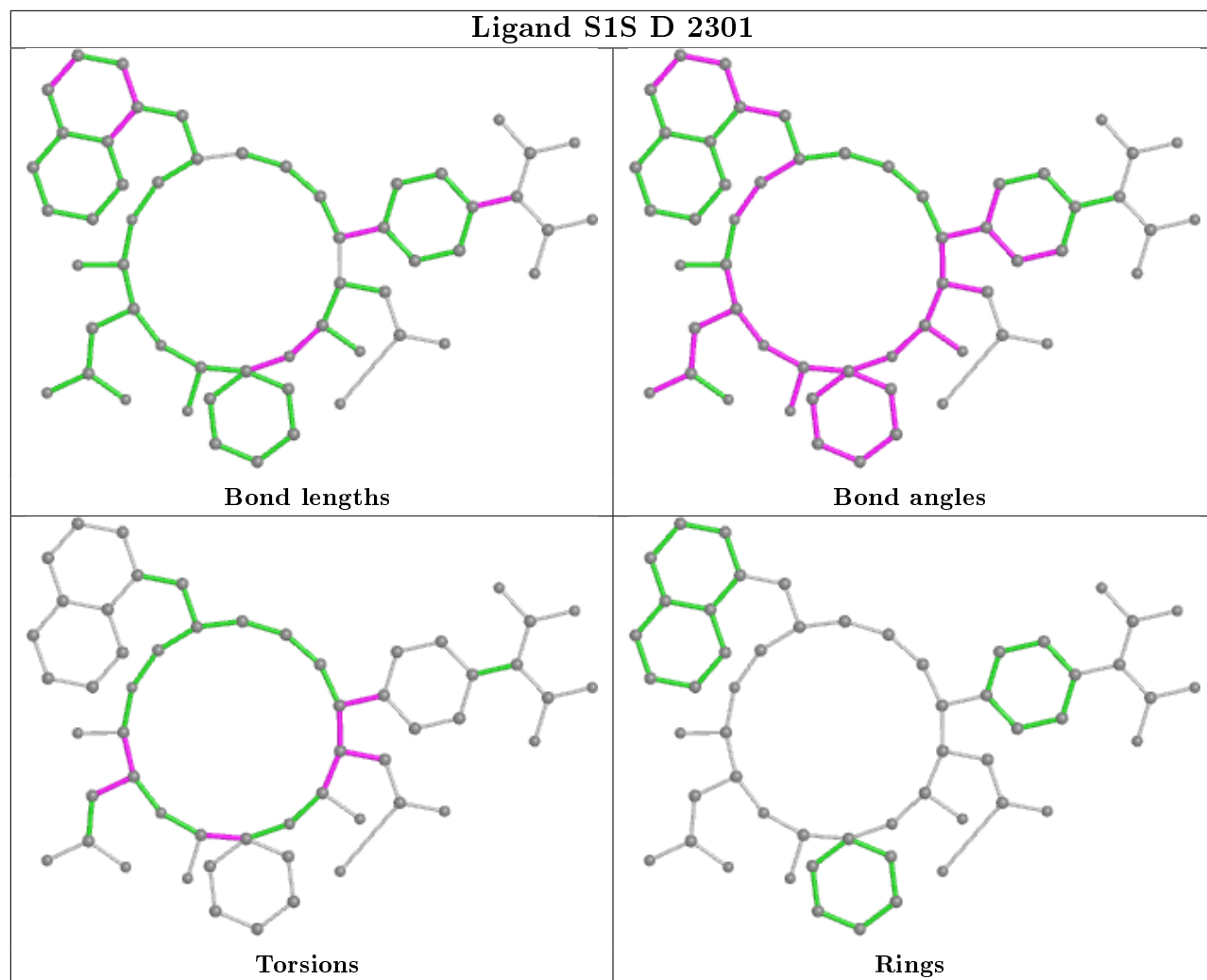


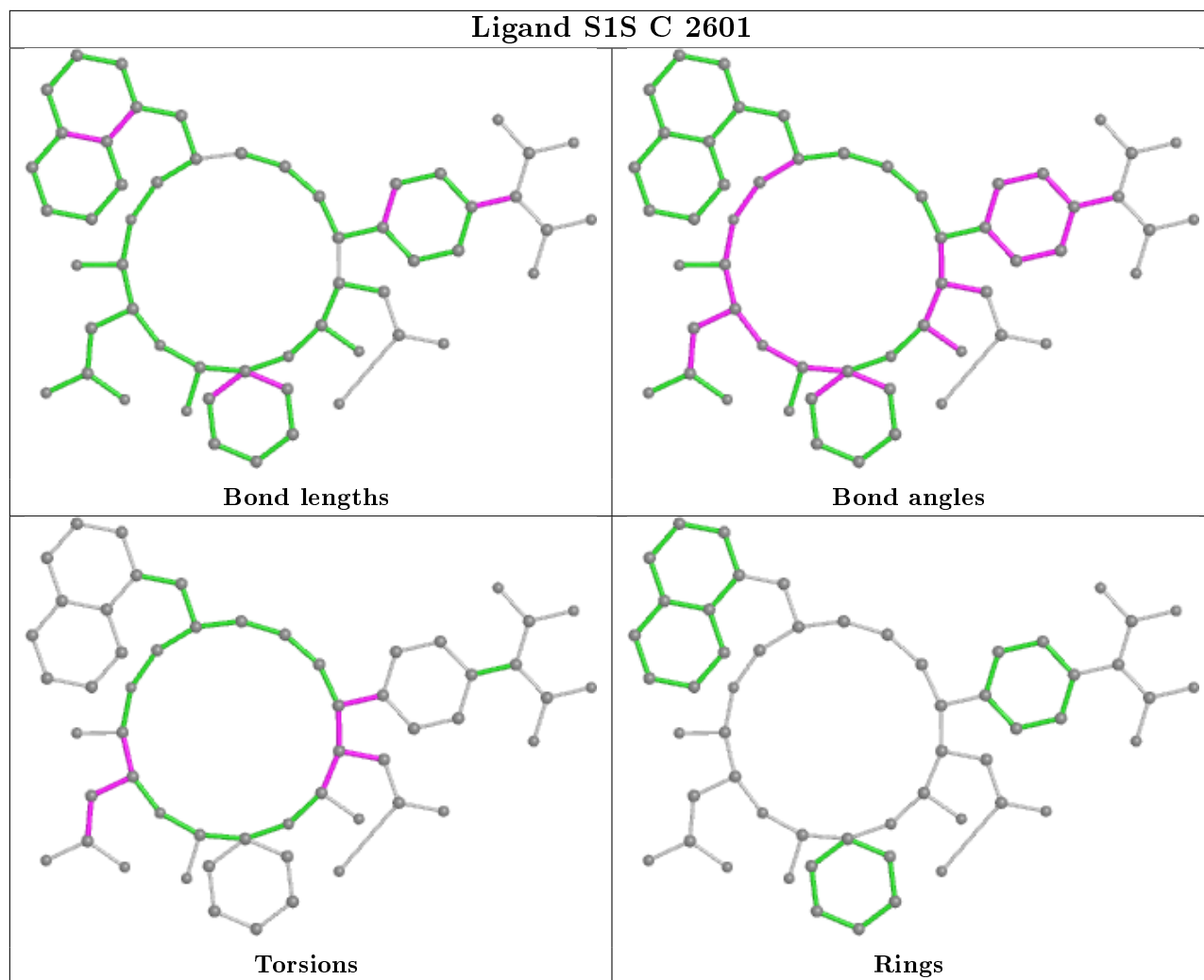


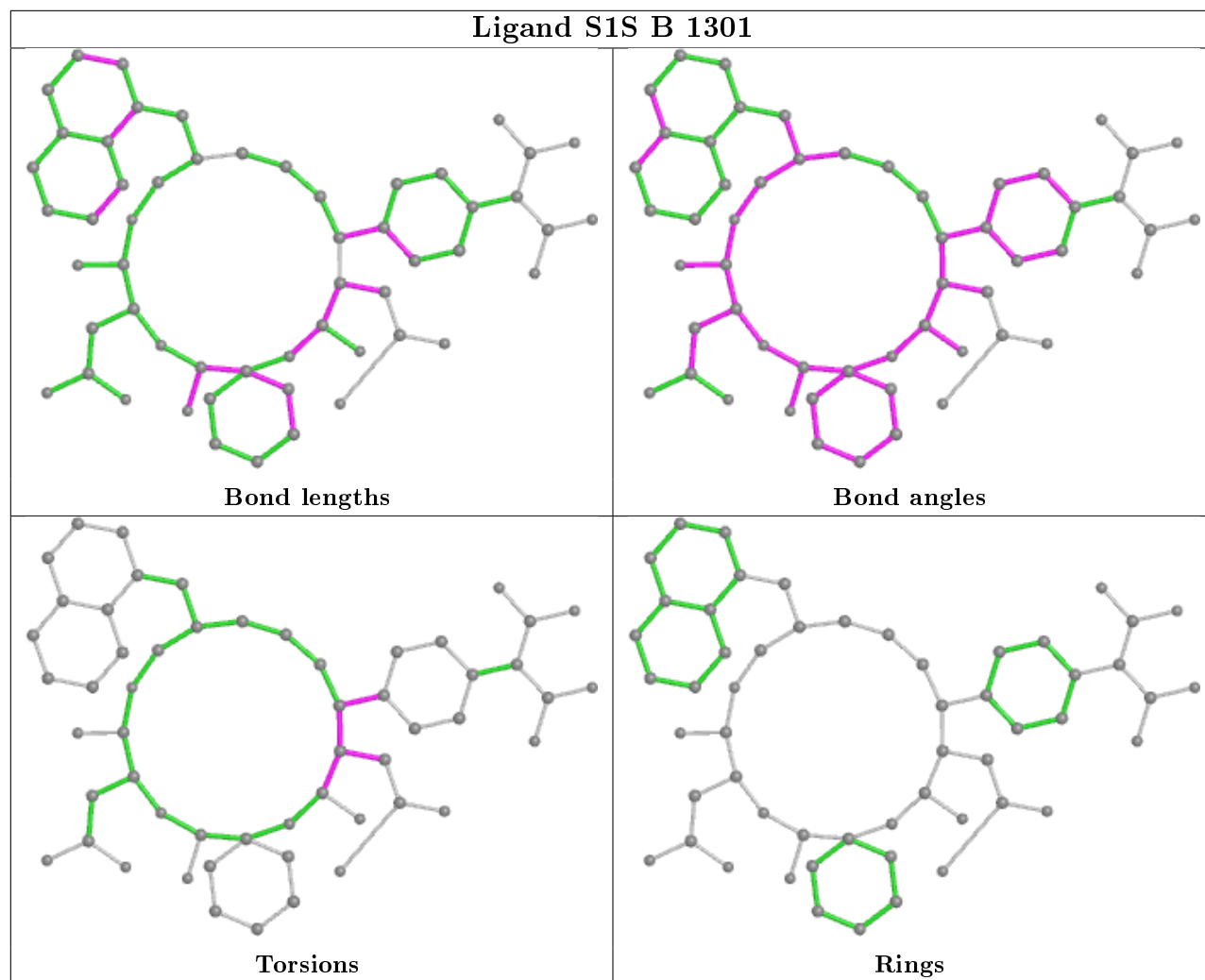


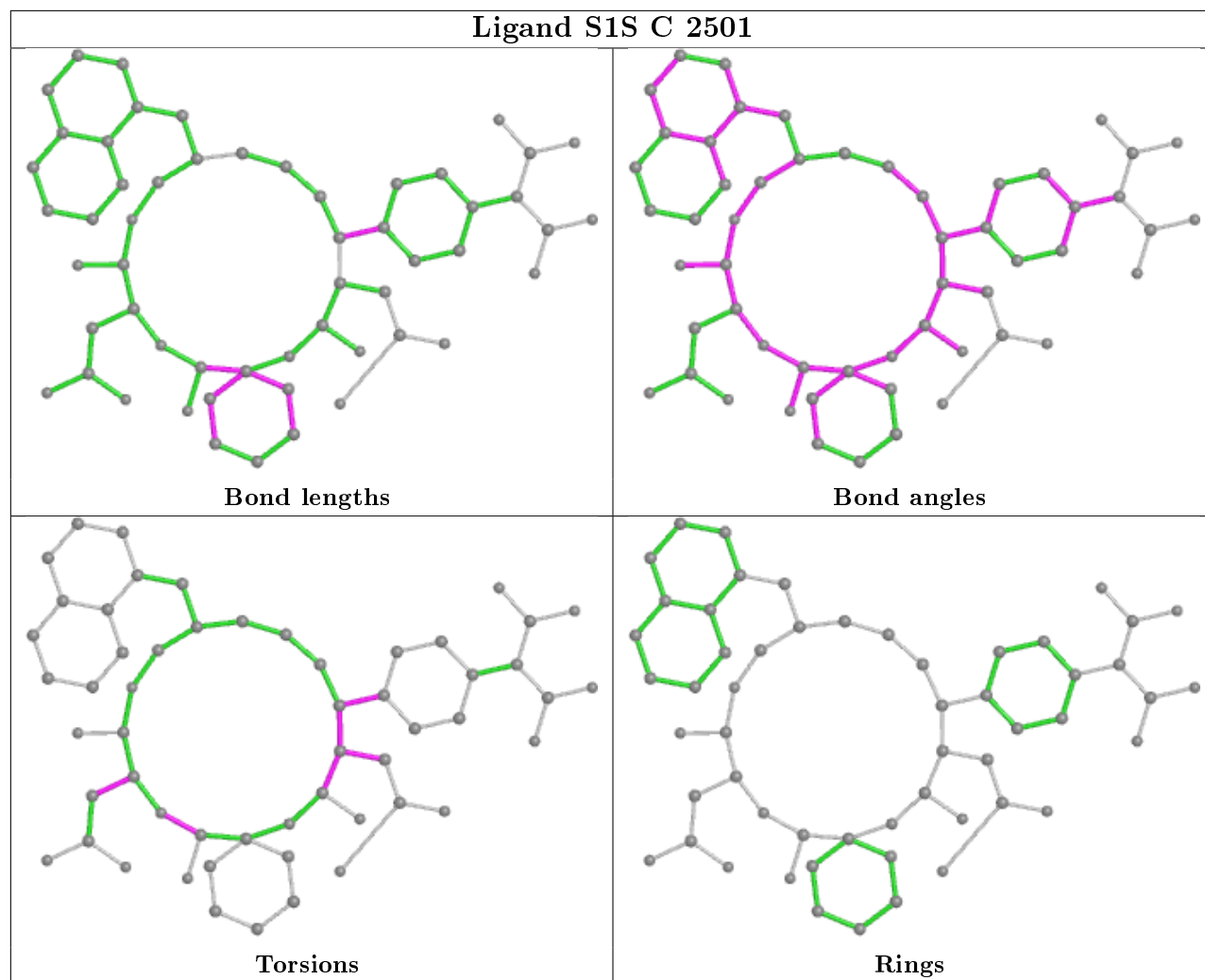


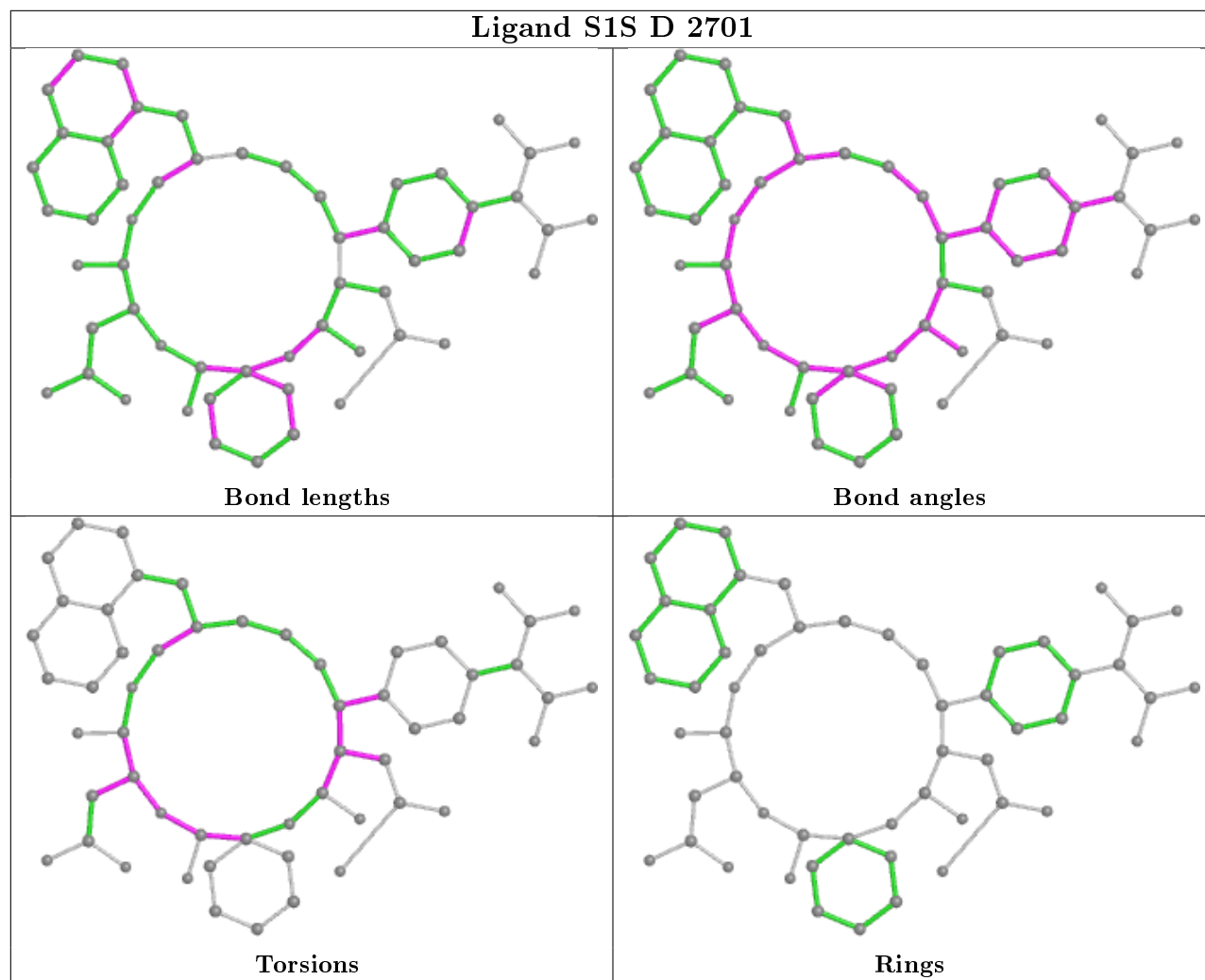


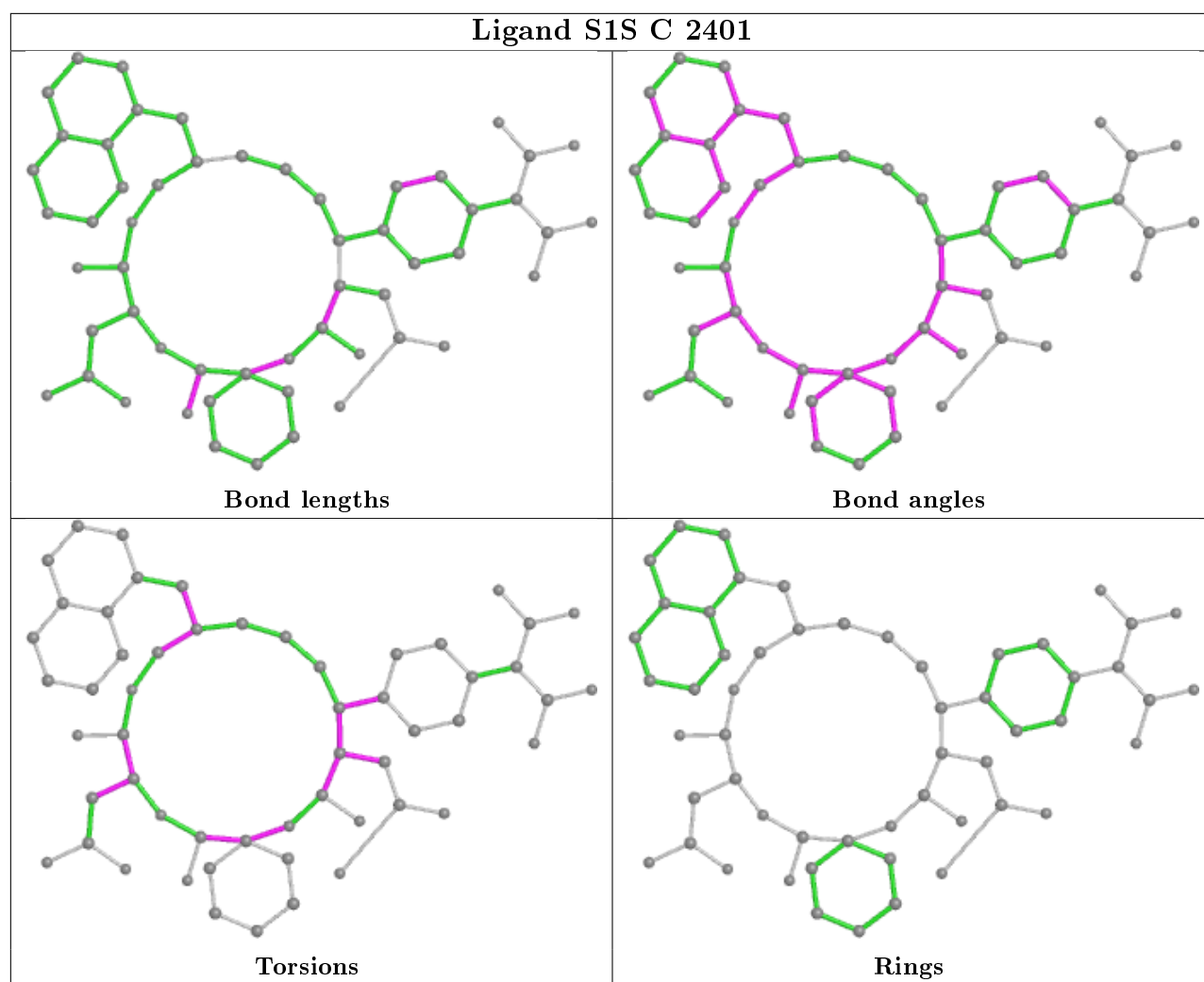












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	96/99 (96%)	1.00	16 (16%) <b>1</b> <b>1</b>	25, 33, 44, 53	0
1	B	93/99 (93%)	1.31	18 (19%) <b>1</b> <b>0</b>	23, 34, 45, 52	0
1	C	96/99 (96%)	0.98	14 (14%) <b>2</b> <b>1</b>	26, 33, 48, 52	0
1	D	93/99 (93%)	1.29	22 (23%) <b>0</b> <b>0</b>	25, 35, 54, 58	0
All	All	378/396 (95%)	1.14	70 (18%) <b>1</b> <b>0</b>	23, 33, 50, 58	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	SER	7.6
1	D	90	SER	5.6
1	B	68	ALA	4.8
1	D	68	ALA	4.6
1	B	89	GLU	4.5
1	B	128	LEU	4.3
1	A	85	ILE	4.3
1	D	66	PRO	4.2
1	D	65	ILE	4.2
1	C	85	ILE	4.2
1	A	97	LEU	4.1
1	B	103	ASN	4.1
1	D	103	ASN	4.0
1	D	128	LEU	3.9
1	B	91	ALA	3.7
1	D	91	ALA	3.7
1	B	131	LEU	3.7
1	C	97	LEU	3.7
1	D	87	GLU	3.7
1	B	66	PRO	3.6
1	C	92	PRO	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	84	LEU	3.4
1	B	151	ILE	3.4
1	A	131	LEU	3.4
1	B	97	LEU	3.3
1	B	132	VAL	3.3
1	D	64	LYS	3.2
1	C	78	ARG	3.2
1	D	89	GLU	3.2
1	C	110	VAL	3.1
1	D	131	LEU	3.0
1	B	61	PHE	3.0
1	D	70	ALA	3.0
1	B	148	LEU	2.9
1	C	61	PHE	2.9
1	A	110	VAL	2.8
1	C	131	LEU	2.8
1	A	140	VAL	2.8
1	C	132	VAL	2.8
1	B	65	ILE	2.8
1	D	93	GLY	2.8
1	B	93	GLY	2.7
1	D	97	LEU	2.6
1	C	104	ASP	2.6
1	D	132	VAL	2.5
1	B	75	SER	2.5
1	A	102	GLY	2.5
1	B	72	GLU	2.5
1	C	134	TYR	2.4
1	A	148	LEU	2.3
1	D	61	PHE	2.3
1	D	69	LYS	2.3
1	D	148	LEU	2.2
1	D	122	VAL	2.2
1	B	121	TRP	2.2
1	A	78	ARG	2.2
1	A	151	ILE	2.2
1	C	79	HIS	2.1
1	C	84	LEU	2.1
1	A	60	TRP	2.1
1	A	104	ASP	2.1
1	D	110	VAL	2.1
1	A	57	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	2.1
1	A	95	PHE	2.1
1	D	85	ILE	2.1
1	D	73	MET	2.0
1	C	123	VAL	2.0
1	C	101	PHE	2.0
1	A	145	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

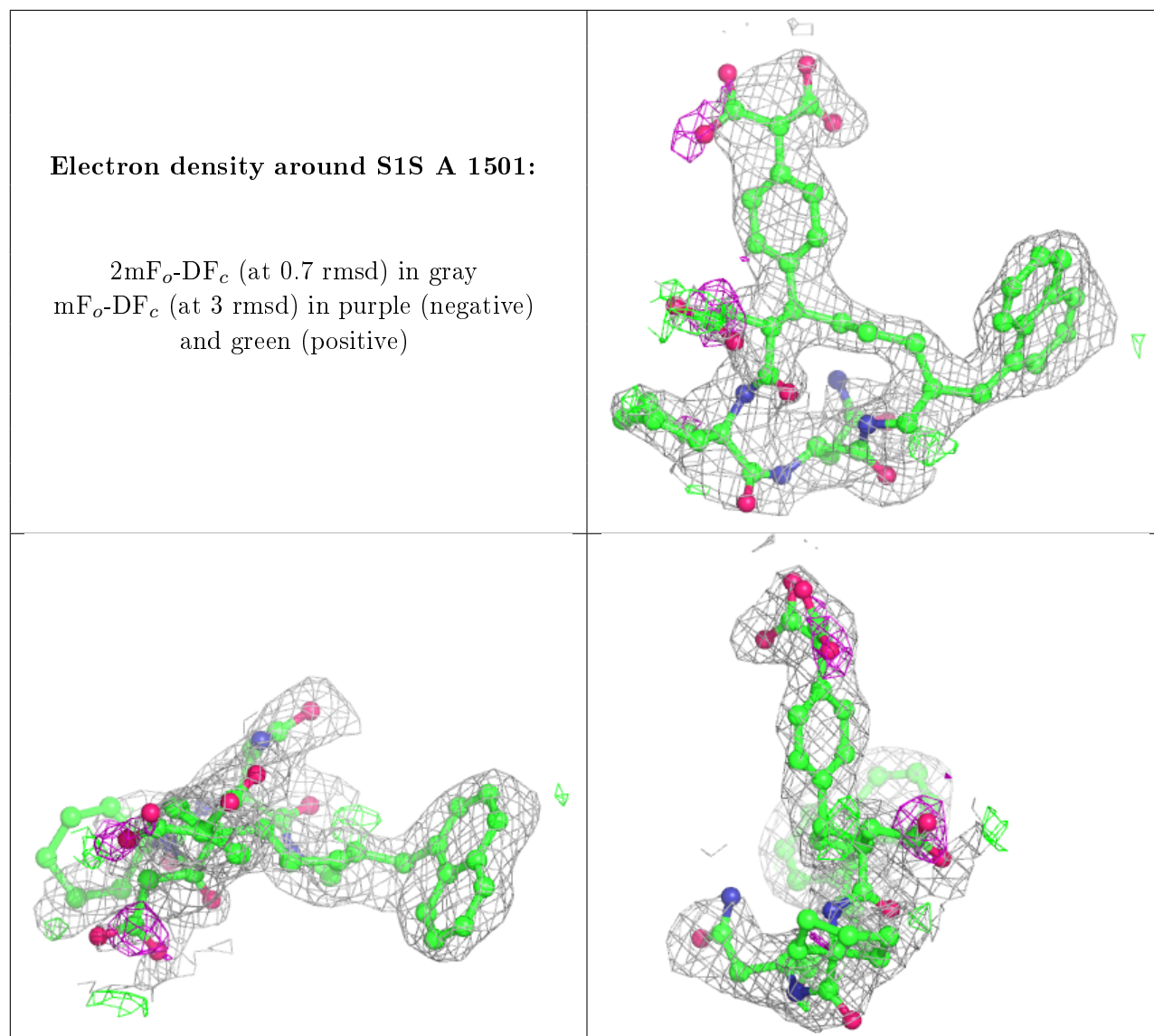
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

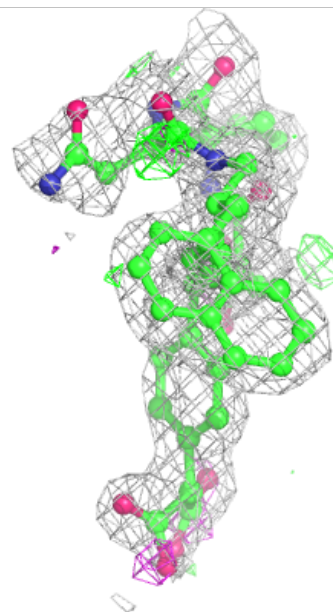
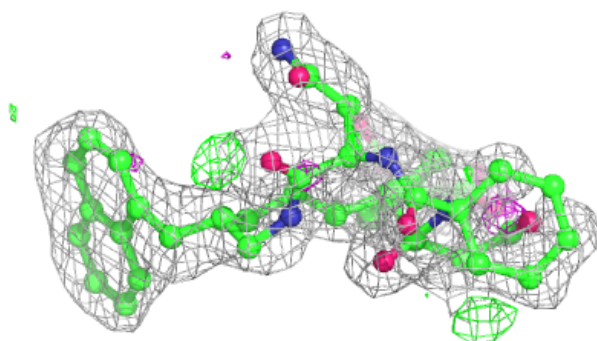
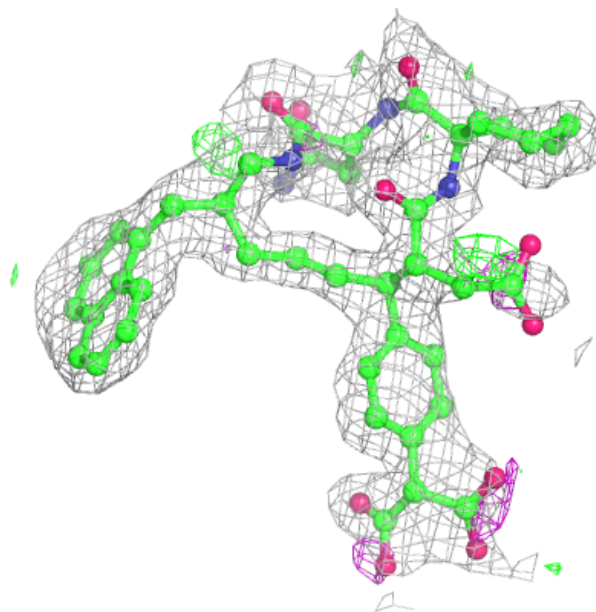
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	S1S	A	1501	55/55	0.79	0.21	35,53,61,61	0
2	S1S	C	2501	55/55	0.79	0.23	31,46,54,62	0
2	S1S	A	1701	55/55	0.80	0.20	21,33,54,56	0
2	S1S	D	2701	55/55	0.82	0.19	20,33,50,53	0
2	S1S	A	1601	55/55	0.86	0.17	19,29,47,55	0
2	S1S	C	2601	55/55	0.88	0.17	20,30,43,47	0
2	S1S	C	2201	55/55	0.89	0.12	22,29,34,35	0
2	S1S	A	1201	55/55	0.91	0.12	21,28,36,38	0
2	S1S	B	1301	55/55	0.91	0.11	16,23,41,47	0
2	S1S	A	1401	55/55	0.92	0.12	16,23,38,40	0
2	S1S	D	2301	55/55	0.92	0.12	15,24,46,50	0
2	S1S	C	2401	55/55	0.93	0.12	16,22,36,38	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.



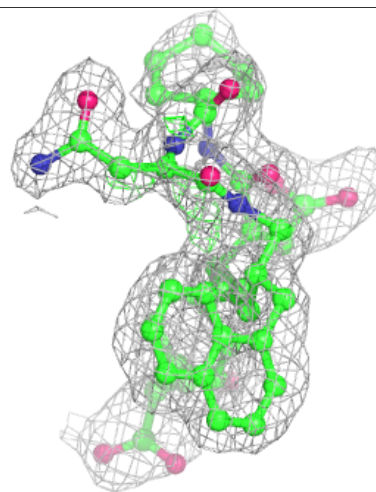
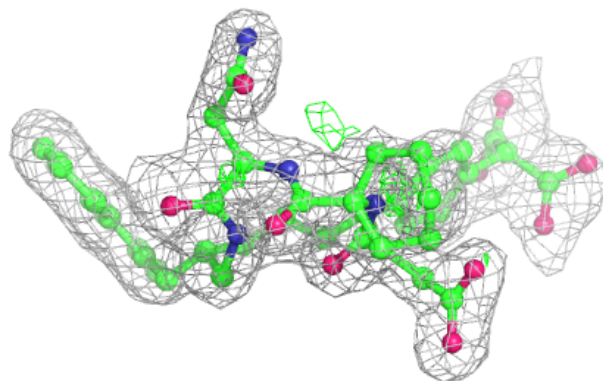
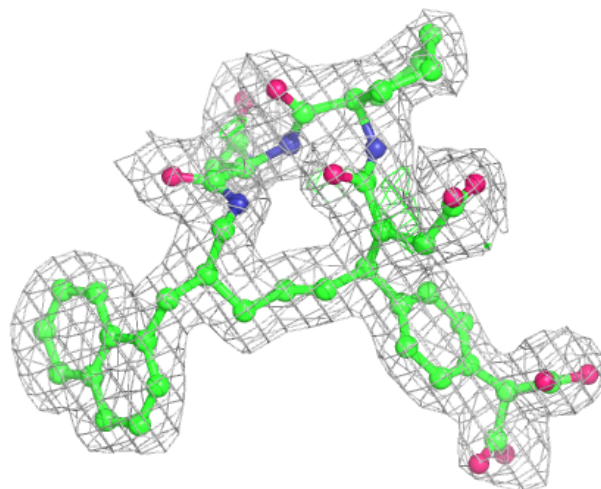
**Electron density around S1S C 2501:**

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



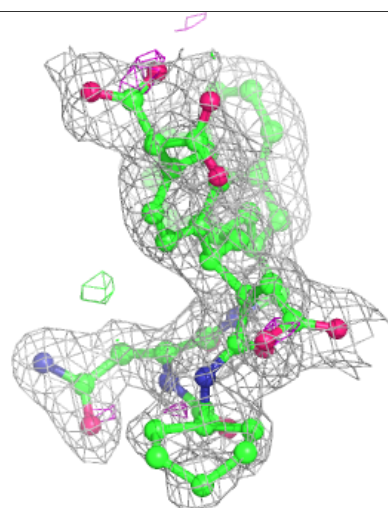
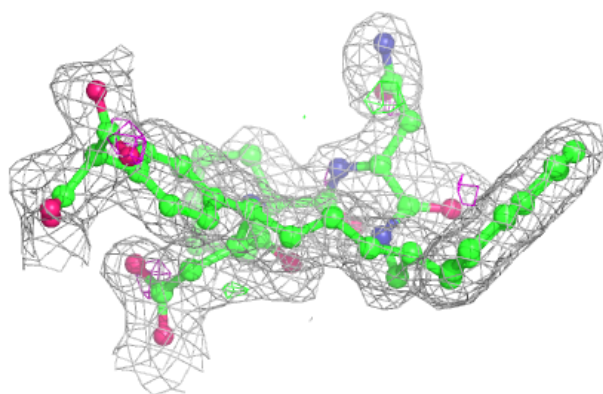
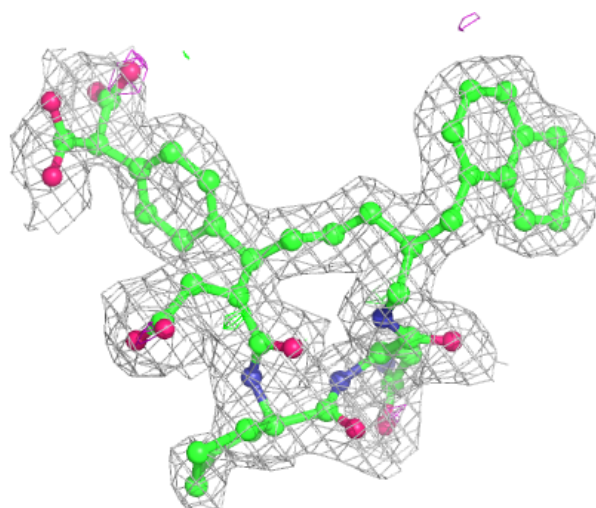
**Electron density around S1S A 1701:**

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

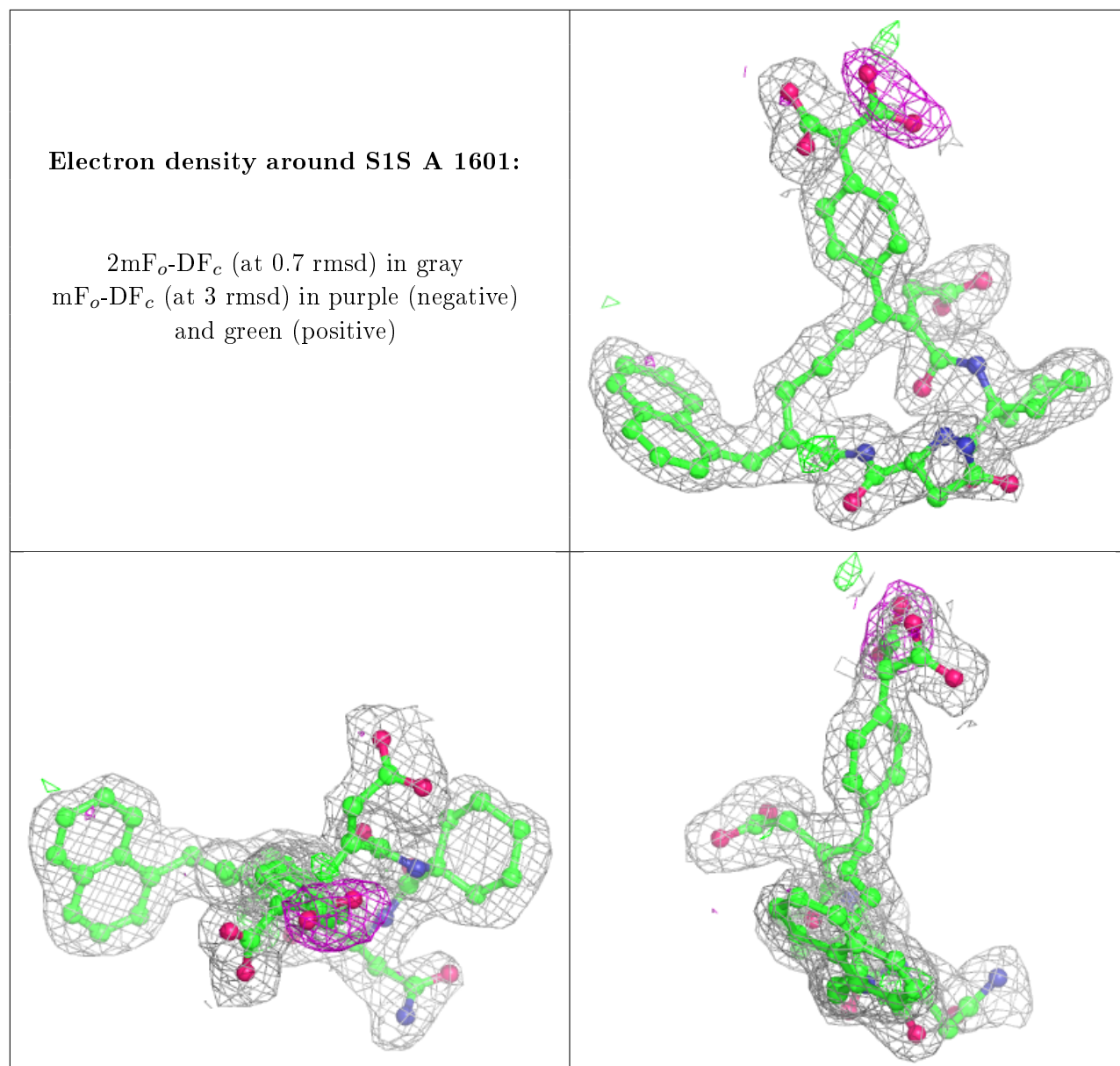


**Electron density around S1S D 2701:**

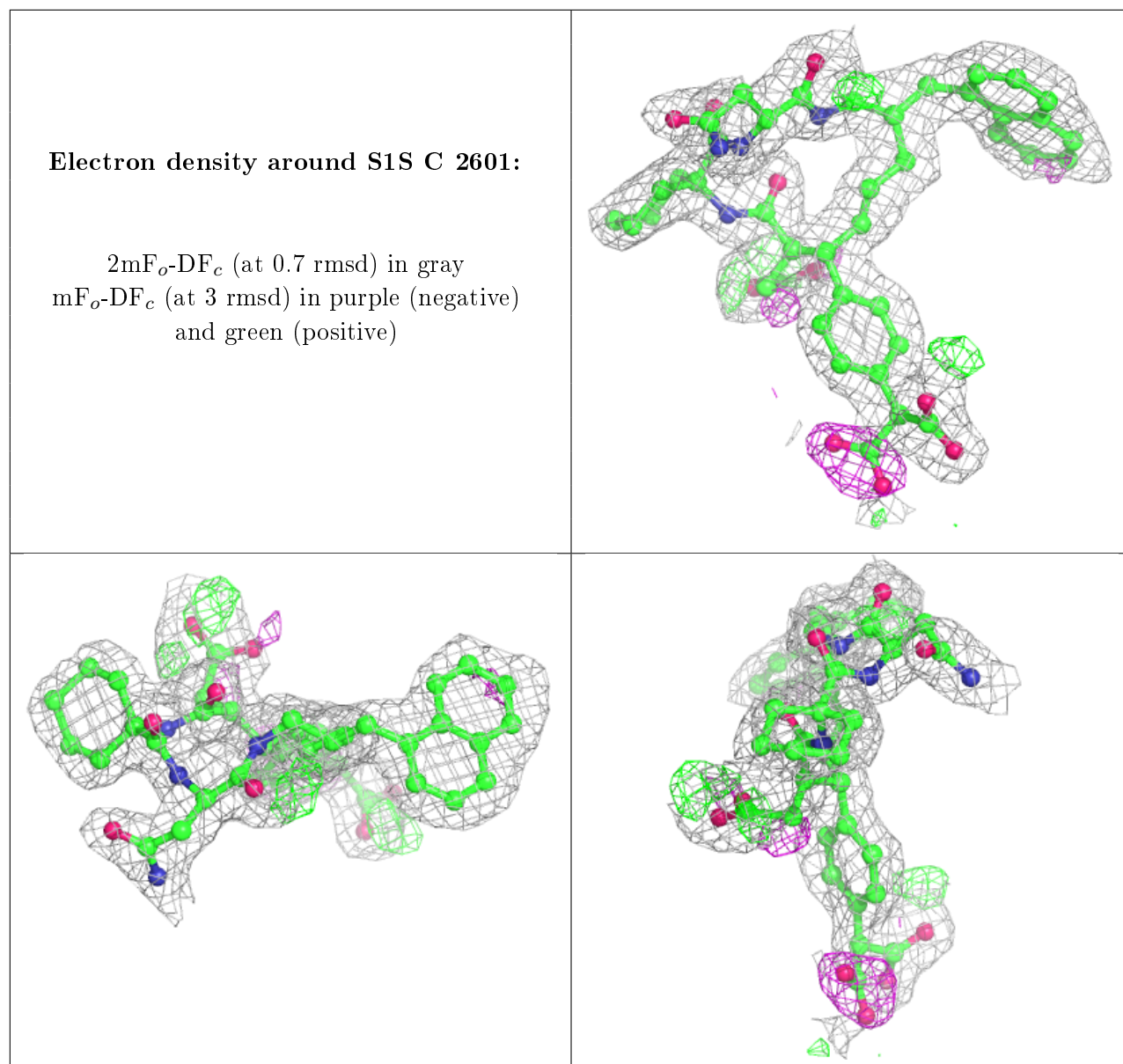
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

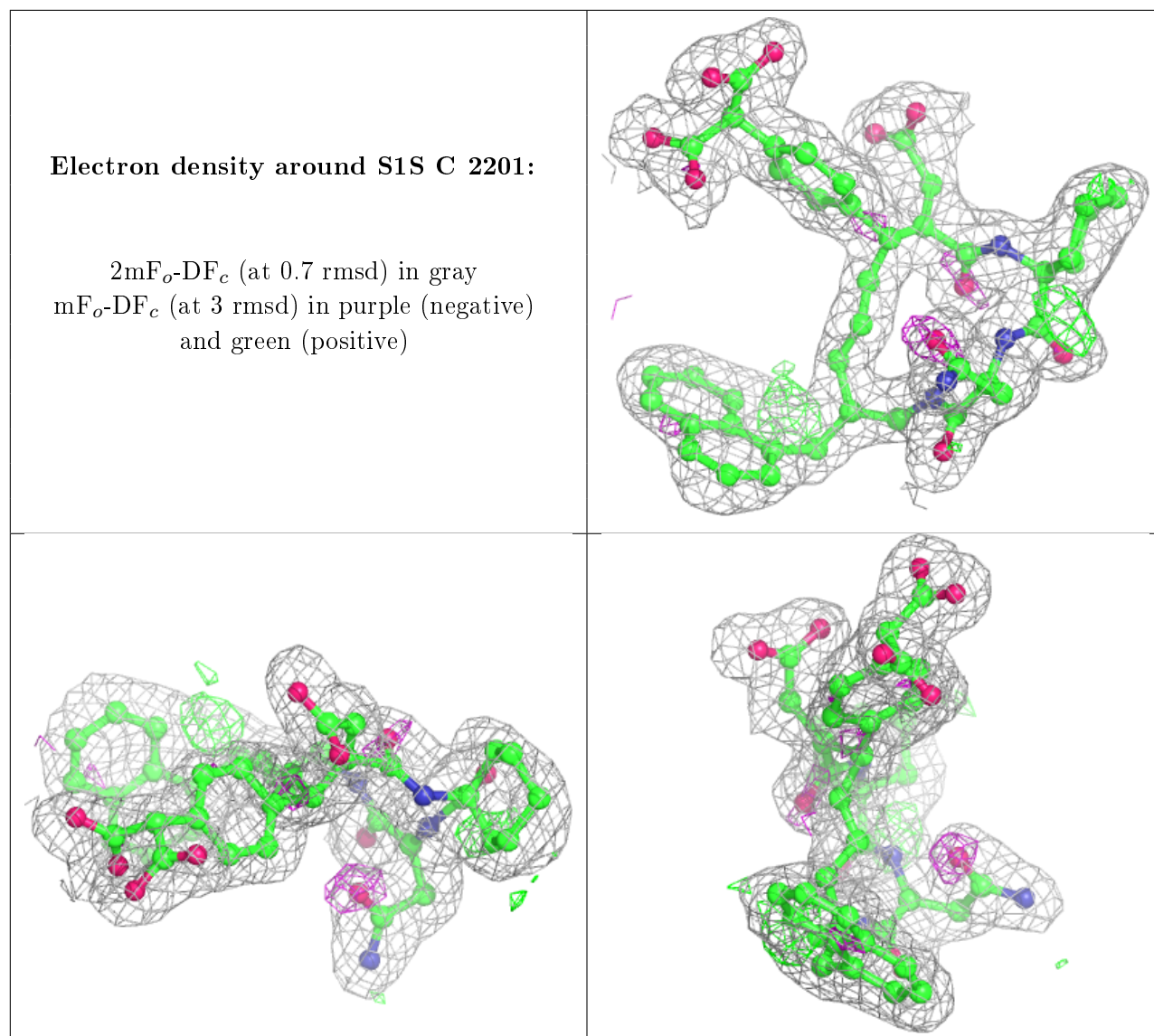






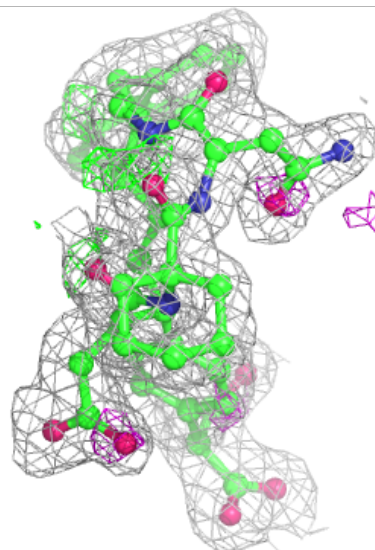
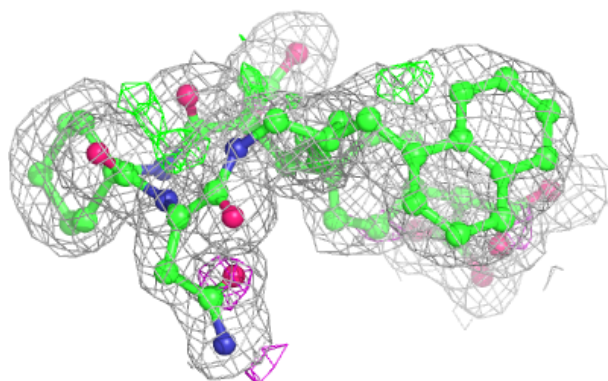
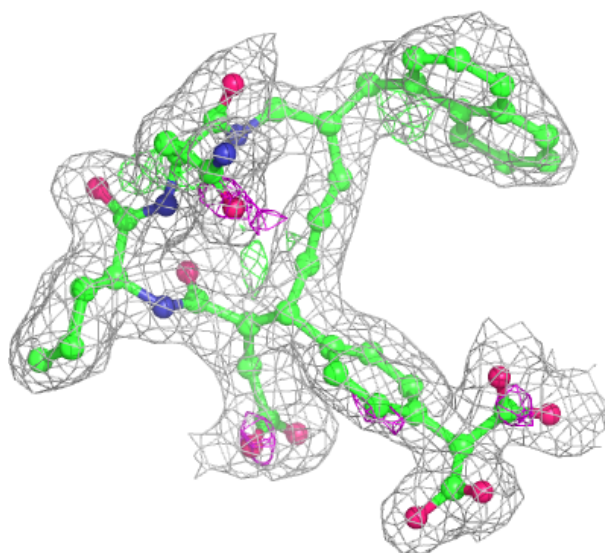






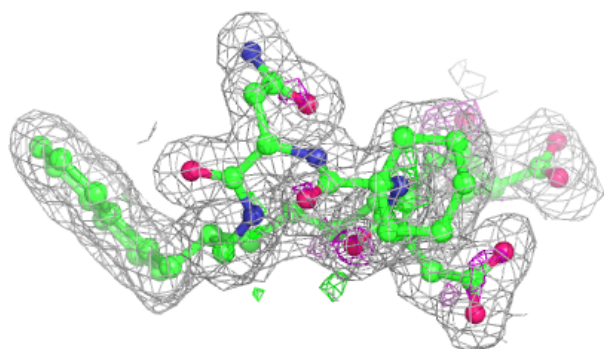
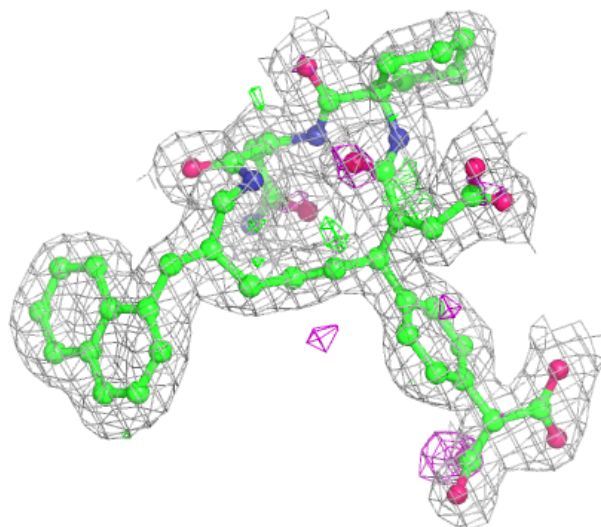
**Electron density around S1S A 1201:**

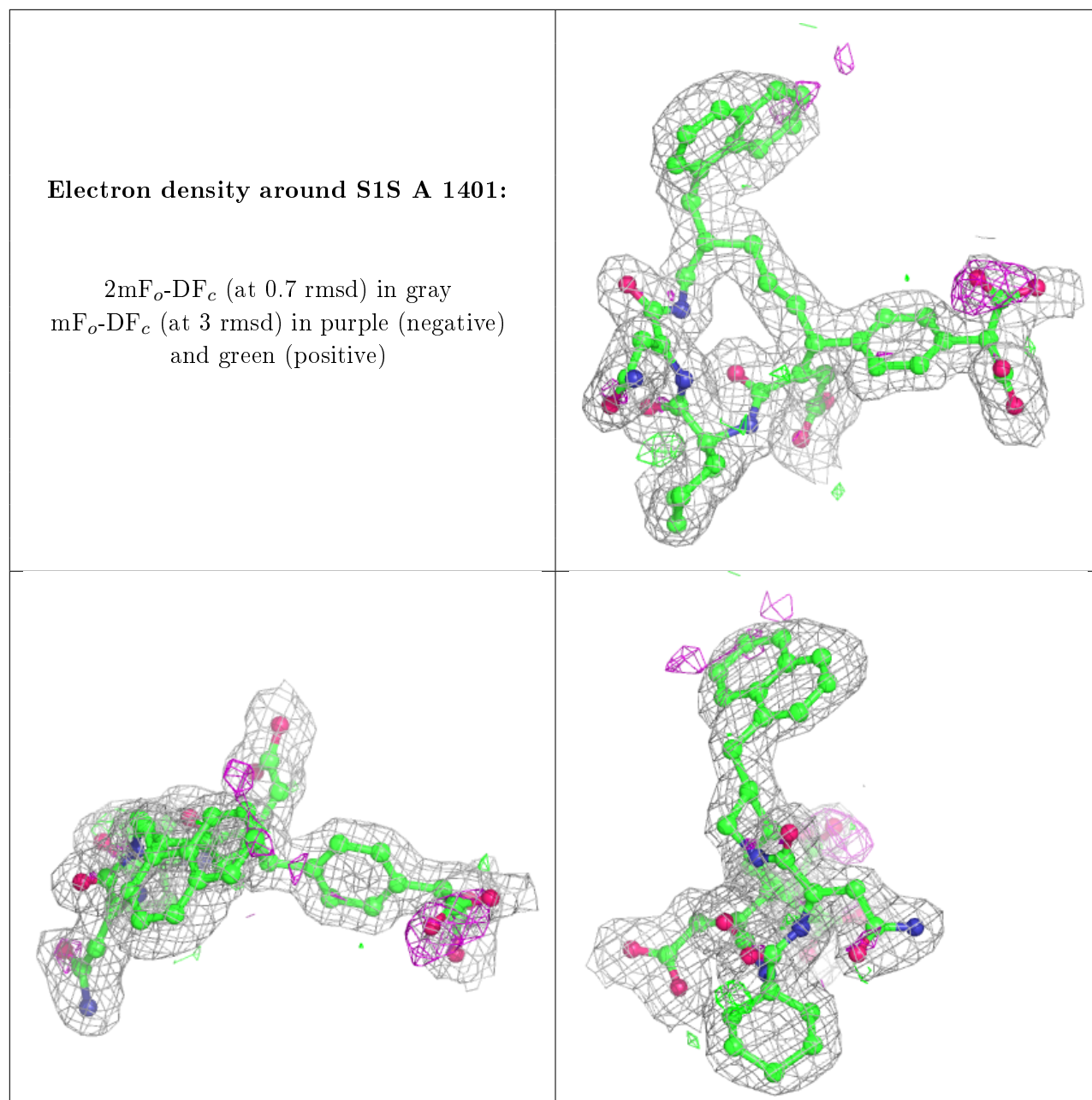
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around S1S B 1301:**

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

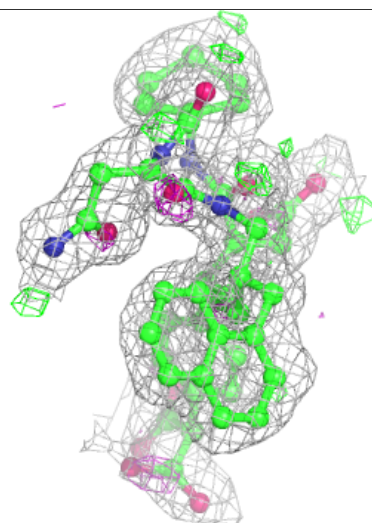
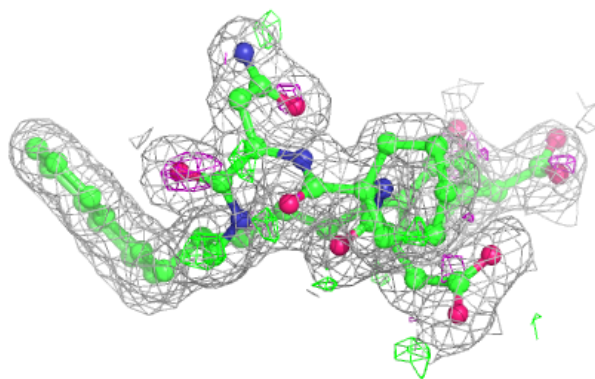
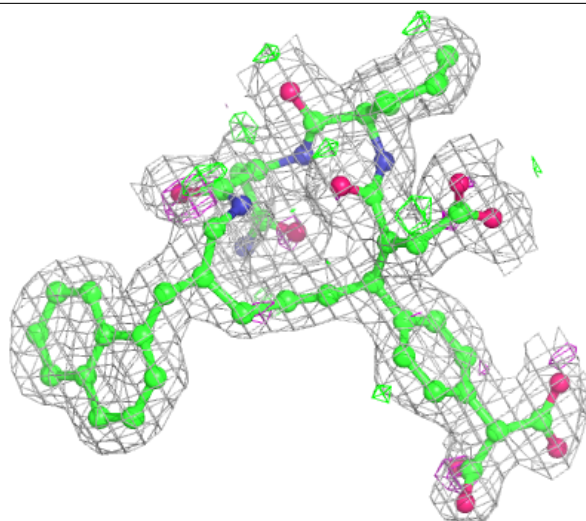


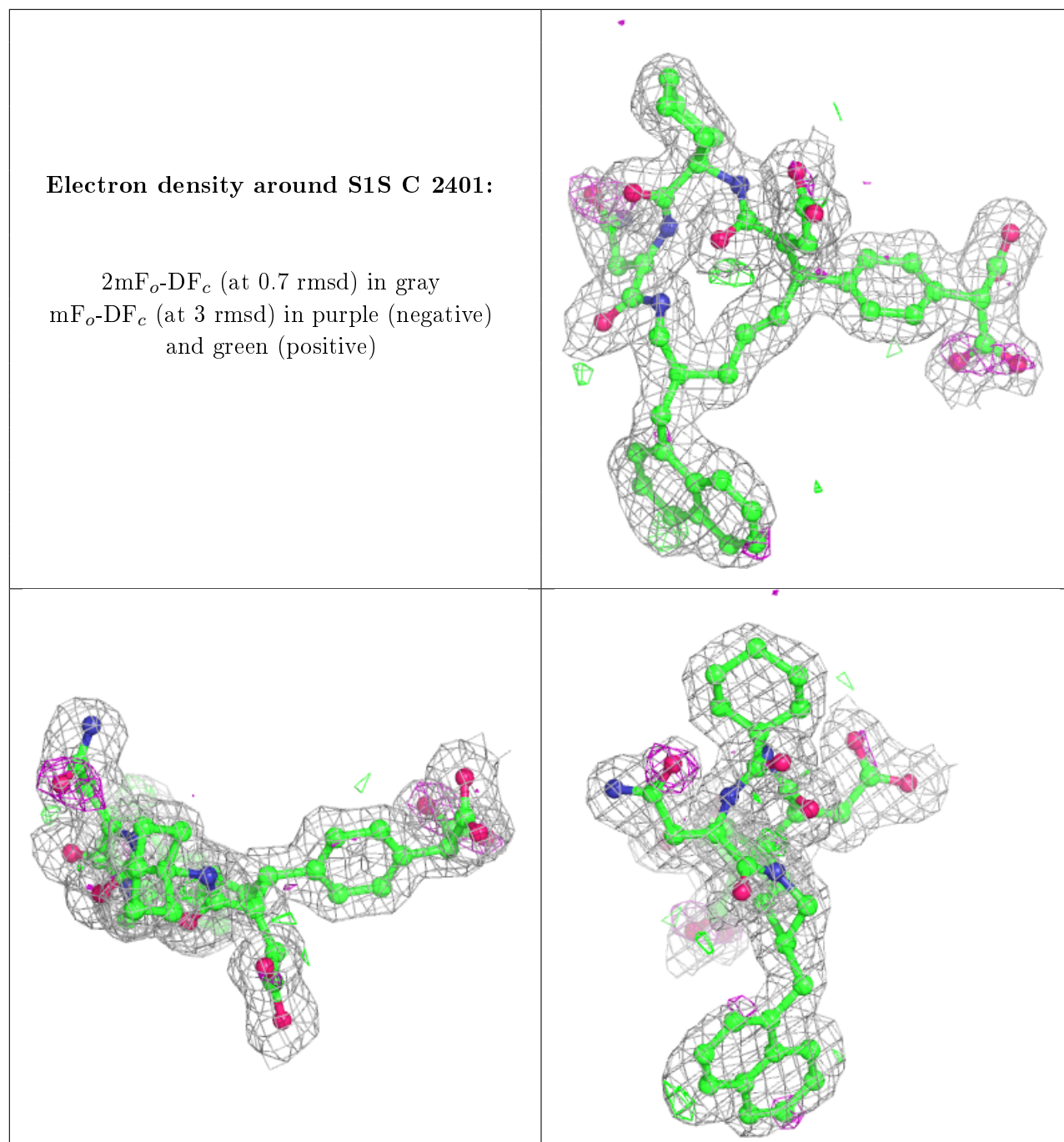




**Electron density around S1S D 2301:**

$2mF_o-DF_c$  (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.