



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 02:41 PM EDT

PDB ID : 2VAX
Title : Crystal structure of deacetylcephalosporin C acetyltransferase (Cephalosporin C-soak)
Authors : Lejon, S.; Ellis, J.; Valegard, K.
Deposited on : 2007-09-04
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

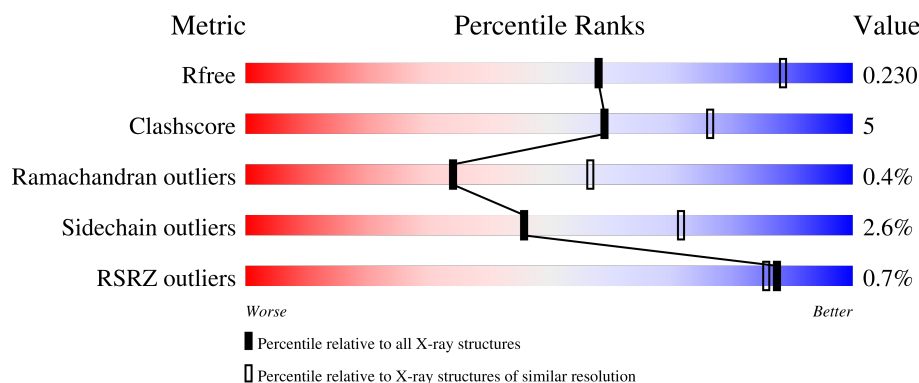
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>11%</div> <div>22%</div> </div> </div>
1	B	444	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>9%</div> <div>21%</div> </div> </div>
1	C	444	<div> <div></div> <div> <div></div> <div>68%</div> <div>10%</div> <div>22%</div> </div> </div>
1	D	444	<div> <div></div> <div> <div></div> <div>68%</div> <div>8%</div> <div>22%</div> </div> </div>
1	E	444	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>8%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	
1	K	444	
1	L	444	

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
2	CSC	A	1383	X	-	-	-
2	CSC	B	1384	X	-	-	-
2	CSC	C	1383	X	-	-	-
2	CSC	D	1383	X	-	-	-
2	CSC	E	1383	X	-	-	-
2	CSC	F	1384	X	-	-	-
2	CSC	G	1383	X	-	-	-
2	CSC	H	1383	X	-	-	-
2	CSC	I	1384	X	-	-	-
2	CSC	J	1385	X	-	-	-
2	CSC	K	1385	X	-	-	-
2	CSC	L	1383	X	-	-	-
3	ACT	C	1384	-	-	X	-
3	ACT	L	1384	-	-	X	-

2 Entry composition

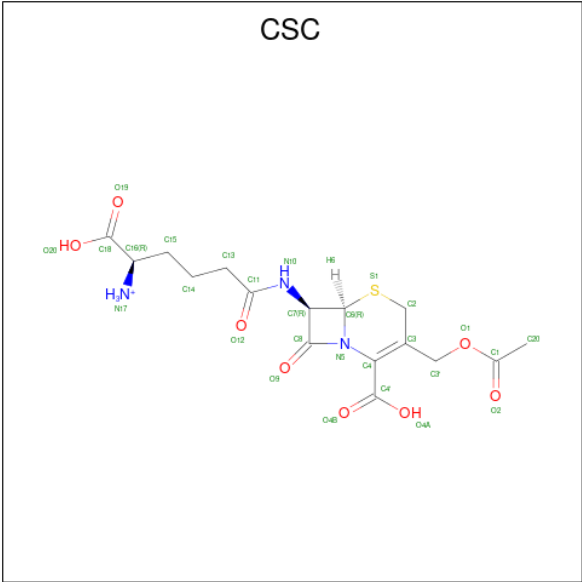
There are 4 unique types of molecules in this entry. The entry contains 33330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE.

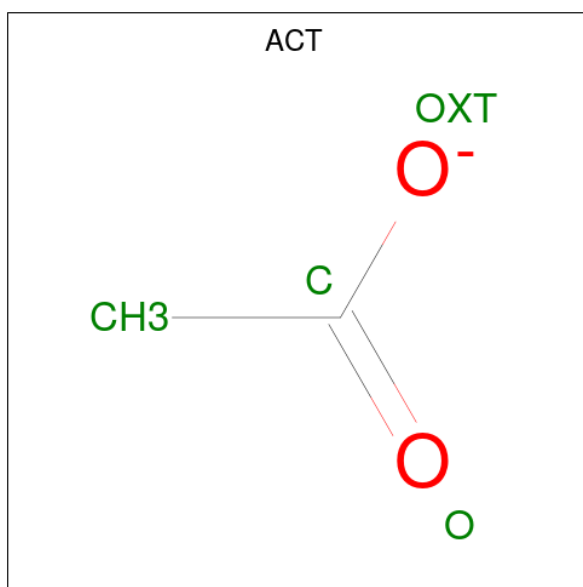
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	3	0
			2739	1728	485	507	19			
1	B	349	Total	C	N	O	S	0	3	0
			2750	1734	487	510	19			
1	C	348	Total	C	N	O	S	0	6	0
			2770	1746	492	513	19			
1	D	345	Total	C	N	O	S	0	4	0
			2742	1730	487	506	19			
1	E	346	Total	C	N	O	S	0	4	0
			2728	1722	481	506	19			
1	F	342	Total	C	N	O	S	0	1	1
			2699	1703	474	503	19			
1	G	342	Total	C	N	O	S	0	6	0
			2726	1720	483	504	19			
1	H	342	Total	C	N	O	S	0	5	0
			2728	1721	486	502	19			
1	I	349	Total	C	N	O	S	0	3	0
			2766	1744	493	510	19			
1	J	344	Total	C	N	O	S	0	1	0
			2719	1716	479	505	19			
1	K	344	Total	C	N	O	S	0	1	0
			2719	1716	479	505	19			
1	L	341	Total	C	N	O	S	0	2	0
			2697	1702	473	503	19			

- Molecule 2 is 4-(3-ACETOXYMETHYL-2-CARBOXY-8-OXO-5-THIA-1-AZA-BICYCLO [4.2.0]OCT-2-EN-7-YLCARBAMOYL)-1-CARBOXY-BUTYL-AMMONIUM (three-letter code: CSC) (formula: C₁₆H₂₂N₃O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	B	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	C	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	D	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	E	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	F	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	G	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	H	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	I	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	J	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	K	1	Total	C	N	O	S	0	0
			25	14	3	7	1		
2	L	1	Total	C	N	O	S	0	0
			25	14	3	7	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	21	Total O 21 21	0	0
4	B	23	Total O 23 23	0	0

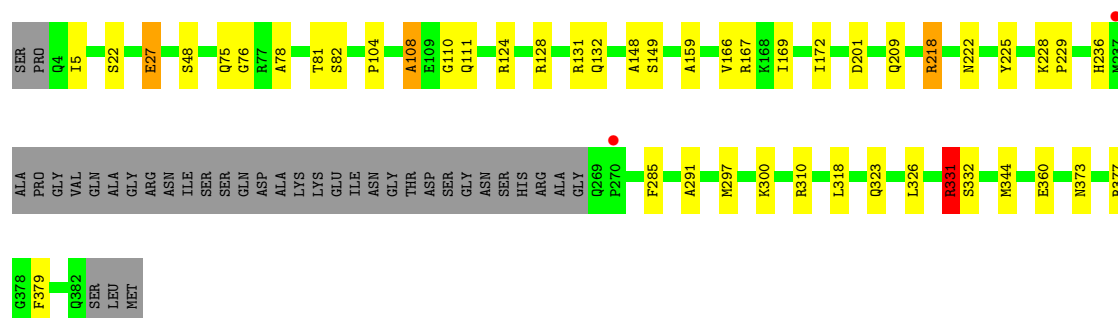
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	22	Total 22	O 22	0	0
4	D	20	Total 20	O 20	0	0
4	E	15	Total 15	O 15	0	0
4	F	13	Total 13	O 13	0	0
4	G	21	Total 21	O 21	0	0
4	H	23	Total 23	O 23	0	0
4	I	24	Total 24	O 24	0	0
4	J	7	Total 7	O 7	0	0
4	K	6	Total 6	O 6	0	0
4	L	12	Total 12	O 12	0	0

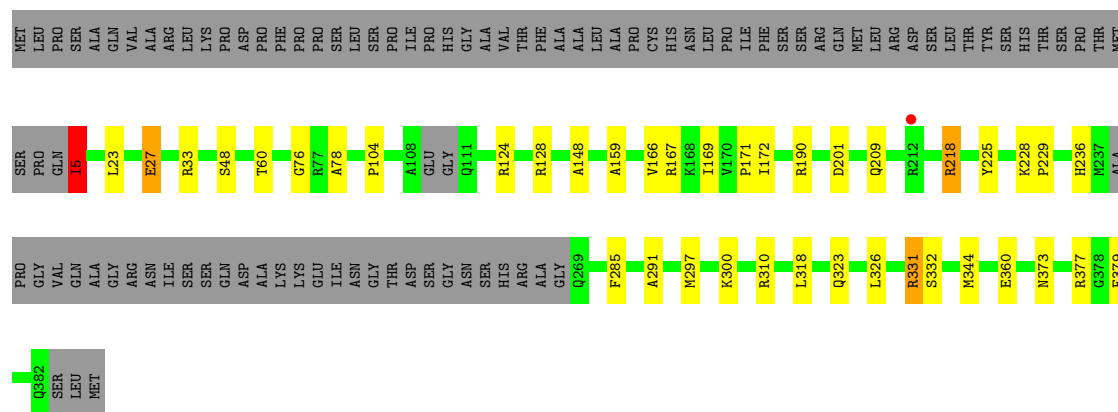
● Molecule 1: ACETYL-CoA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE





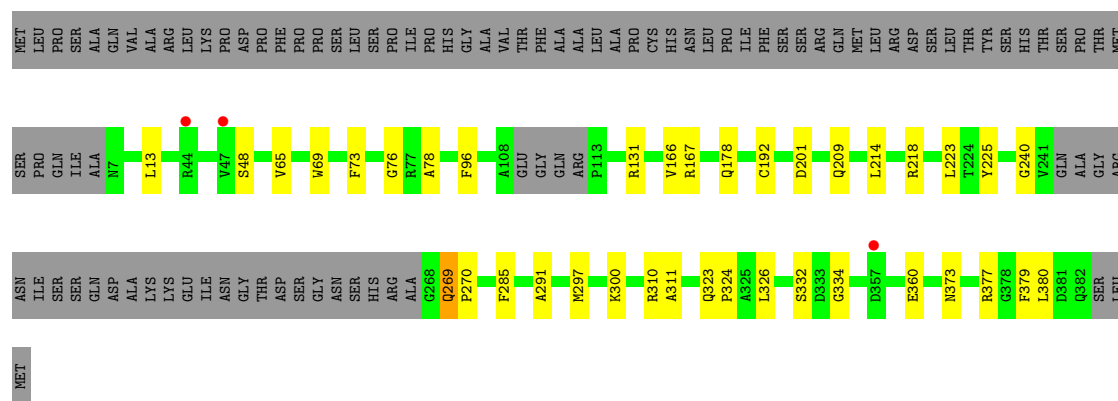
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain D: 68% 8% 22%



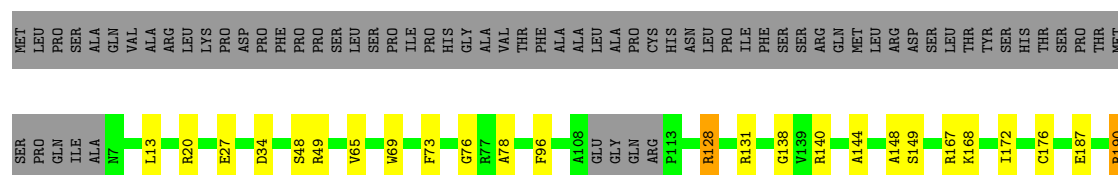
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

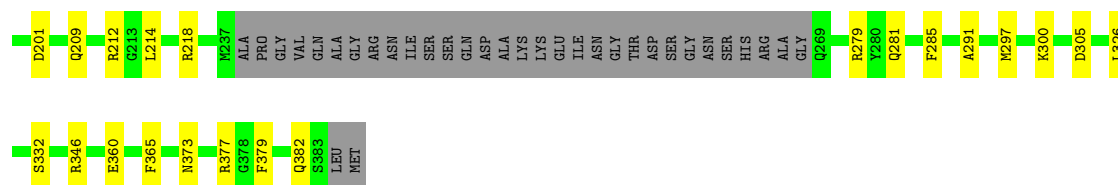
Chain E: 69% 8% 22%



● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

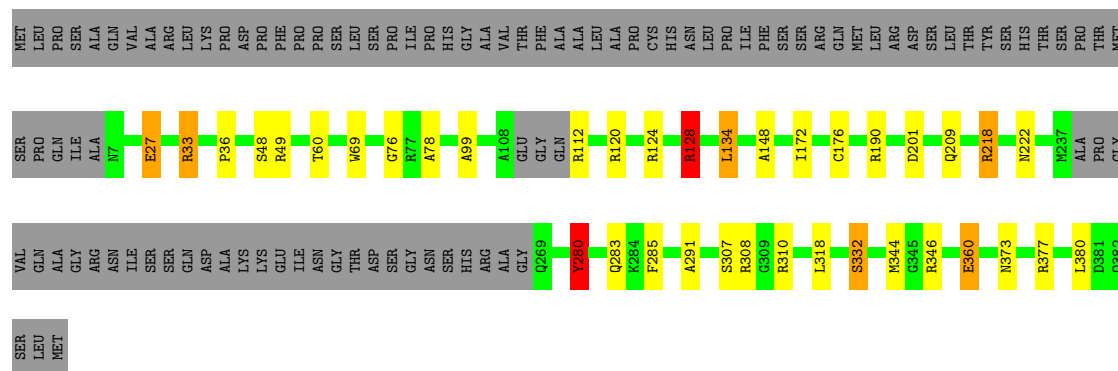
Chain F: 67% 10% 23%





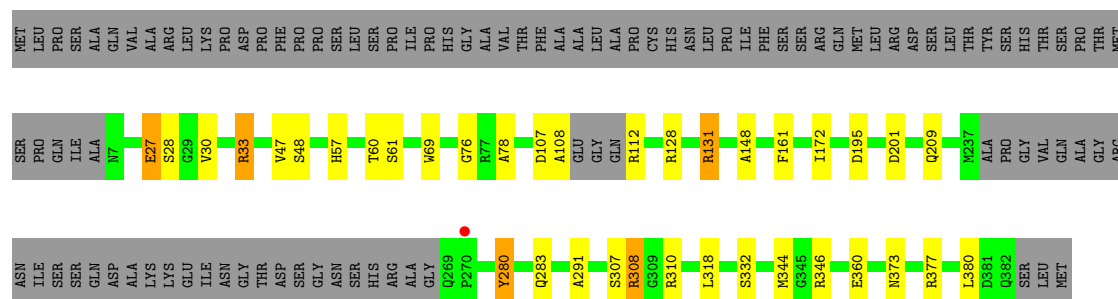
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain G: 68% 7% 23%



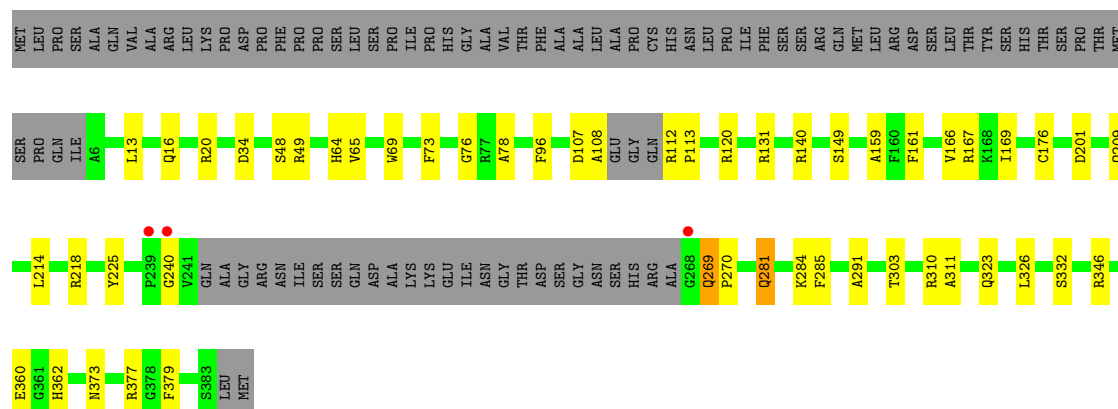
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain H: 69% 7% 23%

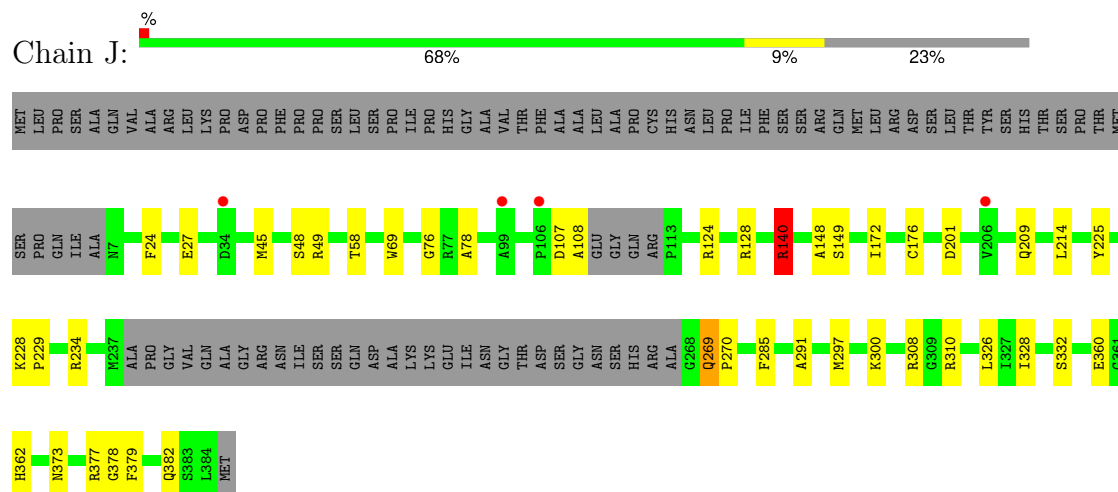


• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

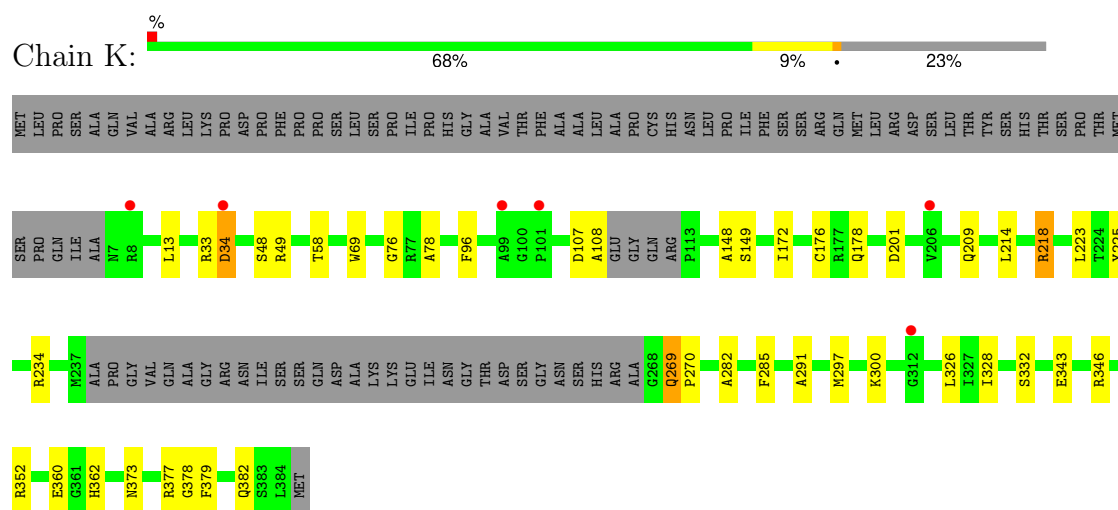
Chain I: 67% 11% 21%



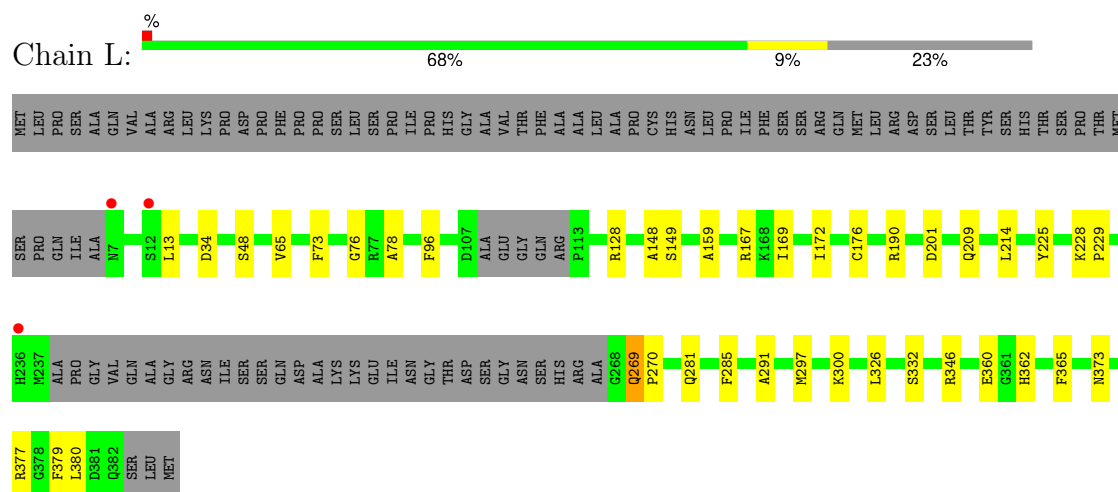
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.36Å 109.29Å 195.39Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	62.75 – 2.60 62.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.75-2.60) 99.6 (62.46-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.240 0.205 , 0.230	Depositor DCC
R_{free} test set	3414 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 7.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33330	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, OAS, CSC

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	0.85	1/2798 (0.0%)	0.92	8/3791 (0.2%)
1	B	0.82	2/2809 (0.1%)	0.97	7/3806 (0.2%)
1	C	0.81	0/2835	0.85	9/3840 (0.2%)
1	D	0.82	0/2803	0.95	11/3796 (0.3%)
1	E	0.84	1/2787 (0.0%)	0.80	5/3776 (0.1%)
1	F	0.89	2/2757 (0.1%)	0.95	8/3736 (0.2%)
1	G	0.85	3/2790 (0.1%)	0.86	8/3778 (0.2%)
1	H	0.84	3/2792 (0.1%)	0.86	6/3780 (0.2%)
1	I	0.84	2/2831 (0.1%)	0.81	4/3834 (0.1%)
1	J	0.90	1/2777 (0.0%)	0.86	4/3761 (0.1%)
1	K	0.90	1/2777 (0.0%)	0.84	1/3761 (0.0%)
1	L	0.85	1/2755 (0.0%)	0.82	4/3732 (0.1%)
All	All	0.85	17/33511 (0.1%)	0.87	75/45391 (0.2%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	360	GLU	C-O	-9.81	1.04	1.23
1	B	360	GLU	C-O	-9.49	1.05	1.23
1	I	360	GLU	C-O	-9.47	1.05	1.23
1	H	360	GLU	C-O	-9.30	1.05	1.23
1	L	176	CYS	CB-SG	-7.98	1.68	1.82

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ARG	NE-CZ-NH2	-21.88	109.36	120.30
1	B	8	ARG	NE-CZ-NH1	21.51	131.05	120.30
1	F	190	ARG	NE-CZ-NH2	-19.76	110.42	120.30
1	D	310	ARG	NE-CZ-NH2	17.52	129.06	120.30
1	D	310	ARG	NE-CZ-NH1	-17.29	111.66	120.30

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	2739	0	2649	27	0
1	B	2750	0	2658	25	0
1	C	2770	0	2682	35	0
1	D	2742	0	2658	25	0
1	E	2728	0	2634	22	0
1	F	2699	0	2605	25	0
1	G	2726	0	2638	22	1
1	H	2728	0	2647	26	1
1	I	2766	0	2689	30	0
1	J	2719	0	2633	24	1
1	K	2719	0	2633	29	1
1	L	2697	0	2601	18	0
2	A	25	0	16	3	0
2	B	25	0	16	2	0
2	C	25	0	17	4	0
2	D	25	0	16	3	0
2	E	25	0	16	2	0
2	F	25	0	17	3	0
2	G	25	0	16	4	0
2	H	25	0	15	3	0
2	I	25	0	16	0	0
2	J	25	0	16	3	0
2	K	25	0	15	4	0
2	L	25	0	17	2	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	2	0
3	D	4	0	3	1	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
3	I	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	4	0	3	3	0
4	A	21	0	0	1	0
4	B	23	0	0	0	0
4	C	22	0	0	0	0
4	D	20	0	0	0	0
4	E	15	0	0	1	0
4	F	13	0	0	1	0
4	G	21	0	0	2	0
4	H	23	0	0	1	0
4	I	24	0	0	0	0
4	J	7	0	0	0	0
4	K	6	0	0	0	0
4	L	12	0	0	0	0
All	All	33330	0	31950	306	2

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 5.

The worst 5 of 306 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:C:75[B]:GLN:HE21	1:F:131:ARG:NH2	1.44	1.16
1:H:108:ALA:HB1	1:H:112:ARG:NH2	1.76	1.00
1:C:75[B]:GLN:NE2	1:F:131:ARG:NH2	2.13	0.97
1:G:33[A]:ARG:HH21	1:G:33[A]:ARG:HG2	1.37	0.88
1:H:108:ALA:HB1	1:H:112:ARG:HH21	1.38	0.88

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:GLN:NE2	1:J:49:ARG:NH2[1_556]	2.09	0.11
1:H:283:GLN:NE2	1:K:49:ARG:NH2[2_655]	2.10	0.10

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	341/444 (77%)	324 (95%)	15 (4%)	2 (1%)	25	47
1	B	343/444 (77%)	331 (96%)	10 (3%)	2 (1%)	25	47
1	C	346/444 (78%)	333 (96%)	12 (4%)	1 (0%)	41	64
1	D	340/444 (77%)	328 (96%)	12 (4%)	0	100	100
1	E	340/444 (77%)	323 (95%)	16 (5%)	1 (0%)	41	64
1	F	336/444 (76%)	323 (96%)	12 (4%)	1 (0%)	41	64
1	G	338/444 (76%)	322 (95%)	15 (4%)	1 (0%)	41	64
1	H	338/444 (76%)	323 (96%)	14 (4%)	1 (0%)	41	64
1	I	345/444 (78%)	333 (96%)	10 (3%)	2 (1%)	25	47
1	J	338/444 (76%)	321 (95%)	16 (5%)	1 (0%)	41	64
1	K	338/444 (76%)	320 (95%)	16 (5%)	2 (1%)	25	47
1	L	335/444 (76%)	324 (97%)	10 (3%)	1 (0%)	41	64
All	All	4078/5328 (76%)	3905 (96%)	158 (4%)	15 (0%)	34	57

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	269	GLN
1	C	108	ALA
1	E	269	GLN
1	I	269	GLN

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	290/371 (78%)	281 (97%)	9 (3%)	40	66
1	B	291/371 (78%)	283 (97%)	8 (3%)	44	71
1	C	294/371 (79%)	286 (97%)	8 (3%)	44	71
1	D	291/371 (78%)	285 (98%)	6 (2%)	53	77
1	E	289/371 (78%)	282 (98%)	7 (2%)	49	74
1	F	287/371 (77%)	277 (96%)	10 (4%)	36	62
1	G	290/371 (78%)	276 (95%)	14 (5%)	25	49
1	H	290/371 (78%)	280 (97%)	10 (3%)	37	63
1	I	293/371 (79%)	287 (98%)	6 (2%)	55	78
1	J	289/371 (78%)	283 (98%)	6 (2%)	53	77
1	K	289/371 (78%)	284 (98%)	5 (2%)	60	81
1	L	287/371 (77%)	279 (97%)	8 (3%)	43	69
All	All	3480/4452 (78%)	3383 (97%)	97 (3%)	46	69

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	218	ARG
1	H	380	LEU
1	G	332	SER
1	H	69	TRP
1	I	281	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	64	HIS
1	J	64	HIS
1	H	209	GLN
1	I	64	HIS
1	J	209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
1	OAS	I	149	1	7,8,9	1.27	1 (14%)	4,9,11	0.78	0
1	OAS	K	149	1	7,8,9	1.76	2 (28%)	4,9,11	1.45	1 (25%)
1	OAS	L	149	1	7,8,9	1.53	1 (14%)	4,9,11	1.39	1 (25%)
1	OAS	A	149	1	7,8,9	1.51	1 (14%)	4,9,11	2.08	1 (25%)
1	OAS	F	149	1	7,8,9	1.53	1 (14%)	4,9,11	1.39	1 (25%)
1	OAS	J	149	1	7,8,9	1.67	2 (28%)	4,9,11	1.60	1 (25%)

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
1	OAS	I	149	1	-	0/5/7/9	-
1	OAS	K	149	1	-	2/5/7/9	-
1	OAS	L	149	1	-	0/5/7/9	-
1	OAS	A	149	1	-	0/5/7/9	-
1	OAS	F	149	1	-	0/5/7/9	-
1	OAS	J	149	1	-	2/5/7/9	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	149	OAS	OG-C1A	3.33	1.49	1.33
1	F	149	OAS	OG-C1A	3.27	1.49	1.33
1	K	149	OAS	OG-C1A	3.16	1.48	1.33
1	J	149	OAS	OG-C1A	3.11	1.48	1.33
1	A	149	OAS	OG-C1A	2.83	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	OAS	CB-OG-C1A	3.97	126.88	117.08
1	J	149	OAS	CB-OG-C1A	3.18	124.92	117.08
1	K	149	OAS	CB-OG-C1A	2.89	124.21	117.08
1	F	149	OAS	CB-OG-C1A	2.72	123.80	117.08
1	L	149	OAS	CB-OG-C1A	2.70	123.75	117.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	149	OAS	C2A-C1A-OG-CB
1	J	149	OAS	C2A-C1A-OG-CB
1	K	149	OAS	OAC-C1A-OG-CB
1	J	149	OAS	OAC-C1A-OG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	B	1385	-	3,3,3	0.71	0	3,3,3	1.50	1 (33%)
2	CSC	H	1383	-	24,26,29	2.32	10 (41%)	31,37,41	2.82	8 (25%)
3	ACT	G	1384	-	3,3,3	1.12	0	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CSC	K	1385	-	24,26,29	2.20	9 (37%)	31,37,41	2.98	12 (38%)
2	CSC	B	1384	-	24,26,29	2.08	9 (37%)	31,37,41	1.95	6 (19%)
2	CSC	D	1383	-	24,26,29	2.09	7 (29%)	31,37,41	2.68	13 (41%)
3	ACT	E	1384	-	3,3,3	0.89	0	3,3,3	0.40	0
2	CSC	G	1383	-	24,26,29	2.04	9 (37%)	31,37,41	2.89	11 (35%)
2	CSC	E	1383	-	24,26,29	2.05	8 (33%)	31,37,41	2.88	16 (51%)
3	ACT	C	1384	-	3,3,3	0.85	0	3,3,3	0.50	0
3	ACT	F	1385	-	3,3,3	1.00	0	3,3,3	0.22	0
2	CSC	C	1383	-	24,26,29	2.24	9 (37%)	31,37,41	2.14	13 (41%)
3	ACT	L	1384	-	3,3,3	0.85	0	3,3,3	0.59	0
2	CSC	L	1383	-	24,26,29	2.19	8 (33%)	31,37,41	2.09	8 (25%)
3	ACT	H	1384	-	3,3,3	0.91	0	3,3,3	0.53	0
2	CSC	F	1384	-	24,26,29	2.23	8 (33%)	31,37,41	2.34	12 (38%)
3	ACT	D	1384	-	3,3,3	0.78	0	3,3,3	0.73	0
2	CSC	A	1383	-	24,26,29	2.01	7 (29%)	31,37,41	2.85	14 (45%)
3	ACT	I	1385	-	3,3,3	1.10	0	3,3,3	0.30	0
2	CSC	J	1385	-	24,26,29	2.09	9 (37%)	31,37,41	2.05	9 (29%)
3	ACT	A	1384	-	3,3,3	0.91	0	3,3,3	0.72	0
2	CSC	I	1384	-	24,26,29	2.08	9 (37%)	31,37,41	2.01	8 (25%)

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	CSC	G	1383	-	1/1/10/12	6/20/49/52	0/2/2/2
2	CSC	L	1383	-	1/1/10/12	7/20/49/52	0/2/2/2
2	CSC	E	1383	-	1/1/10/12	10/20/49/52	0/2/2/2
2	CSC	F	1384	-	1/1/10/12	12/20/49/52	0/2/2/2
2	CSC	H	1383	-	1/1/10/12	11/20/49/52	0/2/2/2
2	CSC	J	1385	-	1/1/10/12	10/20/49/52	0/2/2/2
2	CSC	K	1385	-	1/1/10/12	15/20/49/52	0/2/2/2
2	CSC	C	1383	-	1/1/10/12	13/20/49/52	0/2/2/2
2	CSC	A	1383	-	1/1/10/12	11/20/49/52	0/2/2/2
2	CSC	B	1384	-	1/1/10/12	10/20/49/52	0/2/2/2
2	CSC	D	1383	-	1/1/10/12	9/20/49/52	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSC	I	1384	-	1/1/10/12	14/20/49/52	0/2/2/2

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1383	CSC	C4-C4'	-6.16	1.35	1.48
2	A	1383	CSC	C4-C4'	-5.95	1.35	1.48
2	C	1383	CSC	C4-C4'	-5.66	1.36	1.48
2	J	1385	CSC	C4-C4'	-5.63	1.36	1.48
2	K	1385	CSC	C4-C4'	-5.60	1.36	1.48

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1383	CSC	C7-N10-C11	-8.33	105.35	121.80
2	E	1383	CSC	C7-N10-C11	-7.86	106.28	121.80
2	G	1383	CSC	C7-N10-C11	-7.86	106.28	121.80
2	H	1383	CSC	C8-C7-N10	7.85	137.49	115.29
2	D	1383	CSC	C7-N10-C11	-7.60	106.80	121.80

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1383	CSC	C7
2	B	1384	CSC	C7
2	C	1383	CSC	C7
2	D	1383	CSC	C7
2	E	1383	CSC	C7

5 of 128 torsion outliers are listed below:

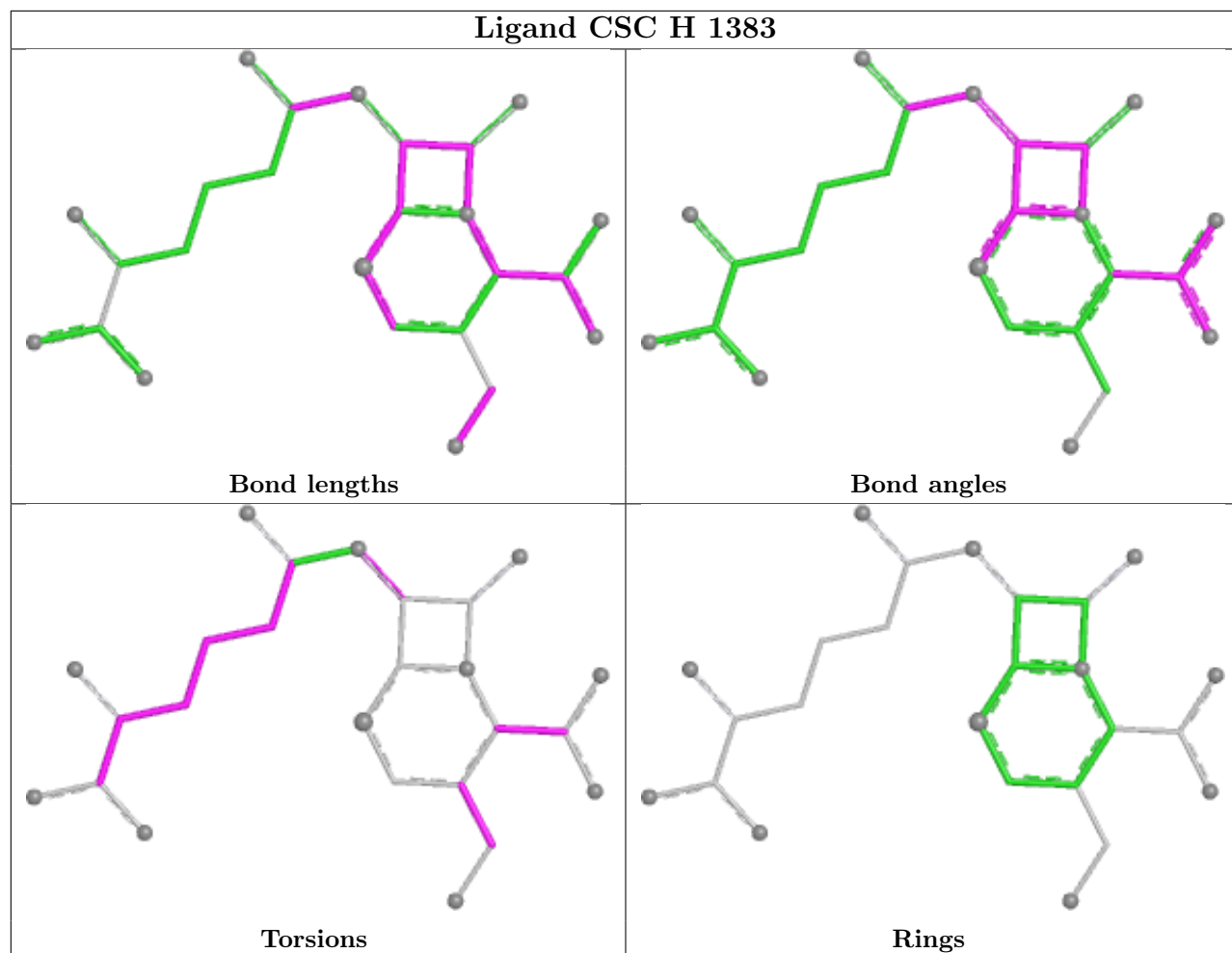
Mol	Chain	Res	Type	Atoms
2	A	1383	CSC	C2-C3-C3'-O1
2	A	1383	CSC	C14-C15-C16-N17
2	A	1383	CSC	C14-C15-C16-C18
2	A	1383	CSC	N17-C16-C18-O19
2	B	1384	CSC	C2-C3-C3'-O1

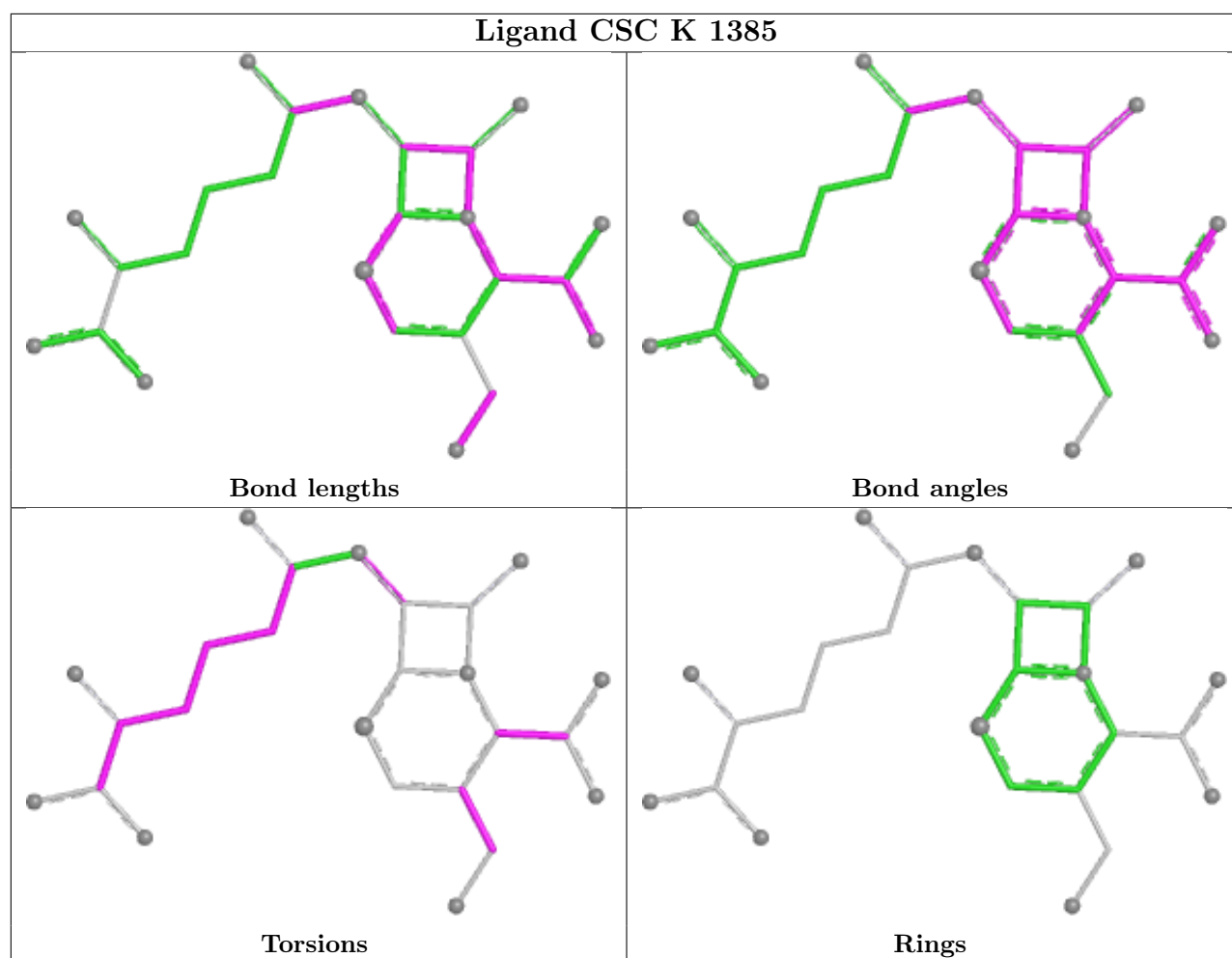
There are no ring outliers.

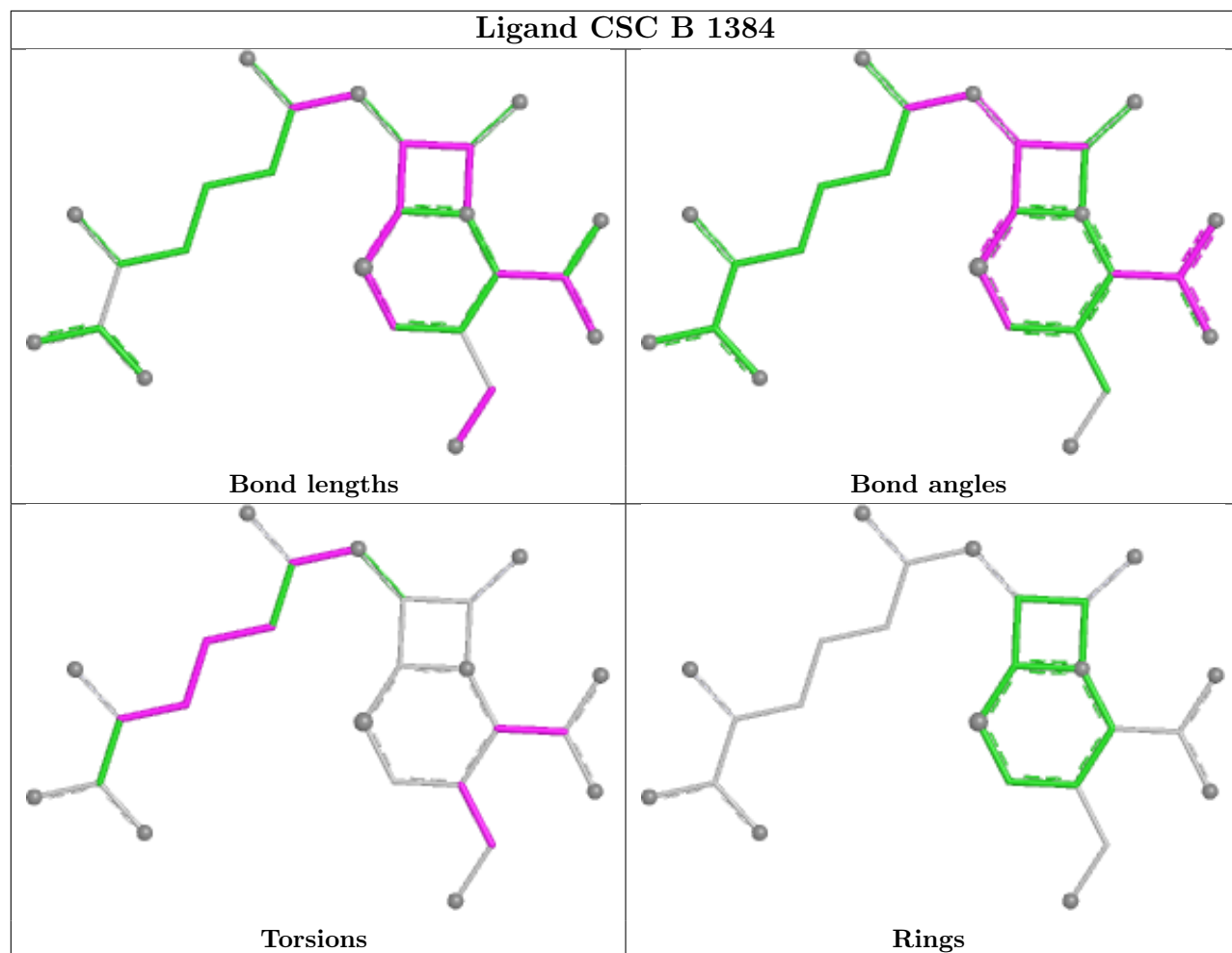
14 monomers are involved in 39 short contacts:

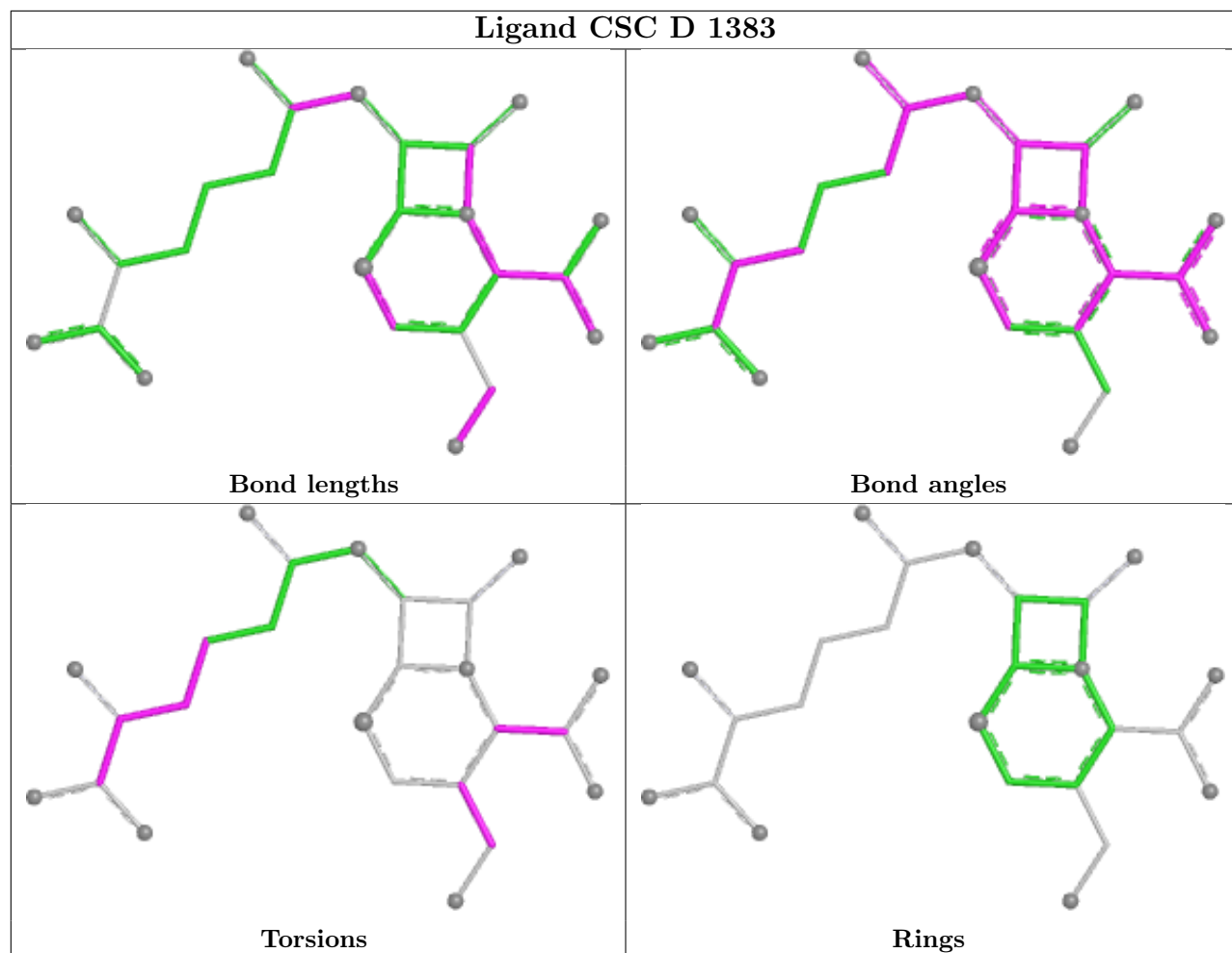
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1383	CSC	3	0
2	K	1385	CSC	4	0
2	B	1384	CSC	2	0
2	D	1383	CSC	3	0
2	G	1383	CSC	4	0
2	E	1383	CSC	2	0
3	C	1384	ACT	2	0
2	C	1383	CSC	4	0
3	L	1384	ACT	3	0
2	L	1383	CSC	2	0
2	F	1384	CSC	3	0
3	D	1384	ACT	1	0
2	A	1383	CSC	3	0
2	J	1385	CSC	3	0

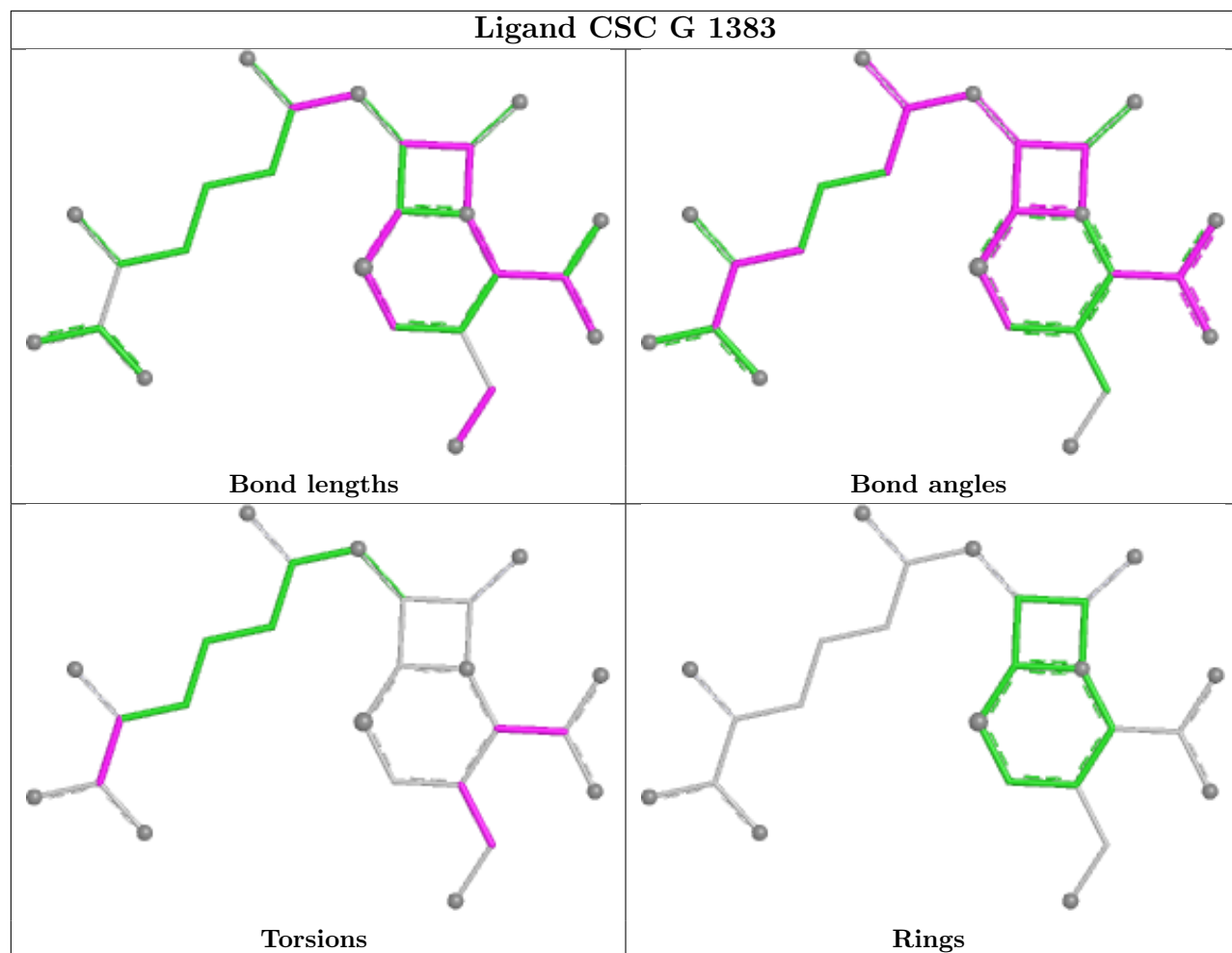
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

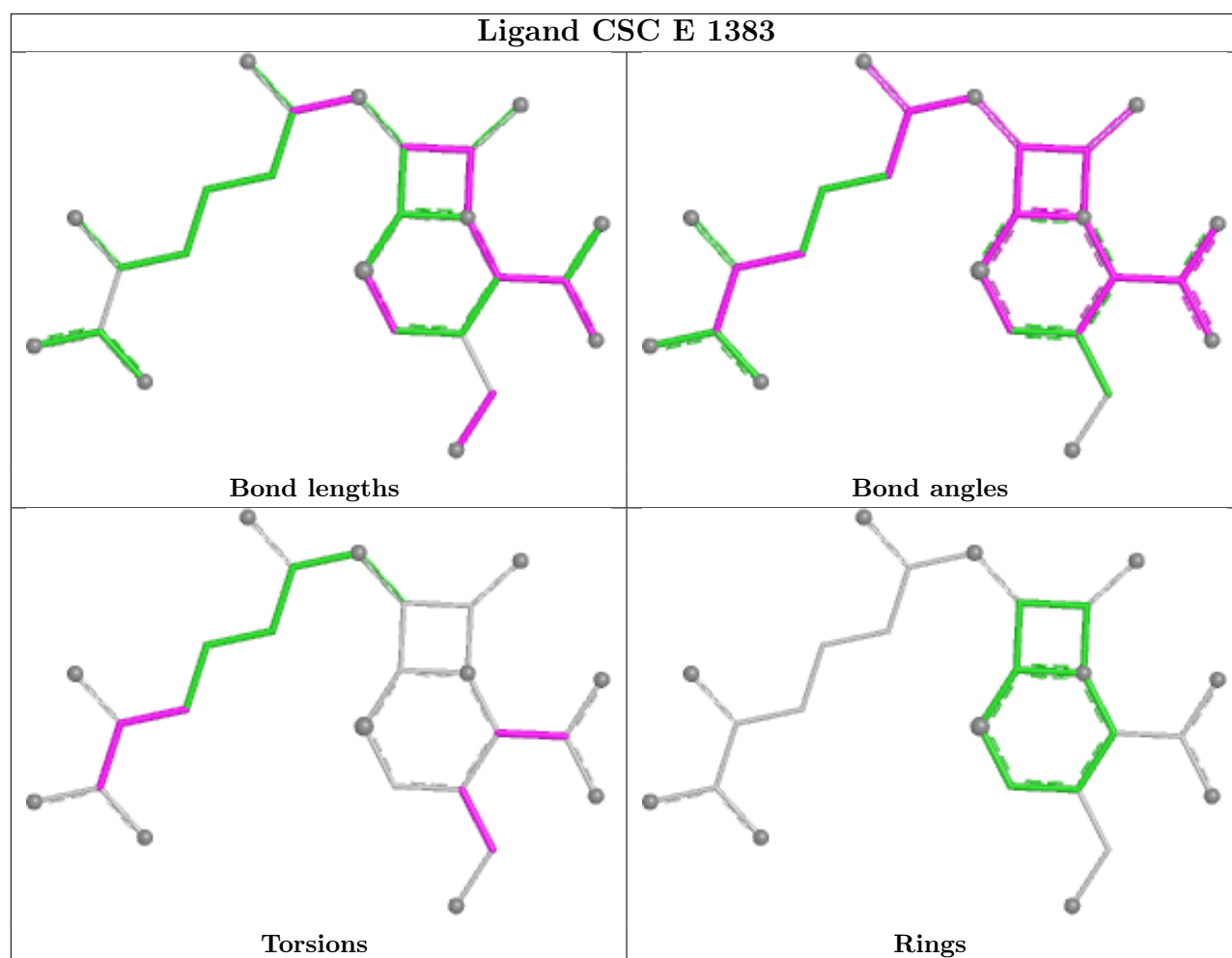


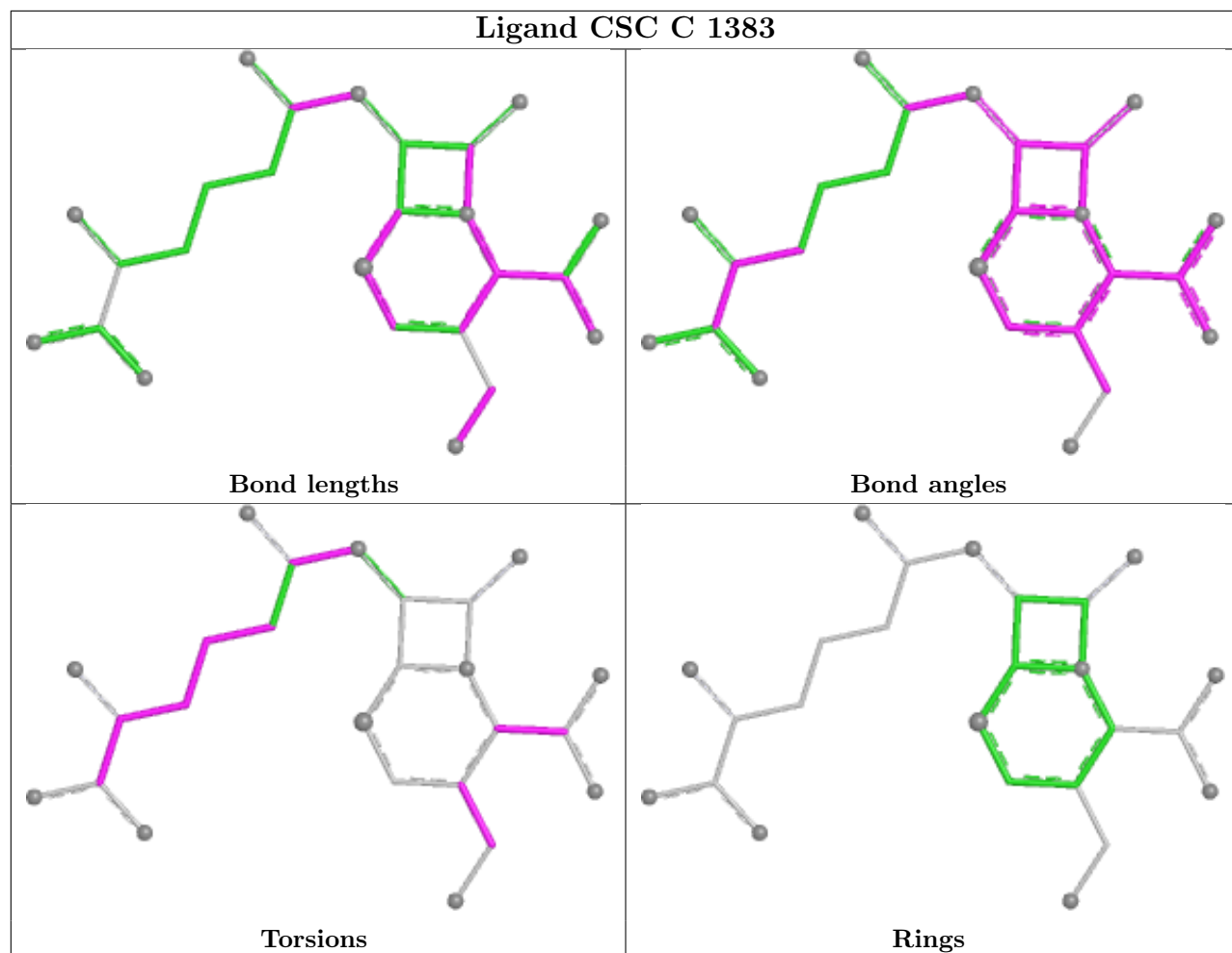


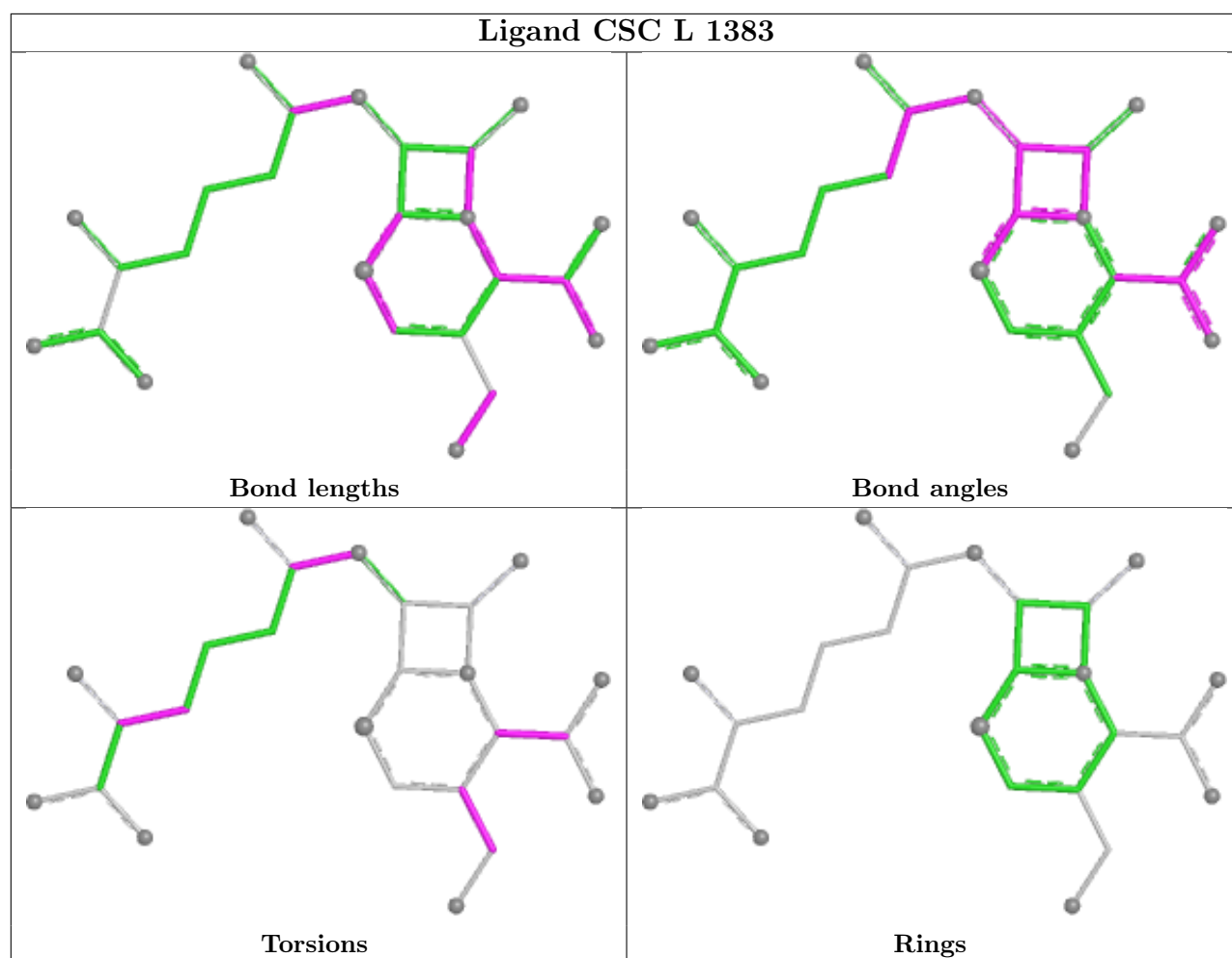


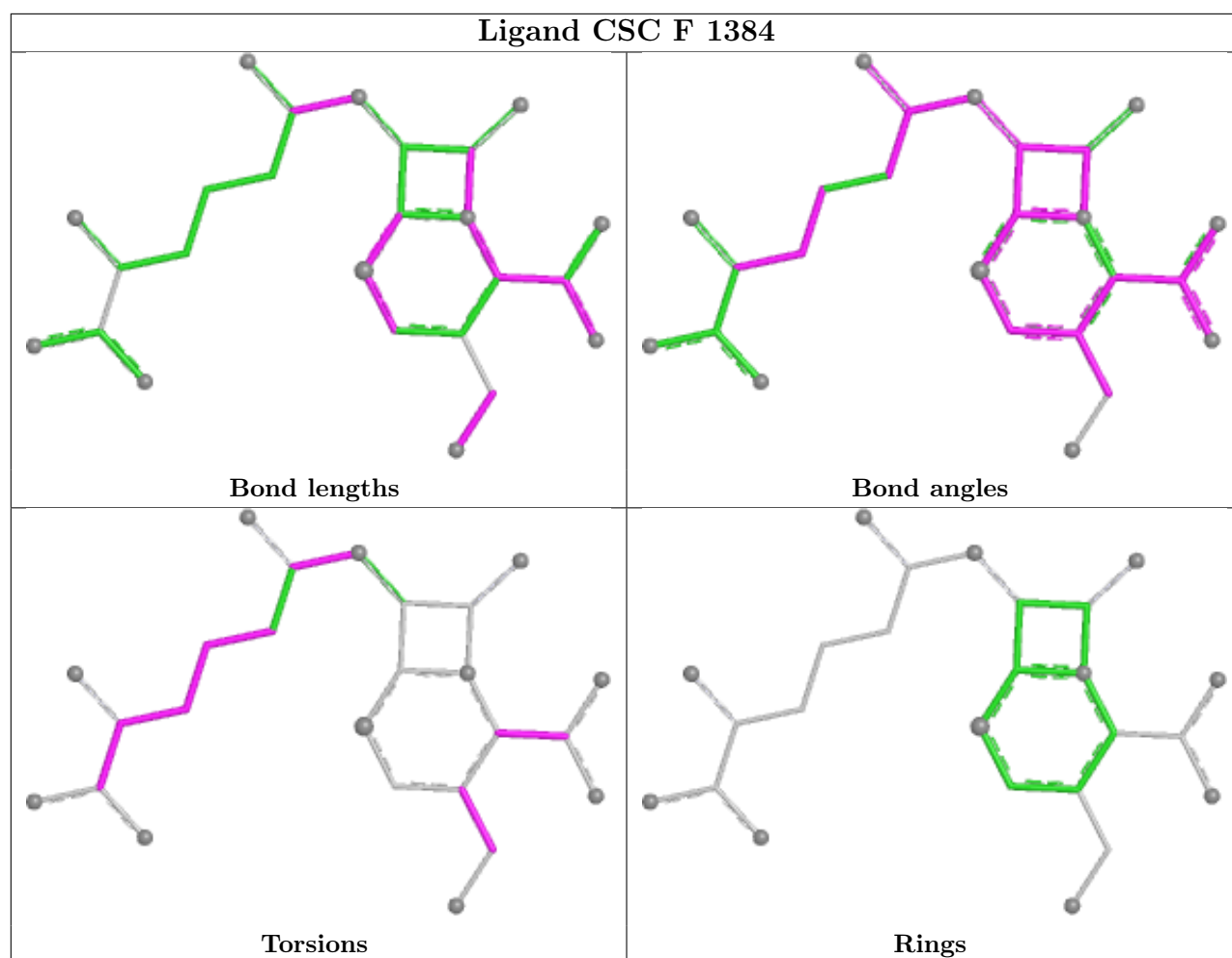


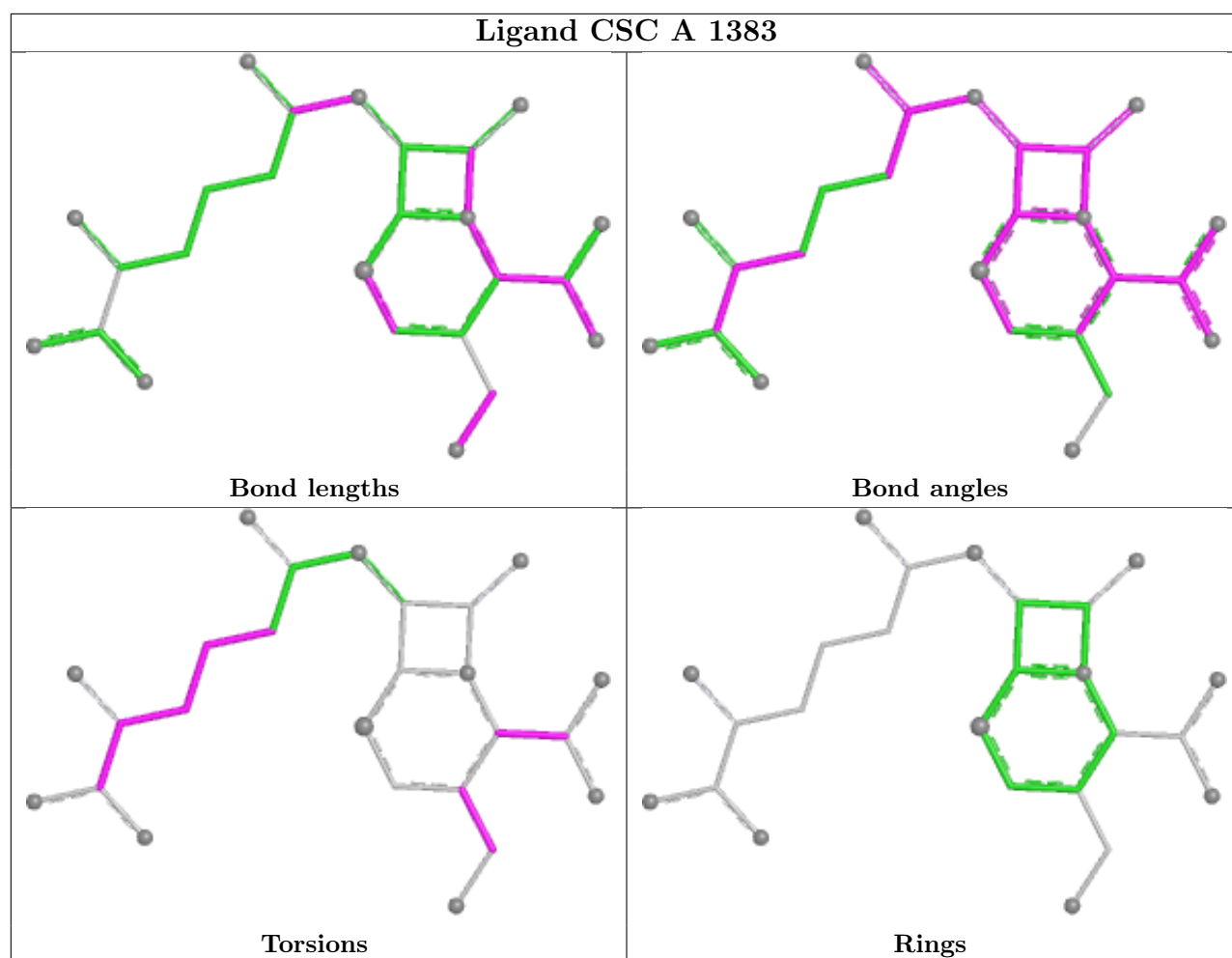


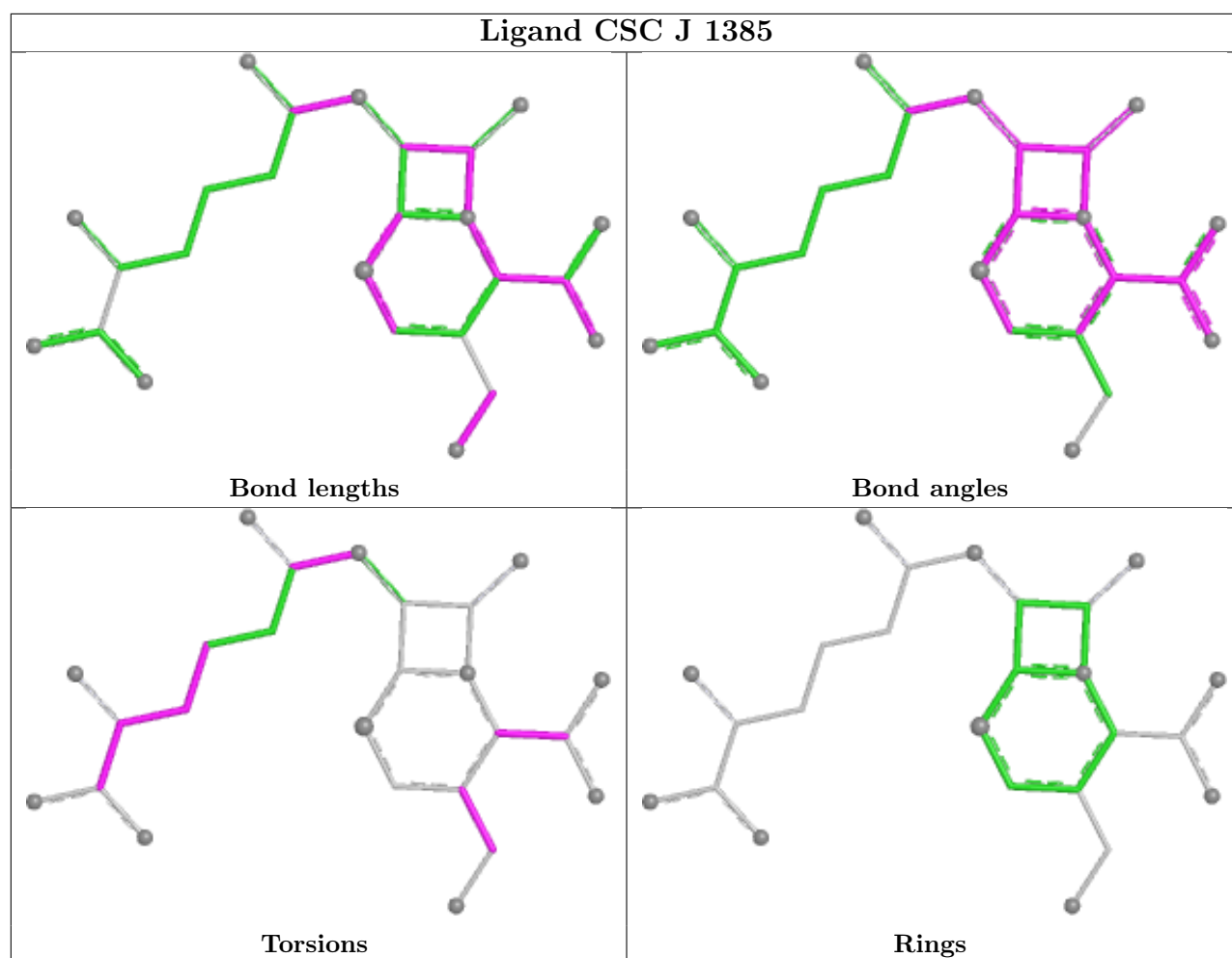


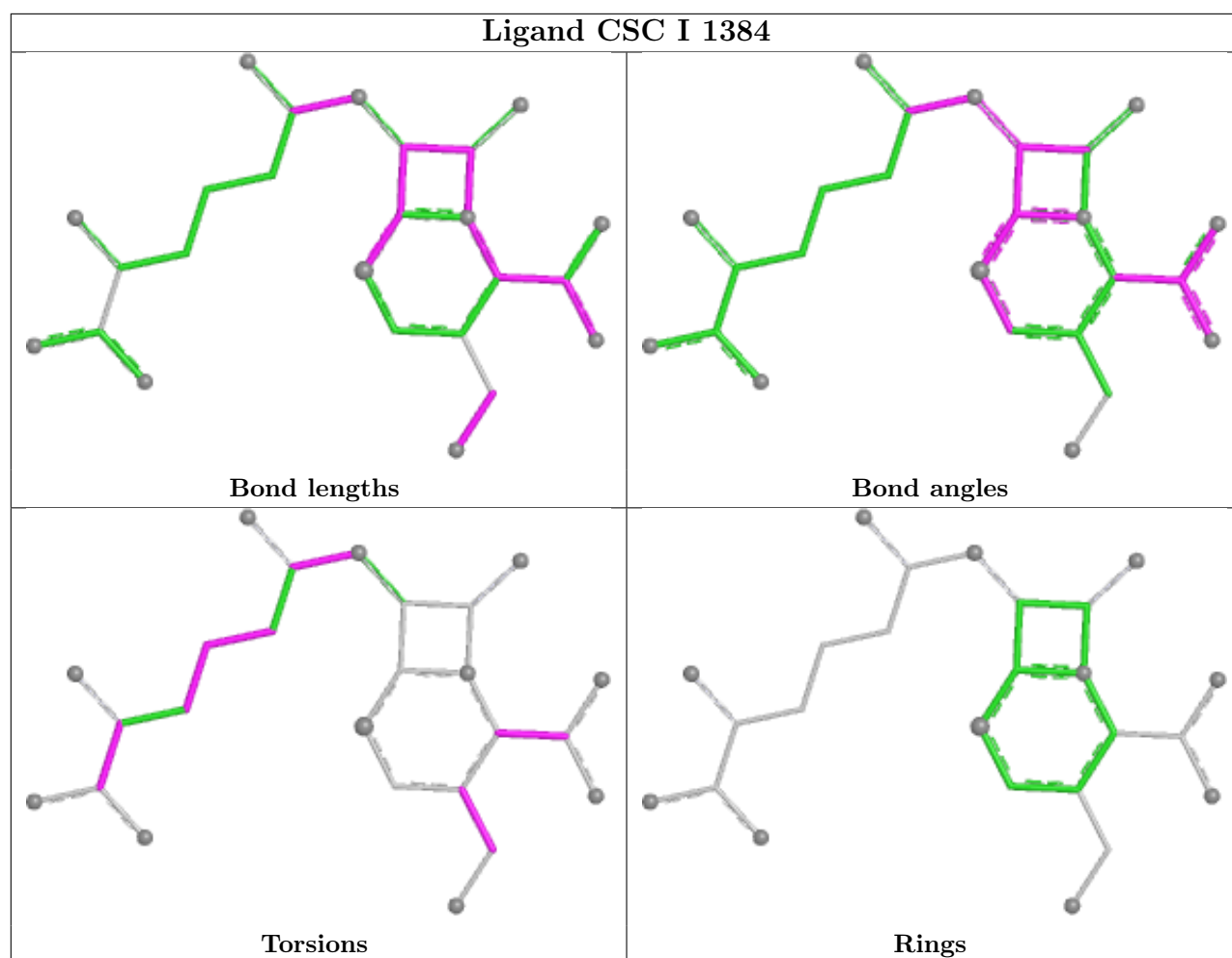












5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/444 (77%)	-0.13	3 (0%) 84 82	16, 28, 44, 62	2 (0%)
1	B	348/444 (78%)	-0.13	3 (0%) 84 82	16, 28, 44, 66	1 (0%)
1	C	347/444 (78%)	-0.02	2 (0%) 89 88	14, 27, 44, 55	2 (0%)
1	D	344/444 (77%)	-0.07	1 (0%) 94 93	14, 27, 43, 55	1 (0%)
1	E	345/444 (77%)	-0.14	3 (0%) 84 82	16, 28, 43, 63	2 (0%)
1	F	341/444 (76%)	-0.13	0 100 100	16, 28, 43, 54	0
1	G	341/444 (76%)	-0.11	0 100 100	16, 27, 42, 53	2 (0%)
1	H	341/444 (76%)	-0.09	1 (0%) 94 93	16, 27, 42, 53	1 (0%)
1	I	348/444 (78%)	-0.14	3 (0%) 84 82	16, 28, 44, 67	0
1	J	343/444 (77%)	0.05	4 (1%) 79 76	16, 28, 43, 53	0
1	K	343/444 (77%)	0.05	6 (1%) 70 66	16, 28, 43, 54	0
1	L	340/444 (76%)	-0.11	3 (0%) 84 82	16, 28, 43, 53	1 (0%)
All	All	4127/5328 (77%)	-0.08	29 (0%) 87 86	14, 28, 43, 67	12 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	PRO	4.9
1	I	239	PRO	4.5
1	A	47	VAL	4.3
1	E	47	VAL	3.7
1	I	268	GLY	3.6

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OAS	J	149	9/10	0.94	0.13	17,18,20,23	0
1	OAS	K	149	9/10	0.94	0.14	17,18,20,23	0
1	OAS	F	149	9/10	0.95	0.14	17,17,20,22	0
1	OAS	E	149[A]	9/10	0.96	0.14	17,18,20,22	0
1	OAS	A	149	9/10	0.96	0.14	17,18,20,22	0
1	OAS	G	149[A]	9/10	0.96	0.17	17,18,20,22	0
1	OAS	C	149[A]	9/10	0.96	0.17	17,18,20,22	3
1	OAS	D	149[A]	9/10	0.96	0.18	17,18,20,22	3
1	OAS	H	149[A]	9/10	0.97	0.16	17,18,20,22	0
1	OAS	I	149	9/10	0.97	0.15	17,18,20,22	0
1	OAS	B	149[A]	9/10	0.98	0.12	17,18,20,22	0
1	OAS	L	149	9/10	0.98	0.11	17,18,20,22	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

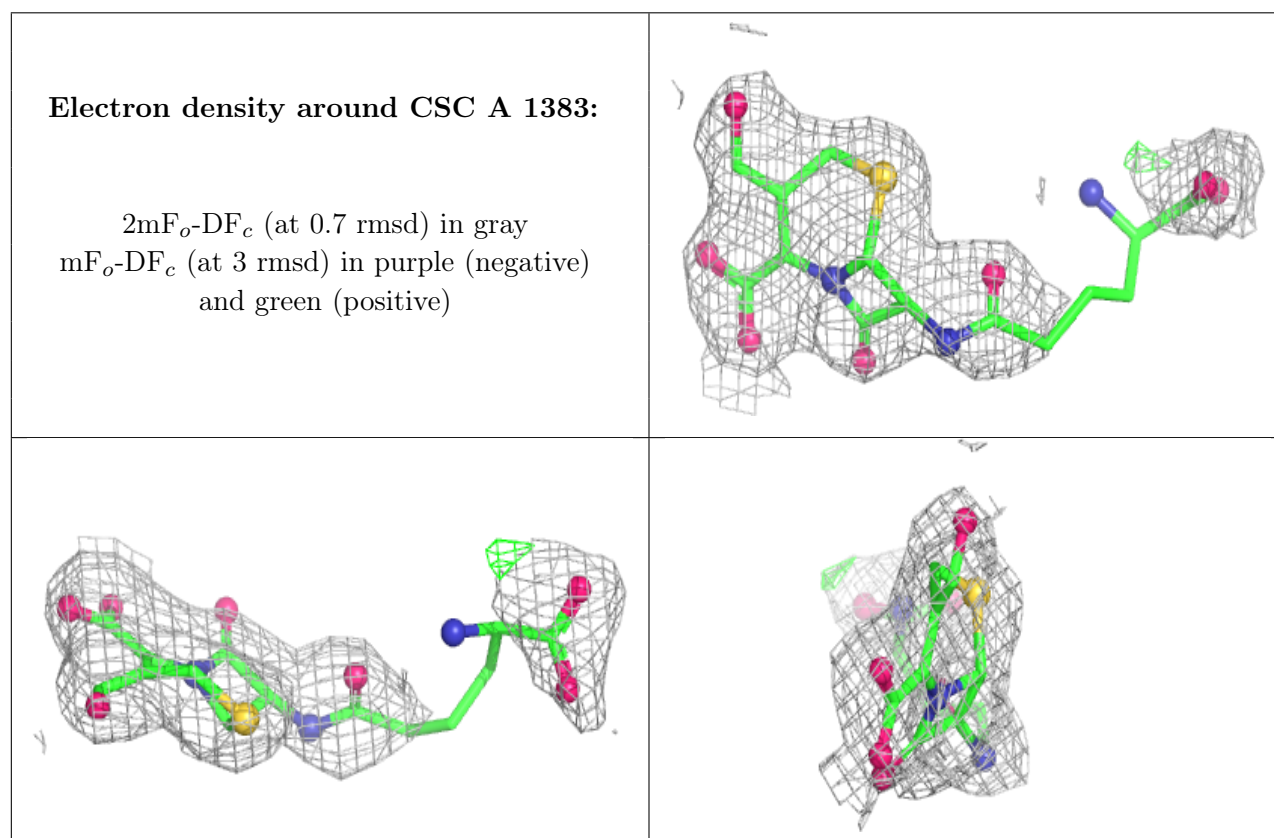
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSC	A	1383	25/28	0.88	0.23	56,65,84,85	0
3	ACT	E	1384	4/4	0.88	0.17	46,47,47,48	0
2	CSC	I	1384	25/28	0.89	0.23	42,51,78,79	0
3	ACT	B	1385	4/4	0.89	0.20	37,38,38,38	0
2	CSC	D	1383	25/28	0.89	0.24	50,54,78,80	0
2	CSC	C	1383	25/28	0.90	0.21	49,54,73,73	0
2	CSC	B	1384	25/28	0.90	0.24	44,51,75,76	0
2	CSC	E	1383	25/28	0.90	0.24	57,67,83,83	0
3	ACT	I	1385	4/4	0.90	0.21	35,36,36,36	0
2	CSC	L	1383	25/28	0.91	0.21	38,44,62,63	0
2	CSC	K	1385	25/28	0.92	0.22	51,59,68,69	0
2	CSC	F	1384	25/28	0.92	0.22	40,44,61,62	0
3	ACT	A	1384	4/4	0.92	0.19	40,42,42,43	0
3	ACT	F	1385	4/4	0.93	0.18	42,43,43,43	0

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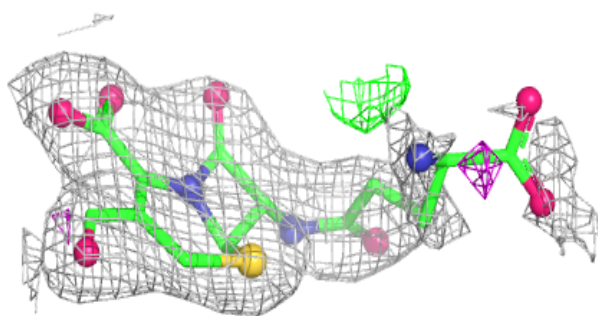
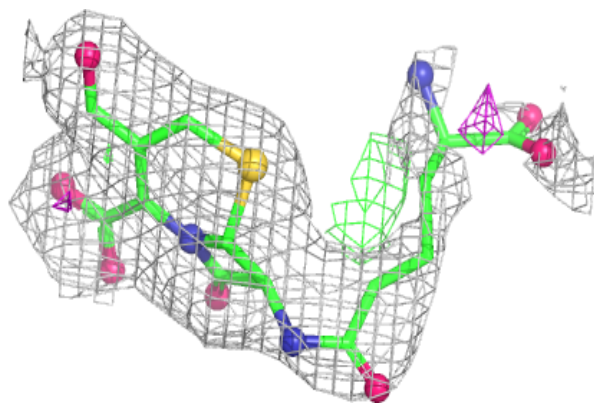
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CSC	J	1385	25/28	0.93	0.22	50,56,71,73	0
2	CSC	H	1383	25/28	0.94	0.23	43,47,78,78	0
3	ACT	G	1384	4/4	0.94	0.14	35,35,36,36	0
2	CSC	G	1383	25/28	0.94	0.19	39,43,73,73	0
3	ACT	H	1384	4/4	0.96	0.12	34,35,35,36	0
3	ACT	D	1384	4/4	0.96	0.18	28,28,28,29	0
3	ACT	L	1384	4/4	0.96	0.19	46,46,47,47	0
3	ACT	C	1384	4/4	0.97	0.15	32,32,32,32	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.

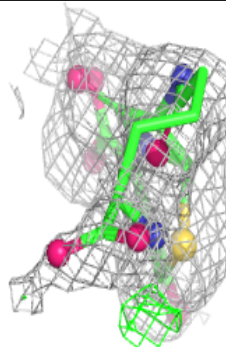
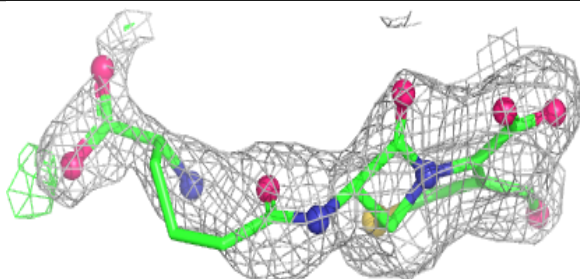
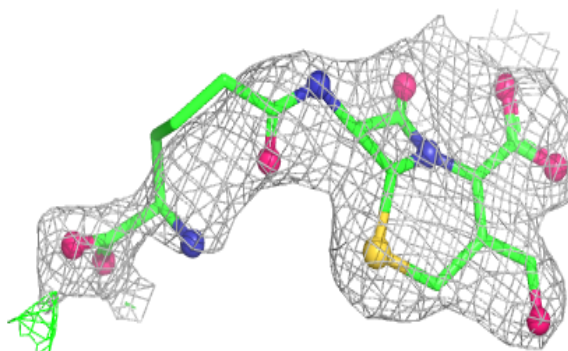


Electron density around CSC I 1384:

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

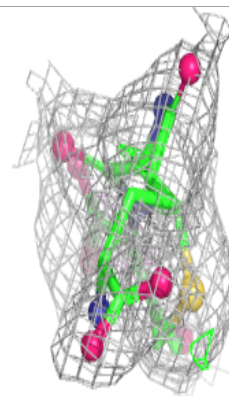
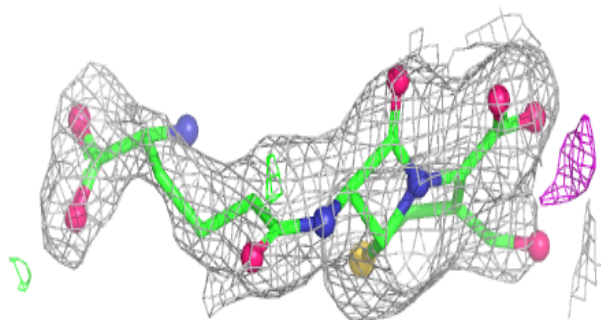
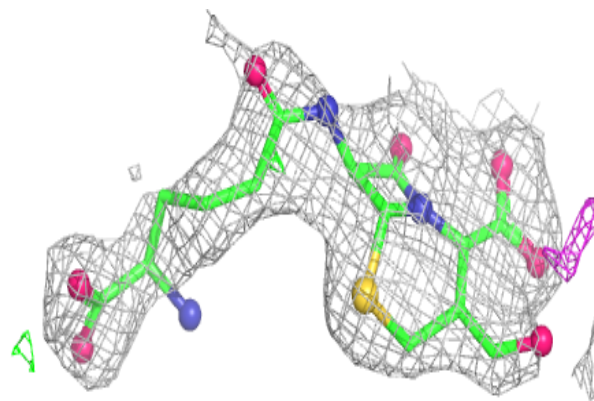
**Electron density around CSC D 1383:**

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



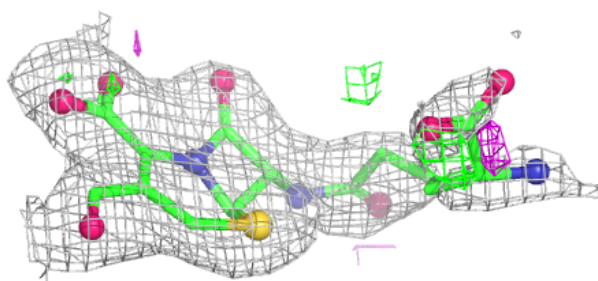
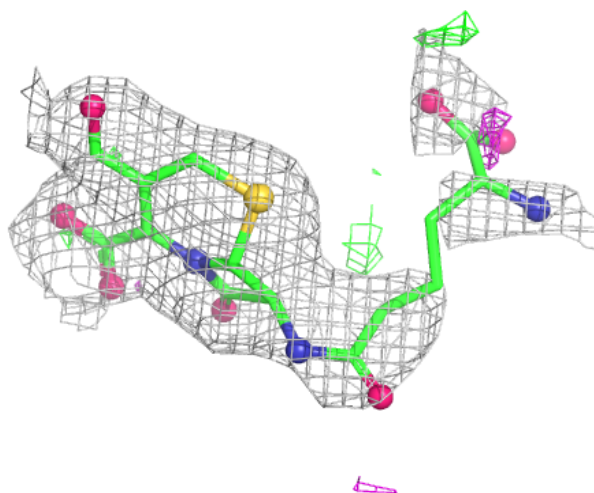
Electron density around CSC C 1383:

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



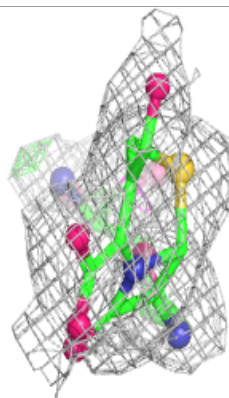
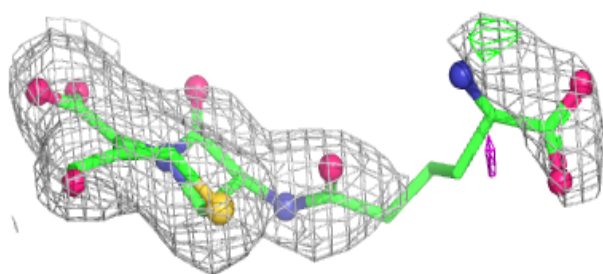
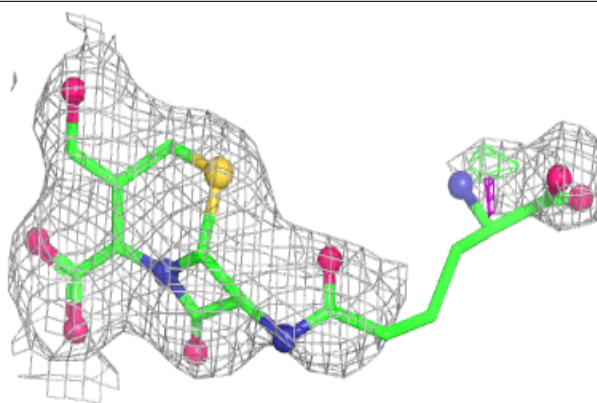
Electron density around CSC B 1384:

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

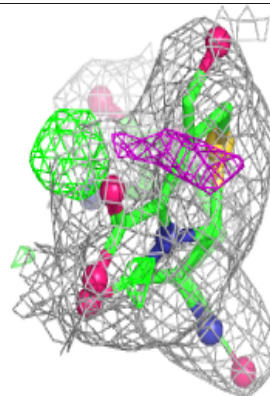
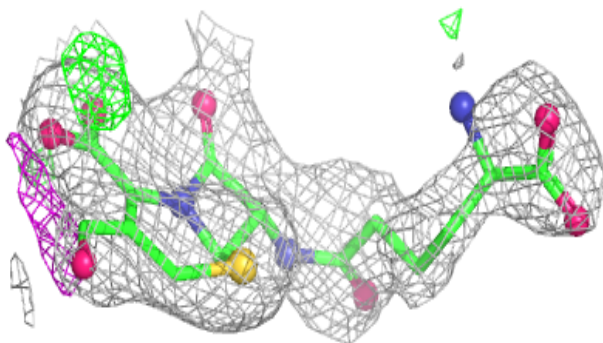
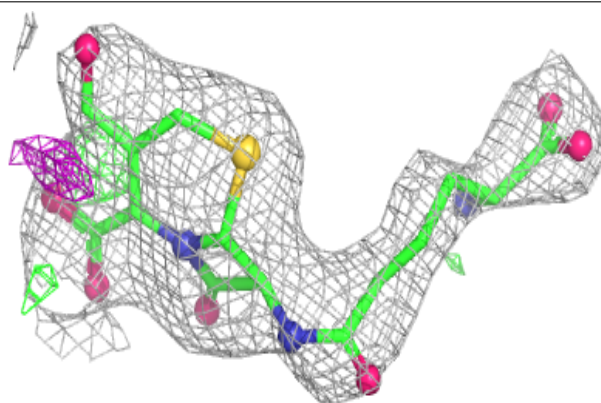


Electron density around CSC E 1383:

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

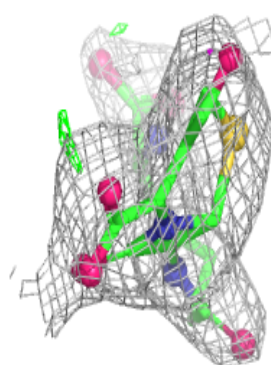
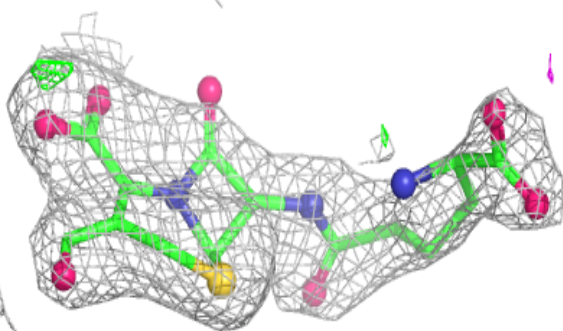
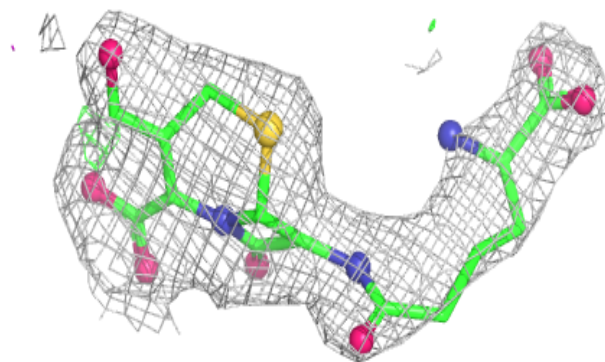
**Electron density around CSC L 1383:**

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

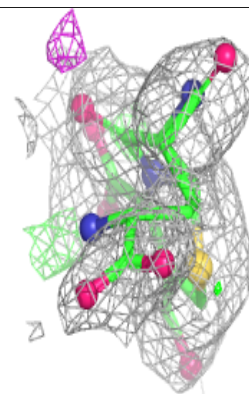
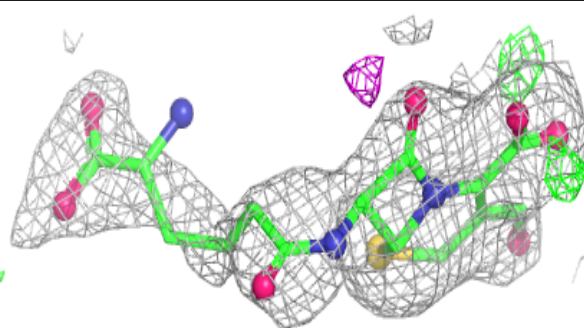
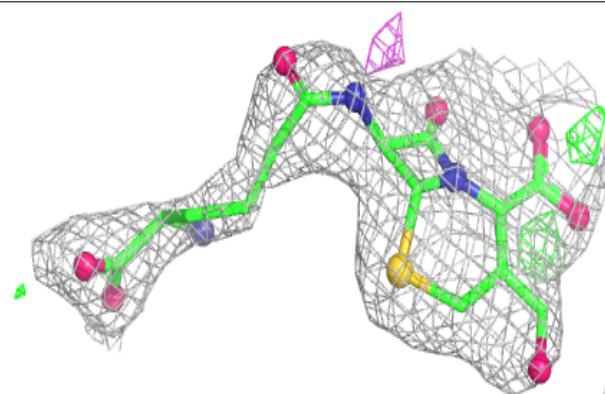


Electron density around CSC K 1385:

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

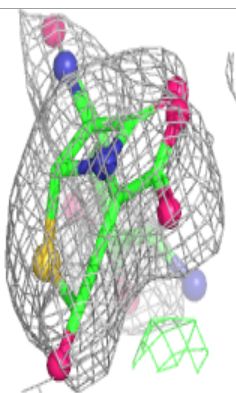
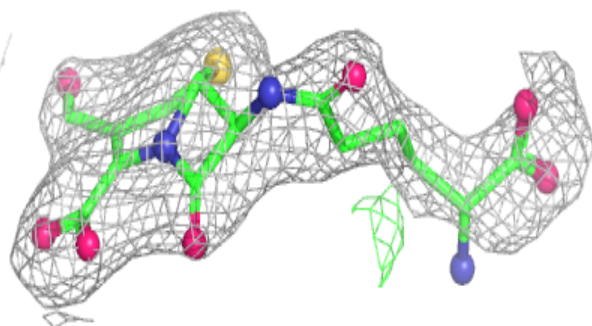
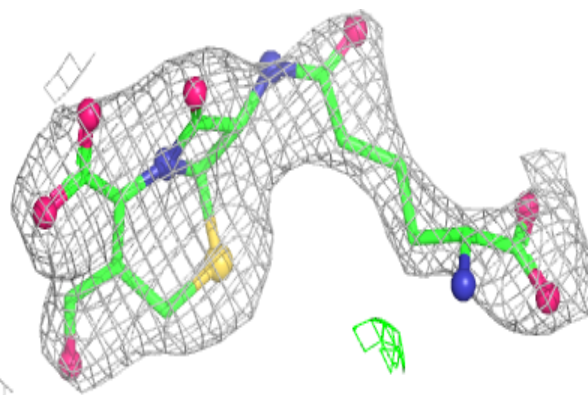
**Electron density around CSC F 1384:**

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

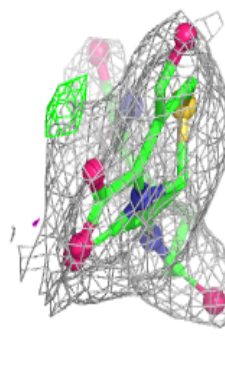
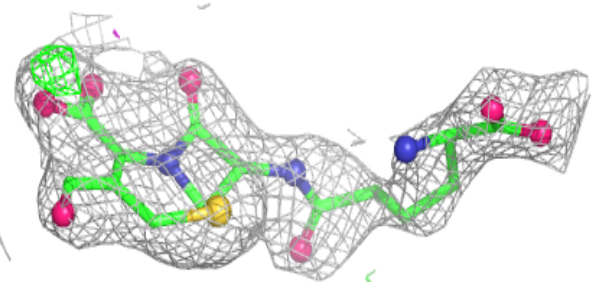
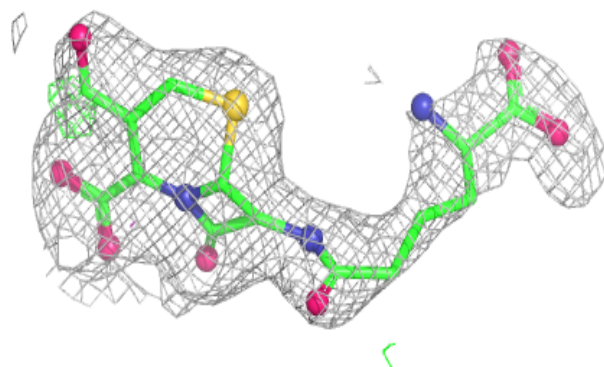


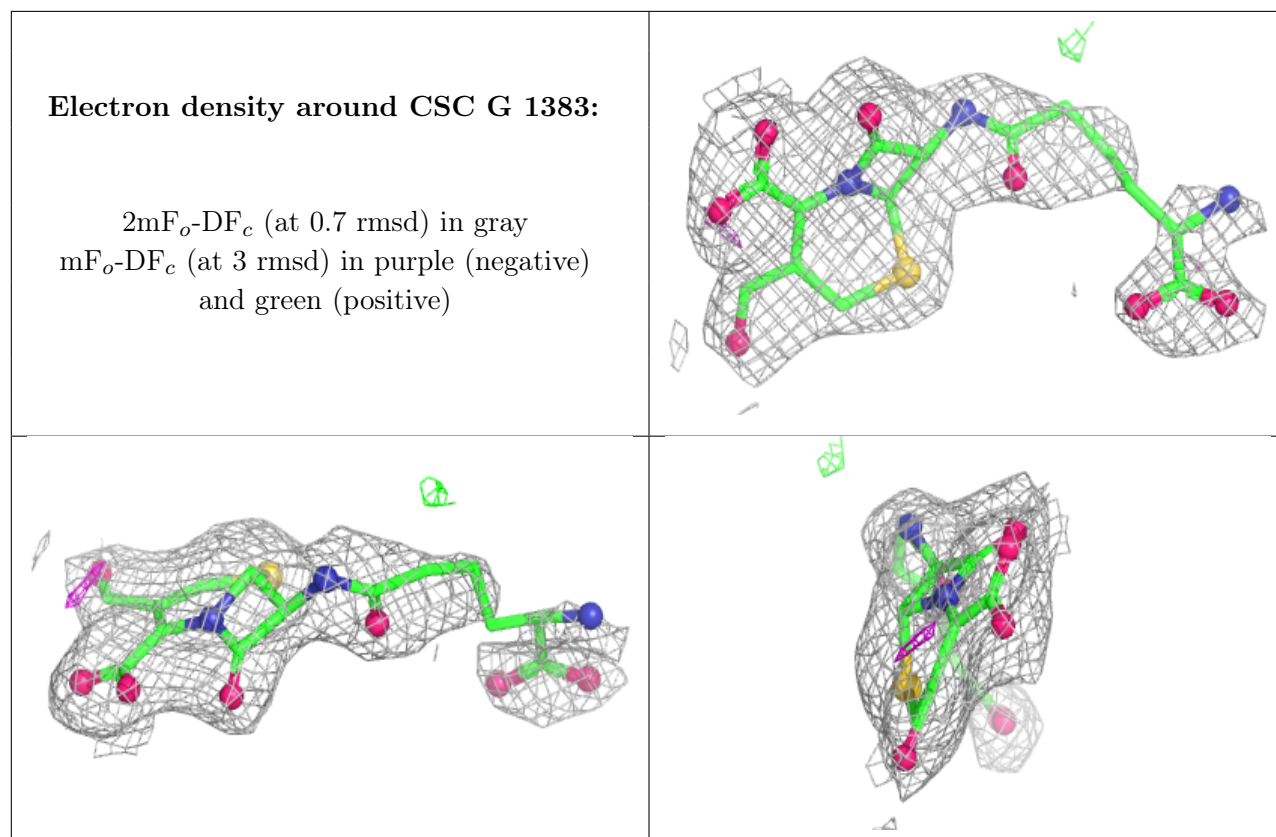
Electron density around CSC J 1385:

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

**Electron density around CSC H 1383:**

$2mF_o-DF_c$ (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.