



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 07:16 pm GMT

PDB ID : 2VAV
Title : Crystal structure of deacetylcephalosporin C acetyltransferase (DAC-Soak)
Authors : Lejon, S.; Ellis, J.; Valegard, K.
Deposited on : 2007-09-04
Resolution : 2.50 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

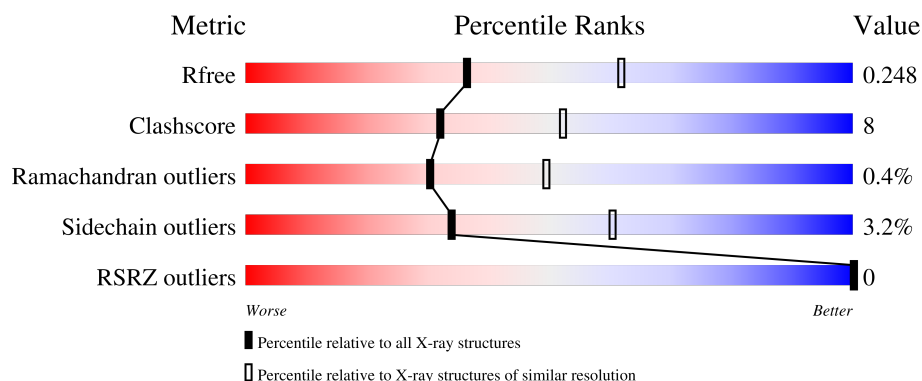
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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>66%</div> <div>11%</div> <div>•</div> <div>22%</div> </div>
1	B	444	<div> <div>68%</div> <div>10%</div> <div>•</div> <div>21%</div> </div>
1	C	444	<div> <div>66%</div> <div>11%</div> <div>•</div> <div>22%</div> </div>
1	D	444	<div> <div>66%</div> <div>11%</div> <div>•</div> <div>22%</div> </div>
1	E	444	<div> <div>68%</div> <div>9%</div> <div>•</div> <div>22%</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
1	OAS	A	149[A]	-	X	-	-
1	OAS	B	149[A]	-	X	-	-
1	OAS	C	149[A]	-	X	-	-
1	OAS	D	149[A]	-	X	-	-
1	OAS	E	149[A]	-	X	-	-
1	OAS	F	149[A]	-	X	X	-
1	OAS	G	149[A]	-	X	-	-
1	OAS	H	149[A]	-	X	-	-
1	OAS	I	149[A]	-	X	-	-
1	OAS	J	149[A]	-	X	-	-
1	OAS	K	149[A]	-	X	-	-
1	OAS	L	149[A]	-	X	-	-
2	CSC	A	1383[B]	-	-	X	-
2	CSC	F	1383[A]	-	-	X	-
3	ACT	A	1384	-	-	X	-
3	ACT	C	1384	-	-	X	-
3	ACT	E	1384	-	-	X	-
3	ACT	H	1384	-	-	X	-

2 Entry composition

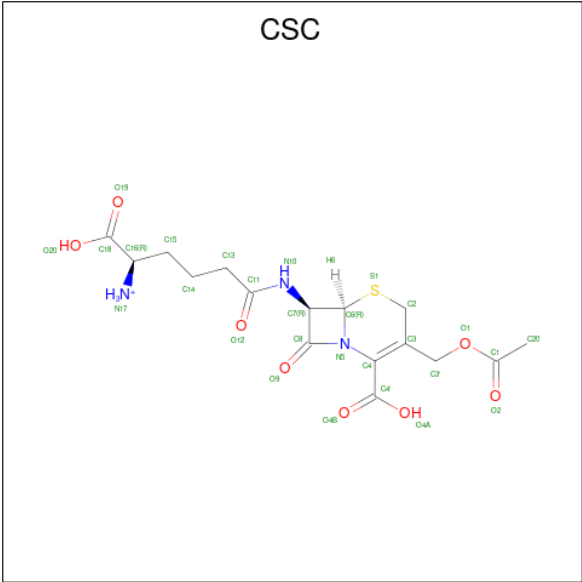
There are 4 unique types of molecules in this entry. The entry contains 33548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	348	Total	C	N	O	S	0	2	0
			2743	1730	483	511	19			
1	B	350	Total	C	N	O	S	0	3	0
			2754	1736	486	513	19			
1	C	347	Total	C	N	O	S	0	4	0
			2758	1739	489	511	19			
1	D	345	Total	C	N	O	S	0	4	0
			2745	1732	487	507	19			
1	E	346	Total	C	N	O	S	0	3	0
			2723	1719	478	507	19			
1	F	341	Total	C	N	O	S	0	2	0
			2696	1702	473	502	19			
1	G	342	Total	C	N	O	S	0	3	0
			2707	1708	477	503	19			
1	H	343	Total	C	N	O	S	0	4	0
			2714	1713	478	504	19			
1	I	348	Total	C	N	O	S	0	3	1
			2735	1725	483	508	19			
1	J	344	Total	C	N	O	S	0	2	0
			2714	1713	476	506	19			
1	K	341	Total	C	N	O	S	0	2	0
			2694	1701	473	501	19			
1	L	340	Total	C	N	O	S	0	3	0
			2691	1699	472	501	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	1
			25	14	3	7	1		
2	B	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	C	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	D	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	E	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	F	1	Total	C	N	O	S	0	1
			30	17	3	9	1		
2	G	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	H	1	Total	C	N	O	S	0	1
			30	17	3	9	1		
2	I	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	J	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	K	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	L	1	Total	C	N	O	S	0	1
			30	17	3	9	1		

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



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

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

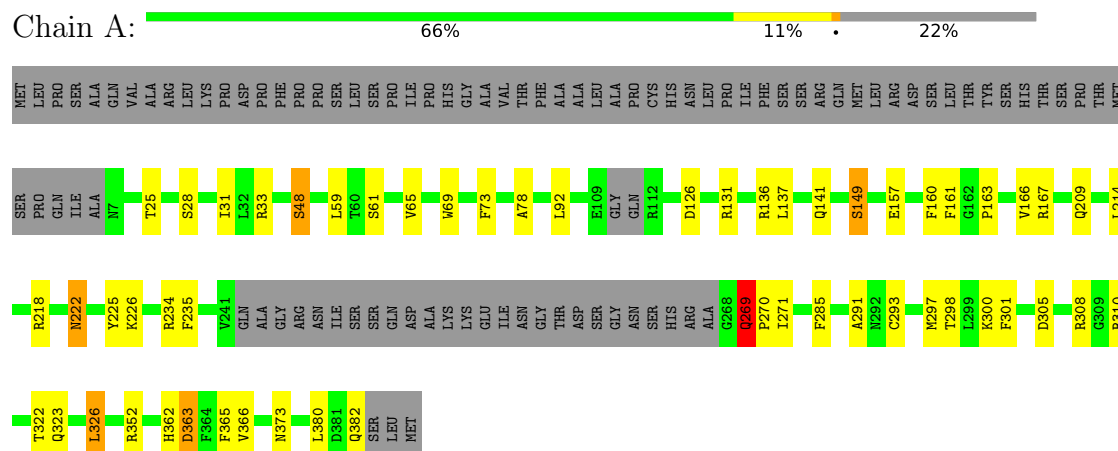
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	51	Total	O	0	0
			51	51		
4	C	43	Total	O	0	0
			43	43		
4	D	49	Total	O	0	0
			49	49		
4	E	46	Total	O	0	0
			46	46		
4	F	41	Total	O	0	0
			41	41		
4	G	52	Total	O	0	0
			52	52		
4	H	48	Total	O	0	0
			48	48		
4	I	56	Total	O	0	0
			56	56		
4	J	17	Total	O	0	0
			17	17		
4	K	11	Total	O	0	0
			11	11		
4	L	37	Total	O	0	0
			37	37		

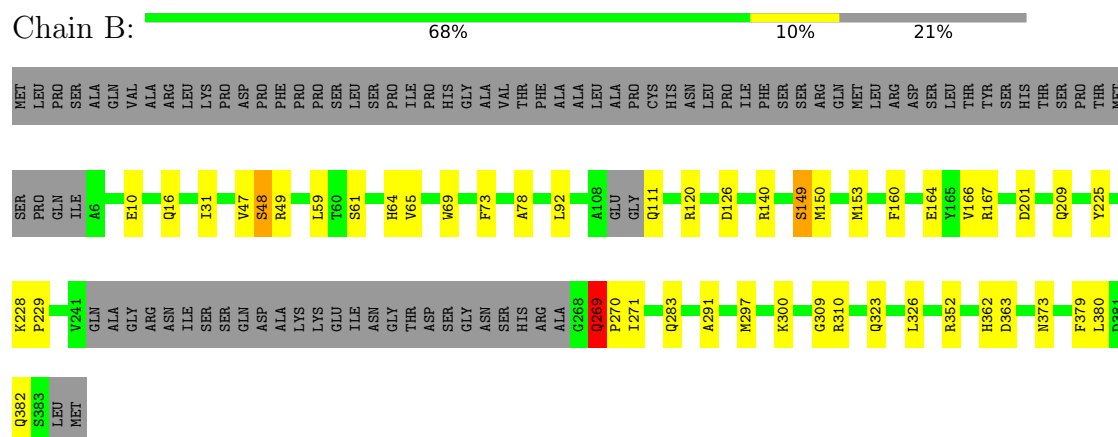
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

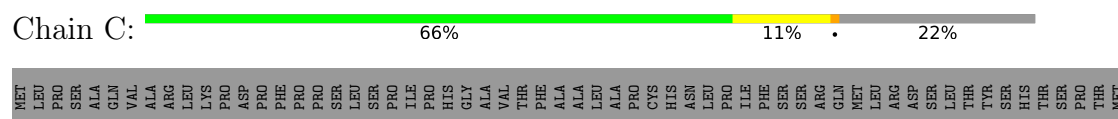
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

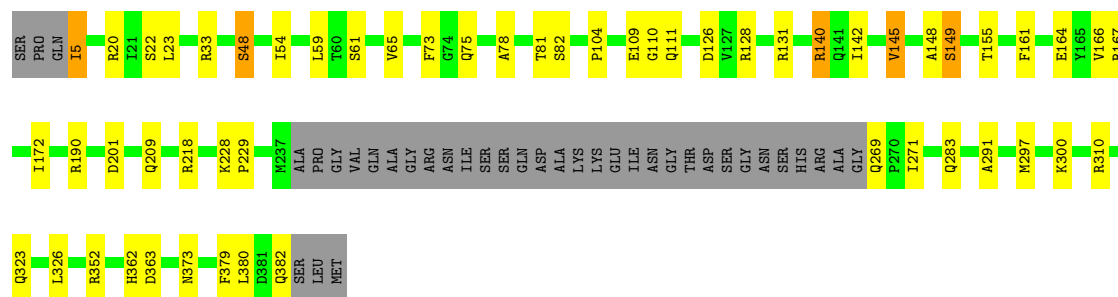


• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



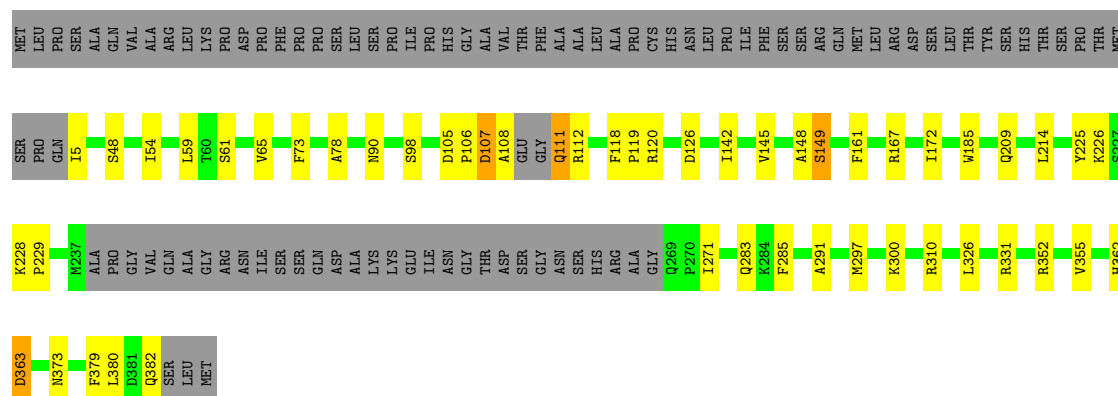
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE





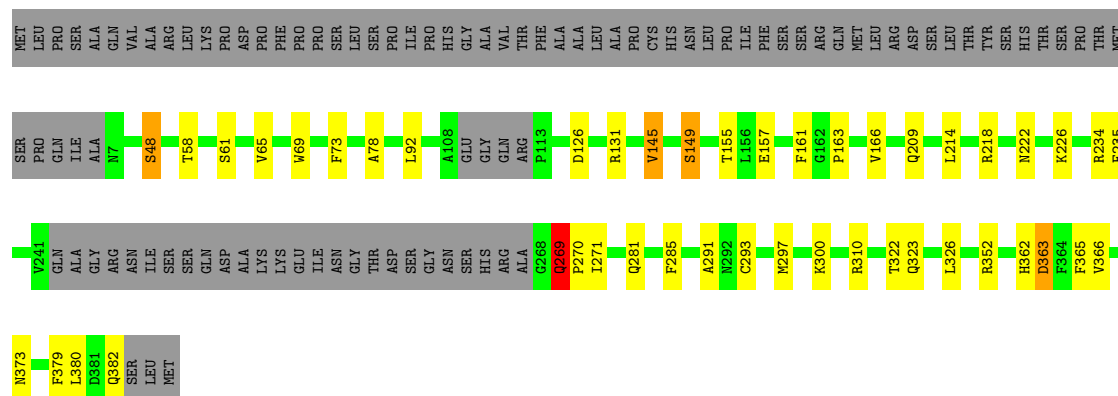
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain D: 66% 11% 22%



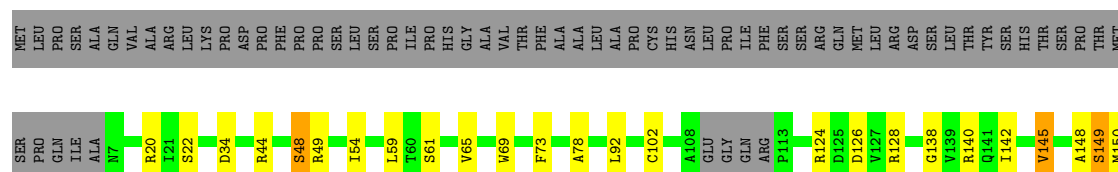
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

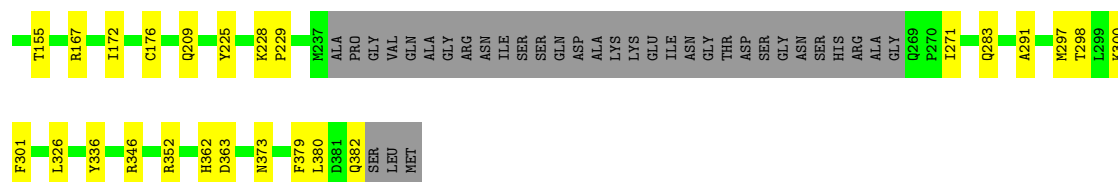
Chain E: 68% 9% 22%



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

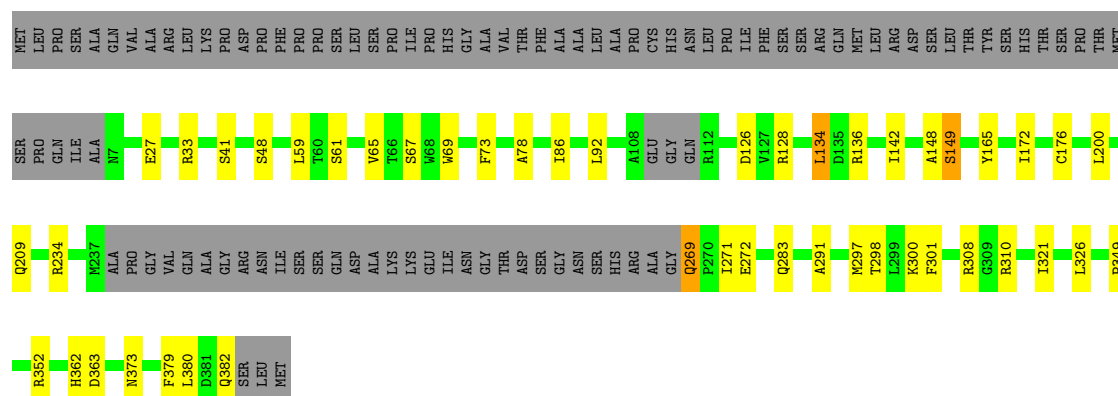
Chain F: 66% 11% 23%





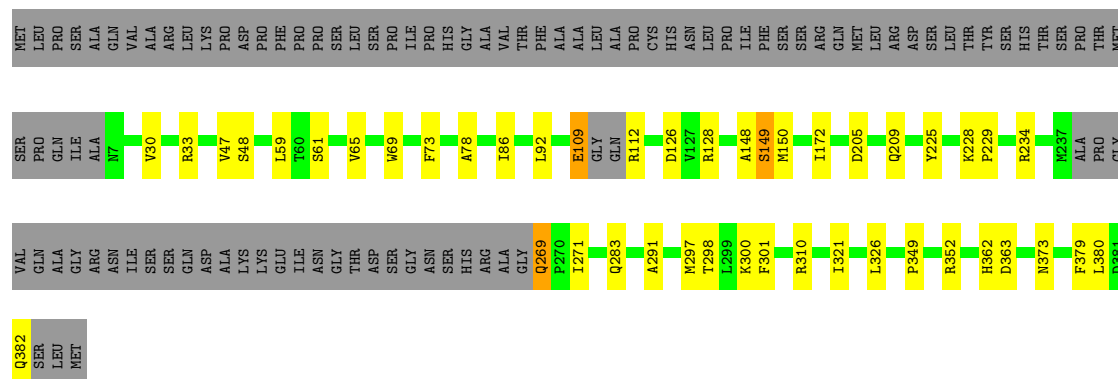
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain G: 66% 10% 23%



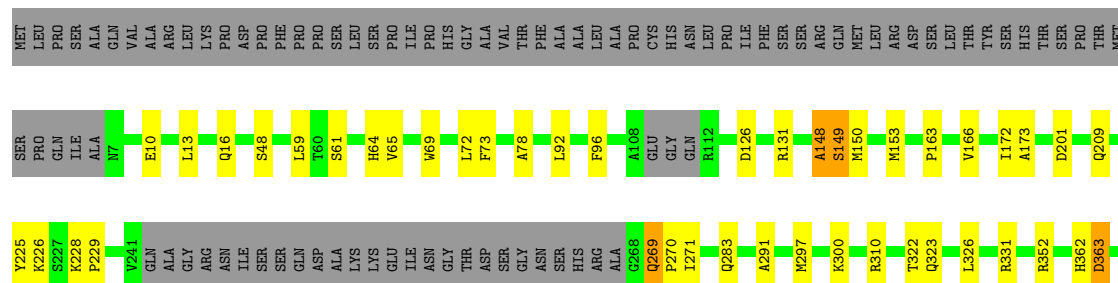
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain H: 67% 9% 23%



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

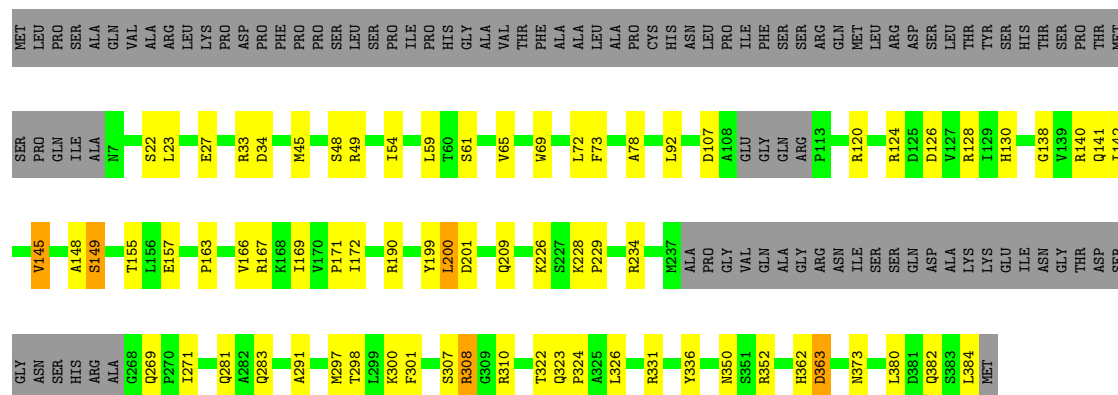
Chain I: 67% 10% 22%





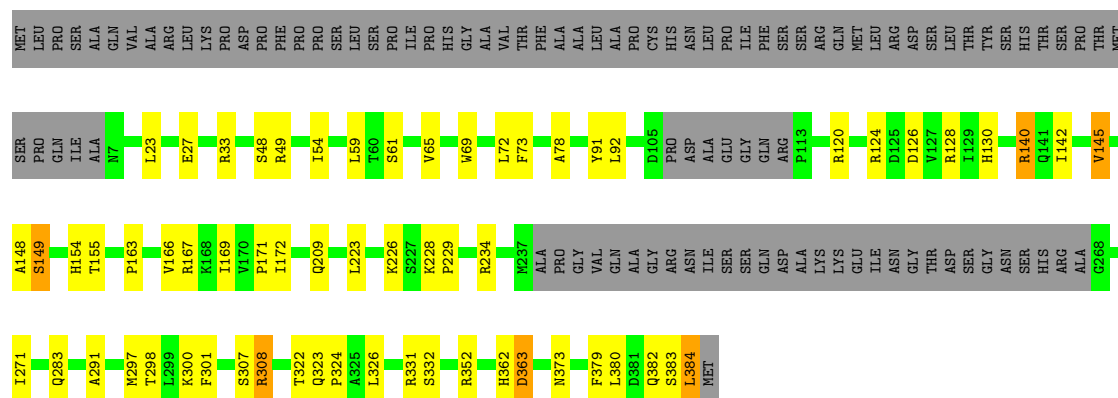
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain J: 61% 15% 23%



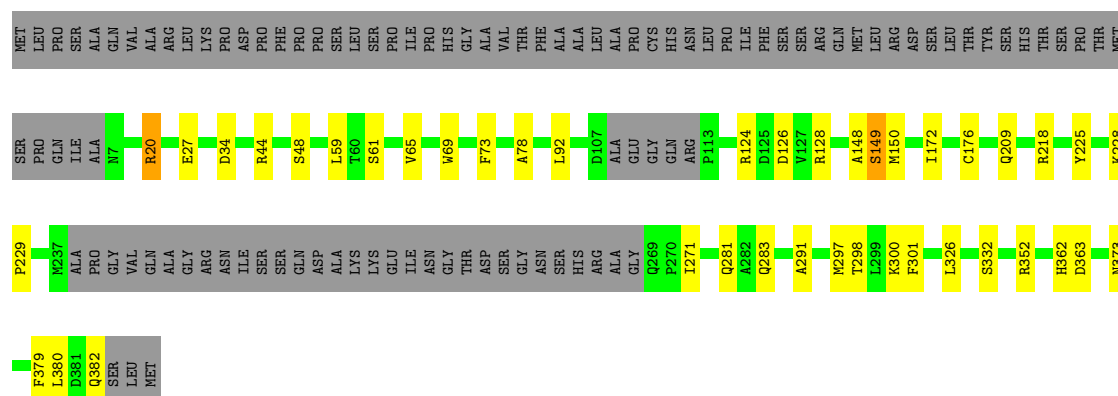
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain K: 63% 13% 23%



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

Chain L: 67% 9% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.06Å 108.86Å 195.79Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	103.70 – 2.50 103.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.70-2.50) 99.7 (103.70-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.255 0.214 , 0.248	Depositor DCC
R_{free} test set	3419 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33548	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 17.42% 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: CSC, OAS, ACT

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	0.70	1/2796 (0.0%)	0.73	1/3789 (0.0%)
1	B	0.68	0/2807	0.72	3/3804 (0.1%)
1	C	0.70	0/2817	0.75	5/3816 (0.1%)
1	D	0.71	0/2803	0.80	5/3796 (0.1%)
1	E	0.70	0/2776	0.73	0/3762
1	F	0.73	1/2748 (0.0%)	0.74	1/3723 (0.0%)
1	G	0.71	1/2759 (0.0%)	0.75	2/3738 (0.1%)
1	H	0.70	0/2766	0.74	3/3747 (0.1%)
1	I	0.69	0/2788	0.73	2/3779 (0.1%)
1	J	0.82	0/2766	0.75	0/3747
1	K	0.83	0/2745	0.76	1/3717 (0.0%)
1	L	0.71	1/2743 (0.0%)	0.74	0/3716
All	All	0.72	4/33314 (0.0%)	0.75	23/45134 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	176	CYS	CB-SG	-7.04	1.70	1.82
1	L	176	CYS	CB-SG	-6.52	1.71	1.82
1	G	176	CYS	CB-SG	-5.73	1.72	1.81
1	A	222	ASN	CB-CG	5.24	1.63	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	310	ARG	NE-CZ-NH1	-13.12	113.74	120.30
1	D	310	ARG	NE-CZ-NH2	13.03	126.82	120.30
1	K	140	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	D	310	ARG	CD-NE-CZ	6.99	133.38	123.60
1	C	310	ARG	NE-CZ-NH1	6.72	123.66	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	148	ALA	Peptide

5.2 Too-close contacts [i](#)

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	2743	0	2645	48	0
1	B	2754	0	2656	37	0
1	C	2758	0	2673	43	0
1	D	2745	0	2661	48	0
1	E	2723	0	2624	39	0
1	F	2696	0	2600	60	0
1	G	2707	0	2610	31	1
1	H	2714	0	2613	41	1
1	I	2735	0	2638	42	0
1	J	2714	0	2618	55	1
1	K	2694	0	2602	47	1
1	L	2691	0	2592	36	0
2	A	25	0	16	9	0
2	B	25	0	17	1	0
2	C	25	0	17	2	0
2	D	25	0	16	2	0
2	E	25	0	16	6	0
2	F	30	0	6	14	0
2	G	25	0	16	3	0
2	H	30	0	4	5	0
2	I	25	0	17	2	0
2	J	25	0	15	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	25	0	15	4	0
2	L	30	0	6	5	0
3	A	8	0	6	2	0
3	B	8	0	6	1	0
3	C	4	0	3	2	0
3	D	4	0	3	1	0
3	E	8	0	6	4	0
3	F	4	0	3	1	0
3	G	4	0	3	1	0
3	H	4	0	3	2	0
3	I	12	0	9	0	0
3	L	4	0	3	0	0
4	A	48	0	0	1	0
4	B	51	0	0	3	0
4	C	43	0	0	5	0
4	D	49	0	0	1	0
4	E	46	0	0	2	0
4	F	41	0	0	5	0
4	G	52	0	0	2	0
4	H	48	0	0	3	0
4	I	56	0	0	1	0
4	J	17	0	0	1	0
4	K	11	0	0	0	0
4	L	37	0	0	3	0
All	All	33548	0	31738	515	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 8.

The worst 5 of 515 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:F:149[A]:OAS:HB2	2:F:1383[A]:CSC:C20	1.24	1.54
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:C20	1.89	1.48
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:H201	1.57	1.27
1:F:149[A]:OAS:OG	2:F:1383[A]:CSC:H202	1.40	1.21
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:H202	1.65	1.11

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:H:283:GLN:OE1	1:K:49:ARG:NH2[2_655]	1.99	0.21
1:G:283:GLN:OE1	1:J:49:ARG:NH2[1_556]	2.13	0.07

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%)	328 (96%)	11 (3%)	2 (1%)	22	39
1	B	343/444 (77%)	329 (96%)	12 (4%)	2 (1%)	22	39
1	C	344/444 (78%)	330 (96%)	13 (4%)	1 (0%)	37	56
1	D	340/444 (77%)	329 (97%)	9 (3%)	2 (1%)	22	39
1	E	339/444 (76%)	327 (96%)	10 (3%)	2 (1%)	22	39
1	F	334/444 (75%)	323 (97%)	10 (3%)	1 (0%)	37	56
1	G	335/444 (76%)	323 (96%)	11 (3%)	1 (0%)	37	56
1	H	336/444 (76%)	324 (96%)	11 (3%)	1 (0%)	37	56
1	I	341/444 (77%)	328 (96%)	11 (3%)	2 (1%)	22	39
1	J	337/444 (76%)	322 (96%)	14 (4%)	1 (0%)	37	56
1	K	334/444 (75%)	319 (96%)	14 (4%)	1 (0%)	37	56
1	L	333/444 (75%)	319 (96%)	13 (4%)	1 (0%)	37	56
All	All	4057/5328 (76%)	3901 (96%)	139 (3%)	17 (0%)	30	49

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ASP
1	B	363	ASP
1	C	363	ASP
1	D	363	ASP
1	E	363	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/371 (78%)	282 (97%)	8 (3%)	38	65
1	B	291/371 (78%)	281 (97%)	10 (3%)	32	58
1	C	292/371 (79%)	278 (95%)	14 (5%)	21	43
1	D	291/371 (78%)	284 (98%)	7 (2%)	44	70
1	E	288/371 (78%)	280 (97%)	8 (3%)	38	65
1	F	286/371 (77%)	279 (98%)	7 (2%)	44	70
1	G	287/371 (77%)	278 (97%)	9 (3%)	35	62
1	H	287/371 (77%)	279 (97%)	8 (3%)	38	65
1	I	289/371 (78%)	280 (97%)	9 (3%)	35	62
1	J	288/371 (78%)	276 (96%)	12 (4%)	25	49
1	K	286/371 (77%)	276 (96%)	10 (4%)	31	57
1	L	286/371 (77%)	278 (97%)	8 (3%)	38	65
All	All	3461/4452 (78%)	3351 (97%)	110 (3%)	34	60

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	69	TRP
1	I	48	SER
1	L	380	LEU
1	K	332	SER
1	G	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	269	GLN
1	L	382	GLN
1	H	382	GLN
1	L	373	ASN

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Mol	Chain	Res	Type
1	K	283	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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	F	149[A]	-	7,5,9	7.40	1 (14%)	5,5,11	7.09	3 (60%)
1	OAS	A	149[B]	-	7,8,9	1.26	1 (14%)	5,9,11	1.03	0
1	OAS	L	149[B]	-	7,8,9	1.21	1 (14%)	5,9,11	0.81	0
1	OAS	F	149[B]	-	7,8,9	1.28	1 (14%)	5,9,11	1.03	0
1	OAS	D	149[A]	-	7,5,9	7.41	1 (14%)	5,5,11	6.91	3 (60%)
1	OAS	D	149[B]	-	7,8,9	1.28	1 (14%)	5,9,11	1.28	1 (20%)
1	OAS	C	149[A]	-	7,5,9	7.41	1 (14%)	5,5,11	6.88	3 (60%)
1	OAS	E	149[A]	-	7,5,9	7.36	1 (14%)	5,5,11	7.17	3 (60%)
1	OAS	C	149[B]	-	7,8,9	1.33	1 (14%)	5,9,11	1.32	1 (20%)
1	OAS	E	149[B]	-	7,8,9	1.18	1 (14%)	5,9,11	1.23	1 (20%)
1	OAS	I	149[A]	-	7,5,9	8.41	1 (14%)	5,5,11	8.02	4 (80%)
1	OAS	G	149[A]	-	7,5,9	7.60	1 (14%)	5,5,11	7.20	3 (60%)
1	OAS	I	149[B]	-	7,8,9	1.30	1 (14%)	5,9,11	2.17	2 (40%)
1	OAS	G	149[B]	-	7,8,9	1.21	1 (14%)	5,9,11	1.16	0
1	OAS	K	149[A]	-	7,5,9	8.63	1 (14%)	5,5,11	7.43	3 (60%)
1	OAS	K	149[B]	-	7,8,9	1.24	1 (14%)	5,9,11	1.52	1 (20%)
1	OAS	L	149[A]	-	7,5,9	7.37	1 (14%)	5,5,11	7.20	3 (60%)
1	OAS	J	149[A]	-	7,5,9	8.35	1 (14%)	5,5,11	7.28	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OAS	H	149[A]	-	7,5,9	7.81	1 (14%)	5,5,11	7.35	3 (60%)
1	OAS	J	149[B]	-	7,8,9	1.30	1 (14%)	5,9,11	1.45	1 (20%)
1	OAS	B	149[A]	-	7,5,9	7.80	1 (14%)	5,5,11	7.35	3 (60%)
1	OAS	H	149[B]	-	7,8,9	1.20	1 (14%)	5,9,11	1.18	0
1	OAS	B	149[B]	-	7,8,9	1.14	1 (14%)	5,9,11	1.36	1 (20%)
1	OAS	A	149[A]	-	7,5,9	7.42	1 (14%)	5,5,11	7.51	3 (60%)

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	F	149[A]	-	-	4/5/4/9	-
1	OAS	A	149[B]	-	-	2/5/7/9	-
1	OAS	L	149[B]	-	-	2/5/7/9	-
1	OAS	F	149[B]	-	-	2/5/7/9	-
1	OAS	D	149[A]	-	-	4/5/4/9	-
1	OAS	D	149[B]	-	-	3/5/7/9	-
1	OAS	C	149[A]	-	-	4/5/4/9	-
1	OAS	E	149[A]	-	-	4/5/4/9	-
1	OAS	C	149[B]	-	-	2/5/7/9	-
1	OAS	E	149[B]	-	-	2/5/7/9	-
1	OAS	I	149[A]	-	-	4/5/4/9	-
1	OAS	G	149[A]	-	-	4/5/4/9	-
1	OAS	I	149[B]	-	-	4/5/7/9	-
1	OAS	G	149[B]	-	-	2/5/7/9	-
1	OAS	K	149[A]	-	-	4/5/4/9	-
1	OAS	K	149[B]	-	-	3/5/7/9	-
1	OAS	L	149[A]	-	-	4/5/4/9	-
1	OAS	J	149[A]	-	-	4/5/4/9	-
1	OAS	H	149[A]	-	-	4/5/4/9	-
1	OAS	J	149[B]	-	-	3/5/7/9	-
1	OAS	B	149[A]	-	-	4/5/4/9	-
1	OAS	H	149[B]	-	-	2/5/7/9	-
1	OAS	B	149[B]	-	-	3/5/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OAS	A	149[A]	-	-	4/5/4/9	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	149[A]	OAS	OG-C1A	22.79	2.43	1.33
1	I	149[A]	OAS	OG-C1A	22.15	2.40	1.33
1	J	149[A]	OAS	OG-C1A	22.02	2.39	1.33
1	H	149[A]	OAS	OG-C1A	20.61	2.33	1.33
1	B	149[A]	OAS	OG-C1A	20.59	2.32	1.33

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149[A]	OAS	CB-OG-C1A	-16.80	74.90	117.10
1	A	149[A]	OAS	CB-OG-C1A	-15.90	77.15	117.10
1	K	149[A]	OAS	CB-OG-C1A	-15.57	77.97	117.10
1	B	149[A]	OAS	CB-OG-C1A	-15.52	78.11	117.10
1	H	149[A]	OAS	CB-OG-C1A	-15.39	78.43	117.10

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149[A]	OAS	C-CA-CB-OG
1	B	149[A]	OAS	C-CA-CB-OG
1	B	149[B]	OAS	C-CA-CB-OG
1	C	149[A]	OAS	C-CA-CB-OG
1	D	149[A]	OAS	C-CA-CB-OG

There are no ring outliers.

21 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	149[A]	OAS	9	0
1	A	149[B]	OAS	3	0
1	L	149[B]	OAS	1	0
1	F	149[B]	OAS	1	0
1	D	149[A]	OAS	1	0
1	D	149[B]	OAS	1	0
1	C	149[A]	OAS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	149[A]	OAS	1	0
1	I	149[A]	OAS	2	0
1	G	149[A]	OAS	1	0
1	I	149[B]	OAS	3	0
1	K	149[A]	OAS	1	0
1	K	149[B]	OAS	1	0
1	L	149[A]	OAS	1	0
1	J	149[A]	OAS	1	0
1	H	149[A]	OAS	1	0
1	J	149[B]	OAS	1	0
1	B	149[A]	OAS	1	0
1	H	149[B]	OAS	1	0
1	B	149[B]	OAS	1	0
1	A	149[A]	OAS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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	C	1384	-	3,3,3	0.87	0	3,3,3	1.10	0
3	ACT	D	1384	-	3,3,3	0.82	0	3,3,3	0.88	0
2	CSC	I	1383[B]	-	25,26,29	1.48	5 (20%)	32,37,41	1.84	6 (18%)
3	ACT	E	1385	-	3,3,3	0.76	0	3,3,3	1.20	0
3	ACT	A	1384	-	3,3,3	0.79	0	3,3,3	1.09	0
3	ACT	F	1384	-	3,3,3	0.84	0	3,3,3	0.58	0
3	ACT	L	1384	-	3,3,3	0.78	0	3,3,3	0.96	0
2	CSC	K	1385[B]	-	25,26,29	1.44	4 (16%)	32,37,41	2.29	9 (28%)
2	CSC	E	1383[B]	-	25,26,29	1.29	4 (16%)	32,37,41	2.14	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	G	1384	-	3,3,3	0.71	0	3,3,3	0.95	0
2	CSC	B	1384[B]	-	25,26,29	1.49	5 (20%)	32,37,41	1.97	7 (21%)
2	CSC	J	1385[B]	-	25,26,29	1.49	4 (16%)	32,37,41	2.20	7 (21%)
2	CSC	H	1383[A]	-	28,29,29	1.39	6 (21%)	36,41,41	1.96	4 (11%)
2	CSC	H	1383[B]	-	28,26,29	1.62	6 (21%)	36,37,41	1.97	4 (11%)
3	ACT	A	1385	-	3,3,3	0.88	0	3,3,3	0.26	0
3	ACT	E	1384	-	3,3,3	0.76	0	3,3,3	1.25	0
2	CSC	G	1383[B]	-	25,26,29	1.49	5 (20%)	32,37,41	2.06	7 (21%)
3	ACT	I	1386	-	3,3,3	0.83	0	3,3,3	0.80	0
3	ACT	I	1384	-	3,3,3	0.93	0	3,3,3	0.25	0
2	CSC	A	1383[B]	-	25,26,29	1.35	5 (20%)	32,37,41	2.00	6 (18%)
3	ACT	B	1386	-	3,3,3	0.74	0	3,3,3	1.16	0
3	ACT	H	1384	-	3,3,3	0.75	0	3,3,3	0.95	0
2	CSC	F	1383[A]	-	28,29,29	1.41	4 (14%)	36,41,41	2.14	4 (11%)
2	CSC	F	1383[B]	-	28,26,29	1.33	3 (10%)	36,37,41	2.28	5 (13%)
3	ACT	B	1385	-	3,3,3	0.97	0	3,3,3	0.25	0
3	ACT	I	1385	-	3,3,3	0.97	0	3,3,3	0.58	0
2	CSC	C	1383[B]	-	25,26,29	1.38	3 (12%)	32,37,41	1.99	3 (9%)

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	B	1384[B]	-	-	8/20/49/52	0/2/2/2
2	CSC	J	1385[B]	-	-	8/20/49/52	0/2/2/2
2	CSC	H	1383[A]	-	-	9/23/52/52	0/2/2/2
2	CSC	F	1383[A]	-	-	10/23/52/52	0/2/2/2
2	CSC	E	1383[B]	-	-	4/20/49/52	0/2/2/2
2	CSC	H	1383[B]	-	-	11/23/49/52	0/2/2/2
2	CSC	F	1383[B]	-	-	8/23/49/52	0/2/2/2
2	CSC	G	1383[B]	-	-	4/20/49/52	0/2/2/2
2	CSC	I	1383[B]	-	-	8/20/49/52	0/2/2/2
2	CSC	K	1385[B]	-	-	9/20/49/52	0/2/2/2
2	CSC	A	1383[B]	-	-	5/20/49/52	0/2/2/2
2	CSC	C	1383[B]	-	-	6/20/49/52	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1383[B]	CSC	O1-C1	5.08	1.58	1.33
2	K	1385[B]	CSC	C4-N5	-4.38	1.32	1.41
2	J	1385[B]	CSC	C4-N5	-4.15	1.33	1.41
2	I	1383[B]	CSC	C4-N5	-4.13	1.33	1.41
2	B	1384[B]	CSC	C4-N5	-4.04	1.33	1.41

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1383[A]	CSC	C6-C7-N10	-8.29	100.16	118.27
2	F	1383[B]	CSC	C6-C7-N10	-8.29	100.16	118.27
2	G	1383[B]	CSC	S1-C6-N5	-6.80	97.02	110.48
2	H	1383[A]	CSC	C6-C7-N10	-6.47	104.12	118.27
2	H	1383[B]	CSC	C6-C7-N10	-6.47	104.12	118.27

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1383[B]	CSC	C2-C3-C3'-O1
2	A	1383[B]	CSC	C14-C15-C16-N17
2	A	1383[B]	CSC	C14-C15-C16-C18
2	B	1384[B]	CSC	C2-C3-C3'-O1
2	B	1384[B]	CSC	C4-C3-C3'-O1

There are no ring outliers.

20 monomers are involved in 63 short contacts:

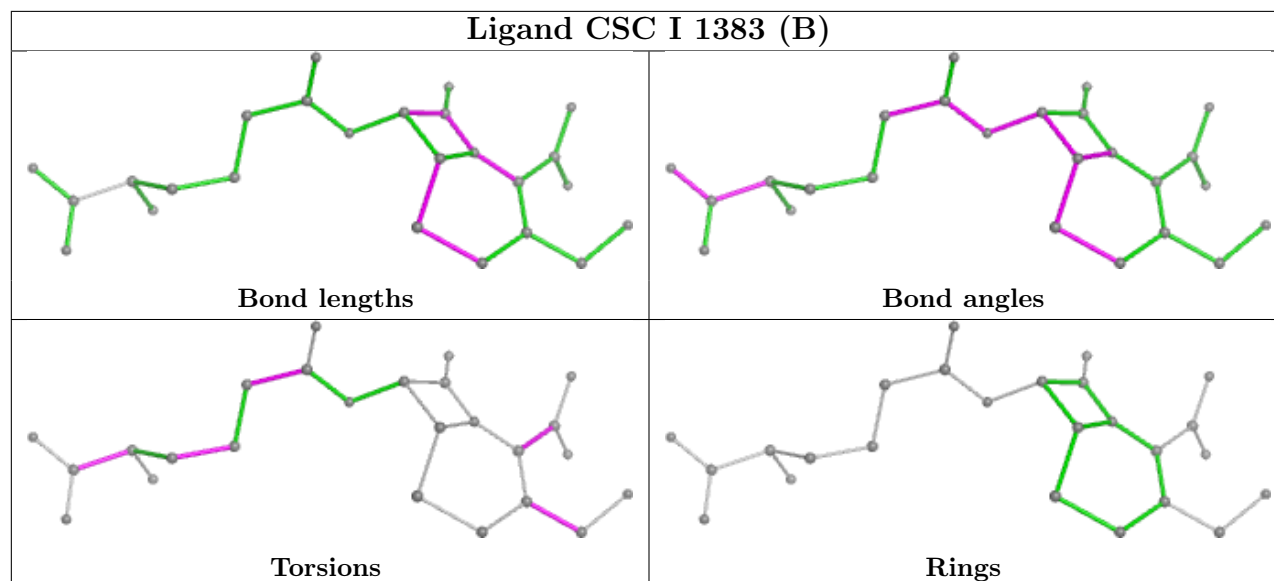
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1384	ACT	2	0
3	D	1384	ACT	1	0
2	I	1383[B]	CSC	2	0
3	A	1384	ACT	2	0
3	F	1384	ACT	1	0
2	K	1385[B]	CSC	4	0
2	E	1383[B]	CSC	6	0
3	G	1384	ACT	1	0
2	B	1384[B]	CSC	1	0
2	J	1385[B]	CSC	3	0
2	H	1383[A]	CSC	3	0

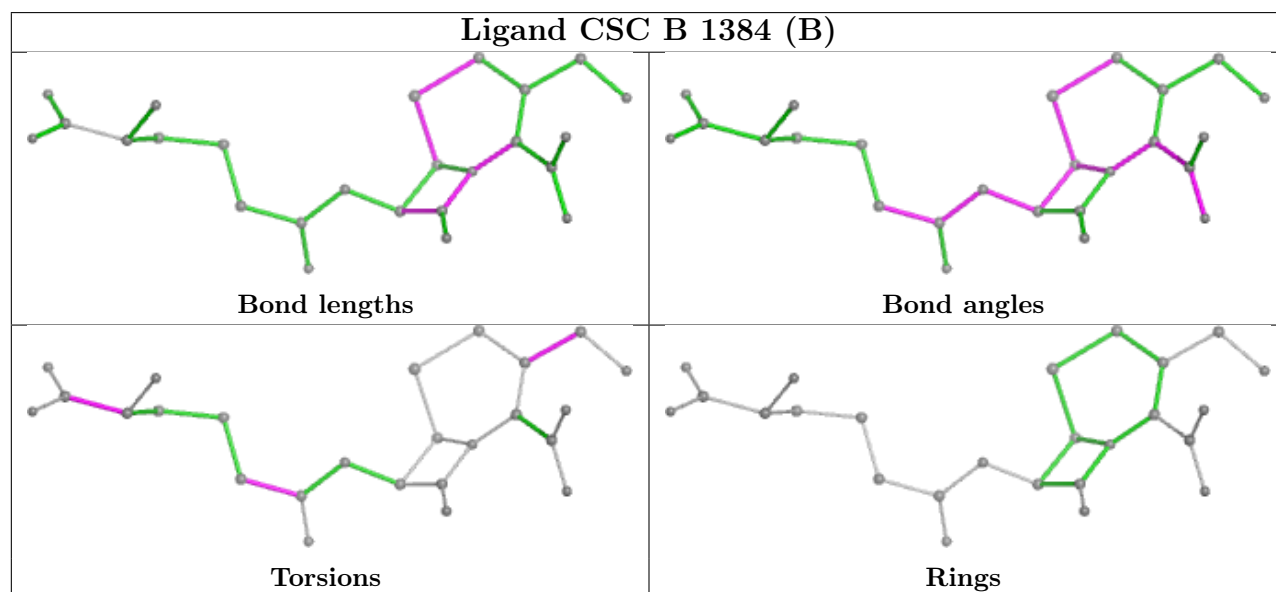
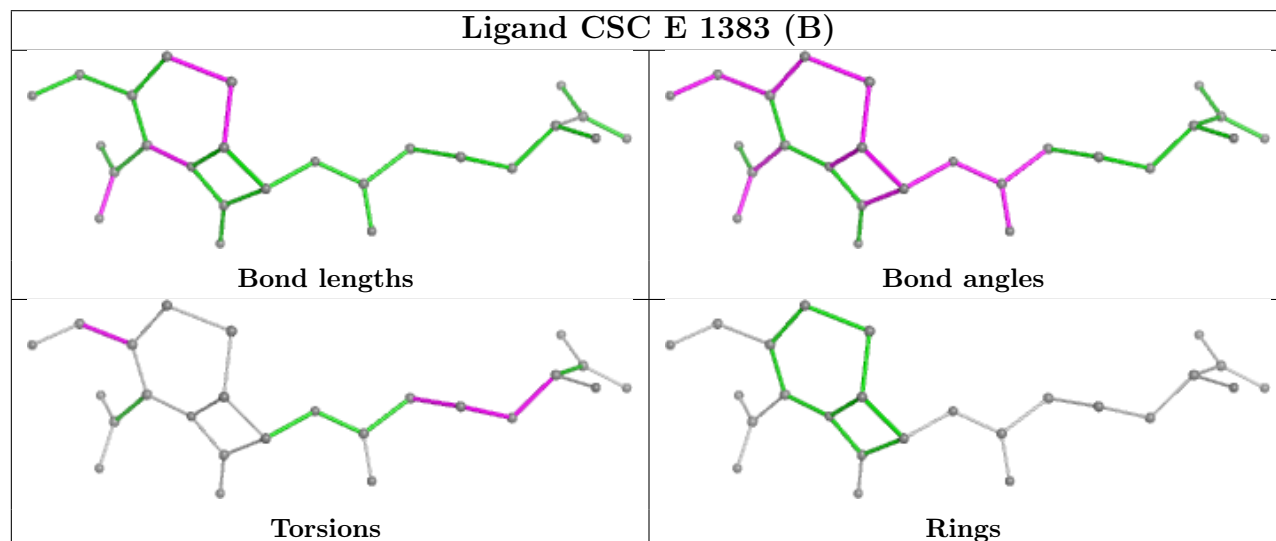
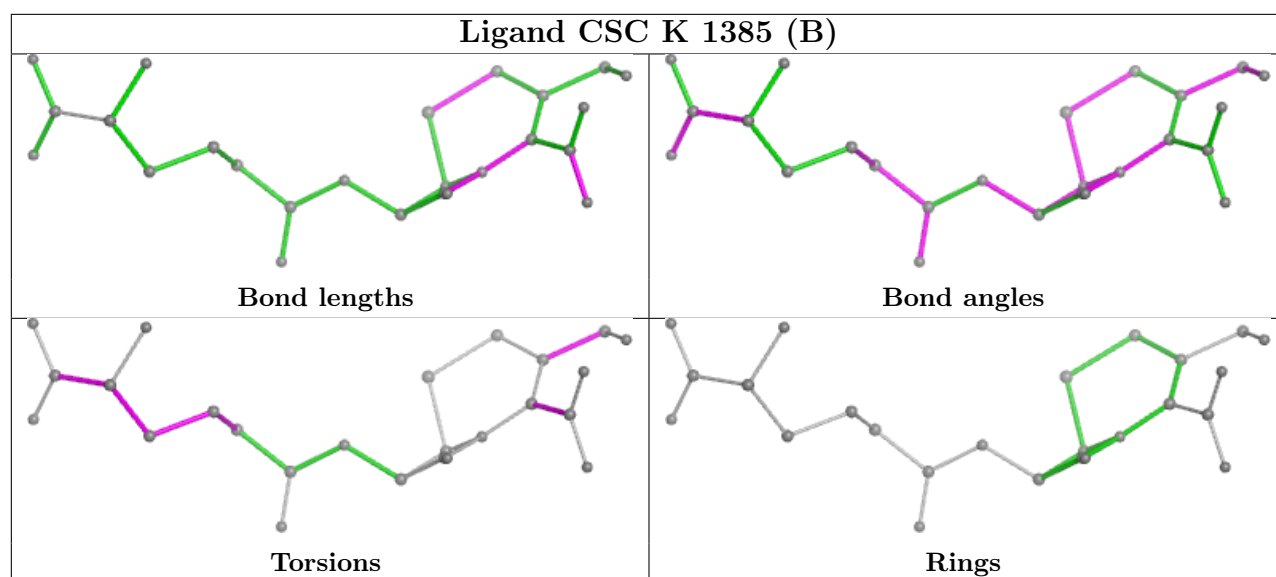
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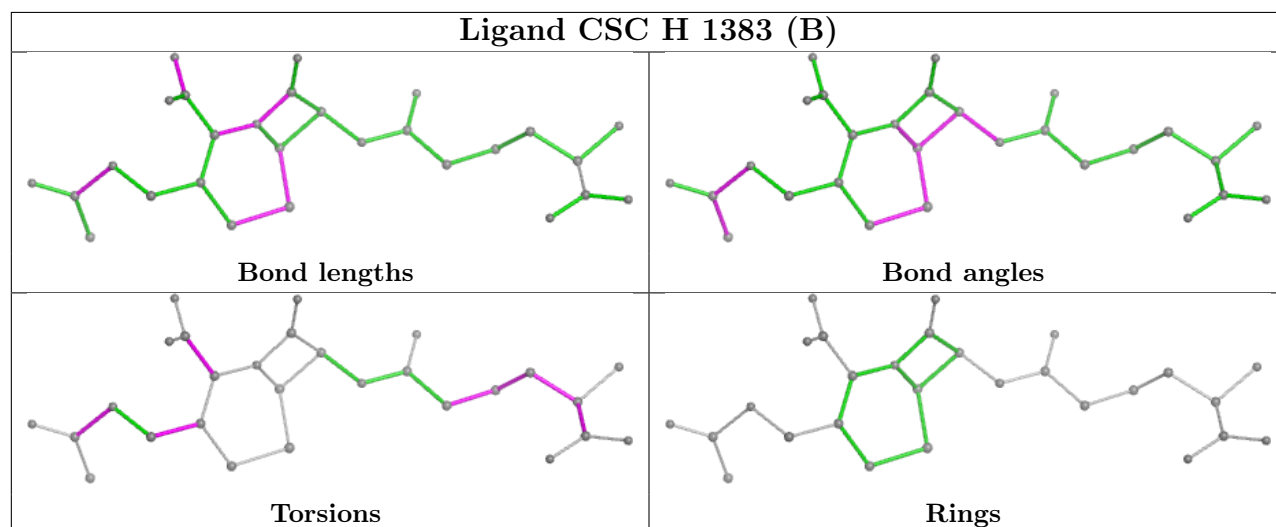
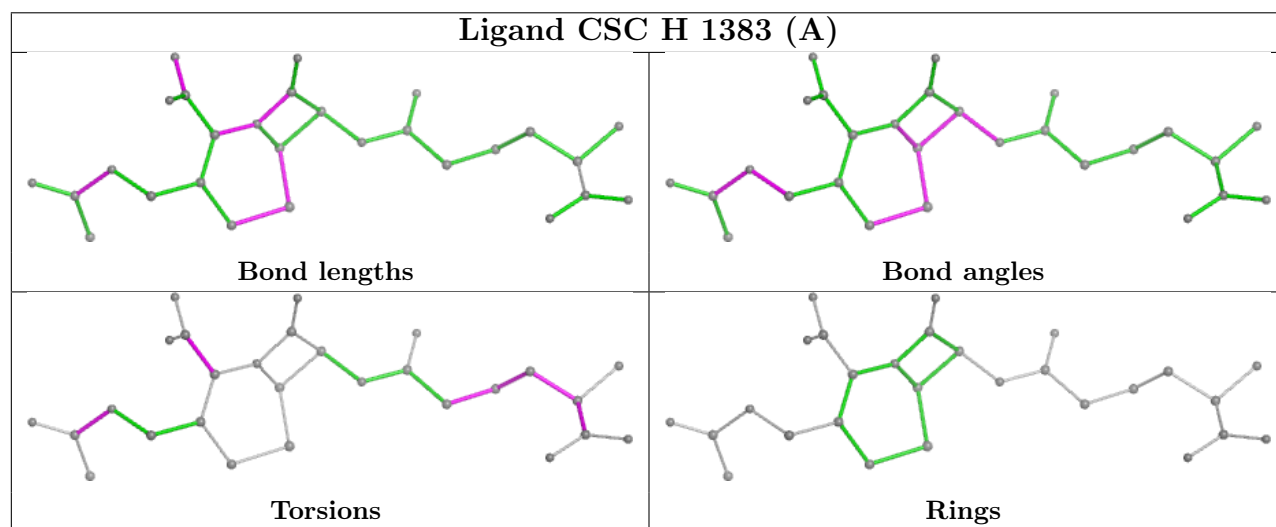
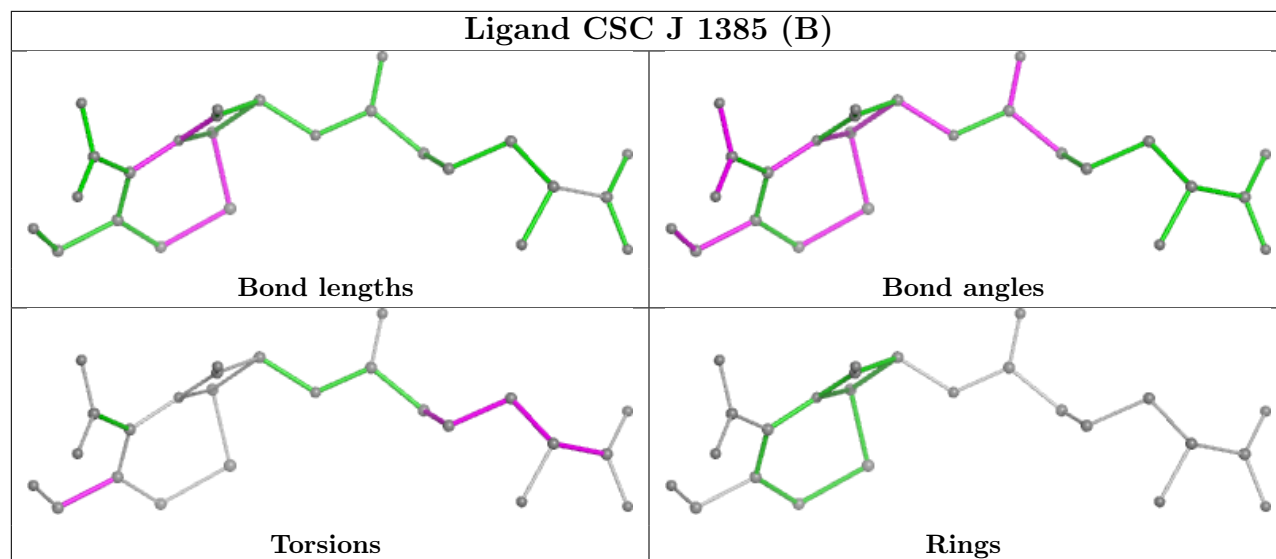
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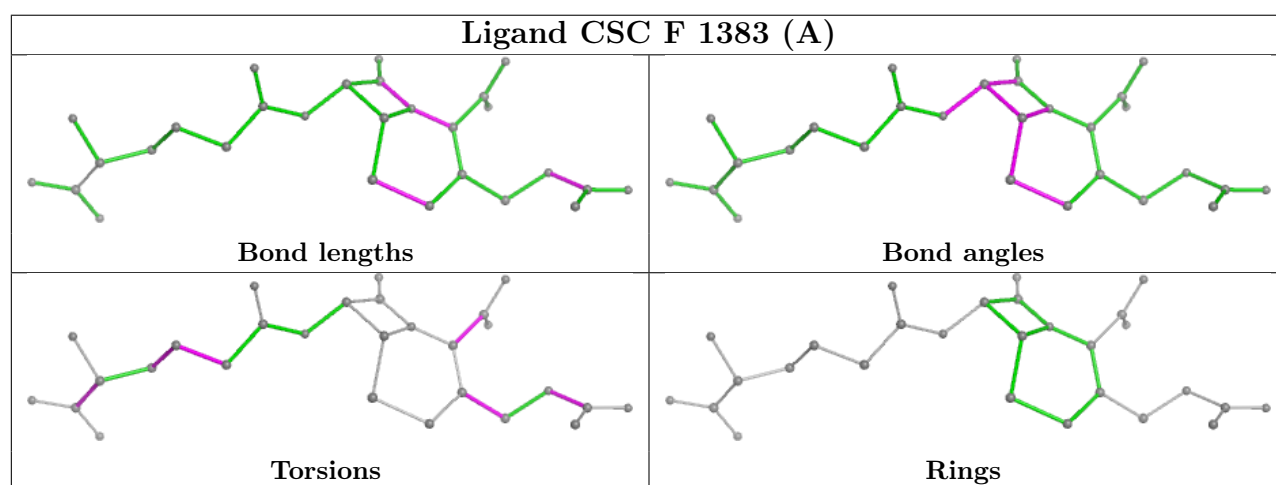
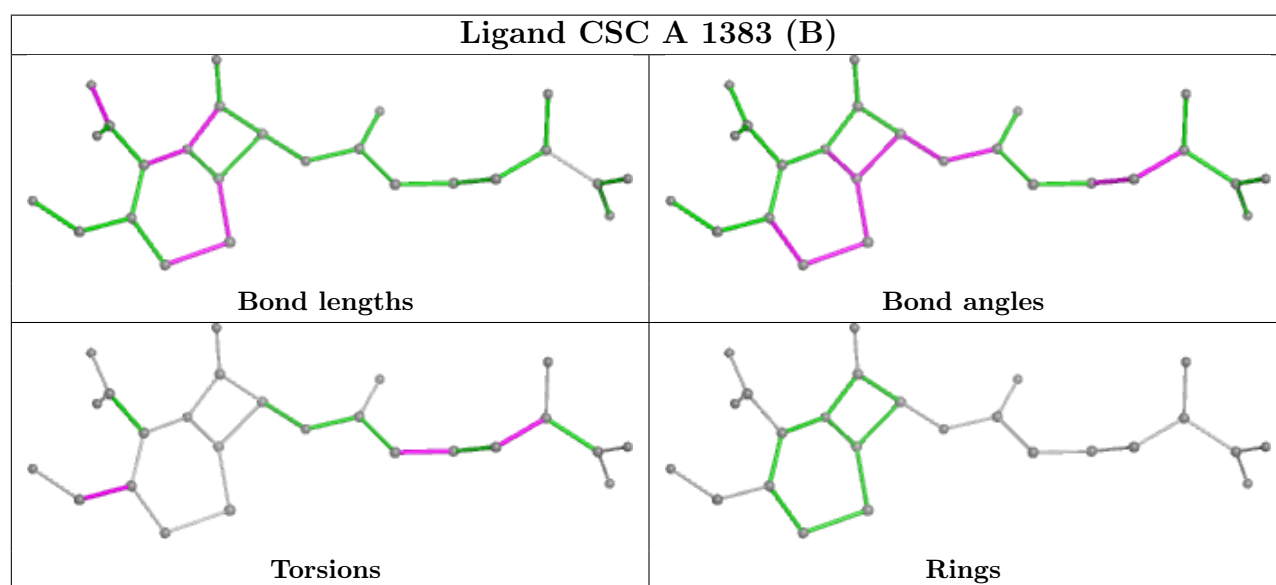
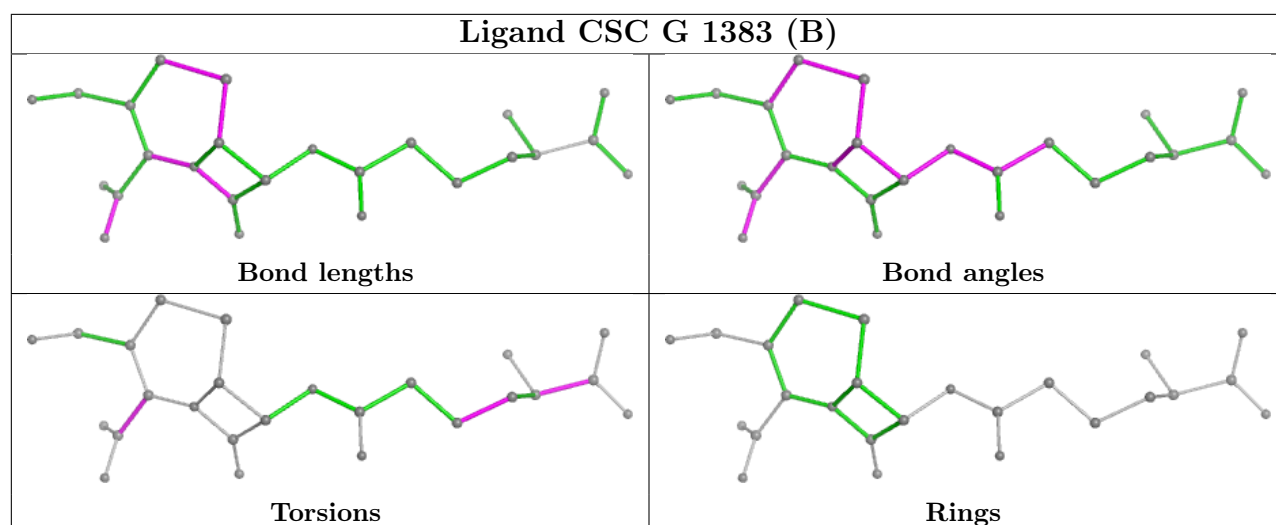
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1383[B]	CSC	2	0
3	E	1384	ACT	4	0
2	G	1383[B]	CSC	3	0
2	A	1383[B]	CSC	9	0
3	H	1384	ACT	2	0
2	F	1383[A]	CSC	12	0
2	F	1383[B]	CSC	2	0
3	B	1385	ACT	1	0
2	C	1383[B]	CSC	2	0

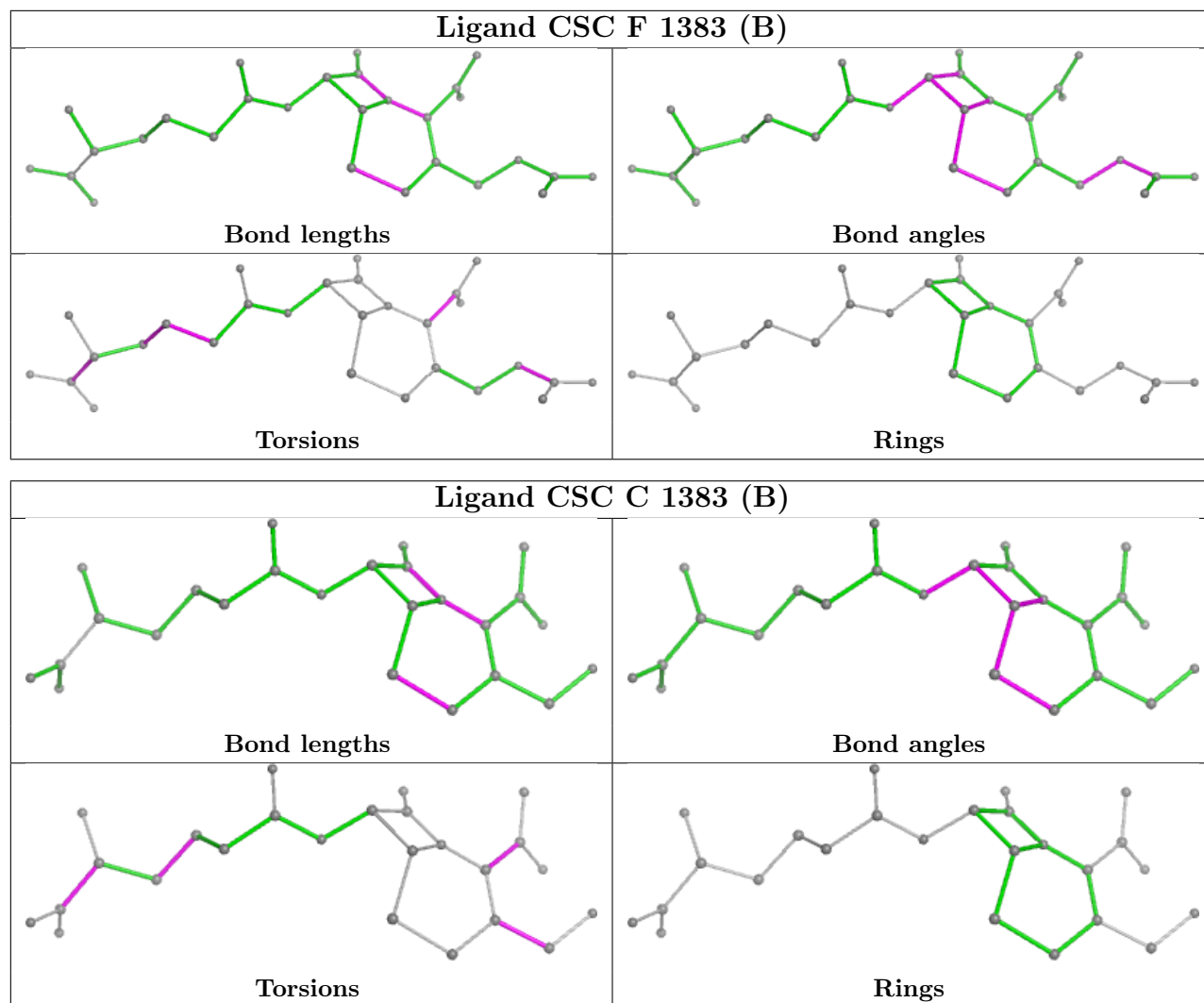
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	347/444 (78%)	-1.59	0 100 100	12, 27, 46, 60	1 (0%)
1	B	349/444 (78%)	-1.58	0 100 100	9, 27, 46, 67	2 (0%)
1	C	346/444 (77%)	-1.57	0 100 100	9, 26, 46, 60	3 (0%)
1	D	344/444 (77%)	-1.56	0 100 100	9, 26, 45, 55	3 (0%)
1	E	345/444 (77%)	-1.56	0 100 100	11, 27, 45, 61	2 (0%)
1	F	340/444 (76%)	-1.55	0 100 100	16, 27, 44, 59	1 (0%)
1	G	341/444 (76%)	-1.56	0 100 100	16, 26, 44, 53	2 (0%)
1	H	342/444 (77%)	-1.61	0 100 100	16, 26, 44, 59	3 (0%)
1	I	347/444 (78%)	-1.60	0 100 100	10, 26, 46, 67	2 (0%)
1	J	343/444 (77%)	-1.44	0 100 100	16, 27, 45, 65	1 (0%)
1	K	340/444 (76%)	-1.43	0 100 100	16, 27, 44, 53	1 (0%)
1	L	339/444 (76%)	-1.56	0 100 100	16, 27, 44, 53	2 (0%)
All	All	4123/5328 (77%)	-1.55	0 100 100	9, 27, 45, 67	23 (0%)

There are no RSRZ outliers to report.

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[A]	6/10	0.97	0.06	15,17,17,18	3
1	OAS	J	149[B]	9/10	0.97	0.06	8,16,17,18	6
1	OAS	C	149[A]	6/10	0.99	0.03	15,17,17,18	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OAS	C	149[B]	9/10	0.99	0.03	8,16,17,18	6
1	OAS	D	149[A]	6/10	0.99	0.03	15,16,17,18	3
1	OAS	D	149[B]	9/10	0.99	0.03	7,16,17,18	6
1	OAS	E	149[A]	6/10	0.99	0.03	15,17,17,17	3
1	OAS	E	149[B]	9/10	0.99	0.03	7,17,17,17	6
1	OAS	G	149[A]	6/10	0.99	0.05	15,17,17,17	3
1	OAS	G	149[B]	9/10	0.99	0.05	8,16,17,17	6
1	OAS	I	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	I	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	B	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	B	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	K	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	K	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	F	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	F	149[B]	9/10	1.00	0.02	8,16,17,17	6
1	OAS	A	149[A]	6/10	1.00	0.03	15,16,17,17	3
1	OAS	A	149[B]	9/10	1.00	0.03	8,16,17,17	6
1	OAS	H	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	H	149[B]	9/10	1.00	0.02	8,16,17,17	6
1	OAS	L	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	L	149[B]	9/10	1.00	0.02	8,16,17,17	6

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
3	ACT	G	1384	4/4	0.97	0.07	37,37,37,38	0
2	CSC	C	1383[B]	25/28	0.98	0.05	11,22,33,34	25
2	CSC	D	1383[B]	25/28	0.98	0.05	7,18,33,35	25
2	CSC	E	1383[B]	25/28	0.98	0.05	14,27,29,31	25
2	CSC	A	1383[B]	25/28	0.98	0.05	29,43,48,48	25
3	ACT	H	1384	4/4	0.98	0.06	37,37,38,38	0
3	ACT	I	1386	4/4	0.98	0.06	41,42,42,42	0

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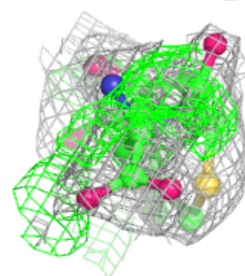
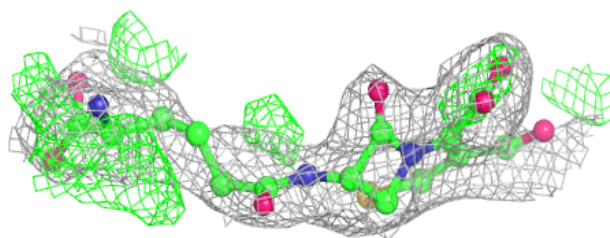
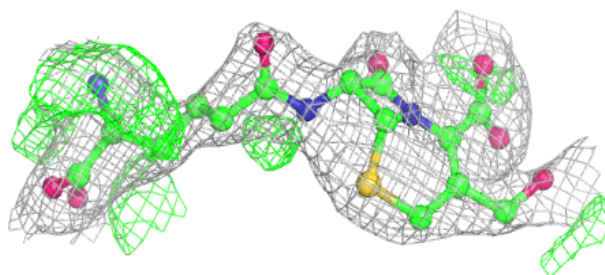
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSC	G	1383[B]	25/28	0.99	0.05	11,21,36,37	25
2	CSC	H	1383[A]	28/28	0.99	0.05	46,60,84,84	5
2	CSC	H	1383[B]	25/28	0.99	0.05	46,60,84,84	2
2	CSC	I	1383[B]	25/28	0.99	0.04	4,16,29,30	25
2	CSC	J	1385[B]	25/28	0.99	0.04	19,23,30,30	25
2	CSC	K	1385[B]	25/28	0.99	0.05	23,26,30,31	25
2	CSC	L	1383[B]	25/28	0.99	0.04	37,46,55,56	2
2	CSC	L	1383[A]	25/28	0.99	0.04	37,50,55,56	5
3	ACT	A	1384	4/4	0.99	0.03	26,26,27,27	0
3	ACT	A	1385	4/4	0.99	0.06	43,44,44,45	0
3	ACT	B	1385	4/4	0.99	0.03	30,31,31,33	0
3	ACT	B	1386	4/4	0.99	0.07	35,37,37,39	0
3	ACT	D	1384	4/4	0.99	0.03	23,24,24,25	0
3	ACT	E	1384	4/4	0.99	0.04	25,26,26,26	0
3	ACT	E	1385	4/4	0.99	0.04	39,39,40,40	0
3	ACT	F	1384	4/4	0.99	0.06	40,40,40,40	0
2	CSC	B	1384[B]	25/28	0.99	0.04	11,19,28,29	25
2	CSC	F	1383[A]	28/28	0.99	0.04	39,51,61,62	5
3	ACT	I	1384	4/4	0.99	0.03	26,28,28,30	0
3	ACT	I	1385	4/4	0.99	0.04	37,37,38,40	0
2	CSC	F	1383[B]	25/28	0.99	0.04	39,49,61,62	2
3	ACT	L	1384	4/4	0.99	0.05	43,43,43,44	0
3	ACT	C	1384	4/4	1.00	0.05	22,22,22,23	0

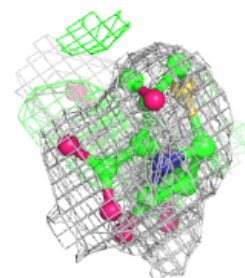
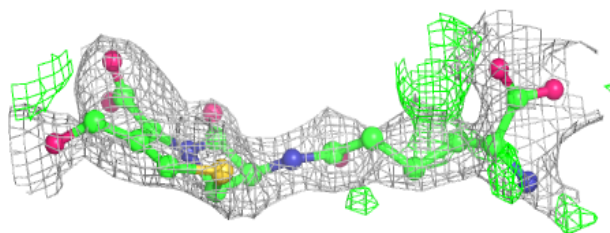
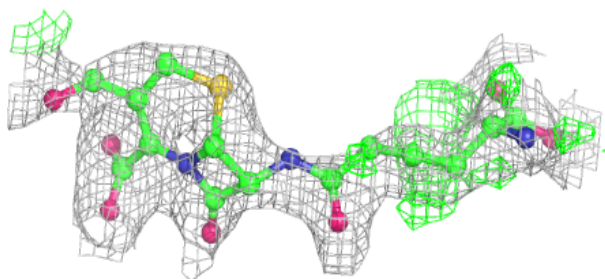
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CSC C 1383 (B):

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

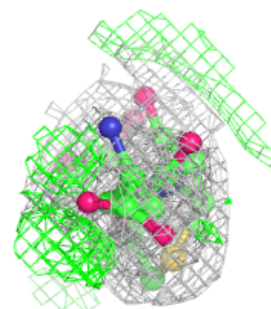
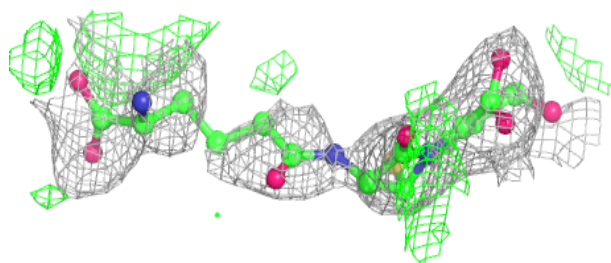
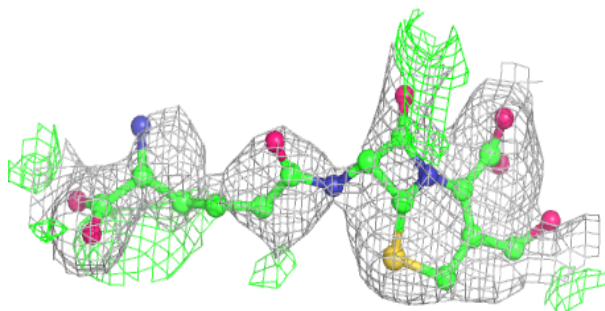
**Electron density around CSC E 1383 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

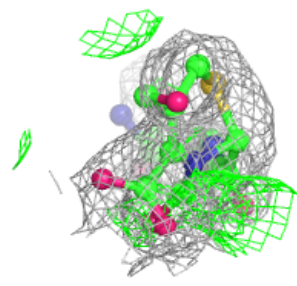
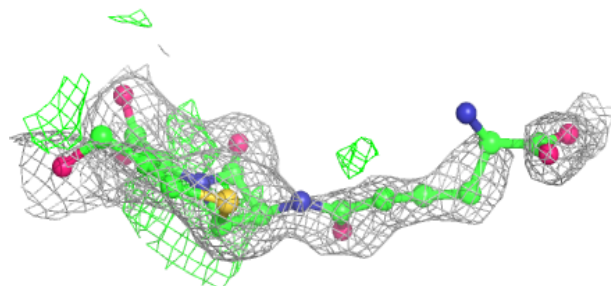
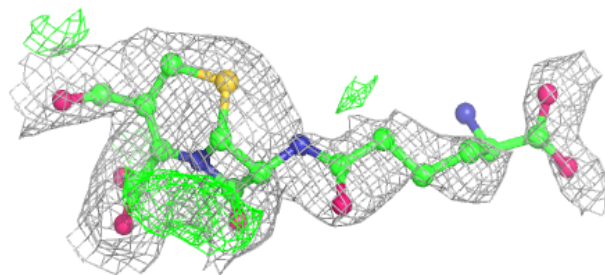


Electron density around CSC A 1383 (B):

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

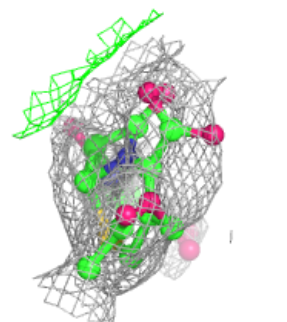
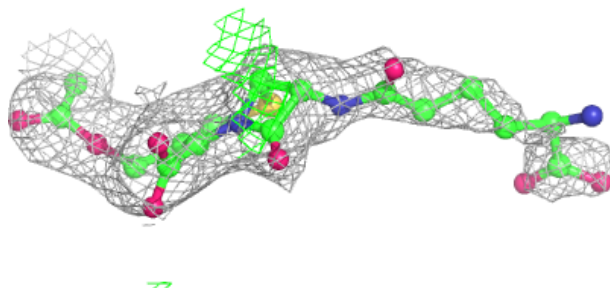
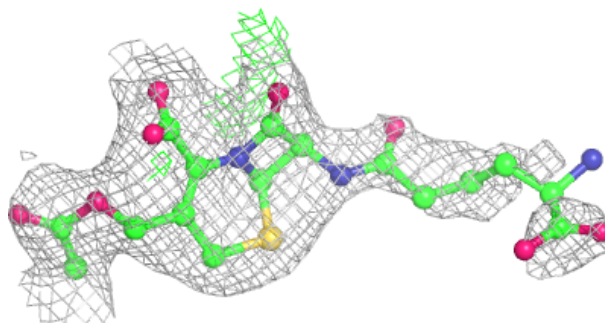
**Electron density around CSC G 1383 (B):**

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

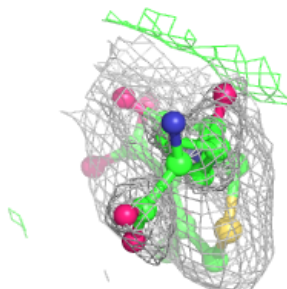
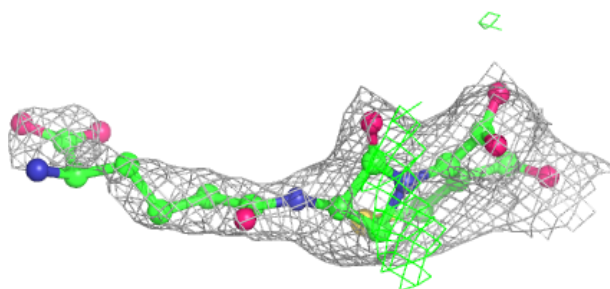
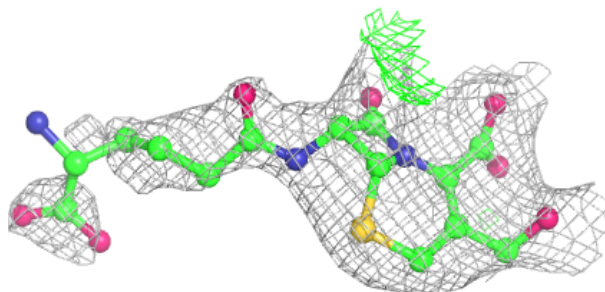


Electron density around CSC H 1383 (A):

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

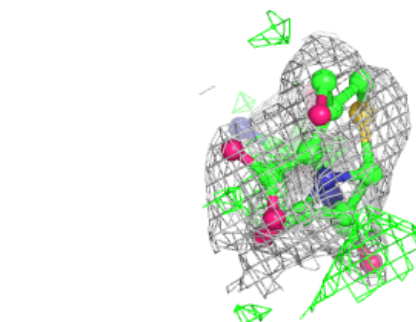
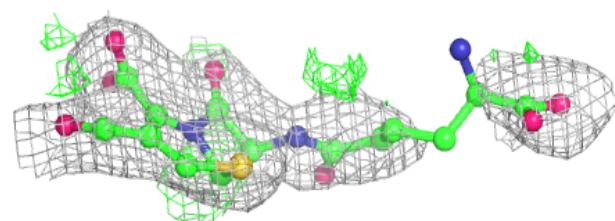
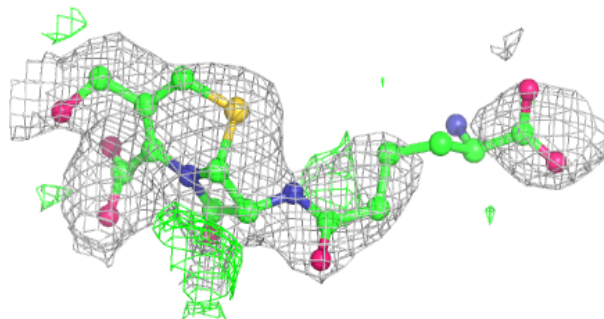
**Electron density around CSC H 1383 (B):**

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and green (positive)

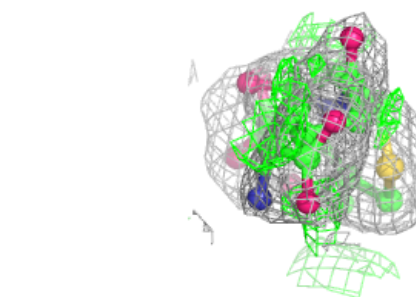
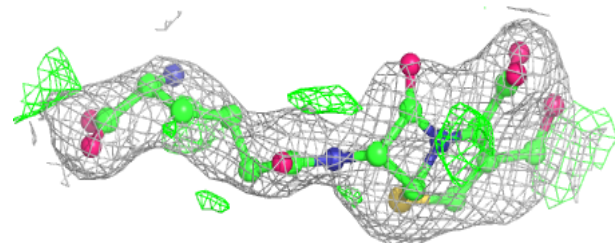
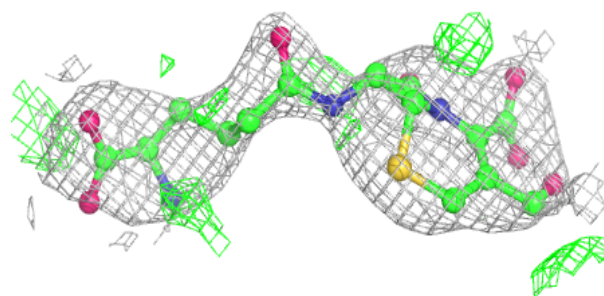


Electron density around CSC I 1383 (B):

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

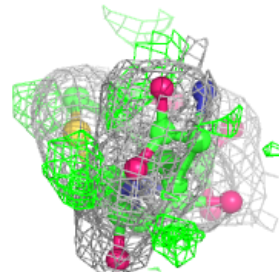
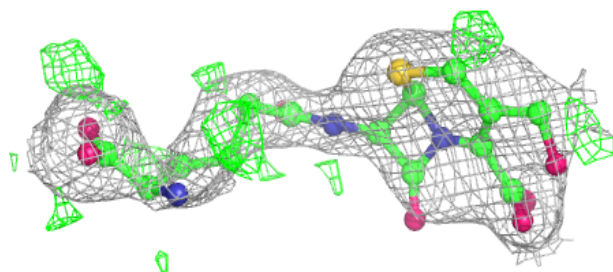
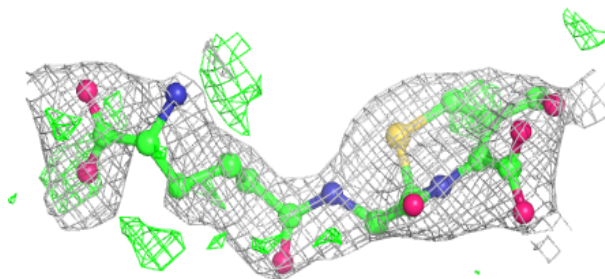
**Electron density around CSC J 1385 (B):**

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and green (positive)

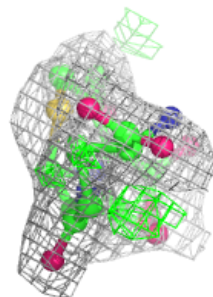
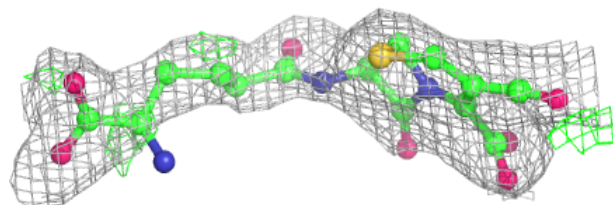
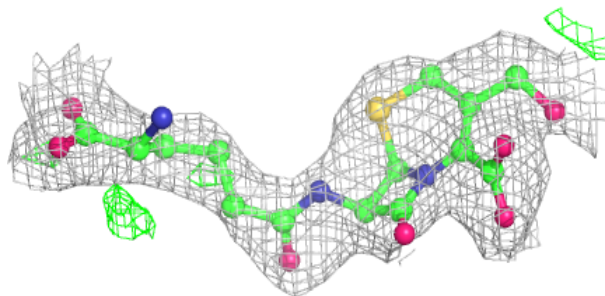


Electron density around CSC K 1385 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

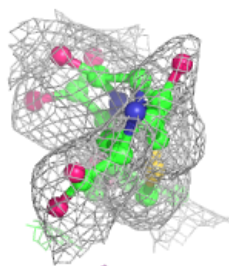
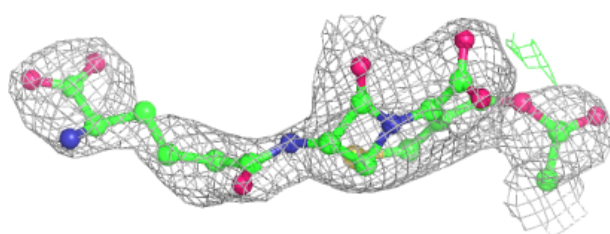
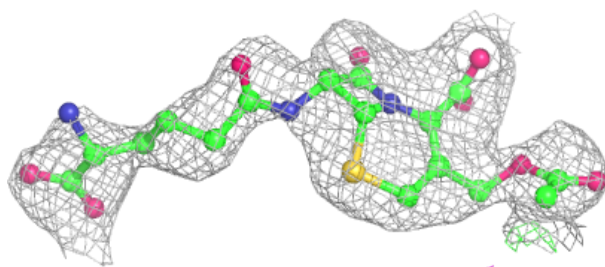
**Electron density around CSC B 1384 (B):**

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

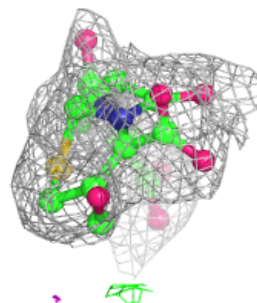
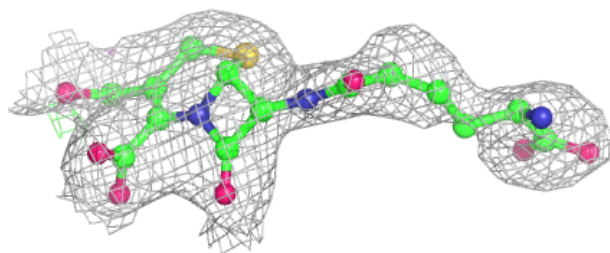
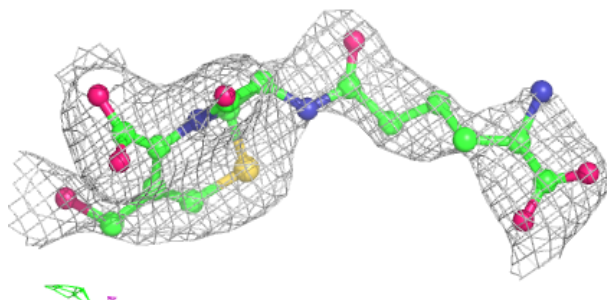


Electron density around CSC F 1383 (A):

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

**Electron density around CSC F 1383 (B):**

$2mF_o-DF_c$ (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.