



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 01:52 PM EDT

PDB ID : 1YAJ / pdb\_00001yaj  
Title : Crystal Structure of Human Liver Carboxylesterase in complex with benzil  
Authors : Fleming, C.D.; Bencharit, S.; Edwards, C.C.; Hyatt, J.L.; Morton, C.M.;  
Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.  
Deposited on : 2004-12-17  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

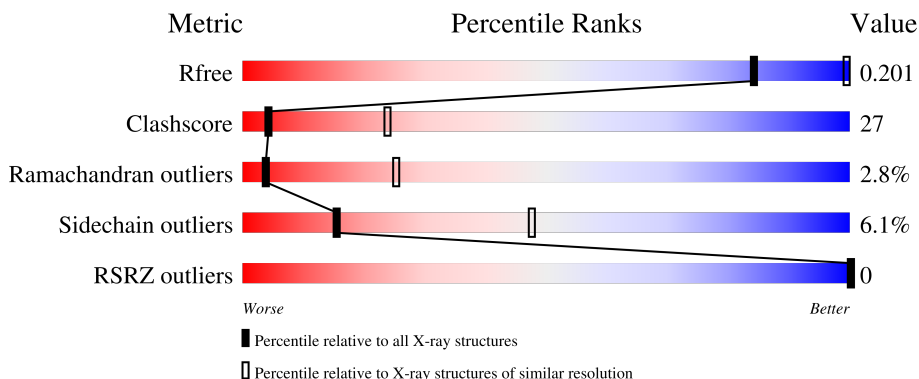
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.





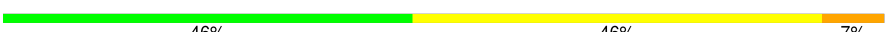



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	532	<div> <div>50%</div> <div>45%</div> <div>6%</div> </div>
1	B	532	<div> <div>54%</div> <div>41%</div> <div>5%</div> </div>
1	C	532	<div> <div>54%</div> <div>41%</div> <div>5%</div> </div>
1	D	532	<div> <div>49%</div> <div>44%</div> <div>6%</div> </div>
1	E	532	<div> <div>51%</div> <div>45%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	532	
1	G	532	
1	H	532	
1	I	532	
1	J	532	
1	K	532	
1	L	532	

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	NAG	B	1279	X	-	-	-
2	NAG	F	2379	X	-	-	-
2	NAG	G	3179	X	-	-	-
2	NAG	J	4179	X	-	-	-
2	NAG	K	4279	X	-	-	-
3	SIA	A	1181	-	-	X	-
5	BEZ	A	11	-	X	-	-
5	BEZ	B	12	-	X	X	-
5	BEZ	D	2385	-	X	-	-
5	BEZ	G	3386	-	X	-	-
5	BEZ	H	3387	-	X	-	-

## 2 Entry composition

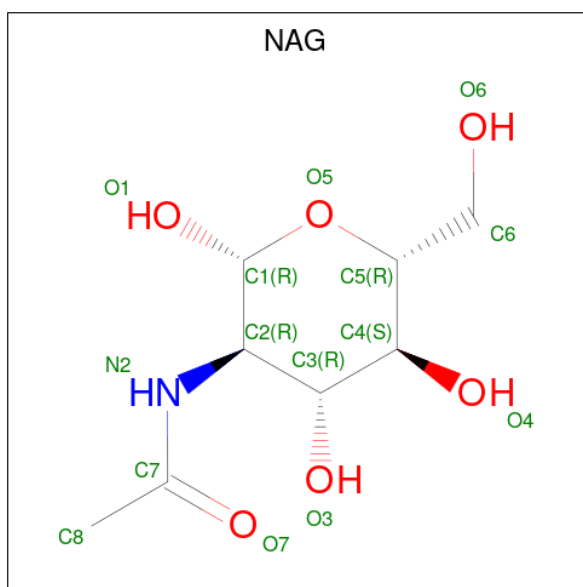
There are 6 unique types of molecules in this entry. The entry contains 50793 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CES1 protein.

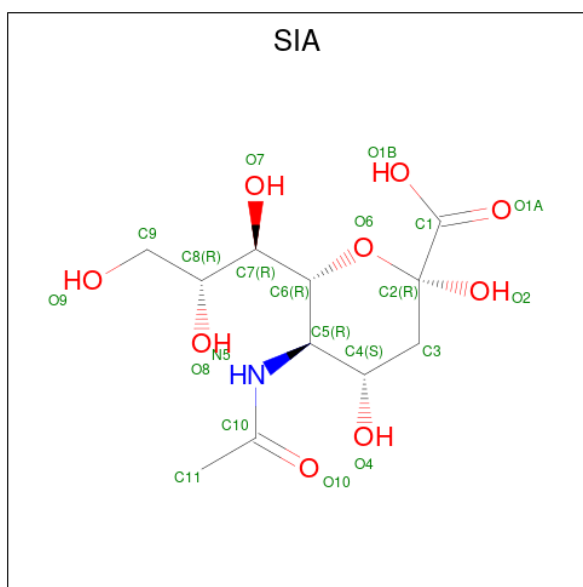
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	C	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	F	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	532	Total	C	N	O	S	0	0	0
			4129	2662	685	762	20			
1	I	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	J	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	K	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	L	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



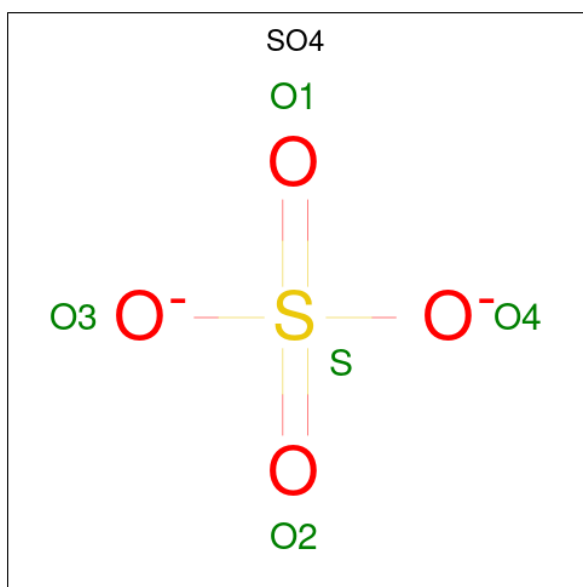
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	D	1	Total	C	N	O	0	0
			21	11	1	9		
3	E	1	Total	C	N	O	0	0
			21	11	1	9		
3	F	1	Total	C	N	O	0	0
			21	11	1	9		
3	G	1	Total	C	N	O	0	0
			21	11	1	9		
3	H	1	Total	C	N	O	0	0
			21	11	1	9		
3	I	1	Total	C	N	O	0	0
			21	11	1	9		
3	J	1	Total	C	N	O	0	0
			21	11	1	9		
3	K	1	Total	C	N	O	0	0
			21	11	1	9		
3	L	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



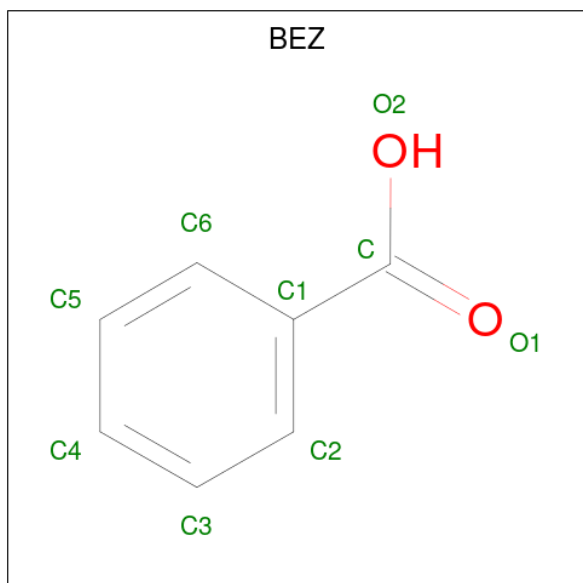
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is BENZOIC ACID (CCD ID: BEZ) (formula:  $C_7H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	C	1	Total	C	O	0	0
			8	7	1		
5	C	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	F	1	Total	C	O	0	0
			8	7	1		
5	F	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	J	1	Total	C	O	0	0
			8	7	1		
5	J	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			9	7	2		
5	L	1	Total	C	O	0	0
			9	7	2		

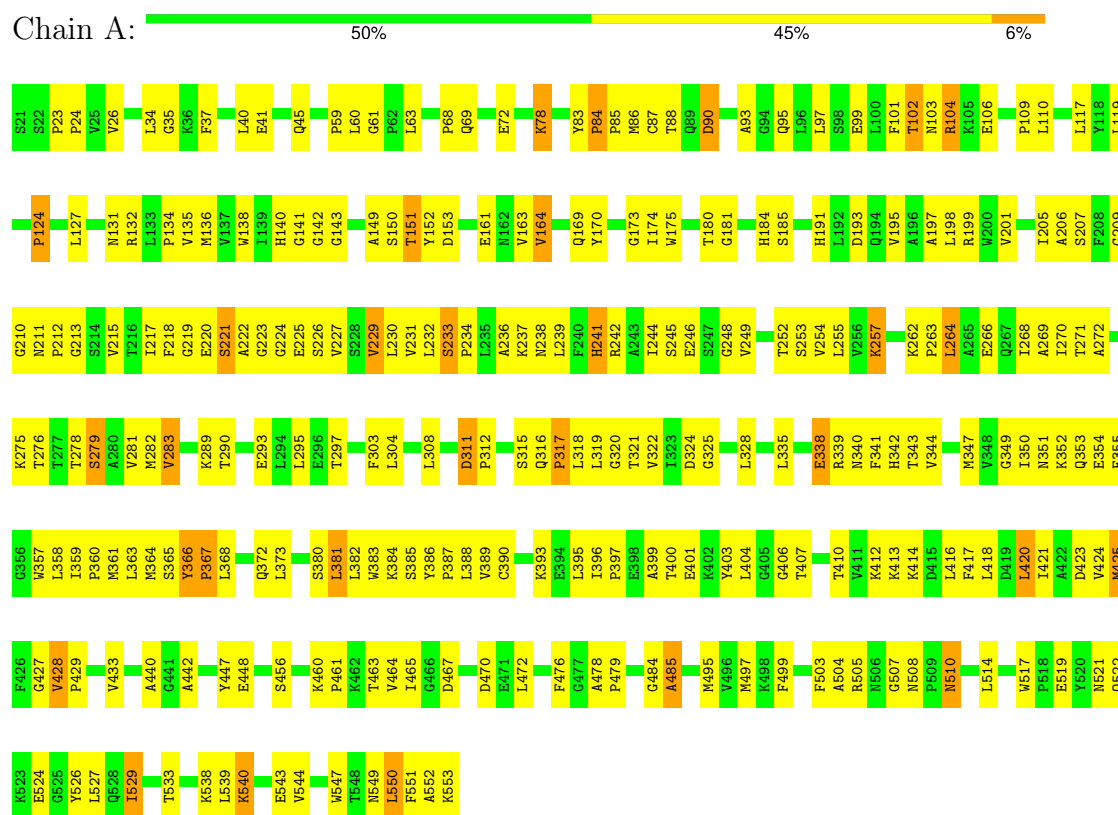
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	30	Total	O	0	0
			30	30		
6	C	33	Total	O	0	0
			33	33		
6	D	49	Total	O	0	0
			49	49		
6	E	38	Total	O	0	0
			38	38		
6	F	42	Total	O	0	0
			42	42		
6	G	41	Total	O	0	0
			41	41		
6	H	37	Total	O	0	0
			37	37		
6	I	34	Total	O	0	0
			34	34		
6	J	38	Total	O	0	0
			38	38		
6	K	50	Total	O	0	0
			50	50		
6	L	39	Total	O	0	0
			39	39		

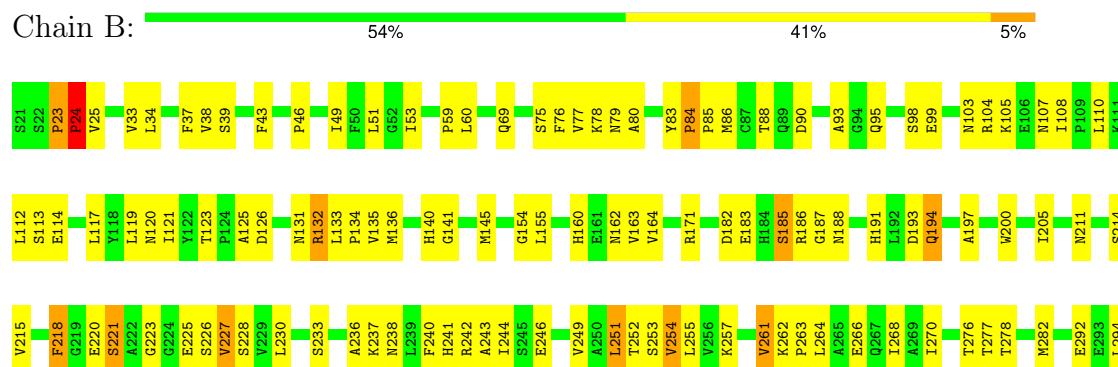
### 3 Residue-property plots

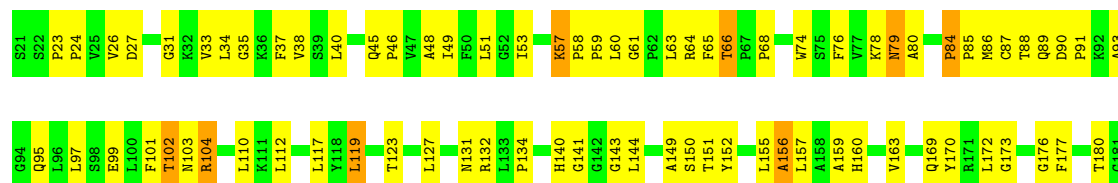
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

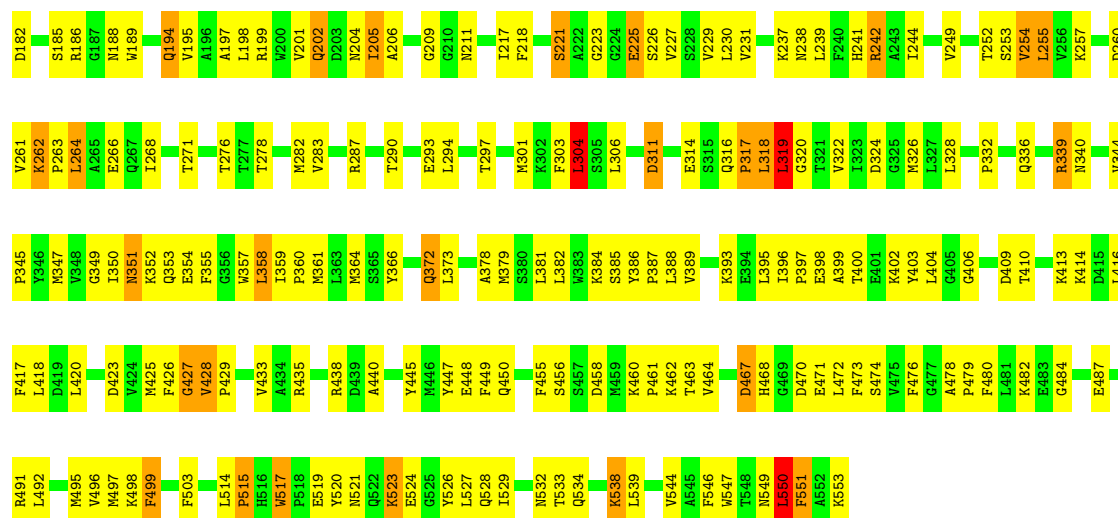
#### • Molecule 1: CES1 protein



#### • Molecule 1: CES1 protein

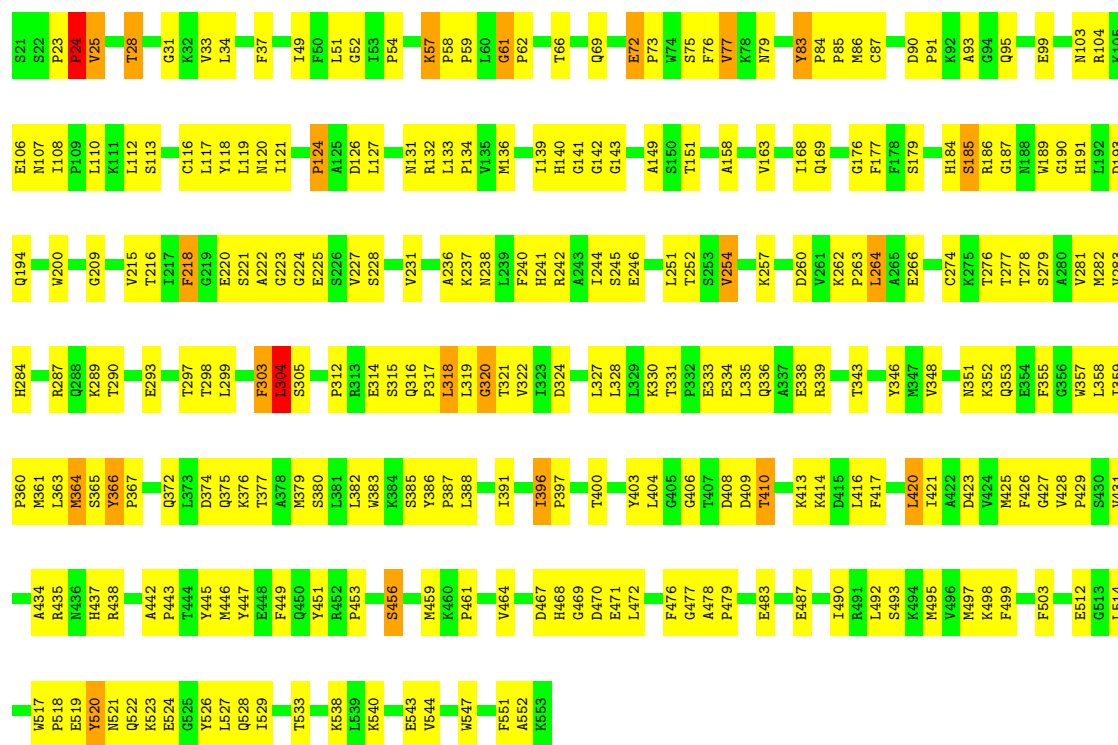






• Molecule 1: CES1 protein

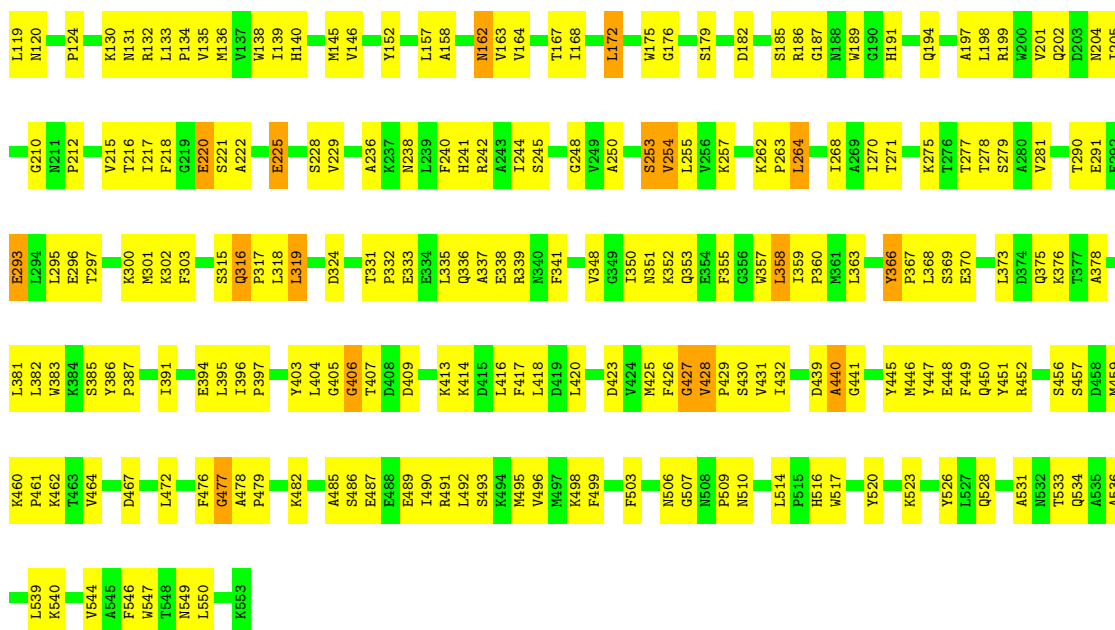
Chain E: 51% 45%



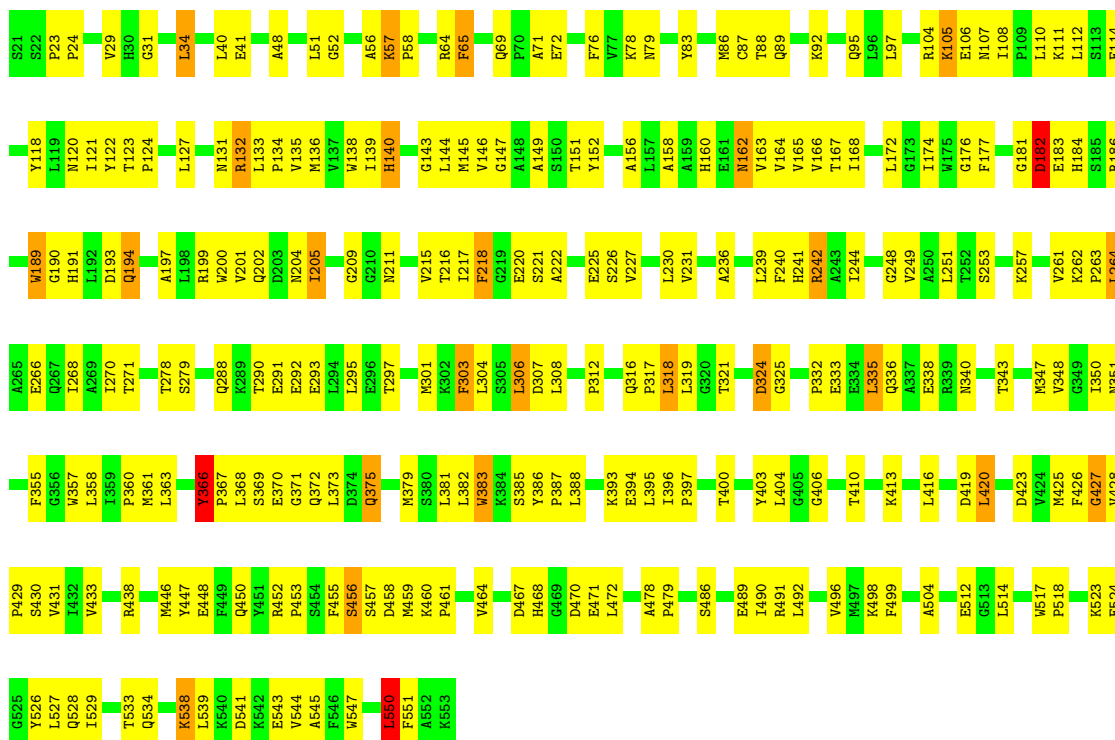
• Molecule 1: CES1 protein

Chain F: 53% 43%



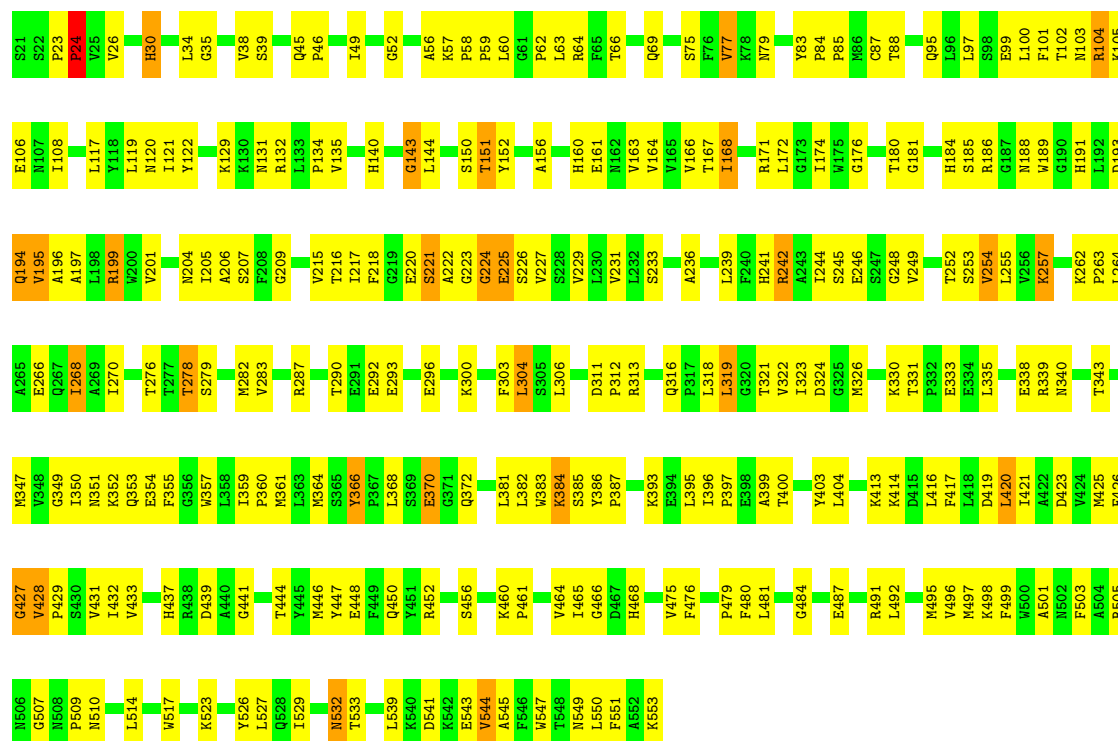


- Molecule 1: CES1 protein



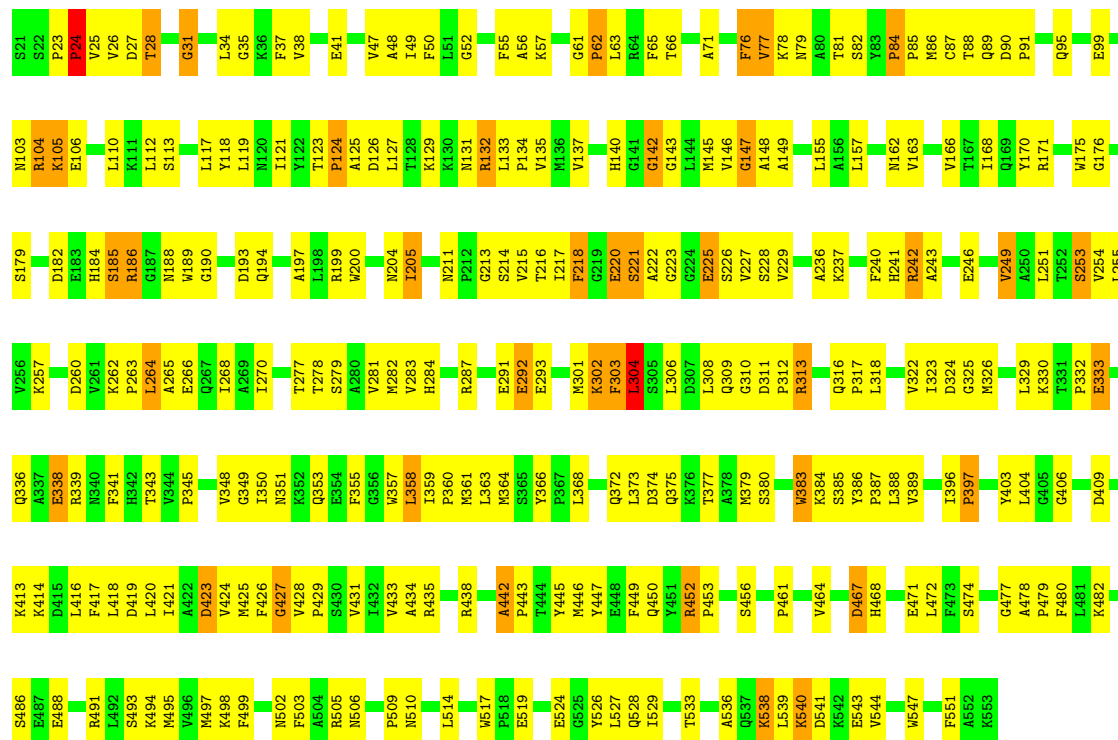
- Molecule 1: CES1 protein





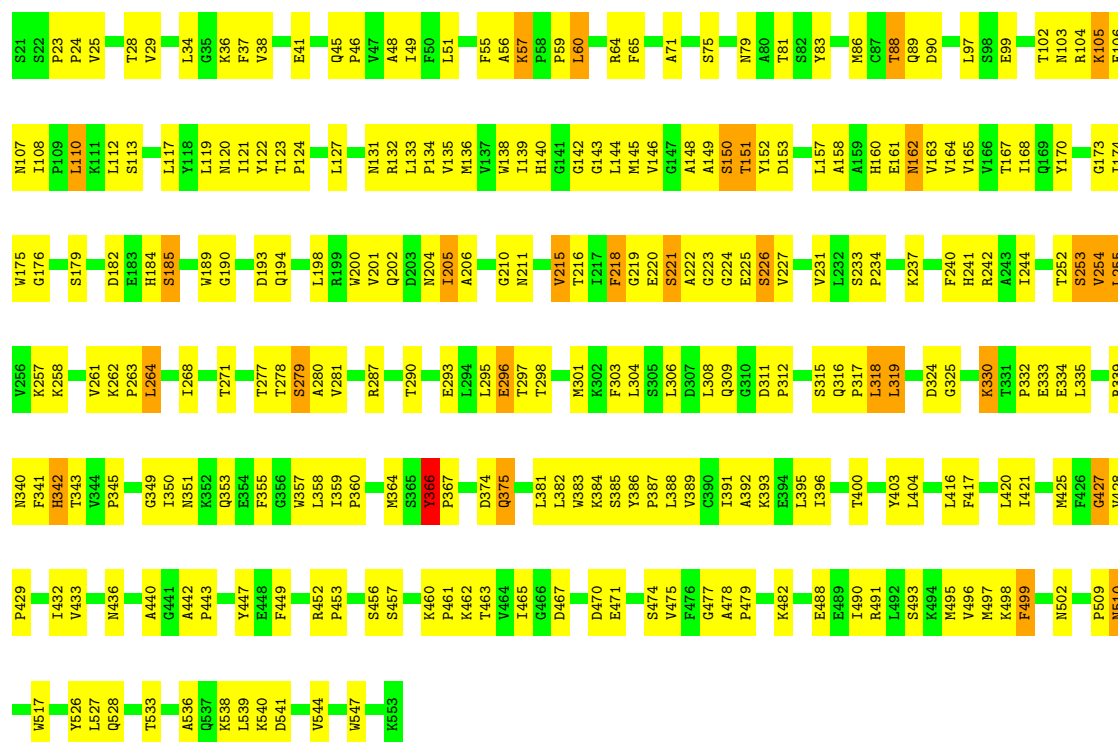
• Molecule 1: CES1 protein

Chain I: 46% 46% 7%



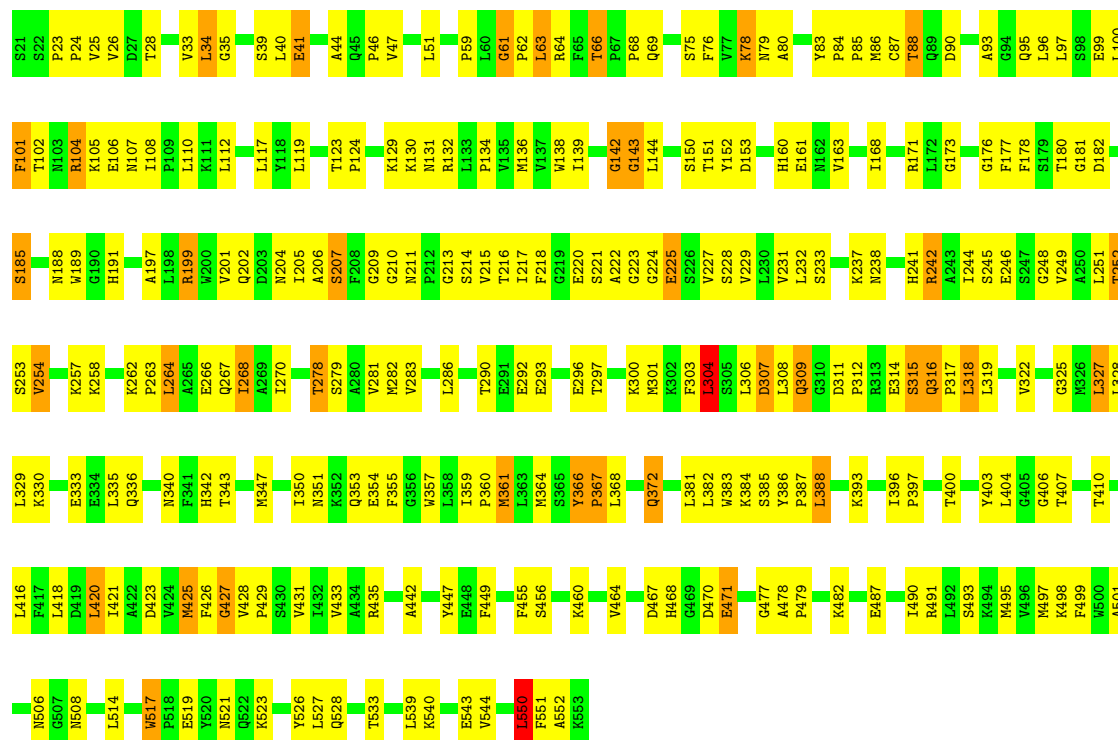
• Molecule 1: CES1 protein

Chain J: 



● Molecule 1: CES1 protein

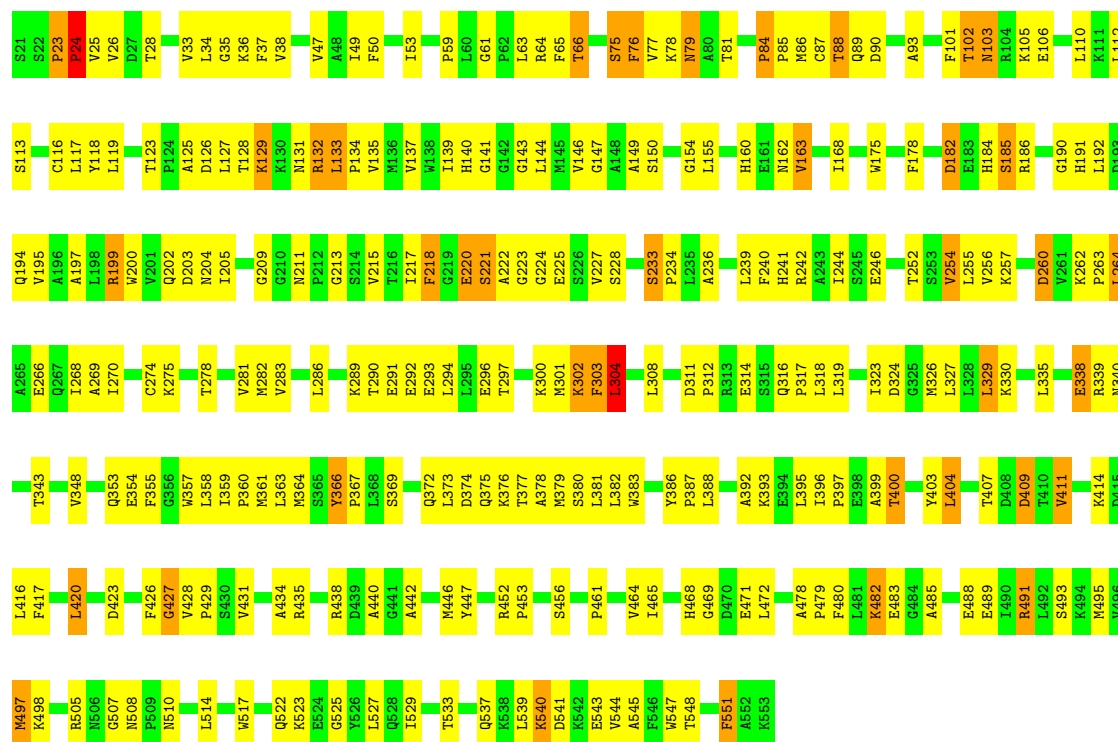
Chain K: 





• Molecule 1: CES1 protein

Chain L:  49% 43% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.56Å 181.49Å 202.71Å 90.12° 89.93° 89.72°	Depositor
Resolution (Å)	54.56 – 3.20 54.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.56-3.20) 95.8 (54.56-3.20)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.287 0.198 , 0.201	Depositor DCC
$R_{free}$ test set	6249 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-l 0.377 for -h,k,-l 0.389 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	50793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BEZ, SO4, SIA

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	0.82	3/4236 (0.1%)	1.09	21/5754 (0.4%)
1	B	0.76	2/4237 (0.0%)	1.02	19/5754 (0.3%)
1	C	0.75	3/4237 (0.1%)	1.01	13/5754 (0.2%)
1	D	0.73	1/4236 (0.0%)	1.04	19/5754 (0.3%)
1	E	0.86	6/4237 (0.1%)	1.09	27/5754 (0.5%)
1	F	0.78	5/4237 (0.1%)	1.01	10/5754 (0.2%)
1	G	0.99	12/4236 (0.3%)	1.15	20/5754 (0.3%)
1	H	0.80	4/4235 (0.1%)	1.06	24/5752 (0.4%)
1	I	0.97	15/4237 (0.4%)	1.10	33/5754 (0.6%)
1	J	0.76	3/4237 (0.1%)	0.99	11/5754 (0.2%)
1	K	0.76	3/4236 (0.1%)	1.04	25/5754 (0.4%)
1	L	0.74	4/4237 (0.1%)	1.02	13/5754 (0.2%)
All	All	0.81	61/50838 (0.1%)	1.05	235/69046 (0.3%)

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	D	0	1
1	G	0	2
1	K	0	1
All	All	0	4

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	550	LEU	CA-C	26.19	1.87	1.52
1	G	550	LEU	C-N	-25.11	1.00	1.33
1	E	24	PRO	CA-C	21.23	1.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	24	PRO	CA-C	20.29	1.77	1.52
1	B	24	PRO	CA-C	18.73	1.76	1.52

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	550	LEU	CA-C-O	-25.60	93.51	120.90
1	G	550	LEU	O-C-N	21.68	144.63	122.09
1	G	181	GLY	N-CA-C	-16.07	94.02	114.92
1	G	303	PHE	N-CA-C	15.51	128.19	111.28
1	E	303	PHE	N-CA-C	14.48	130.20	112.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	550	LEU	Mainchain
1	G	550	LEU	Mainchain
1	G	57	LYS	Mainchain
1	K	550	LEU	Mainchain

## 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	4130	0	4131	240	0
1	B	4131	0	4130	193	0
1	C	4131	0	4130	213	0
1	D	4130	0	4130	221	0
1	E	4131	0	4131	215	0
1	F	4131	0	4130	198	0
1	G	4130	0	4129	198	0
1	H	4129	0	4131	216	0
1	I	4131	0	4131	240	0
1	J	4131	0	4129	227	0
1	K	4130	0	4130	234	0
1	L	4131	0	4131	245	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	3	0
2	G	14	0	13	1	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	1	0
2	K	14	0	13	2	0
2	L	14	0	13	0	0
3	A	42	0	36	13	0
3	B	21	0	18	5	0
3	D	21	0	18	8	0
3	E	21	0	18	2	0
3	F	21	0	18	1	0
3	G	21	0	18	6	0
3	H	21	0	18	1	0
3	I	21	0	18	6	0
3	J	21	0	18	5	0
3	K	21	0	18	7	0
3	L	21	0	18	7	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	1	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
5	A	18	0	10	2	0
5	B	18	0	11	6	0
5	C	17	0	10	4	0
5	D	18	0	11	3	0
5	E	18	0	10	0	0
5	F	17	0	10	0	0
5	G	18	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	18	0	10	1	0
5	I	18	0	10	1	0
5	J	17	0	10	0	0
5	K	18	0	10	0	0
5	L	18	0	10	1	0
6	A	43	0	0	11	0
6	B	30	0	0	5	0
6	C	33	0	0	5	0
6	D	49	0	0	9	0
6	E	38	0	0	16	0
6	F	42	0	0	4	0
6	G	41	0	0	8	0
6	H	37	0	0	8	0
6	I	34	0	0	10	0
6	J	38	0	0	9	0
6	K	50	0	0	11	0
6	L	39	0	0	12	0
All	All	50793	0	50057	2672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 2672 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)
5:B:12:BEZ:C2	5:B:12:BEZ:C3	1.76	1.62
1:B:24:PRO:C	1:B:24:PRO:CA	1.76	1.59
5:B:12:BEZ:C2	5:B:12:BEZ:C1	1.78	1.59
5:B:12:BEZ:C5	5:B:12:BEZ:C6	1.74	1.58
1:I:24:PRO:CA	1:I:24:PRO:C	1.77	1.57

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/532 (100%)	451 (85%)	67 (13%)	12 (2%)	5	29
1	B	530/532 (100%)	448 (84%)	65 (12%)	17 (3%)	3	22
1	C	530/532 (100%)	467 (88%)	54 (10%)	9 (2%)	7	36
1	D	530/532 (100%)	454 (86%)	60 (11%)	16 (3%)	3	23
1	E	530/532 (100%)	438 (83%)	80 (15%)	12 (2%)	5	29
1	F	530/532 (100%)	464 (88%)	51 (10%)	15 (3%)	4	25
1	G	530/532 (100%)	445 (84%)	62 (12%)	23 (4%)	2	16
1	H	530/532 (100%)	449 (85%)	71 (13%)	10 (2%)	6	34
1	I	530/532 (100%)	451 (85%)	60 (11%)	19 (4%)	3	20
1	J	530/532 (100%)	444 (84%)	74 (14%)	12 (2%)	5	29
1	K	530/532 (100%)	451 (85%)	64 (12%)	15 (3%)	4	25
1	L	530/532 (100%)	434 (82%)	80 (15%)	16 (3%)	3	23
All	All	6360/6384 (100%)	5396 (85%)	788 (12%)	176 (3%)	4	25

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	SER
1	B	358	LEU
1	E	185	SER
1	E	358	LEU
1	E	456	SER

### 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	448/448 (100%)	423 (94%)	25 (6%)	17	50
1	B	448/448 (100%)	423 (94%)	25 (6%)	17	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	448/448 (100%)	419 (94%)	29 (6%)	14	45
1	D	448/448 (100%)	419 (94%)	29 (6%)	14	45
1	E	448/448 (100%)	418 (93%)	30 (7%)	13	44
1	F	448/448 (100%)	429 (96%)	19 (4%)	25	58
1	G	448/448 (100%)	417 (93%)	31 (7%)	13	43
1	H	448/448 (100%)	425 (95%)	23 (5%)	20	53
1	I	448/448 (100%)	420 (94%)	28 (6%)	15	46
1	J	448/448 (100%)	424 (95%)	24 (5%)	18	51
1	K	448/448 (100%)	417 (93%)	31 (7%)	13	43
1	L	448/448 (100%)	415 (93%)	33 (7%)	11	40
All	All	5376/5376 (100%)	5049 (94%)	327 (6%)	15	47

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	313	ARG
1	K	372	GLN
1	I	506	ASN
1	J	457	SER
1	L	129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	528	GLN
1	J	131	ASN
1	H	549	ASN
1	I	372	GLN
1	J	353	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

72 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
5	BEZ	I	3380	-	9,9,9	1.55	1 (11%)	11,11,11	1.62	4 (36%)
5	BEZ	K	4387	-	9,9,9	3.36	6 (66%)	11,11,11	1.24	2 (18%)
4	SO4	I	3285	-	4,4,4	0.43	0	6,6,6	0.12	0
3	SIA	D	2180	-	21,21,21	0.91	0	24,31,31	1.00	1 (4%)
2	NAG	H	3279	1	14,14,15	0.76	0	17,19,21	0.88	0
5	BEZ	D	2385	-	9,9,9	14.32	9 (100%)	11,11,11	3.19	9 (81%)
5	BEZ	E	2387	-	9,9,9	1.57	1 (11%)	11,11,11	1.47	4 (36%)
4	SO4	B	1284	-	4,4,4	0.42	0	6,6,6	0.05	0
2	NAG	E	2279	1	14,14,15	0.55	0	17,19,21	1.10	1 (5%)
3	SIA	I	982	-	21,21,21	0.85	1 (4%)	24,31,31	1.00	2 (8%)
5	BEZ	G	3385	-	9,9,9	1.86	1 (11%)	11,11,11	1.71	4 (36%)
2	NAG	L	4379	1	14,14,15	0.57	0	17,19,21	0.85	1 (5%)
3	SIA	A	1180	-	21,21,21	0.82	0	24,31,31	1.07	1 (4%)
4	SO4	C	1285	-	4,4,4	0.43	0	6,6,6	0.11	0
4	SO4	F	2185	-	4,4,4	0.42	0	6,6,6	0.19	0
5	BEZ	D	2386	-	9,9,9	3.61	7 (77%)	11,11,11	1.26	1 (9%)
5	BEZ	F	5023	1	8,8,9	2.33	5 (62%)	9,9,11	0.70	0
4	SO4	A	1184	-	4,4,4	0.36	0	6,6,6	0.08	0
5	BEZ	J	5041	1	8,8,9	2.37	4 (50%)	9,9,11	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	H	3385	-	4,4,4	0.43	0	6,6,6	0.13	0
5	BEZ	K	4386	-	9,9,9	1.68	1 (11%)	11,11,11	1.41	2 (18%)
5	BEZ	G	3386	-	9,9,9	5.57	7 (77%)	11,11,11	4.35	6 (54%)
4	SO4	D	2384	-	4,4,4	0.45	0	6,6,6	0.16	0
5	BEZ	H	3387	-	9,9,9	4.05	5 (55%)	11,11,11	5.05	7 (63%)
4	SO4	F	2285	-	4,4,4	0.42	0	6,6,6	0.12	0
4	SO4	D	2184	-	4,4,4	0.38	0	6,6,6	0.08	0
4	SO4	J	4185	-	4,4,4	0.42	0	6,6,6	0.26	0
2	NAG	G	3179	1	14,14,15	0.85	0	17,19,21	0.93	1 (5%)
2	NAG	A	1179	1	14,14,15	0.70	0	17,19,21	0.73	1 (5%)
5	BEZ	H	3386	-	9,9,9	1.62	1 (11%)	11,11,11	1.55	3 (27%)
3	SIA	B	1280	-	21,21,21	0.84	0	24,31,31	1.36	4 (16%)
2	NAG	K	4279	1	14,14,15	0.86	0	17,19,21	0.69	0
5	BEZ	C	5014	-	9,9,9	2.30	3 (33%)	11,11,11	1.55	2 (18%)
5	BEZ	J	5042	-	9,9,9	5.25	4 (44%)	11,11,11	3.14	3 (27%)
5	BEZ	E	2386	-	9,9,9	1.50	1 (11%)	11,11,11	1.36	2 (18%)
5	BEZ	I	3381	-	9,9,9	2.18	5 (55%)	11,11,11	0.89	1 (9%)
2	NAG	D	2179	1	14,14,15	0.73	0	17,19,21	0.68	1 (5%)
4	SO4	K	4284	-	4,4,4	0.40	0	6,6,6	0.08	0
2	NAG	F	2379	1	14,14,15	1.24	2 (14%)	17,19,21	1.61	4 (23%)
2	NAG	J	4179	1	14,14,15	0.81	0	17,19,21	1.38	4 (23%)
3	SIA	F	682	-	21,21,21	1.16	3 (14%)	24,31,31	1.12	3 (12%)
4	SO4	L	4285	-	4,4,4	0.42	0	6,6,6	0.07	0
5	BEZ	B	1386	-	9,9,9	2.42	4 (44%)	11,11,11	0.92	1 (9%)
4	SO4	H	3284	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	J	4384	-	4,4,4	0.44	0	6,6,6	0.09	0
3	SIA	G	782	-	21,21,21	0.97	0	24,31,31	1.06	1 (4%)
3	SIA	L	1282	-	21,21,21	0.88	0	24,31,31	1.20	2 (8%)
4	SO4	B	1385	-	4,4,4	0.38	0	6,6,6	0.12	0
4	SO4	A	1384	-	4,4,4	0.41	0	6,6,6	0.10	0
3	SIA	A	1181	-	21,21,21	1.10	2 (9%)	24,31,31	1.00	1 (4%)
4	SO4	G	3184	-	4,4,4	0.38	0	6,6,6	0.13	0
5	BEZ	L	4381	-	9,9,9	1.47	1 (11%)	11,11,11	1.40	3 (27%)
4	SO4	K	4385	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SIA	E	582	-	21,21,21	0.90	1 (4%)	24,31,31	1.20	2 (8%)
2	NAG	C	1379	1	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
2	NAG	I	3379	1	14,14,15	0.65	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BEZ	B	12	-	9,9,9	19.07	9 (100%)	11,11,11	4.13	4 (36%)
3	SIA	K	1182	-	21,21,21	0.95	1 (4%)	24,31,31	1.12	2 (8%)
2	NAG	B	1279	1	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
3	SIA	J	1082	-	21,21,21	1.07	2 (9%)	24,31,31	1.12	2 (8%)
4	SO4	G	3384	-	4,4,4	0.41	0	6,6,6	0.11	0
4	SO4	I	3185	-	4,4,4	0.38	0	6,6,6	0.16	0
5	BEZ	A	1385	-	9,9,9	4.58	4 (44%)	11,11,11	2.07	1 (9%)
5	BEZ	F	5024	-	9,9,9	2.00	3 (33%)	11,11,11	1.04	1 (9%)
3	SIA	H	882	-	21,21,21	1.09	2 (9%)	24,31,31	1.15	3 (12%)
4	SO4	E	2385	-	4,4,4	0.38	0	6,6,6	0.15	0
5	BEZ	A	11	-	9,9,9	3.48	6 (66%)	11,11,11	1.80	4 (36%)
5	BEZ	C	5013	1	8,8,9	2.33	4 (50%)	9,9,11	0.83	1 (11%)
5	BEZ	L	4380	-	9,9,9	1.69	1 (11%)	11,11,11	1.24	2 (18%)
4	SO4	E	2284	-	4,4,4	0.41	0	6,6,6	0.16	0
4	SO4	C	1185	-	4,4,4	0.42	0	6,6,6	0.20	0
4	SO4	J	4184	-	4,4,4	0.39	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	I	3380	-	-	0/4/4/4	0/1/1/1
5	BEZ	K	4387	-	-	0/4/4/4	0/1/1/1
3	SIA	D	2180	-	-	7/20/38/38	0/1/1/1
2	NAG	H	3279	1	-	5/6/23/26	0/1/1/1
5	BEZ	D	2385	-	-	0/4/4/4	0/1/1/1
5	BEZ	E	2387	-	-	0/4/4/4	0/1/1/1
2	NAG	E	2279	1	-	2/6/23/26	0/1/1/1
3	SIA	I	982	-	-	12/20/38/38	0/1/1/1
5	BEZ	G	3385	-	-	0/4/4/4	0/1/1/1
2	NAG	L	4379	1	-	6/6/23/26	0/1/1/1
3	SIA	A	1180	-	-	7/20/38/38	0/1/1/1
5	BEZ	D	2386	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5023	1	-	0/2/2/4	0/1/1/1
5	BEZ	J	5041	1	-	0/2/2/4	0/1/1/1
5	BEZ	K	4386	-	-	0/4/4/4	0/1/1/1
5	BEZ	G	3386	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	H	3387	-	-	0/4/4/4	0/1/1/1
2	NAG	G	3179	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1179	1	-	5/6/23/26	0/1/1/1
5	BEZ	H	3386	-	-	0/4/4/4	0/1/1/1
3	SIA	B	1280	-	-	9/20/38/38	0/1/1/1
2	NAG	K	4279	1	1/1/5/7	3/6/23/26	0/1/1/1
5	BEZ	C	5014	-	-	0/4/4/4	0/1/1/1
5	BEZ	J	5042	-	-	2/4/4/4	0/1/1/1
5	BEZ	I	3381	-	-	0/4/4/4	0/1/1/1
2	NAG	D	2179	1	-	2/6/23/26	0/1/1/1
2	NAG	F	2379	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	4179	1	1/1/5/7	4/6/23/26	0/1/1/1
3	SIA	F	682	-	-	9/20/38/38	0/1/1/1
5	BEZ	B	1386	-	-	0/4/4/4	0/1/1/1
3	SIA	G	782	-	-	9/20/38/38	0/1/1/1
3	SIA	L	1282	-	-	9/20/38/38	0/1/1/1
3	SIA	A	1181	-	-	8/20/38/38	0/1/1/1
5	BEZ	L	4381	-	-	0/4/4/4	0/1/1/1
3	SIA	E	582	-	-	10/20/38/38	0/1/1/1
2	NAG	C	1379	1	-	3/6/23/26	0/1/1/1
2	NAG	I	3379	1	-	2/6/23/26	0/1/1/1
5	BEZ	B	12	-	-	0/4/4/4	0/1/1/1
3	SIA	K	1182	-	-	14/20/38/38	0/1/1/1
2	NAG	B	1279	1	1/1/5/7	4/6/23/26	0/1/1/1
3	SIA	J	1082	-	-	11/20/38/38	0/1/1/1
5	BEZ	A	1385	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5024	-	-	0/4/4/4	0/1/1/1
3	SIA	H	882	-	-	7/20/38/38	0/1/1/1
5	BEZ	C	5013	1	-	0/2/2/4	0/1/1/1
5	BEZ	A	11	-	-	0/4/4/4	0/1/1/1
5	BEZ	E	2386	-	-	0/4/4/4	0/1/1/1
5	BEZ	L	4380	-	-	0/4/4/4	0/1/1/1

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	12	BEZ	C6-C1	25.95	1.78	1.39
5	B	12	BEZ	C2-C1	25.70	1.78	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	12	BEZ	C3-C2	22.14	1.76	1.38
5	B	12	BEZ	C4-C3	21.53	1.85	1.38
5	B	12	BEZ	C5-C4	21.16	1.84	1.38

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3387	BEZ	O2-C-O1	-13.35	94.64	123.35
5	B	12	BEZ	O2-C-O1	11.24	147.52	123.35
5	J	5042	BEZ	C6-C1-C2	-8.15	108.20	118.57
5	G	3386	BEZ	C5-C4-C3	-7.58	109.49	119.87
5	H	3387	BEZ	O2-C-C1	7.31	133.59	114.84

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1279	NAG	C1
2	F	2379	NAG	C1
2	G	3179	NAG	C1
2	J	4179	NAG	C1
2	K	4279	NAG	C1

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1179	NAG	C8-C7-N2-C2
2	A	1179	NAG	O7-C7-N2-C2
2	B	1279	NAG	C1-C2-N2-C7
2	B	1279	NAG	C8-C7-N2-C2
2	B	1279	NAG	O7-C7-N2-C2

There are no ring outliers.

27 monomers are involved in 89 short contacts:

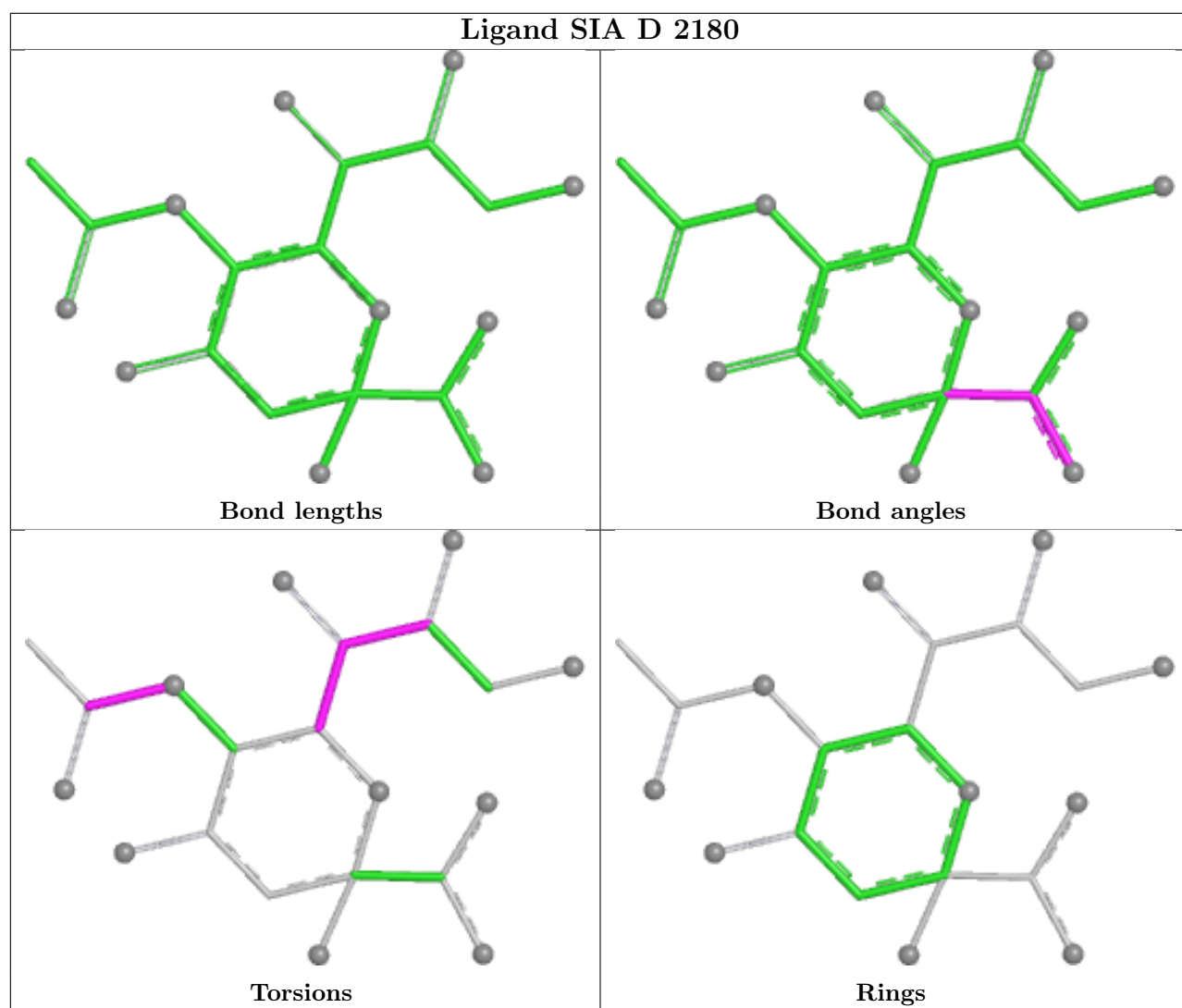
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	3380	BEZ	1	0
4	I	3285	SO4	1	0
3	D	2180	SIA	8	0
5	D	2385	BEZ	3	0
3	I	982	SIA	6	0
5	G	3385	BEZ	1	0

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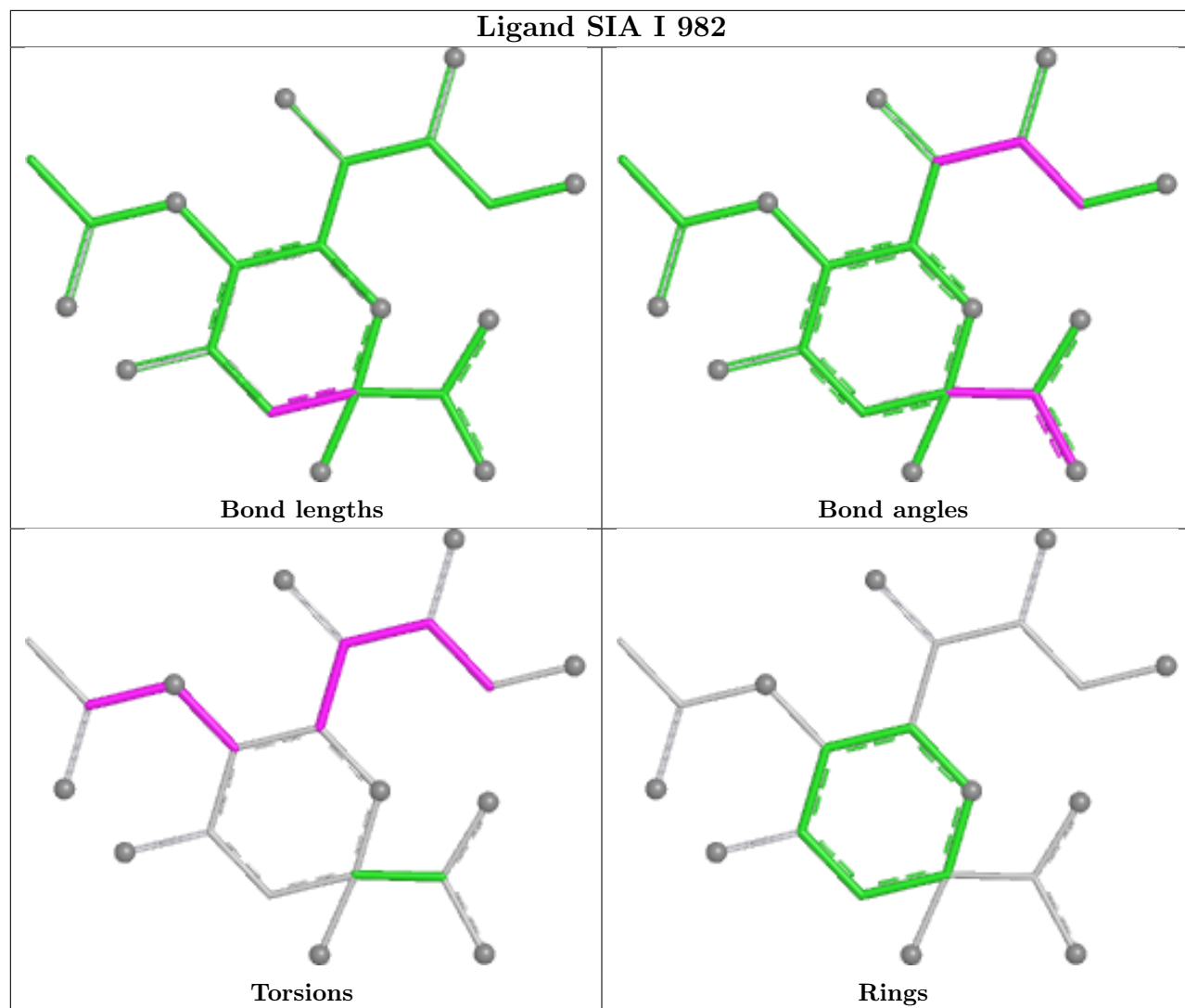
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1180	SIA	3	0
2	G	3179	NAG	1	0
5	H	3386	BEZ	1	0
3	B	1280	SIA	5	0
2	K	4279	NAG	2	0
5	C	5014	BEZ	1	0
2	F	2379	NAG	3	0
2	J	4179	NAG	1	0
3	F	682	SIA	1	0
3	G	782	SIA	6	0
3	L	1282	SIA	7	0
3	A	1181	SIA	10	0
3	E	582	SIA	2	0
5	B	12	BEZ	6	0
3	K	1182	SIA	7	0
2	B	1279	NAG	1	0
3	J	1082	SIA	5	0
5	A	1385	BEZ	2	0
3	H	882	SIA	1	0
5	C	5013	BEZ	3	0
5	L	4380	BEZ	1	0

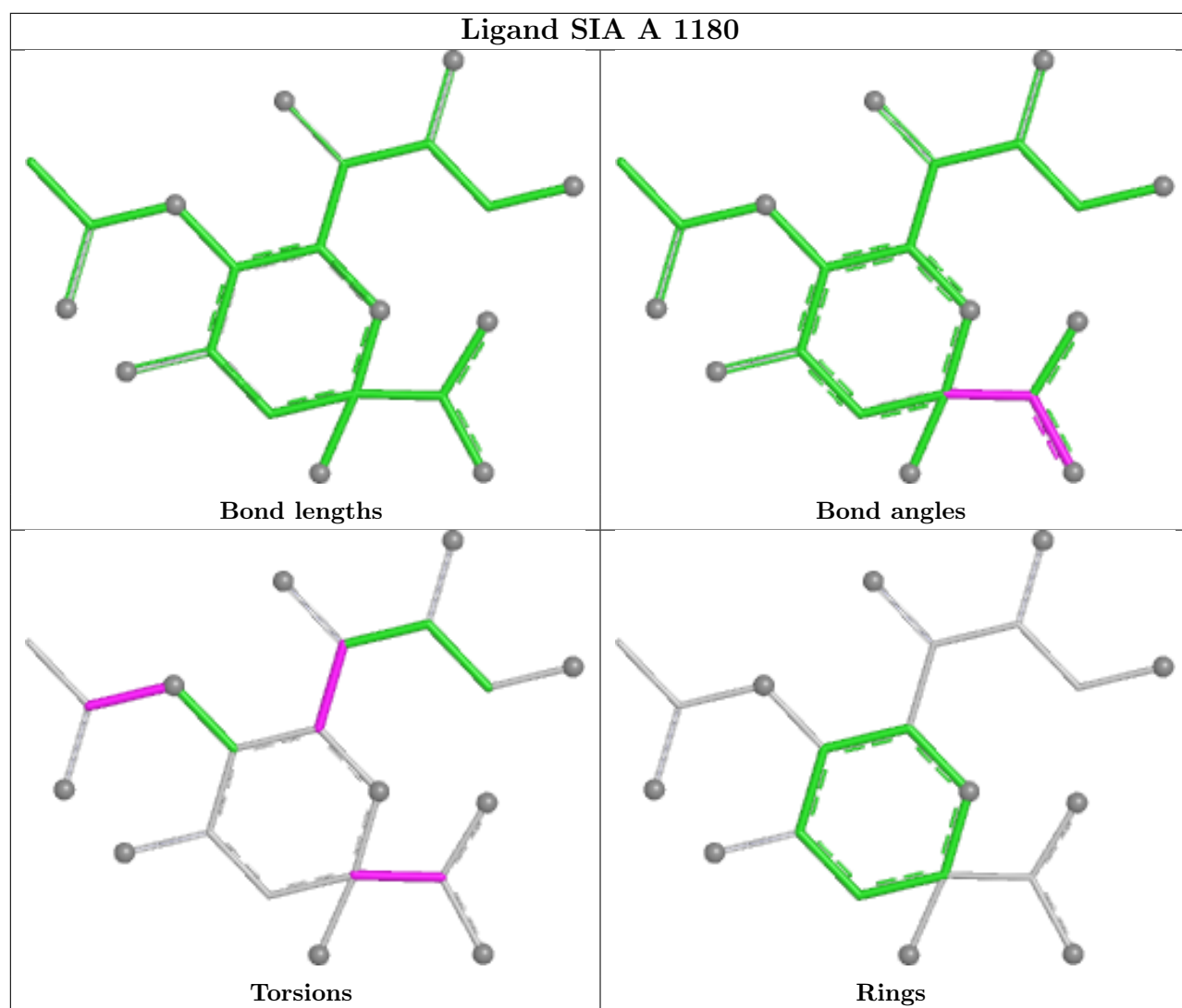
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

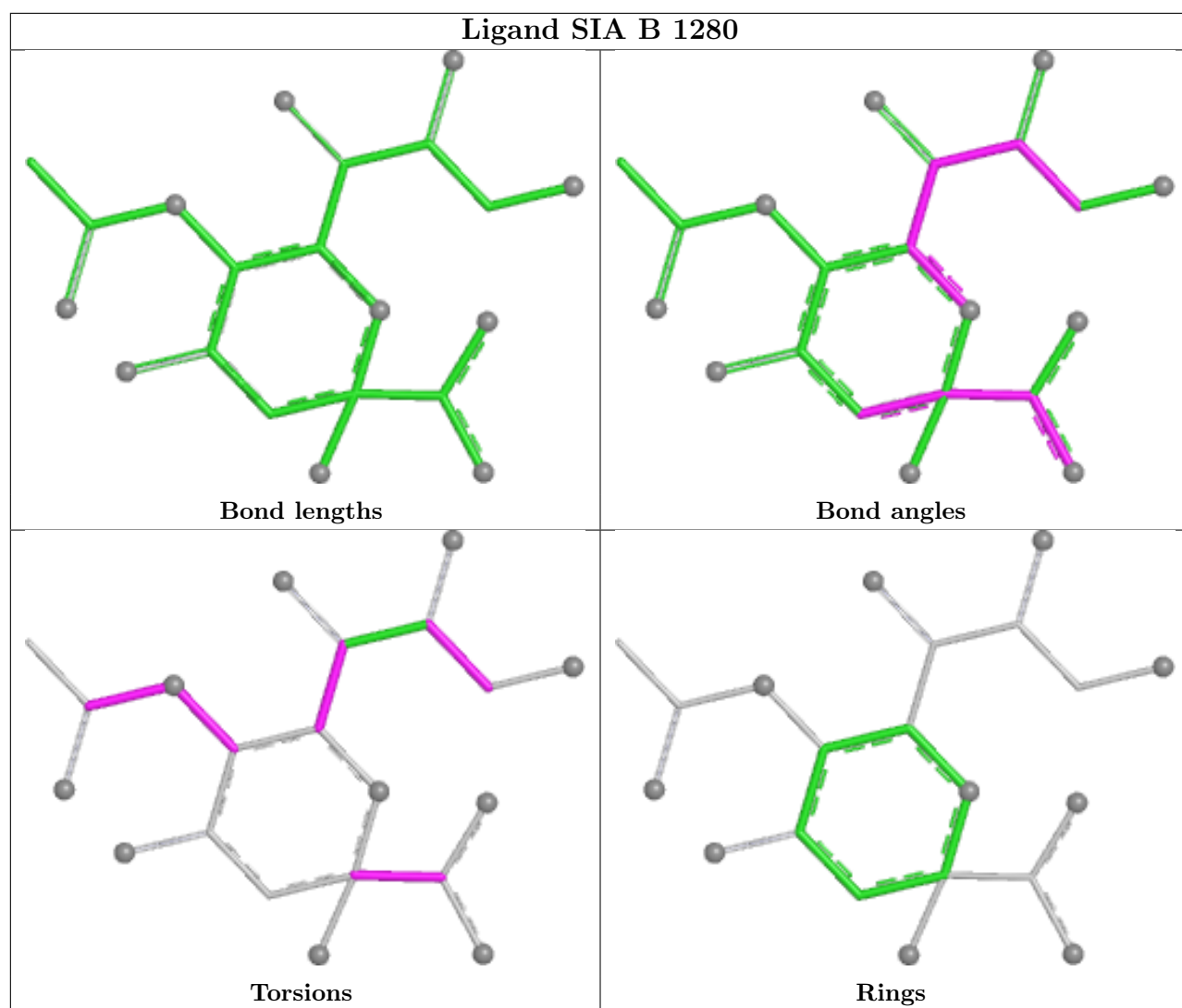


## Ligand SIA I 982

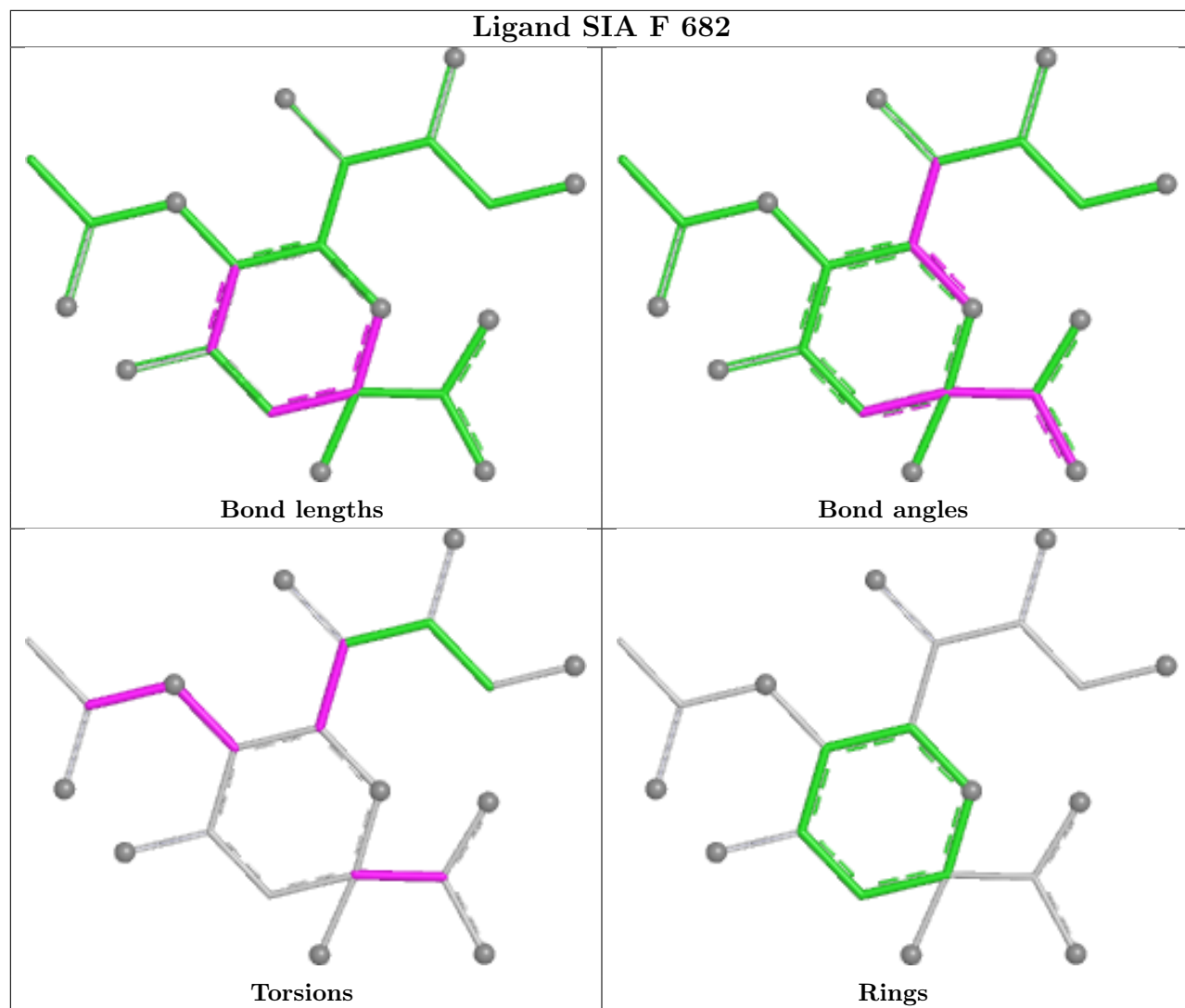




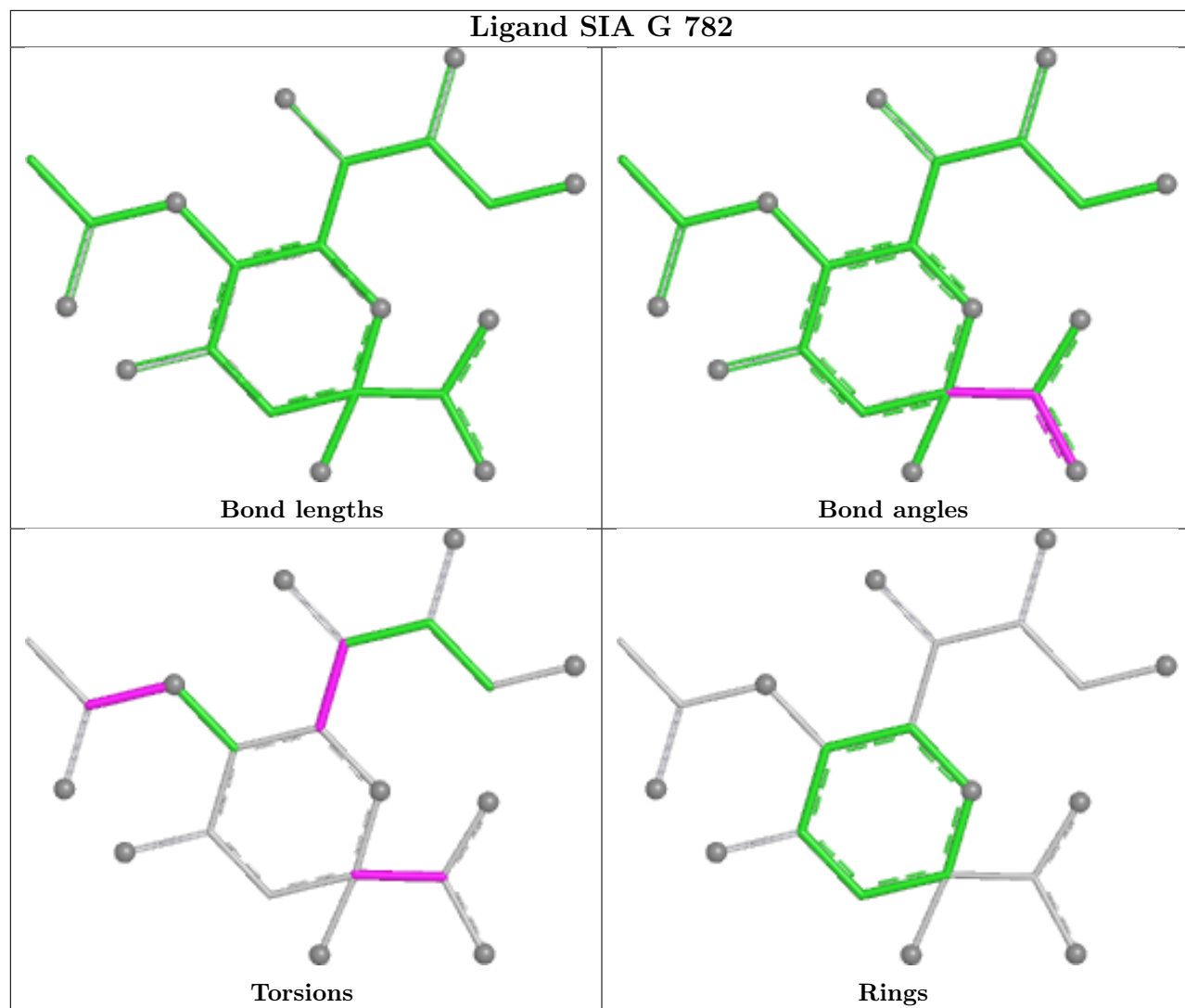




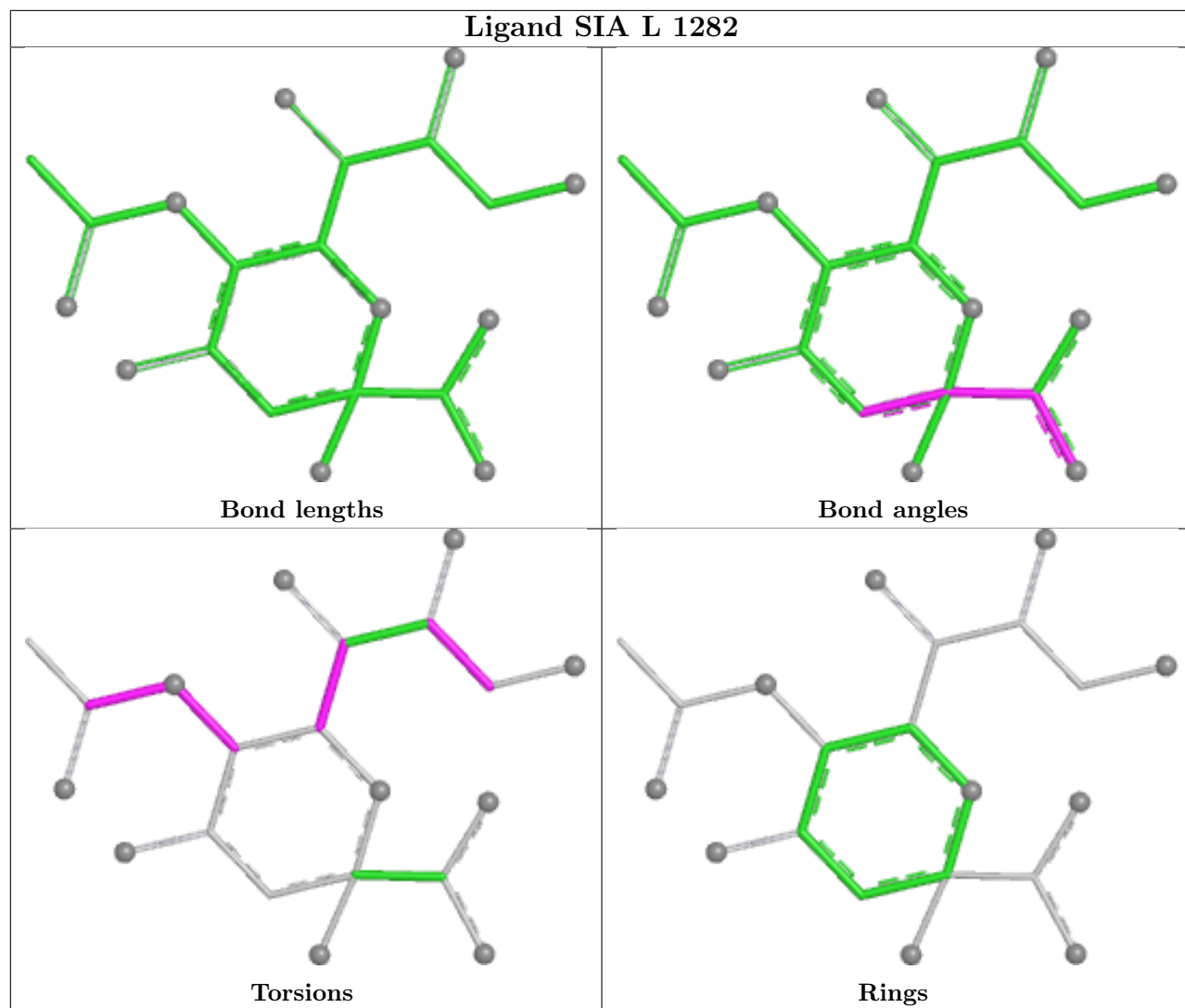
## Ligand SIA F 682

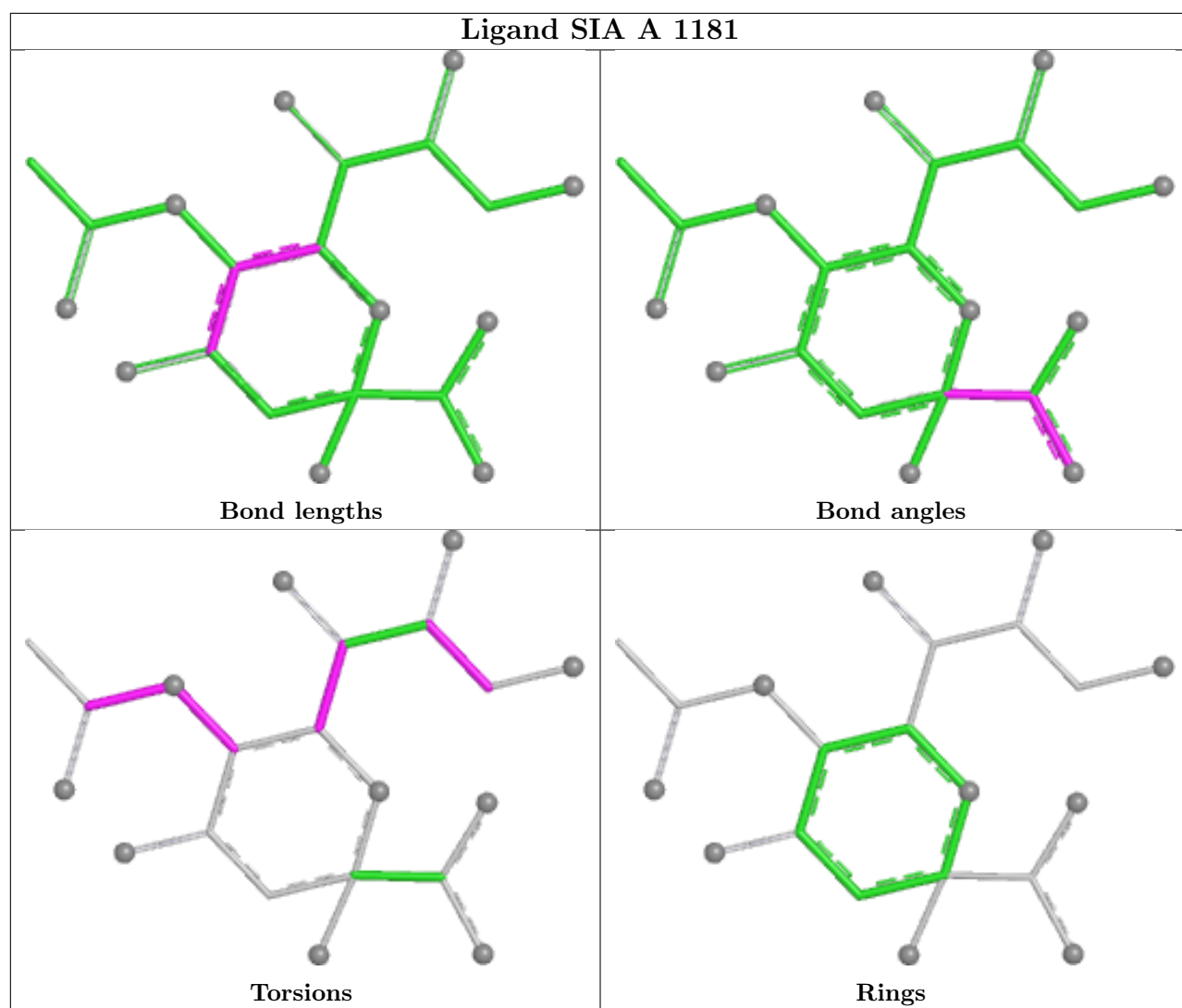


## Ligand SIA G 782

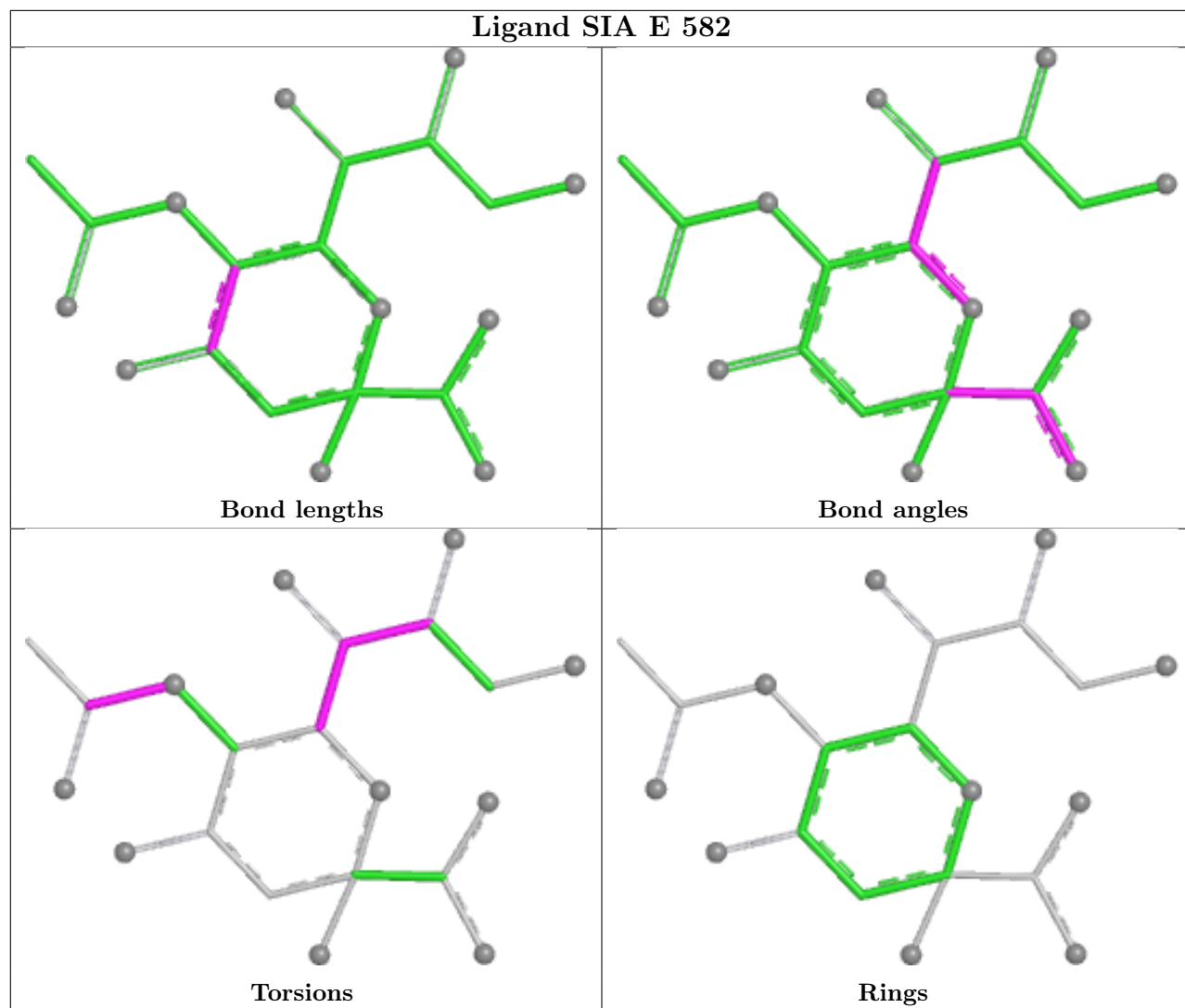


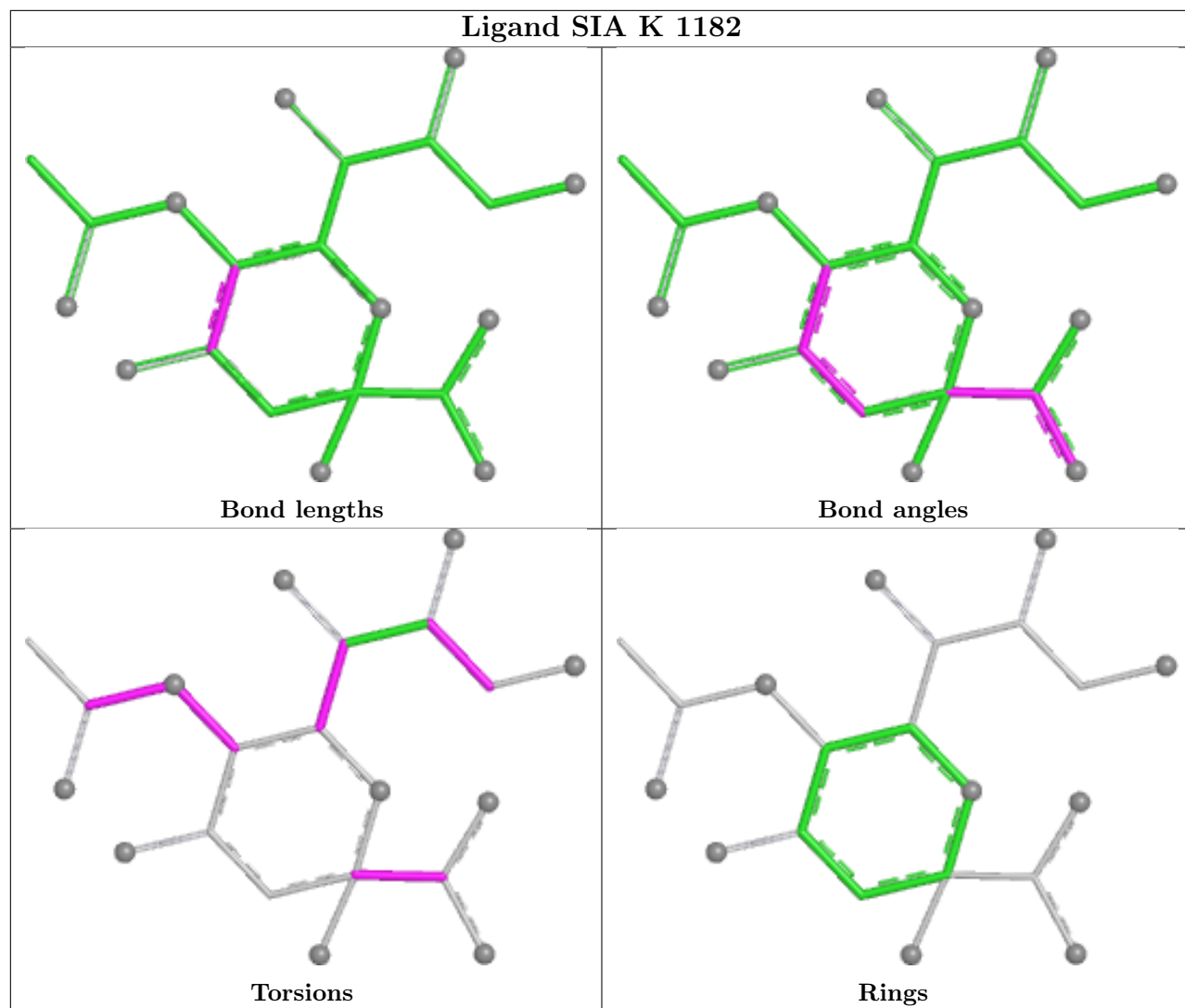
## Ligand SIA L 1282





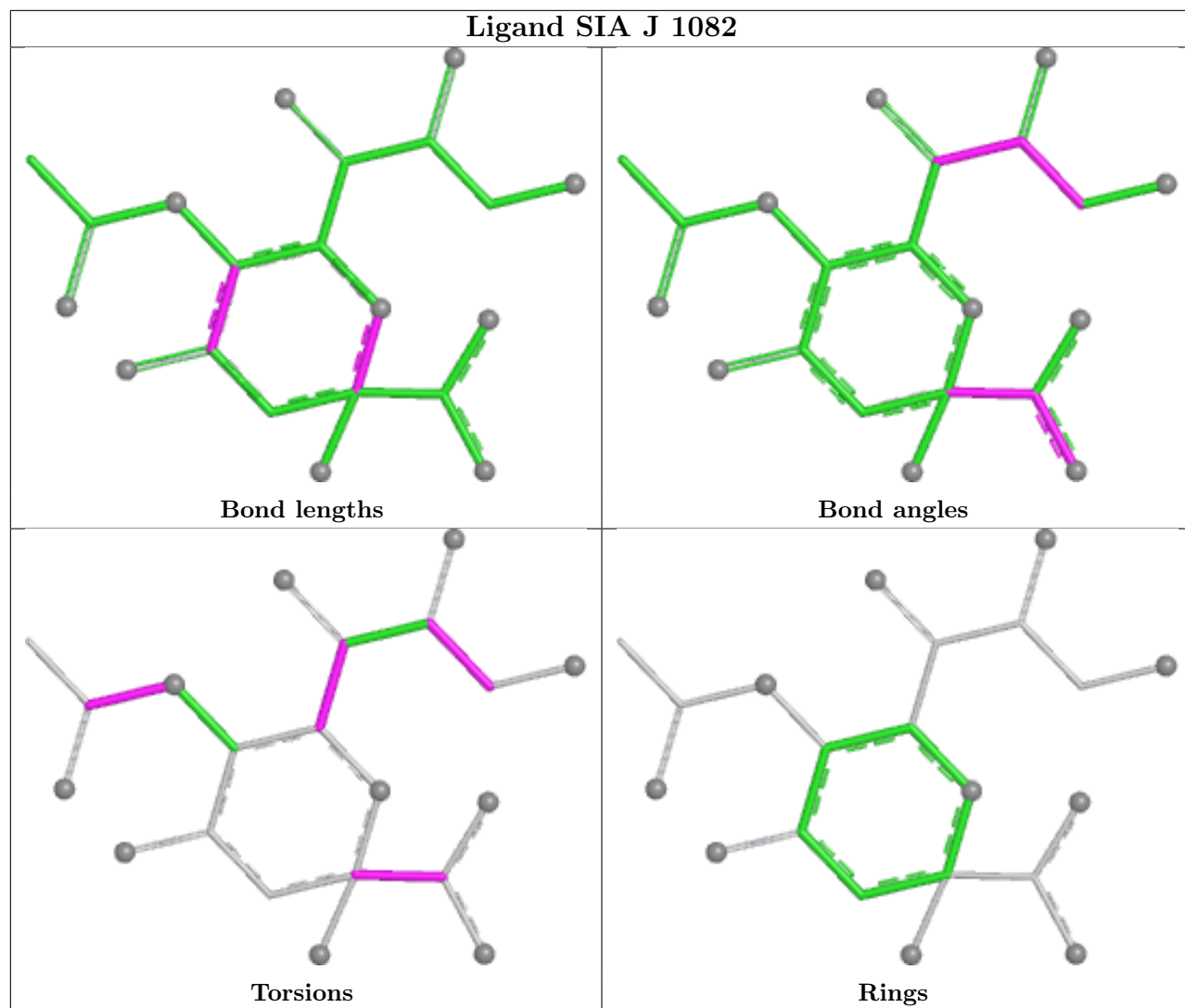
## Ligand SIA E 582

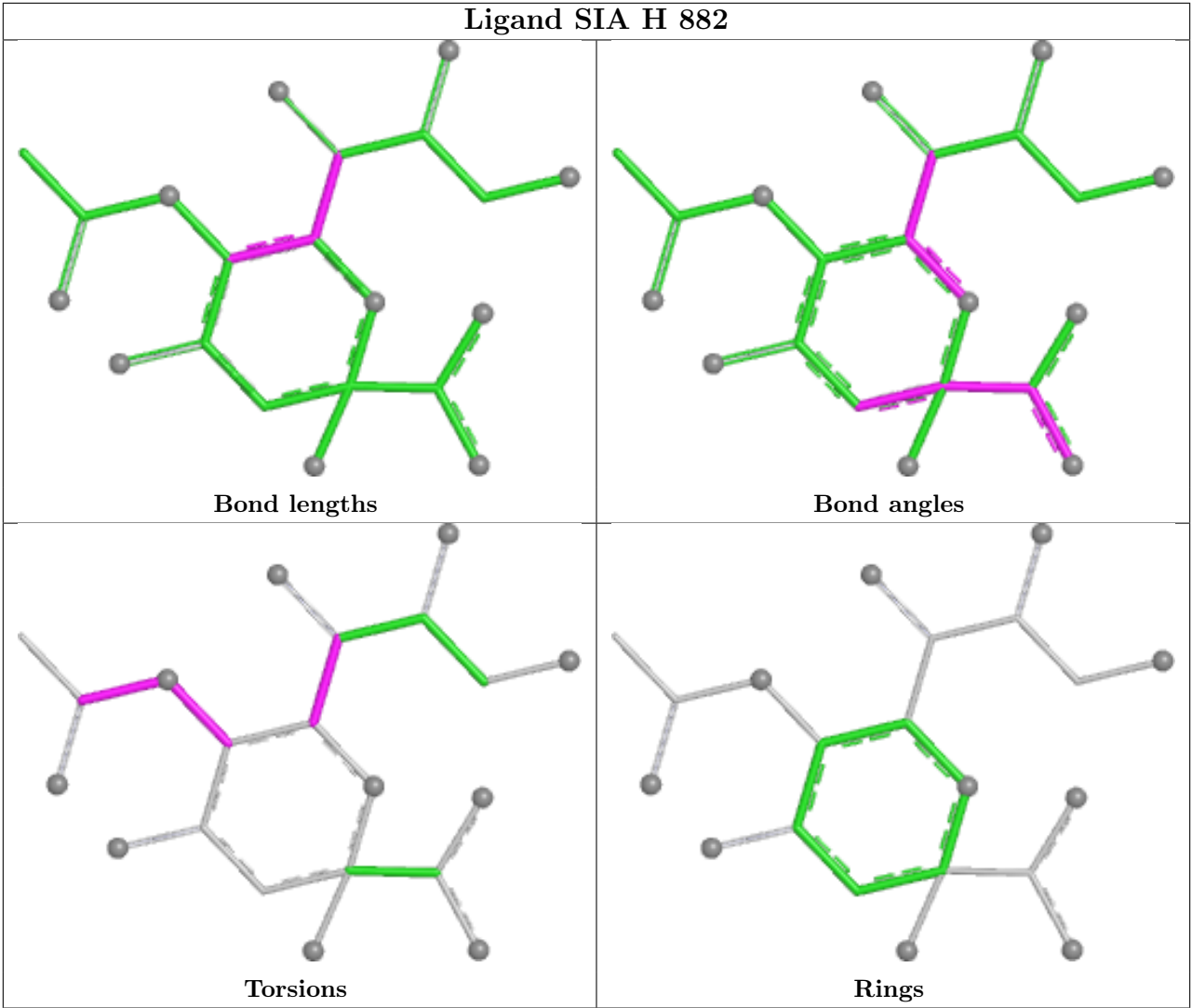






## Ligand SIA J 1082





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	550:LEU	C	551:PHE	N	1.00

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	532/532 (100%)	-1.77	0 100 100	2, 25, 69, 83	0
1	B	532/532 (100%)	-1.76	0 100 100	4, 29, 74, 86	0
1	C	532/532 (100%)	-1.76	0 100 100	2, 26, 64, 85	0
1	D	532/532 (100%)	-1.77	0 100 100	2, 25, 70, 84	0
1	E	532/532 (100%)	-1.76	0 100 100	4, 30, 73, 86	0
1	F	532/532 (100%)	-1.76	0 100 100	3, 26, 65, 81	0
1	G	532/532 (100%)	-1.77	0 100 100	3, 26, 67, 85	0
1	H	532/532 (100%)	-1.74	0 100 100	2, 27, 71, 84	0
1	I	532/532 (100%)	-1.73	0 100 100	3, 31, 74, 85	0
1	J	532/532 (100%)	-1.78	0 100 100	2, 26, 64, 83	0
1	K	532/532 (100%)	-1.74	0 100 100	3, 27, 71, 85	0
1	L	532/532 (100%)	-1.75	0 100 100	2, 31, 73, 83	0
All	All	6384/6384 (100%)	-1.76	0 100 100	2, 27, 70, 86	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1179	14/15	0.96	0.08	70,76,78,78	0
2	NAG	D	2179	14/15	0.96	0.06	70,76,78,79	0
5	BEZ	L	4381	9/9	0.96	0.06	54,55,55,55	0
4	SO4	C	1185	5/5	0.97	0.08	100,100,101,101	0
5	BEZ	E	2386	9/9	0.97	0.07	47,47,49,50	0
5	BEZ	L	4380	9/9	0.97	0.08	59,59,60,60	0
2	NAG	B	1279	14/15	0.97	0.05	59,64,68,70	0
2	NAG	H	3279	14/15	0.98	0.05	63,66,69,69	0
2	NAG	I	3379	14/15	0.98	0.05	57,61,62,63	0
2	NAG	J	4179	14/15	0.98	0.05	69,75,78,78	0
2	NAG	K	4279	14/15	0.98	0.04	63,67,71,71	0
2	NAG	L	4379	14/15	0.98	0.04	56,59,62,63	0
3	SIA	B	1280	21/21	0.98	0.05	45,61,66,67	0
2	NAG	C	1379	14/15	0.98	0.05	59,64,68,68	0
5	BEZ	A	1385	9/9	0.98	0.07	49,50,52,52	0
5	BEZ	B	1386	9/9	0.98	0.06	54,55,56,56	0
5	BEZ	C	5014	9/9	0.98	0.08	36,40,40,41	0
5	BEZ	D	2386	9/9	0.98	0.07	44,45,46,46	0
2	NAG	E	2279	14/15	0.98	0.04	57,60,62,63	0
5	BEZ	E	2387	9/9	0.98	0.06	42,43,43,44	0
5	BEZ	F	5024	9/9	0.98	0.11	42,44,46,46	0
5	BEZ	H	3387	9/9	0.98	0.07	41,43,45,46	0
5	BEZ	I	3381	9/9	0.98	0.08	52,52,53,54	0
5	BEZ	J	5042	9/9	0.98	0.09	44,45,46,46	0
5	BEZ	K	4387	9/9	0.98	0.09	36,39,40,41	0
2	NAG	F	2379	14/15	0.98	0.04	59,64,66,66	0
2	NAG	G	3179	14/15	0.98	0.04	67,72,75,75	0
4	SO4	B	1385	5/5	0.99	0.03	96,97,97,98	0
3	SIA	A	1181	21/21	0.99	0.04	44,57,67,68	0
4	SO4	D	2184	5/5	0.99	0.10	100,100,101,101	0
4	SO4	D	2384	5/5	0.99	0.07	76,77,77,77	0
4	SO4	E	2385	5/5	0.99	0.04	94,94,94,95	0
4	SO4	F	2185	5/5	0.99	0.04	106,106,106,106	0
4	SO4	F	2285	5/5	0.99	0.06	80,80,81,81	0
4	SO4	G	3184	5/5	0.99	0.06	86,86,87,88	0
4	SO4	G	3384	5/5	0.99	0.06	81,81,81,81	0
4	SO4	H	3284	5/5	0.99	0.12	84,84,85,85	0

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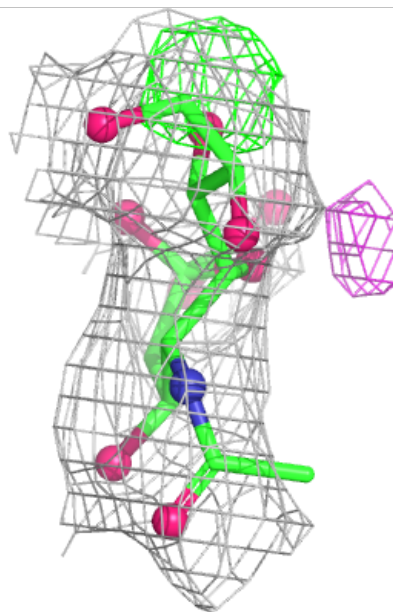
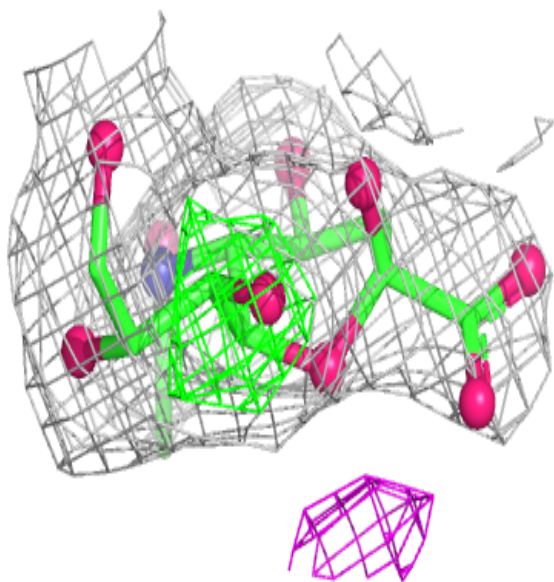
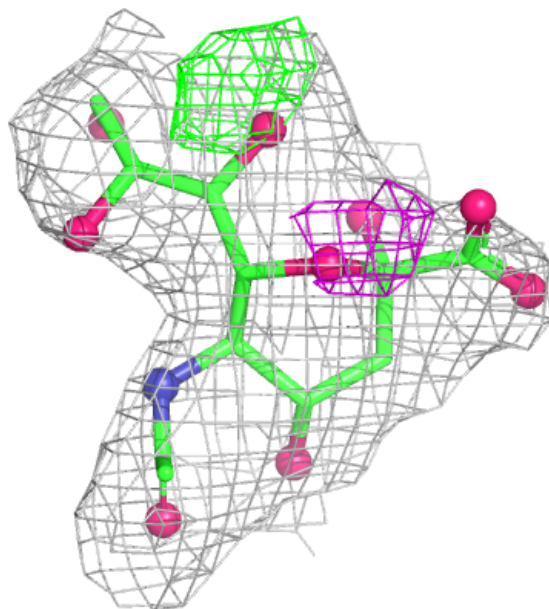
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	3385	5/5	0.99	0.05	97,97,97,97	0
4	SO4	I	3185	5/5	0.99	0.07	95,95,96,96	0
4	SO4	I	3285	5/5	0.99	0.05	79,79,79,80	0
4	SO4	J	4185	5/5	0.99	0.06	96,96,97,97	0
4	SO4	J	4384	5/5	0.99	0.04	84,85,85,86	0
4	SO4	K	4284	5/5	0.99	0.10	85,85,86,86	0
4	SO4	K	4385	5/5	0.99	0.08	97,98,98,99	0
4	SO4	L	4285	5/5	0.99	0.05	74,74,75,75	0
5	BEZ	A	11	9/9	0.99	0.05	49,51,52,52	0
3	SIA	A	1180	21/21	0.99	0.05	64,71,74,75	0
3	SIA	D	2180	21/21	0.99	0.04	57,69,72,73	0
5	BEZ	B	12	9/9	0.99	0.09	52,53,54,55	0
5	BEZ	C	5013	8/9	0.99	0.08	40,44,46,46	0
3	SIA	E	582	21/21	0.99	0.04	42,60,70,70	0
5	BEZ	D	2385	9/9	0.99	0.09	51,51,53,53	0
3	SIA	F	682	21/21	0.99	0.04	52,56,62,62	0
3	SIA	G	782	21/21	0.99	0.04	61,69,73,74	0
3	SIA	H	882	21/21	0.99	0.03	52,66,69,70	0
5	BEZ	F	5023	8/9	0.99	0.06	46,49,50,51	0
3	SIA	I	982	21/21	0.99	0.03	51,60,64,65	0
5	BEZ	G	3385	9/9	0.99	0.09	58,59,60,60	0
5	BEZ	G	3386	9/9	0.99	0.09	45,47,48,49	0
5	BEZ	H	3386	9/9	0.99	0.09	49,51,51,51	0
3	SIA	J	1082	21/21	0.99	0.05	59,71,76,77	0
5	BEZ	I	3380	9/9	0.99	0.07	53,53,54,55	0
3	SIA	K	1182	21/21	0.99	0.03	60,63,67,69	0
5	BEZ	J	5041	8/9	0.99	0.04	41,45,45,46	0
3	SIA	L	1282	21/21	0.99	0.05	50,55,63,65	0
5	BEZ	K	4386	9/9	0.99	0.05	48,49,50,50	0
4	SO4	A	1184	5/5	0.99	0.08	94,94,94,95	0
4	SO4	A	1384	5/5	0.99	0.09	76,76,77,77	0
4	SO4	B	1284	5/5	0.99	0.04	80,80,81,81	0
4	SO4	J	4184	5/5	1.00	0.03	94,94,95,95	0
4	SO4	E	2284	5/5	1.00	0.03	85,86,86,86	0
4	SO4	C	1285	5/5	1.00	0.04	76,76,77,77	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.

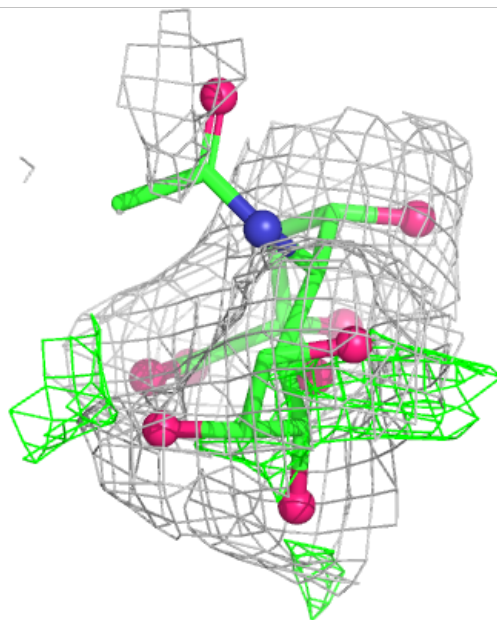
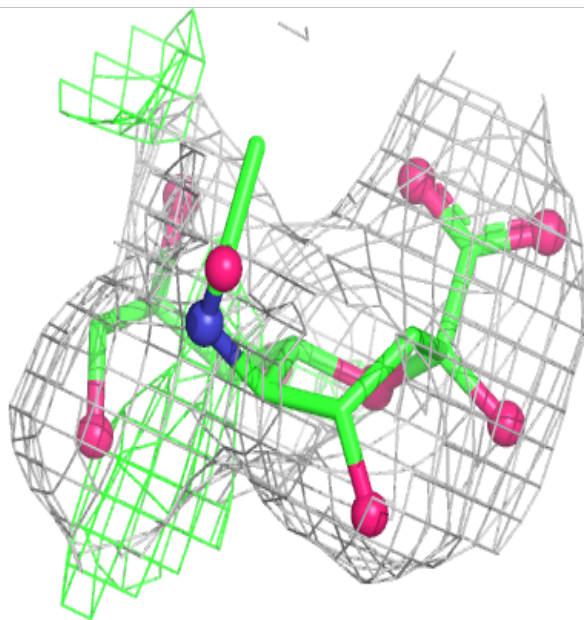
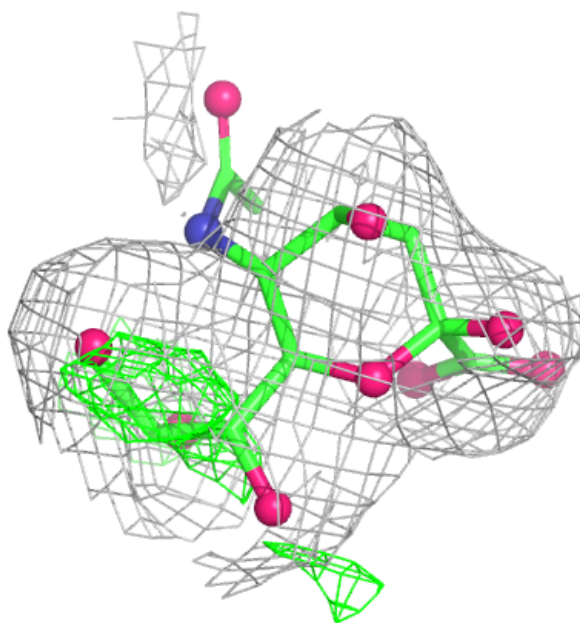
**Electron density around SIA B 1280:**

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



**Electron density around SIA A 1181:**

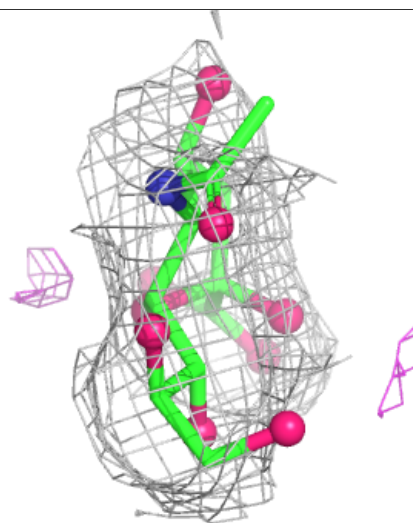
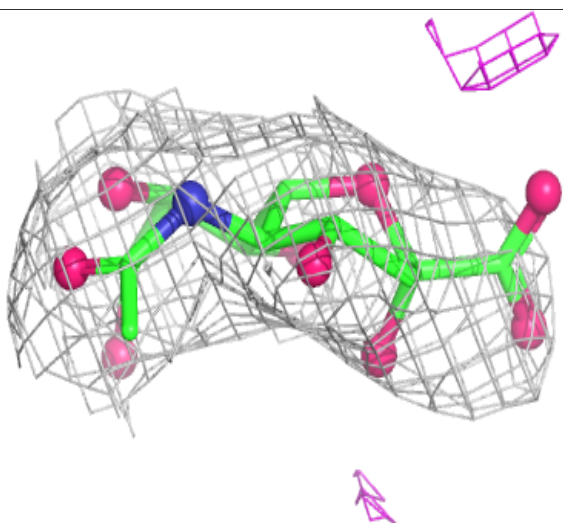
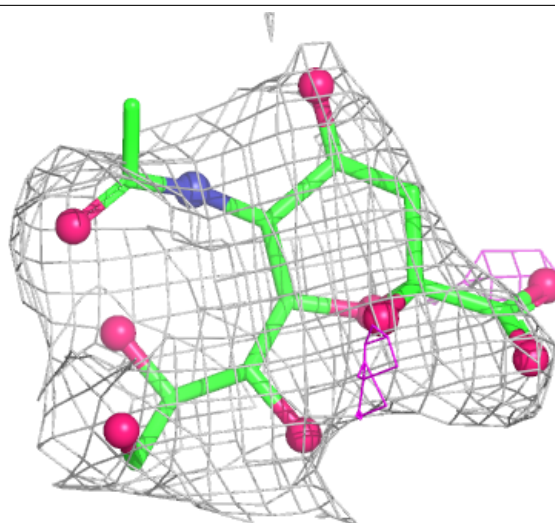
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SIA A 1180:**

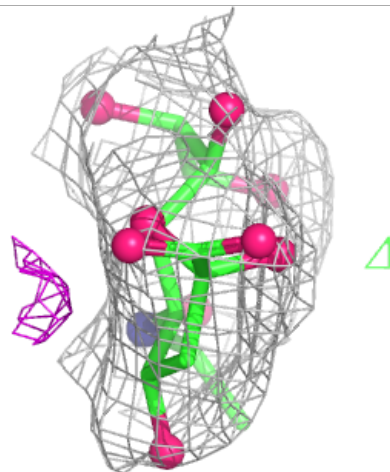
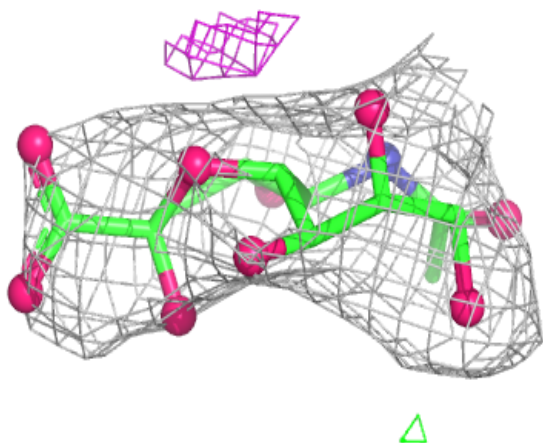
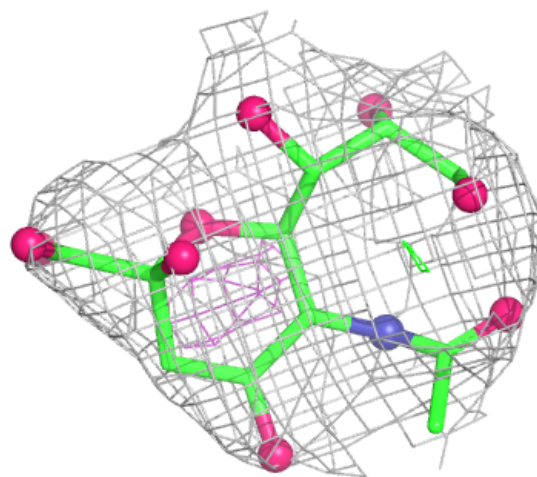
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





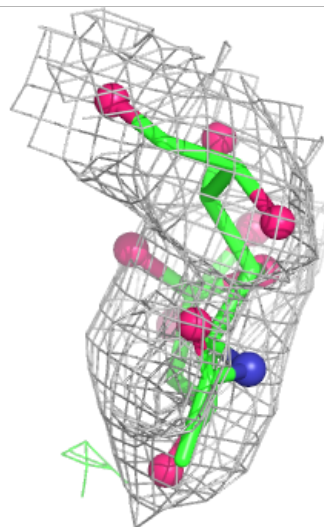
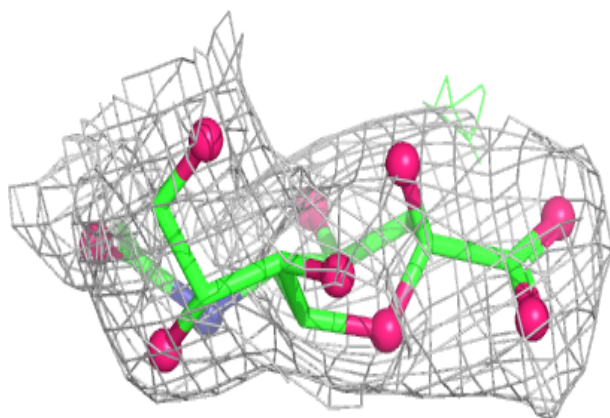
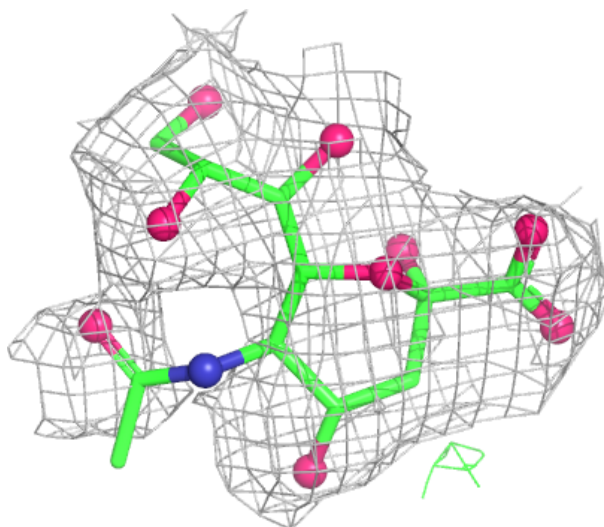
**Electron density around SIA D 2180:**

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



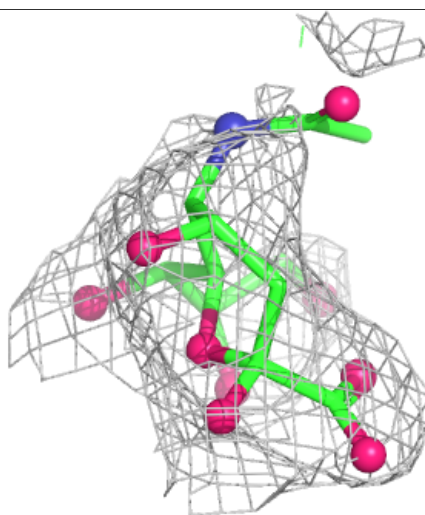
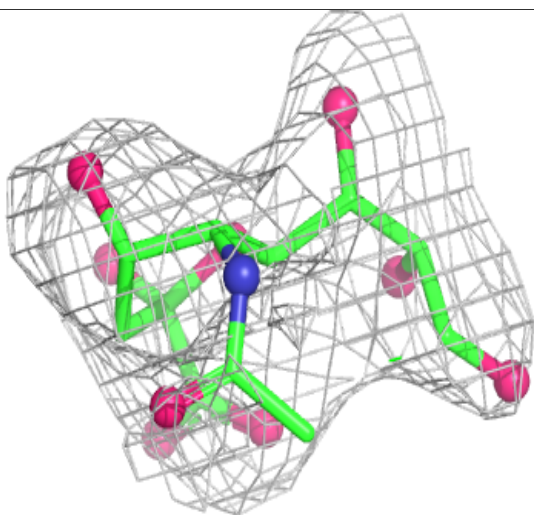
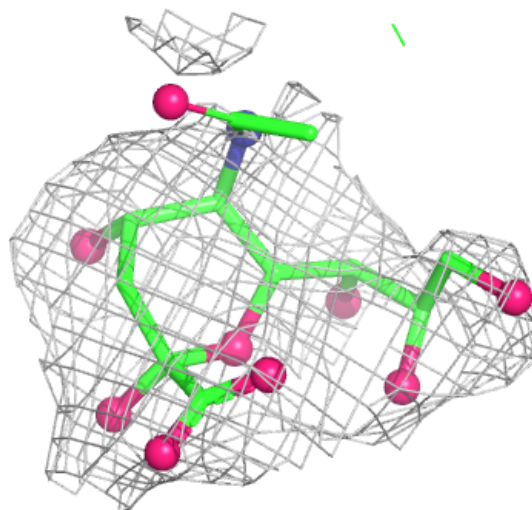
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



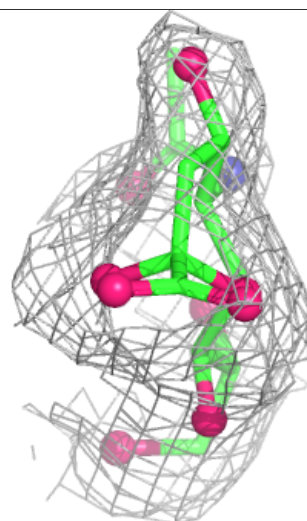
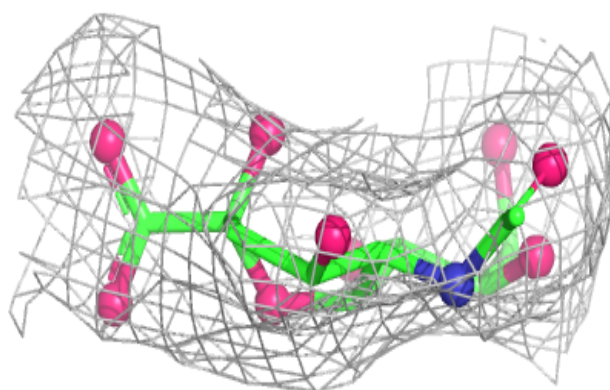
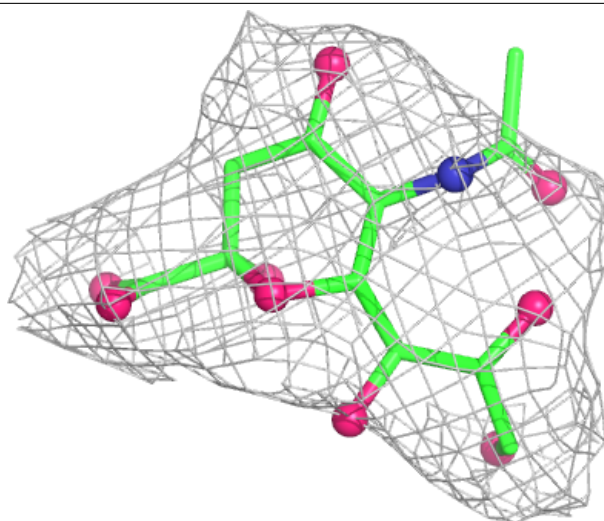
**Electron density around SIA F 682:**

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and green (positive)



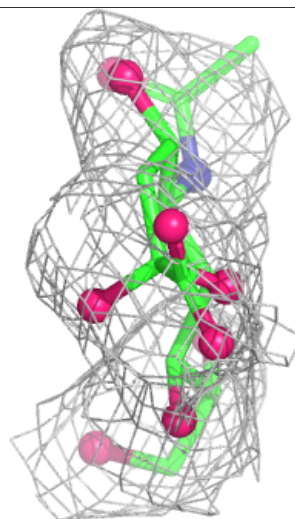
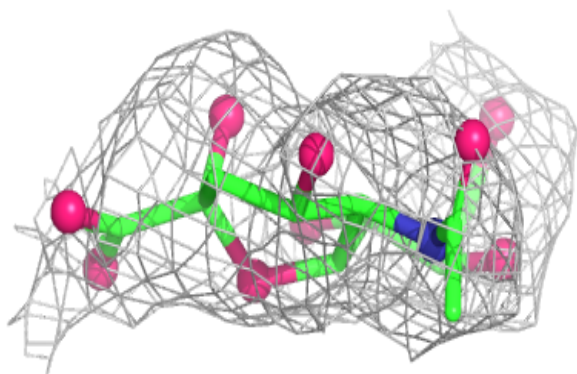
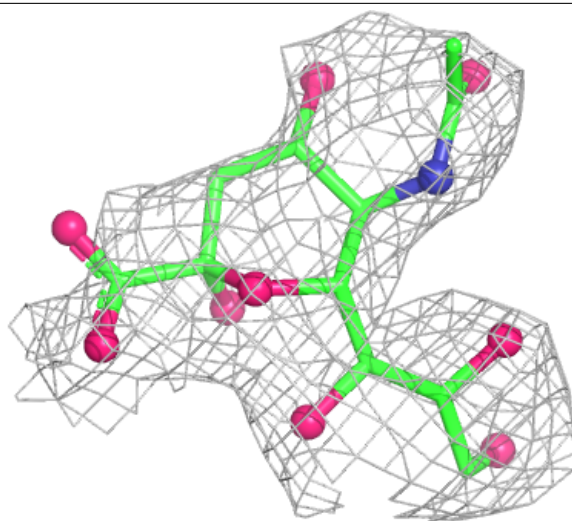
**Electron density around SIA G 782:**

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



**Electron density around SIA H 882:**

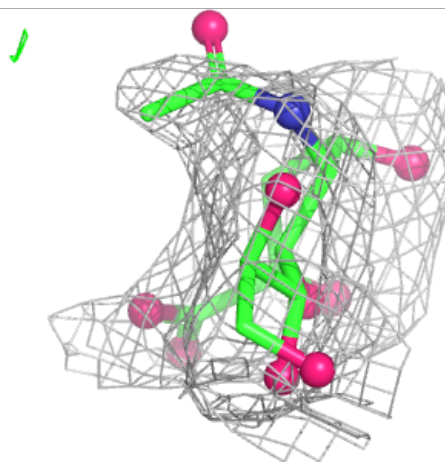
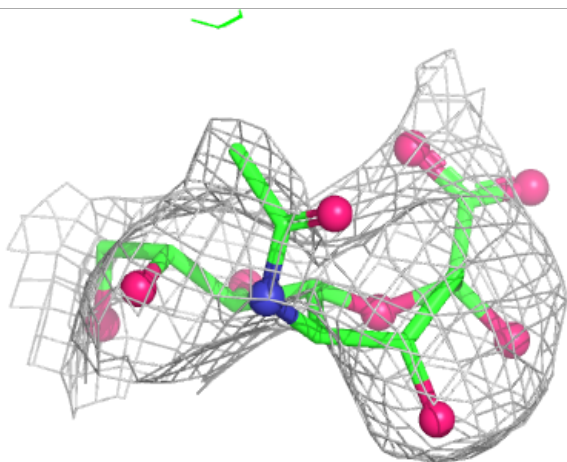
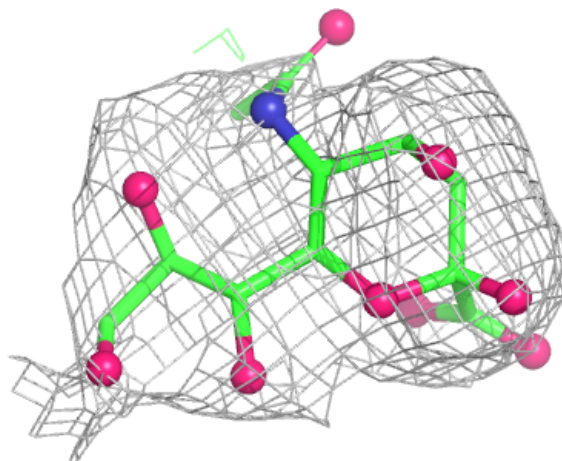
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





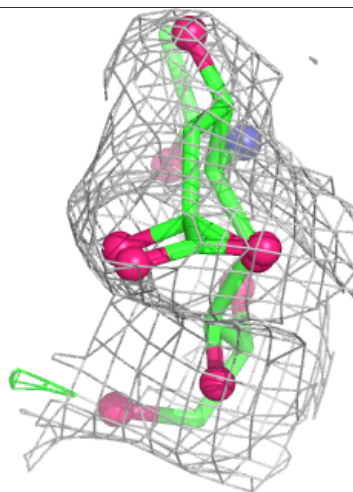
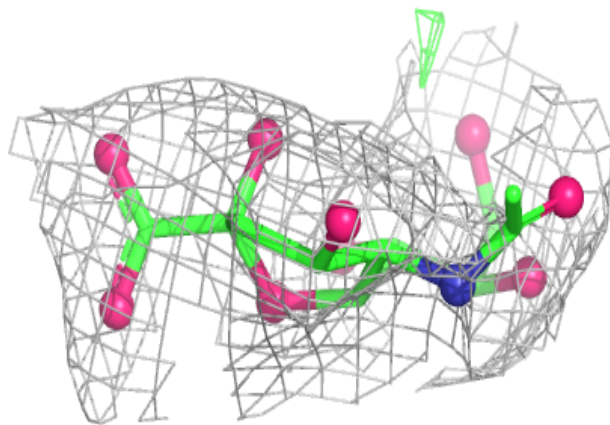
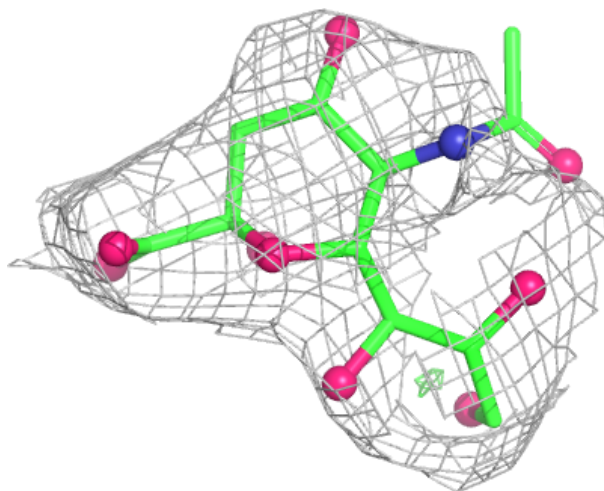
**Electron density around SIA I 982:**

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



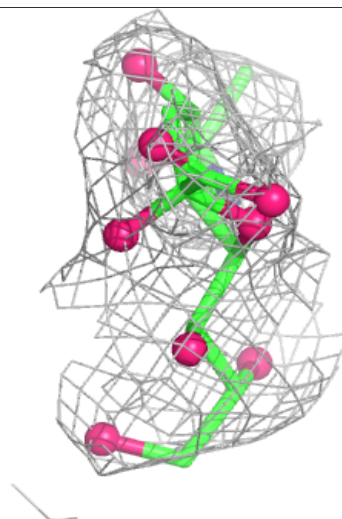
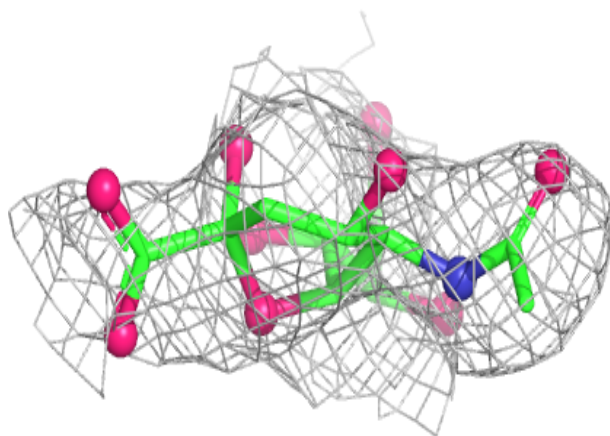
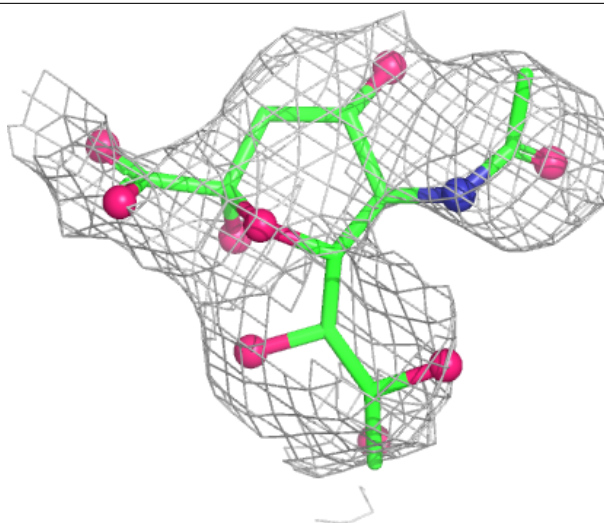
**Electron density around SIA J 1082:**

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



**Electron density around SIA K 1182:**

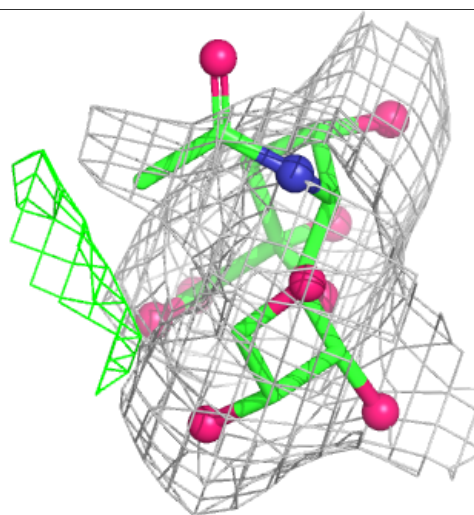
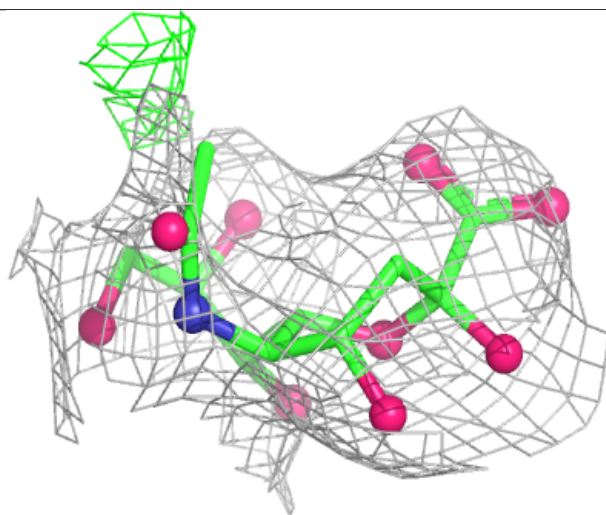
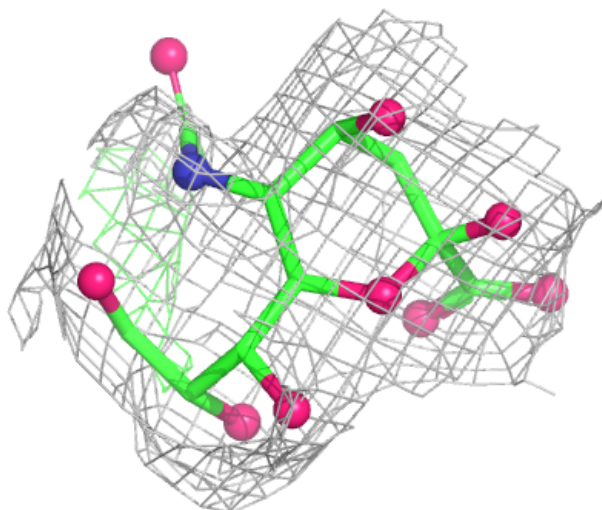
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SIA L 1282:**

$2mF_o-DF_c$  (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.