wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 02:32 AM EDT

PDB ID	:	1YAJ
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

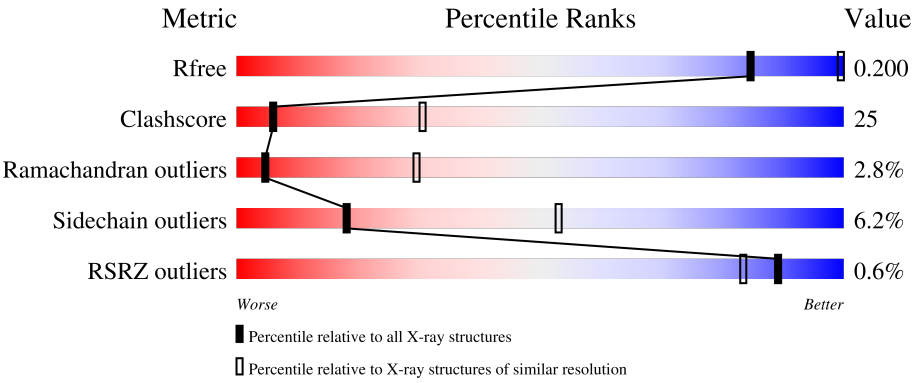
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	52% 44% .
1	B	532	% 56% 40% .
1	C	532	% 56% 40% .
1	D	532	% 52% 42% 5%
1	E	532	% 54% 42% .

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Mol	Chain	Length	Quality of chain
1	F	532	55% 41%
1	G	532	55% 41%
1	H	532	54% 43%
1	I	532	50% 44% 6%
1	J	532	53% 43%
1	K	532	53% 41% 6%
1	L	532	51% 42% 7%

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	A	1179	-	-	-	X
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	B	12	-	X	X	-
5	BEZ	D	2385	-	X	-	-
5	BEZ	G	3386	-	X	-	-
5	BEZ	H	3387	-	X	-	-

2 Entry composition (i)

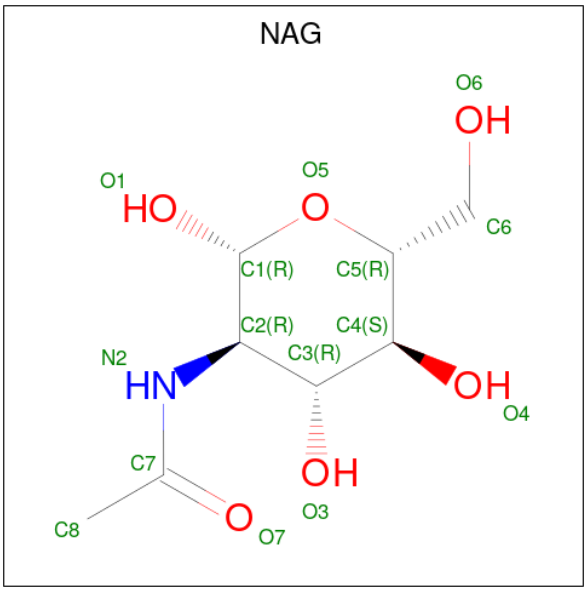
There are 6 unique types of molecules in this entry. The entry contains 50793 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

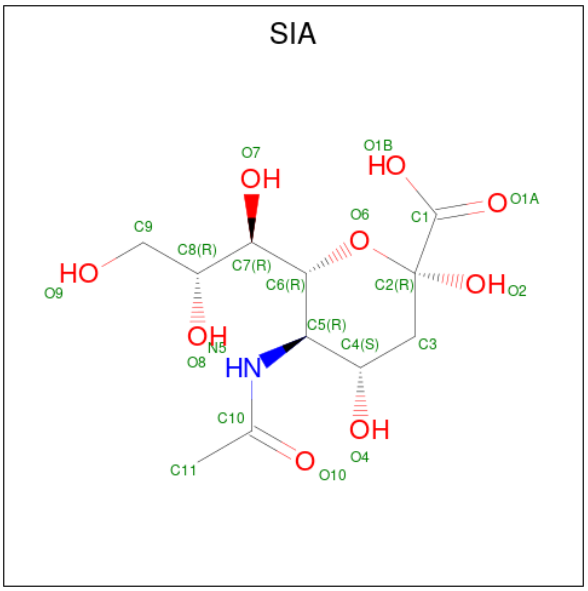
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	C	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	532	Total	C	N	O	S	0	0	0
			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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



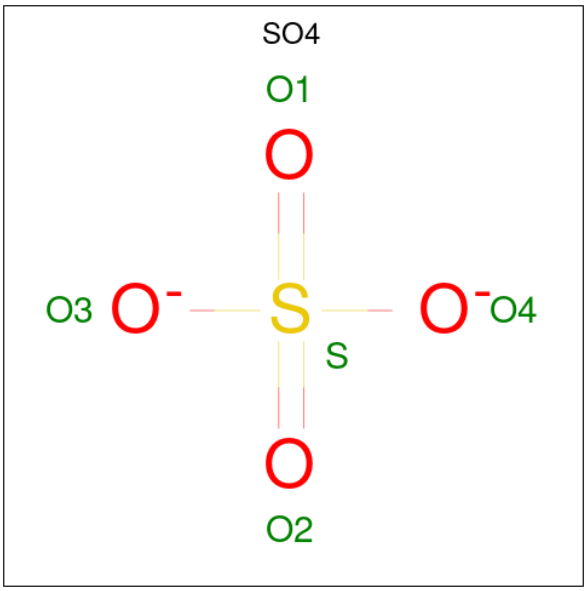
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	H	1	Total C N O 14 8 1 5	0	0
2	I	1	Total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

- Molecule 3 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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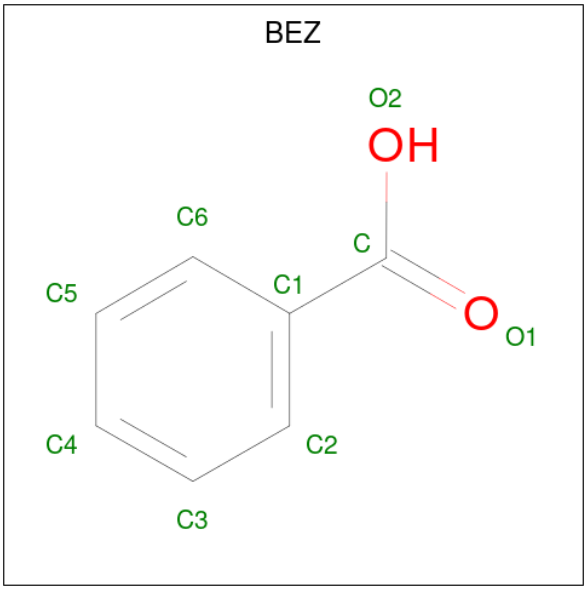
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

- Molecule 5 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



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

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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 9 7 2	0	0
5	L	1	Total C O 9 7 2	0	0

- Molecule 6 is water.

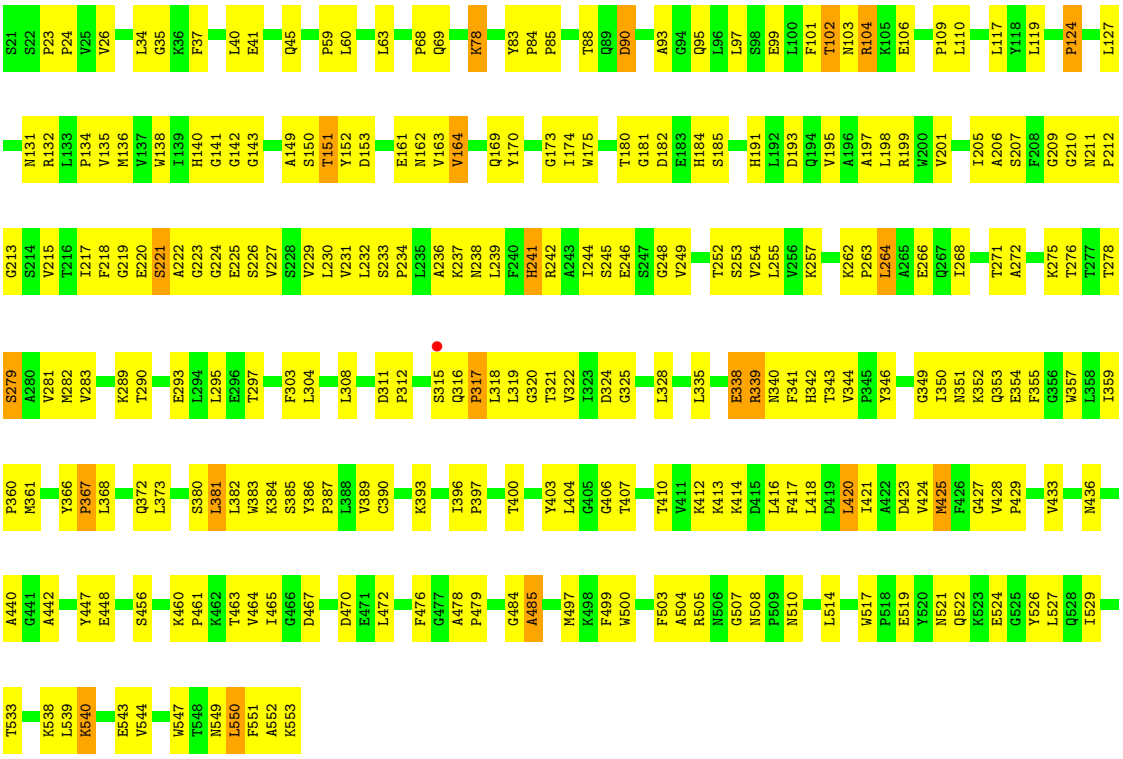
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	30	Total O 30 30	0	0
6	C	33	Total O 33 33	0	0
6	D	49	Total O 49 49	0	0
6	E	38	Total O 38 38	0	0
6	F	42	Total O 42 42	0	0
6	G	41	Total O 41 41	0	0
6	H	37	Total O 37 37	0	0
6	I	34	Total O 34 34	0	0
6	J	38	Total O 38 38	0	0
6	K	50	Total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

3 Residue-property plots (i)

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

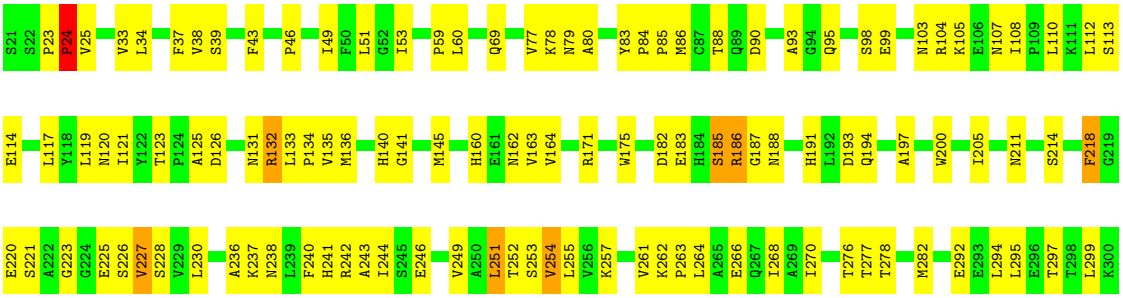
- Molecule 1: CES1 protein

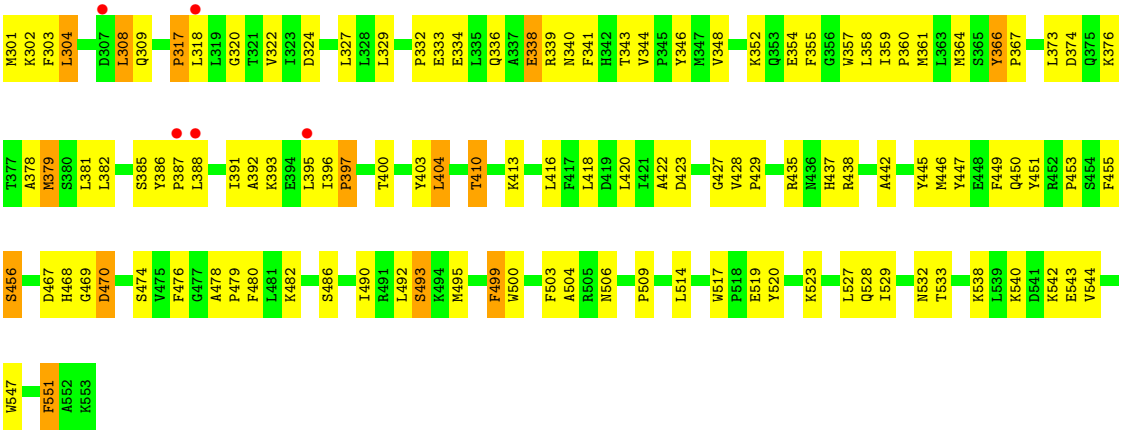
Chain A:



- Molecule 1: CES1 protein

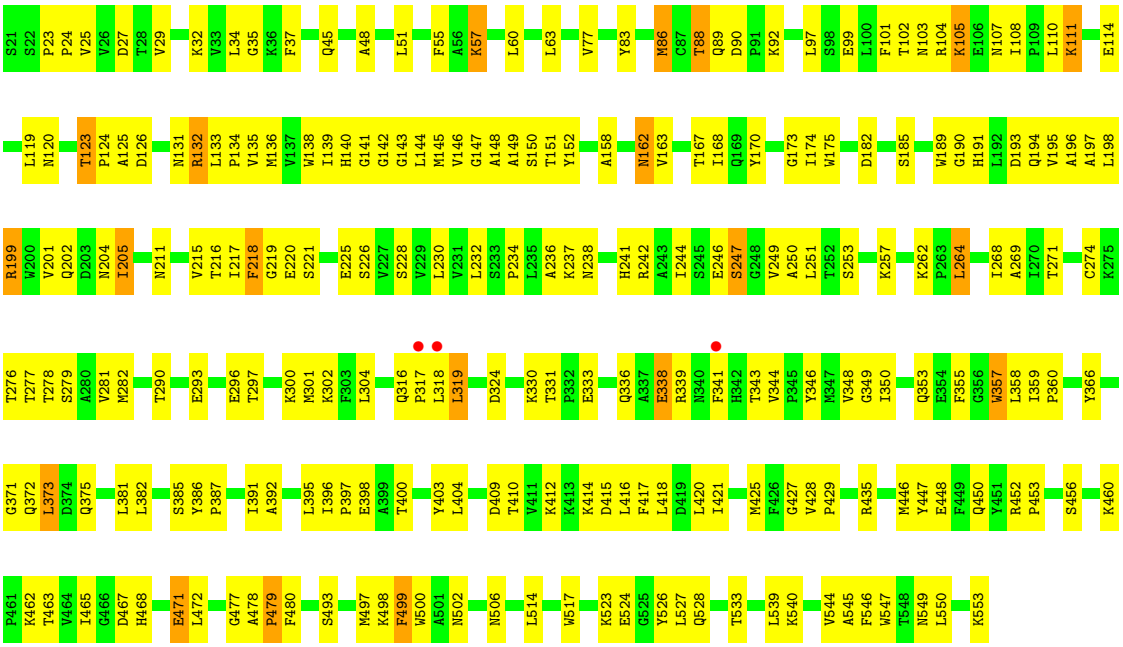
Chain B:





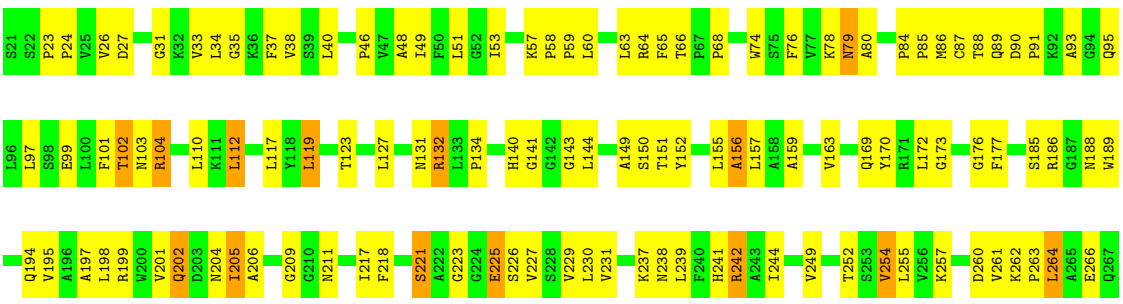
• Molecule 1: CES1 protein

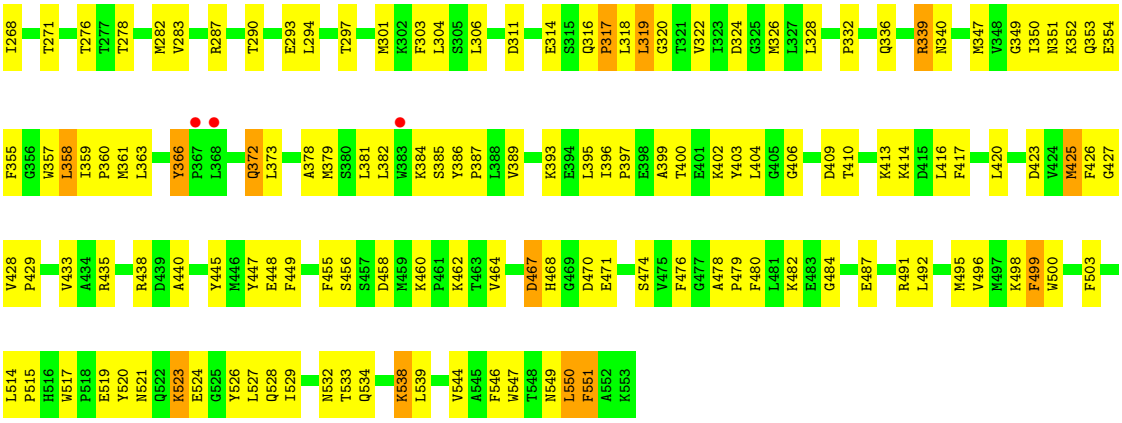
Chain C:



• Molecule 1: CES1 protein

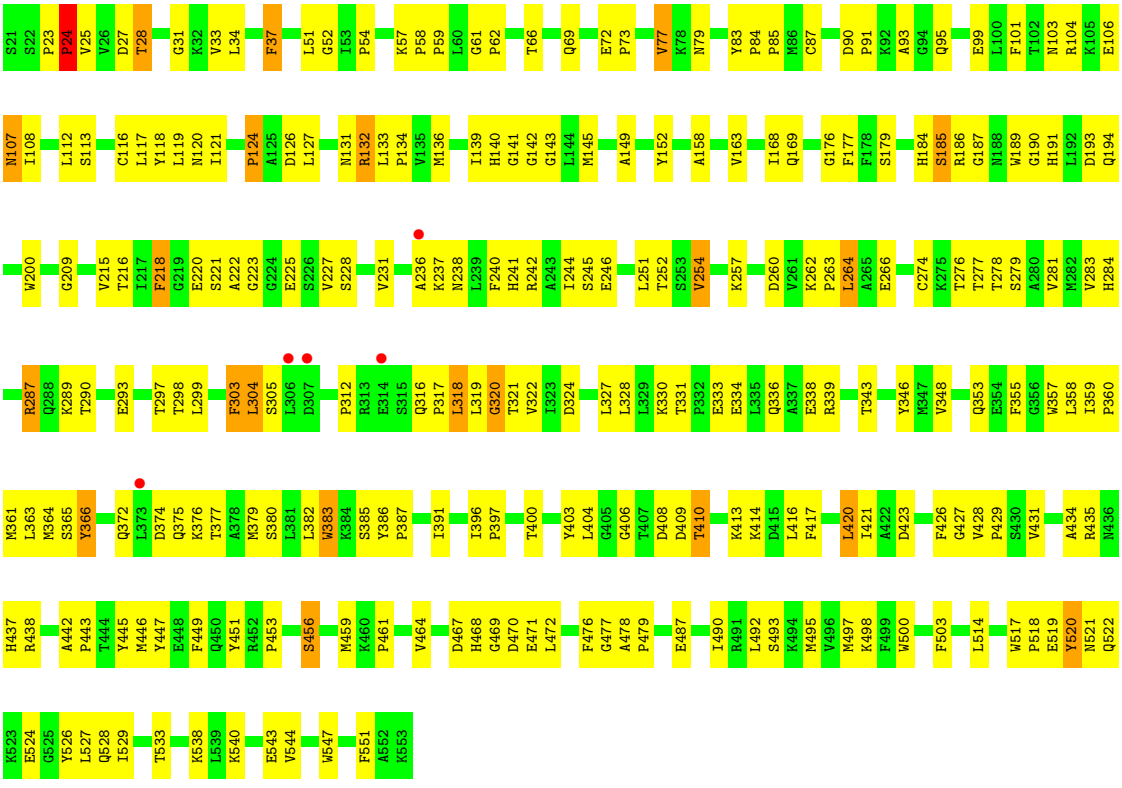
Chain D:





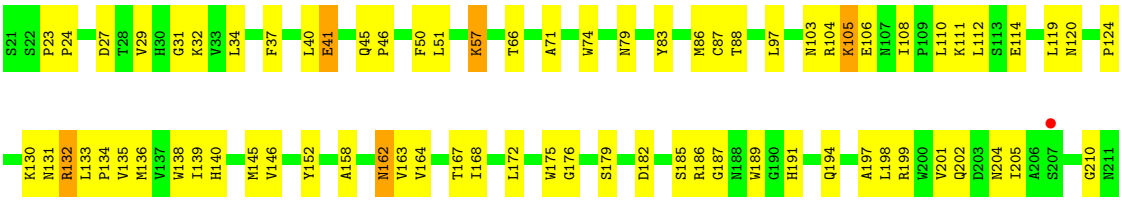
• Molecule 1: CES1 protein

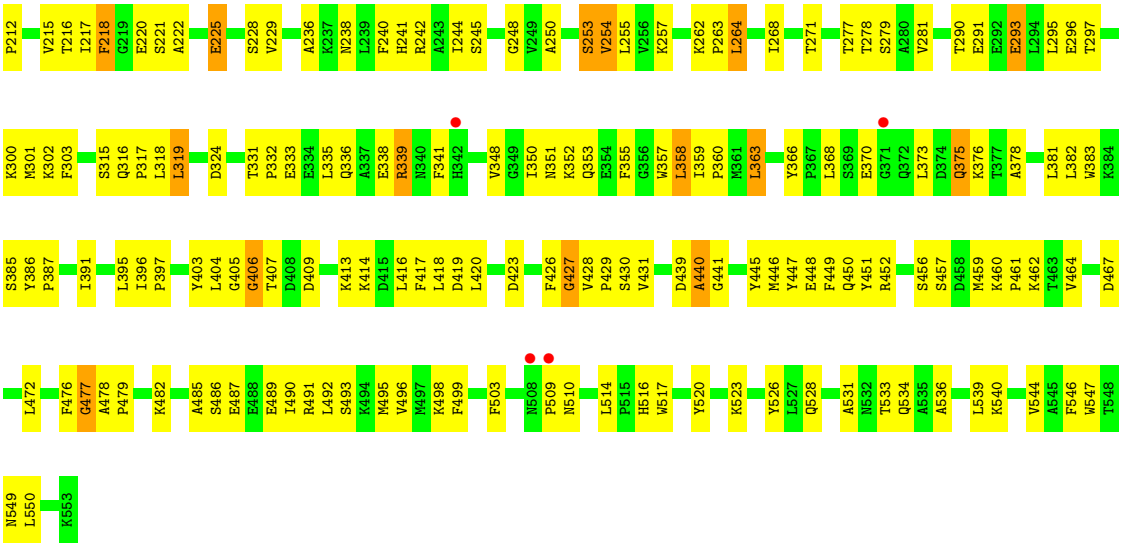
Chain E:



• Molecule 1: CES1 protein

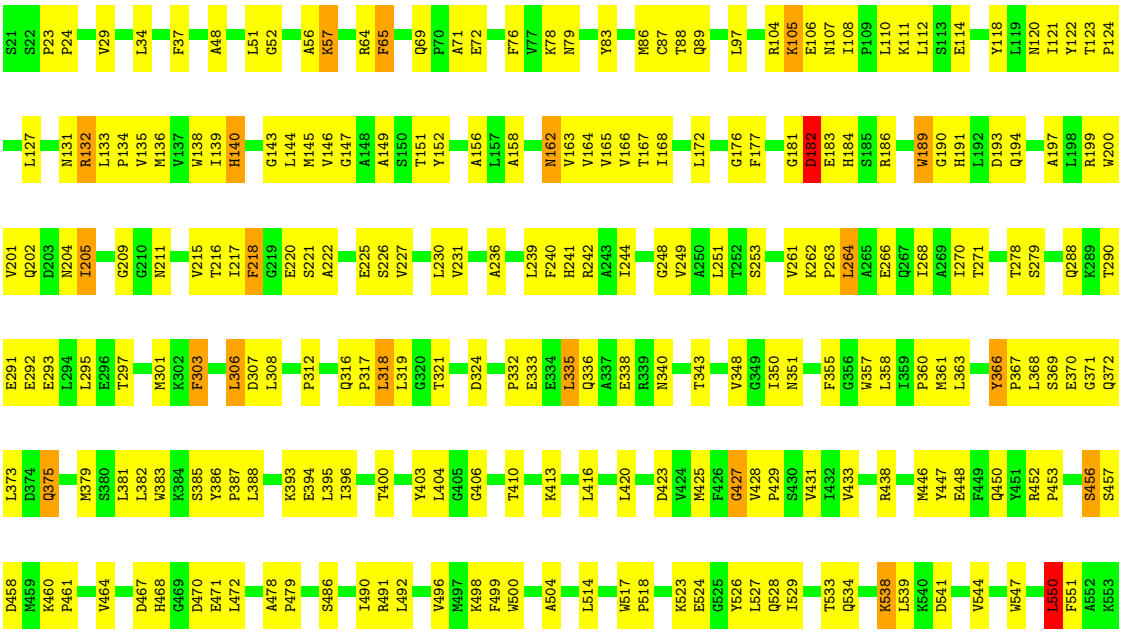
Chain F:





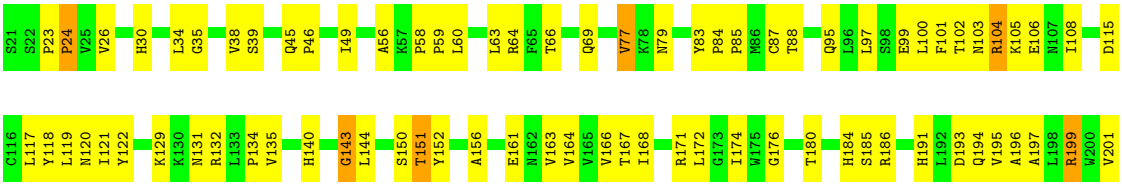
• Molecule 1: CES1 protein

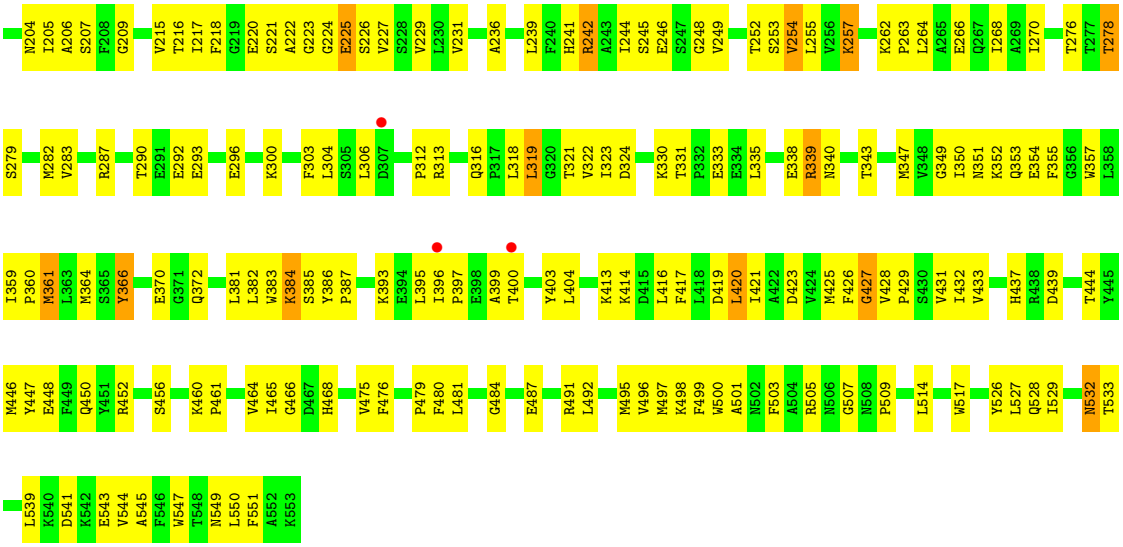
Chain G:



• Molecule 1: CES1 protein

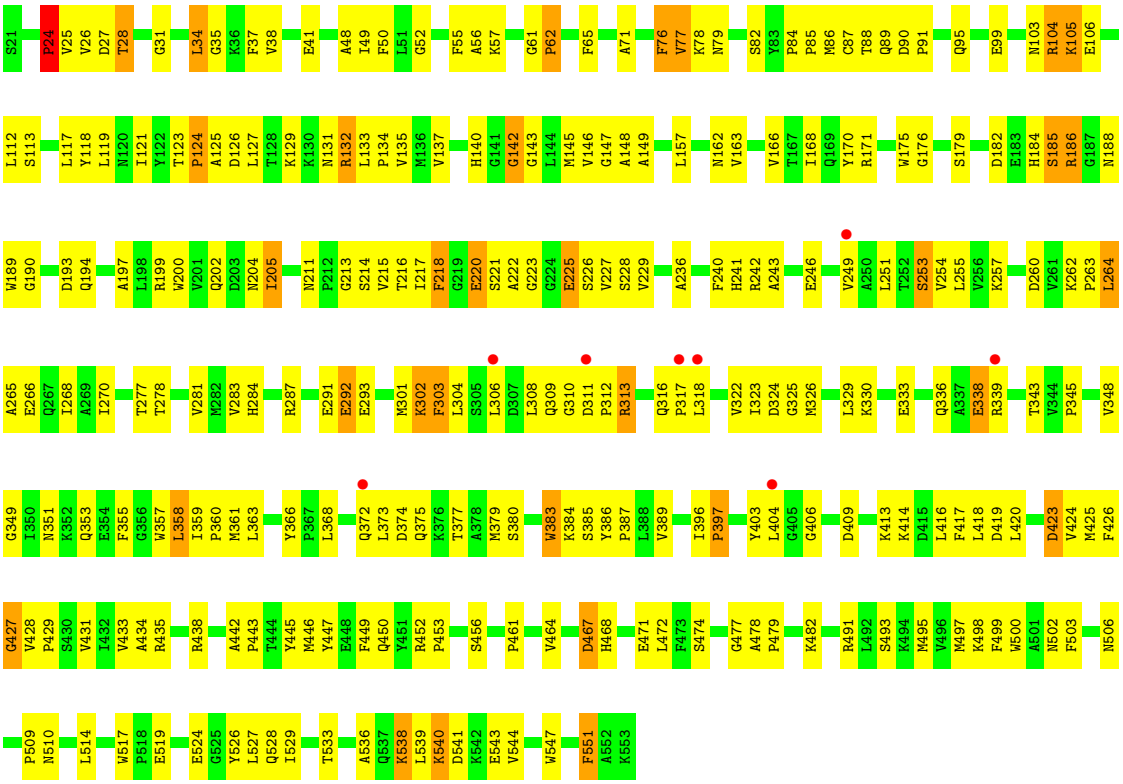
Chain H:





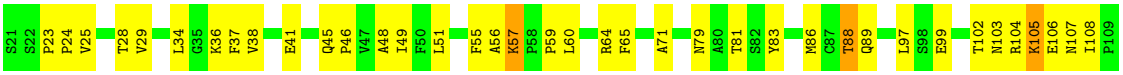
• Molecule 1: CES1 protein

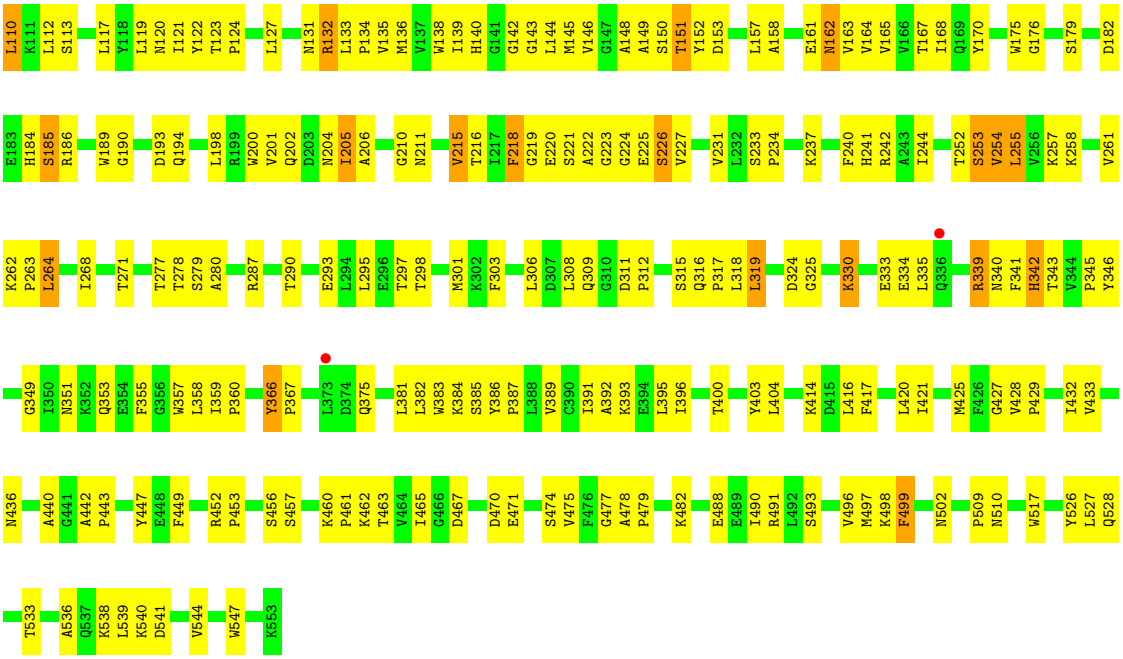
Chain I:



• Molecule 1: CES1 protein

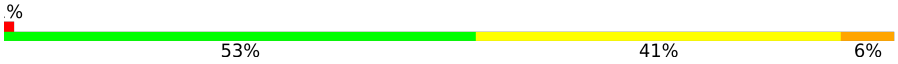
Chain J:

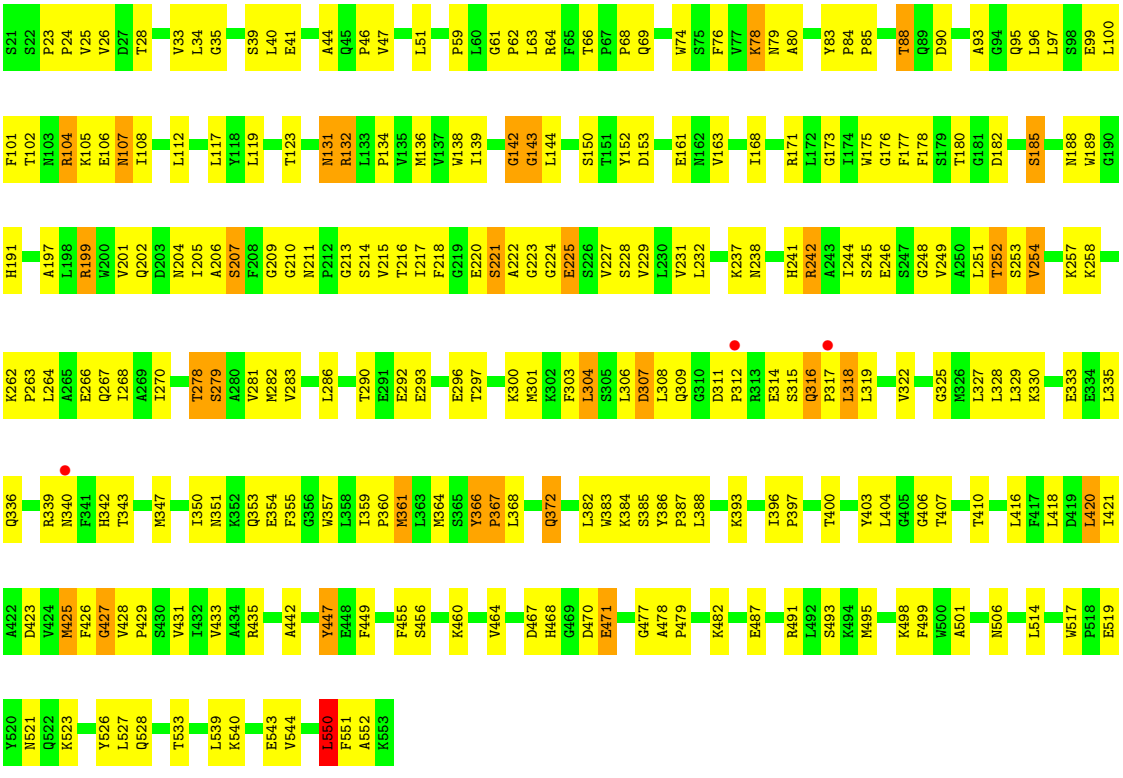




• Molecule 1: CES1 protein

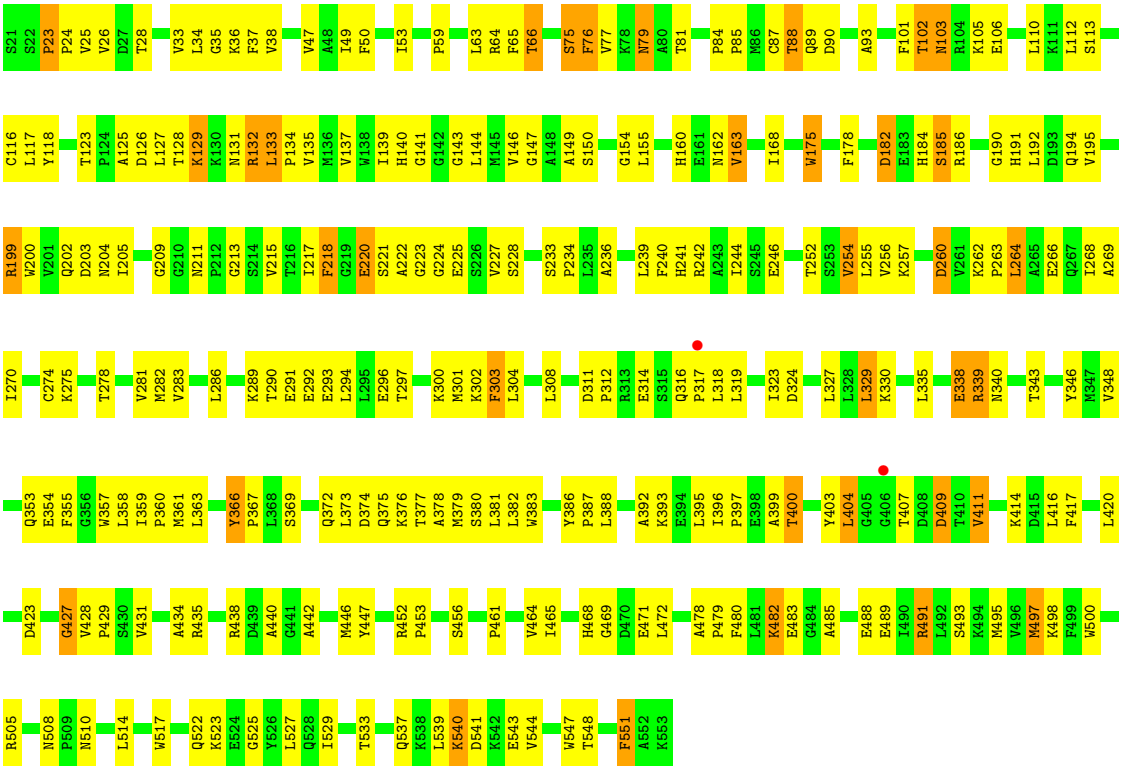
Chain K:





• Molecule 1: CES1 protein

Chain L:


S21 S22 P23 P24 V25 V26 D27 T28 V33 L34 G35 K36 F37 V38 V47 A48 I49 F50 I53 P59 L63 R64 F65 T66 S75 F76 V77 K78 N79 A80 T81 P84 P85 M86 C87 T88 Q89 D90 A93 F101 T102 N103 R104 K105 E106 L110 K111 L112 S113
C116 L117 Y118 T123 P124 A125 D126 L127 T128 K129 K130 N131 R132 L133 P134 V135 M136 V137 W138 I139 H140 G141 G142 G143 L144 M145 V146 G147 A148 A149 S150 G154 L155 H160 E161 N162 V163 I168 W175 F178 D182 E183 H184 S185 R186 G190 H191 L192 D193 Q194 V195
R199 W200 V201 Q202 D203 N204 I205 G209 G210 N211 P212 G213 S214 V215 T216 I217 F218 G219 E220 S221 A222 G223 G224 E225 S226 V227 S228 S233 P234 L235 A236 L239 F240 H241 R242 A243 I244 S245 E246 T252 S253 V254 L255 V256 K257 D260 V261 K262 P263 L264 A265 E266 Q267 I268 A269
I270 C274 K275 T278 V281 M282 V283 L286 K289 T290 E291 E292 E293 L294 L295 E296 T297 K300 M301 K302 F303 L304 L308 D311 P312 R313 E314 S315 Q316 P317 L318 L319 I323 D324 L327 L328 L329 K330 L335 E338 R339 N340 T343 Y346 M347 V348
Q353 E354 F355 G356 W357 L358 I359 P360 M361 L363 Y366 P367 L368 S369 Q372 L373 D374 Q375 K376 T377 A378 M379 S380 L381 L382 W383 Y386 P387 L388 A392 K393 E394 L395 I396 P397 E398 A399 T400 Y403 L404 G405 G406 T407 D408 D409 T410 V411 K414 D415 L416 F417 L420
D423 G427 V428 P429 S430 V431 A434 R435 R438 D439 A440 G441 A442 M446 Y447 R452 P453 S456 P461 V464 I465 H468 G469 D470 E471 L472 A478 P479 F480 L481 K482 E483 G484 A485 E488 E489 I490 R491 L492 S493 K494 M495 V496 M497 K498 F499 W500
R505 N508 P509 N510 L514 W517 Q522 K523 E524 G525 Y526 L527 Q528 I529 T533 Q537 K538 L539 K540 D541 K542 E543 V544 W547 T548 F551 A552 K553

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.287 0.196 , 0.200	Depositor DCC
R_{free} test set	6249 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 27.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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	0.92	EDS
Total number of atoms	50793	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.64	4/4236 (0.1%)	0.70	2/5754 (0.0%)
1	B	0.62	3/4237 (0.1%)	0.66	3/5754 (0.1%)
1	C	0.62	3/4237 (0.1%)	0.66	0/5754
1	D	0.60	0/4236	0.67	1/5754 (0.0%)
1	E	0.71	6/4237 (0.1%)	0.69	4/5754 (0.1%)
1	F	0.63	3/4237 (0.1%)	0.67	2/5754 (0.0%)
1	G	0.73	10/4236 (0.2%)	0.78	9/5754 (0.2%)
1	H	0.70	2/4235 (0.0%)	0.70	1/5752 (0.0%)
1	I	0.92	12/4237 (0.3%)	0.76	13/5754 (0.2%)
1	J	0.61	3/4237 (0.1%)	0.68	2/5754 (0.0%)
1	K	0.60	4/4236 (0.1%)	0.68	1/5754 (0.0%)
1	L	0.64	4/4237 (0.1%)	0.68	3/5754 (0.1%)
All	All	0.67	54/50838 (0.1%)	0.69	41/69046 (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	D	0	1
1	G	0	2
1	K	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CD2-CE2	21.55	1.67	1.41
1	I	383	TRP	CE3-CZ3	20.67	1.73	1.38
1	H	77	VAL	CB-CG1	19.61	1.94	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	383	TRP	CE2-CZ2	17.00	1.68	1.39
1	E	77	VAL	CB-CG1	15.91	1.86	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	550	LEU	O-C-N	13.71	144.63	122.70
1	G	550	LEU	CA-C-O	-12.66	93.51	120.10
1	G	182	ASP	CB-CG-OD1	11.15	128.34	118.30
1	A	550	LEU	O-C-N	8.86	136.88	122.70
1	I	186	ARG	NE-CZ-NH1	8.76	124.68	120.30

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 (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	4130	0	4131	221	0
1	B	4131	0	4130	180	0
1	C	4131	0	4130	199	0
1	D	4130	0	4130	199	0
1	E	4131	0	4131	202	0
1	F	4131	0	4130	184	0
1	G	4130	0	4129	192	0
1	H	4129	0	4131	206	0
1	I	4131	0	4131	212	0
1	J	4131	0	4129	214	0
1	K	4130	0	4130	219	0
1	L	4131	0	4131	227	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	5	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	1	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	8	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	9	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	2486	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 25.

The worst 5 of 2486 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
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
5:B:12:BEZ:C1	5:B:12:BEZ:C6	1.78	1.57
1:B:24:PRO:C	1:B:24:PRO:CA	1.76	1.54

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%)	6 34
1	B	530/532 (100%)	448 (84%)	65 (12%)	17 (3%)	4 26
1	C	530/532 (100%)	467 (88%)	54 (10%)	9 (2%)	9 42
1	D	530/532 (100%)	454 (86%)	60 (11%)	16 (3%)	4 28
1	E	530/532 (100%)	438 (83%)	80 (15%)	12 (2%)	6 34
1	F	530/532 (100%)	464 (88%)	51 (10%)	15 (3%)	5 29
1	G	530/532 (100%)	445 (84%)	62 (12%)	23 (4%)	2 20
1	H	530/532 (100%)	449 (85%)	71 (13%)	10 (2%)	8 39
1	I	530/532 (100%)	451 (85%)	60 (11%)	19 (4%)	3 23
1	J	530/532 (100%)	444 (84%)	74 (14%)	12 (2%)	6 34
1	K	530/532 (100%)	451 (85%)	64 (12%)	15 (3%)	5 29
1	L	530/532 (100%)	434 (82%)	80 (15%)	16 (3%)	4 28
All	All	6360/6384 (100%)	5396 (85%)	788 (12%)	176 (3%)	5 29

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/448 (100%)	423 (94%)	25 (6%)	21 57
1	B	448/448 (100%)	419 (94%)	29 (6%)	17 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	448/448 (100%)	419 (94%)	29 (6%)	17 51
1	D	448/448 (100%)	418 (93%)	30 (7%)	16 50
1	E	448/448 (100%)	417 (93%)	31 (7%)	15 49
1	F	448/448 (100%)	430 (96%)	18 (4%)	31 66
1	G	448/448 (100%)	423 (94%)	25 (6%)	21 57
1	H	448/448 (100%)	423 (94%)	25 (6%)	21 57
1	I	448/448 (100%)	418 (93%)	30 (7%)	16 50
1	J	448/448 (100%)	424 (95%)	24 (5%)	22 58
1	K	448/448 (100%)	417 (93%)	31 (7%)	15 49
1	L	448/448 (100%)	413 (92%)	35 (8%)	12 43
All	All	5376/5376 (100%)	5044 (94%)	332 (6%)	18 53

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	313	ARG
1	K	318	LEU
1	I	471	GLU
1	J	346	TYR
1	L	81	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	549	ASN
1	J	549	ASN
1	I	241	HIS
1	J	107	ASN
1	K	267	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 monosaccharides 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	E	2386	-	9,9,9	1.45	1 (11%)	11,11,11	1.24	2 (18%)
2	NAG	J	4179	1	14,14,15	0.79	0	17,19,21	1.33	4 (23%)
3	SIA	B	1280	-	21,21,21	0.82	0	25,31,31	1.33	4 (16%)
4	SO4	E	2284	-	4,4,4	0.31	0	6,6,6	0.15	0
4	SO4	G	3184	-	4,4,4	0.27	0	6,6,6	0.13	0
2	NAG	E	2279	1	14,14,15	0.54	0	17,19,21	1.05	1 (5%)
4	SO4	A	1384	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SIA	E	582	-	21,21,21	0.90	1 (4%)	25,31,31	1.17	1 (4%)
3	SIA	H	882	-	21,21,21	1.08	2 (9%)	25,31,31	1.13	2 (8%)
3	SIA	L	1282	-	21,21,21	0.86	0	25,31,31	1.17	2 (8%)
5	BEZ	A	11	-	9,9,9	3.02	5 (55%)	11,11,11	1.50	1 (9%)
2	NAG	D	2179	1	14,14,15	0.72	0	17,19,21	0.65	1 (5%)
4	SO4	B	1284	-	4,4,4	0.32	0	6,6,6	0.08	0
5	BEZ	D	2386	-	9,9,9	3.16	7 (77%)	11,11,11	1.09	0
4	SO4	D	2384	-	4,4,4	0.35	0	6,6,6	0.14	0
5	BEZ	L	4380	-	9,9,9	1.57	1 (11%)	11,11,11	1.15	2 (18%)
5	BEZ	F	5023	1	8,8,9	2.14	4 (50%)	9,9,11	0.66	0
5	BEZ	B	1386	-	9,9,9	2.19	3 (33%)	11,11,11	0.87	0
3	SIA	J	1082	-	21,21,21	1.06	2 (9%)	25,31,31	1.09	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BEZ	J	5041	1	8,8,9	2.21	3 (37%)	9,9,11	0.63	0
4	SO4	J	4185	-	4,4,4	0.31	0	6,6,6	0.23	0
4	SO4	J	4184	-	4,4,4	0.28	0	6,6,6	0.14	0
4	SO4	I	3185	-	4,4,4	0.27	0	6,6,6	0.13	0
4	SO4	K	4385	-	4,4,4	0.29	0	6,6,6	0.07	0
2	NAG	C	1379	1	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
4	SO4	C	1285	-	4,4,4	0.33	0	6,6,6	0.17	0
5	BEZ	A	1385	-	9,9,9	4.16	4 (44%)	11,11,11	1.86	1 (9%)
5	BEZ	H	3386	-	9,9,9	1.57	1 (11%)	11,11,11	1.41	2 (18%)
5	BEZ	I	3381	-	9,9,9	1.96	3 (33%)	11,11,11	0.85	1 (9%)
5	BEZ	K	4387	-	9,9,9	2.92	6 (66%)	11,11,11	1.05	0
4	SO4	K	4284	-	4,4,4	0.29	0	6,6,6	0.05	0
4	SO4	I	3285	-	4,4,4	0.33	0	6,6,6	0.13	0
2	NAG	K	4279	1	14,14,15	0.84	0	17,19,21	0.67	0
4	SO4	J	4384	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SIA	G	782	-	21,21,21	0.97	1 (4%)	25,31,31	1.04	1 (4%)
4	SO4	L	4285	-	4,4,4	0.32	0	6,6,6	0.07	0
5	BEZ	C	5013	1	8,8,9	2.18	3 (37%)	9,9,11	0.78	1 (11%)
5	BEZ	F	5024	-	9,9,9	1.85	3 (33%)	11,11,11	0.98	1 (9%)
5	BEZ	G	3385	-	9,9,9	1.81	1 (11%)	11,11,11	1.57	3 (27%)
2	NAG	H	3279	1	14,14,15	0.75	0	17,19,21	0.86	0
4	SO4	H	3284	-	4,4,4	0.34	0	6,6,6	0.10	0
5	BEZ	L	4381	-	9,9,9	1.40	1 (11%)	11,11,11	1.26	2 (18%)
5	BEZ	J	5042	-	9,9,9	4.75	4 (44%)	11,11,11	2.75	3 (27%)
5	BEZ	C	5014	-	9,9,9	2.23	1 (11%)	11,11,11	1.43	2 (18%)
5	BEZ	B	12	-	9,9,9	16.30	9 (100%)	11,11,11	4.00	3 (27%)
3	SIA	A	1180	-	21,21,21	0.83	1 (4%)	25,31,31	1.04	1 (4%)
2	NAG	L	4379	1	14,14,15	0.57	0	17,19,21	0.82	1 (5%)
3	SIA	D	2180	-	21,21,21	0.91	0	25,31,31	0.98	1 (4%)
3	SIA	F	682	-	21,21,21	1.17	3 (14%)	25,31,31	1.10	3 (12%)
5	BEZ	E	2387	-	9,9,9	1.50	1 (11%)	11,11,11	1.32	3 (27%)
5	BEZ	K	4386	-	9,9,9	1.61	1 (11%)	11,11,11	1.29	2 (18%)
3	SIA	I	982	-	21,21,21	0.86	1 (4%)	25,31,31	0.97	2 (8%)
4	SO4	B	1385	-	4,4,4	0.27	0	6,6,6	0.13	0
2	NAG	G	3179	1	14,14,15	0.84	0	17,19,21	0.92	1 (5%)
4	SO4	C	1185	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	D	2184	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	A	1184	-	4,4,4	0.25	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1179	1	14,14,15	0.70	0	17,19,21	0.70	1 (5%)
4	SO4	F	2185	-	4,4,4	0.31	0	6,6,6	0.15	0
4	SO4	G	3384	-	4,4,4	0.30	0	6,6,6	0.16	0
5	BEZ	G	3386	-	9,9,9	5.13	7 (77%)	11,11,11	3.63	6 (54%)
5	BEZ	H	3387	-	9,9,9	3.71	5 (55%)	11,11,11	4.83	6 (54%)
5	BEZ	D	2385	-	9,9,9	12.09	9 (100%)	11,11,11	2.90	8 (72%)
3	SIA	A	1181	-	21,21,21	1.10	3 (14%)	25,31,31	0.99	2 (8%)
4	SO4	F	2285	-	4,4,4	0.32	0	6,6,6	0.13	0
5	BEZ	I	3380	-	9,9,9	1.49	1 (11%)	11,11,11	1.47	3 (27%)
3	SIA	K	1182	-	21,21,21	0.95	1 (4%)	25,31,31	1.12	1 (4%)
4	SO4	E	2385	-	4,4,4	0.27	0	6,6,6	0.12	0
2	NAG	B	1279	1	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
4	SO4	H	3385	-	4,4,4	0.33	0	6,6,6	0.11	0
2	NAG	F	2379	1	14,14,15	1.18	2 (14%)	17,19,21	1.56	3 (17%)
2	NAG	I	3379	1	14,14,15	0.64	0	17,19,21	0.89	1 (5%)

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	E	2386	-	-	0/4/4/4	0/1/1/1
2	NAG	J	4179	1	1/1/5/7	4/6/23/26	0/1/1/1
3	SIA	B	1280	-	-	11/20/38/38	0/1/1/1
2	NAG	E	2279	1	-	2/6/23/26	0/1/1/1
3	SIA	E	582	-	-	13/20/38/38	0/1/1/1
3	SIA	H	882	-	-	7/20/38/38	0/1/1/1
3	SIA	L	1282	-	-	9/20/38/38	0/1/1/1
5	BEZ	A	11	-	-	0/4/4/4	0/1/1/1
2	NAG	D	2179	1	-	2/6/23/26	0/1/1/1
5	BEZ	D	2386	-	-	0/4/4/4	0/1/1/1
5	BEZ	L	4380	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5023	1	-	0/2/2/4	0/1/1/1
5	BEZ	B	1386	-	-	0/4/4/4	0/1/1/1
3	SIA	J	1082	-	-	10/20/38/38	0/1/1/1
5	BEZ	J	5041	1	-	0/2/2/4	0/1/1/1
5	BEZ	H	3386	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1379	1	-	3/6/23/26	0/1/1/1
5	BEZ	A	1385	-	-	0/4/4/4	0/1/1/1
5	BEZ	I	3381	-	-	0/4/4/4	0/1/1/1
5	BEZ	K	4387	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5024	-	-	0/4/4/4	0/1/1/1
2	NAG	K	4279	1	1/1/5/7	3/6/23/26	0/1/1/1
3	SIA	G	782	-	-	9/20/38/38	0/1/1/1
5	BEZ	C	5013	1	-	0/2/2/4	0/1/1/1
5	BEZ	G	3385	-	-	0/4/4/4	0/1/1/1
2	NAG	H	3279	1	-	6/6/23/26	0/1/1/1
5	BEZ	L	4381	-	-	0/4/4/4	0/1/1/1
5	BEZ	C	5014	-	-	0/4/4/4	0/1/1/1
5	BEZ	B	12	-	-	0/4/4/4	0/1/1/1
3	SIA	A	1180	-	-	7/20/38/38	0/1/1/1
2	NAG	L	4379	1	-	6/6/23/26	0/1/1/1
3	SIA	D	2180	-	-	9/20/38/38	0/1/1/1
3	SIA	F	682	-	-	8/20/38/38	0/1/1/1
5	BEZ	E	2387	-	-	0/4/4/4	0/1/1/1
5	BEZ	K	4386	-	-	0/4/4/4	0/1/1/1
3	SIA	I	982	-	-	11/20/38/38	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	-	6/6/23/26	0/1/1/1
5	BEZ	G	3386	-	-	0/4/4/4	0/1/1/1
5	BEZ	H	3387	-	-	0/4/4/4	0/1/1/1
5	BEZ	D	2385	-	-	0/4/4/4	0/1/1/1
3	SIA	A	1181	-	-	8/20/38/38	0/1/1/1
5	BEZ	I	3380	-	-	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
5	BEZ	J	5042	-	-	2/4/4/4	0/1/1/1
2	NAG	F	2379	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	I	3379	1	-	3/6/23/26	0/1/1/1

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	12	BEZ	C6-C1	23.03	1.78	1.39
5	B	12	BEZ	C2-C1	22.80	1.78	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	12	BEZ	C3-C2	17.98	1.76	1.38
5	B	12	BEZ	C4-C3	17.92	1.85	1.38
5	B	12	BEZ	C5-C4	17.62	1.84	1.38

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3387	BEZ	O2-C-O1	-12.93	94.64	123.35
5	B	12	BEZ	O2-C-O1	10.89	147.52	123.35
5	J	5042	BEZ	C6-C1-C2	-7.29	108.20	118.59
5	H	3387	BEZ	O2-C-C1	7.22	133.59	114.85
5	D	2385	BEZ	O2-C-O1	6.19	137.09	123.35

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 163 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	C8-C7-N2-C2
2	B	1279	NAG	O7-C7-N2-C2
2	C	1379	NAG	C8-C7-N2-C2

There are no ring outliers.

28 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	4179	NAG	1	0
3	B	1280	SIA	5	0
3	E	582	SIA	2	0
3	H	882	SIA	1	0
3	L	1282	SIA	7	0
5	L	4380	BEZ	1	0

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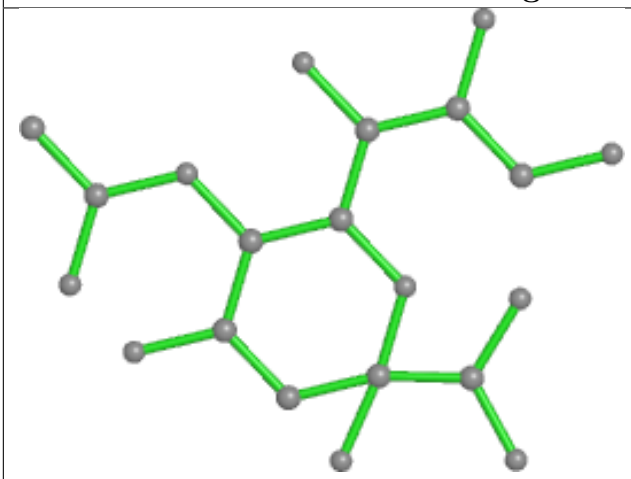
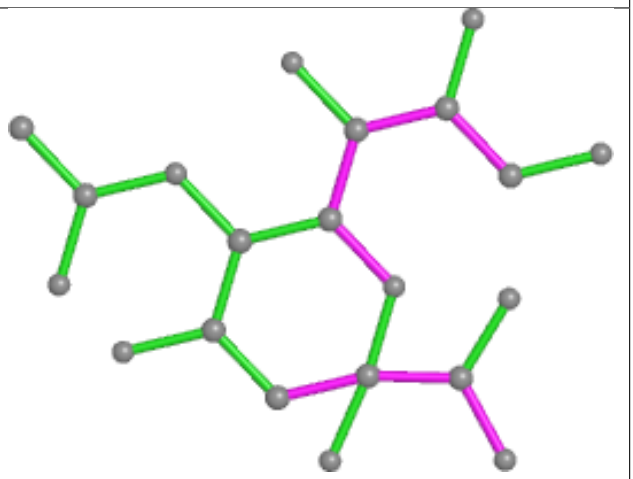
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1082	SIA	5	0
5	A	1385	BEZ	2	0
5	H	3386	BEZ	1	0
4	I	3285	SO4	1	0
2	K	4279	NAG	2	0
3	G	782	SIA	6	0
5	C	5013	BEZ	3	0
5	G	3385	BEZ	1	0
5	J	5042	BEZ	1	0
5	C	5014	BEZ	1	0
5	B	12	BEZ	6	0
3	A	1180	SIA	3	0
3	D	2180	SIA	8	0
3	F	682	SIA	1	0
3	I	982	SIA	5	0
2	G	3179	NAG	1	0
5	D	2385	BEZ	3	0
3	A	1181	SIA	10	0
5	I	3380	BEZ	1	0
3	K	1182	SIA	7	0
2	B	1279	NAG	1	0
2	F	2379	NAG	3	0

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

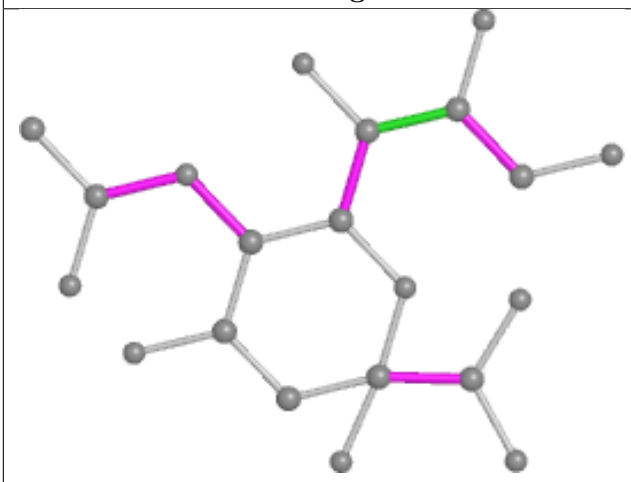
Ligand SIA B 1280



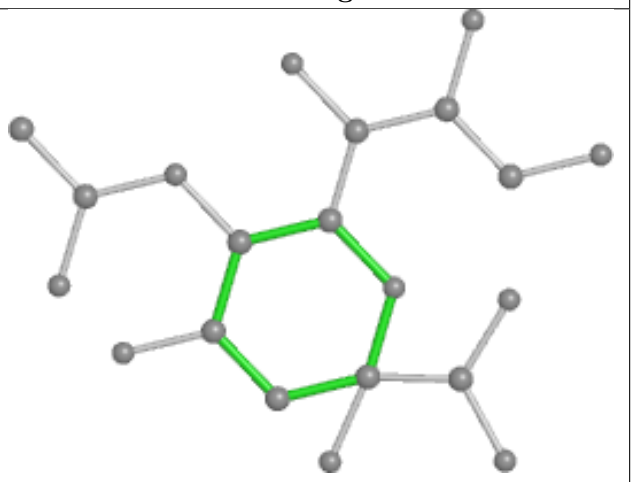
Bond lengths



Bond angles

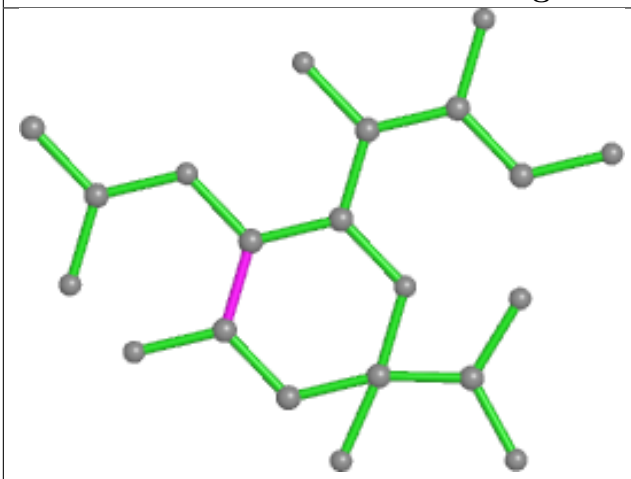


Torsions

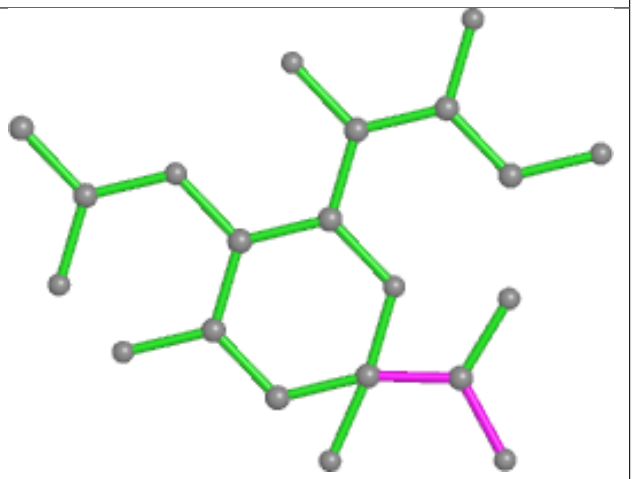


Rings

Ligand SIA E 582



Bond lengths



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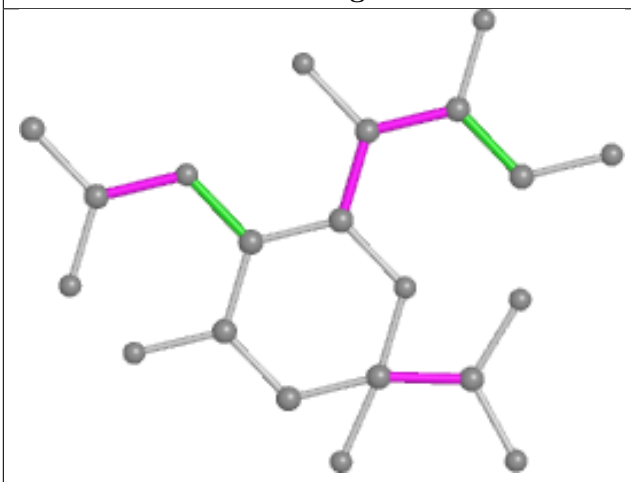

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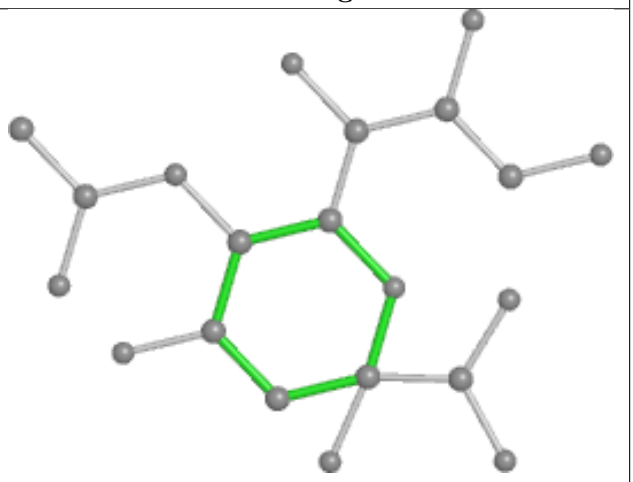
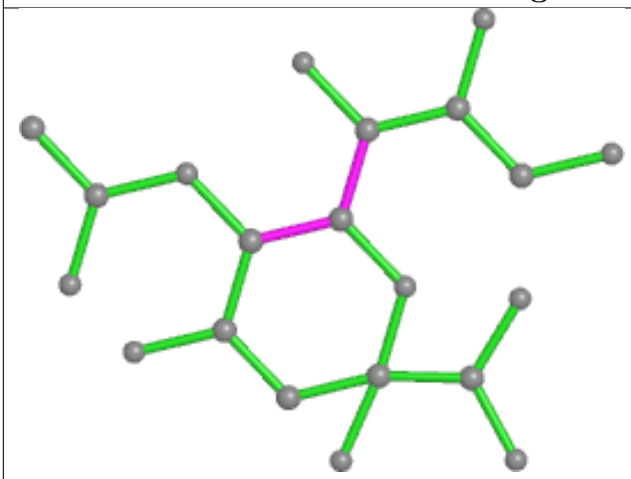


Rings

Ligand SIA H 882



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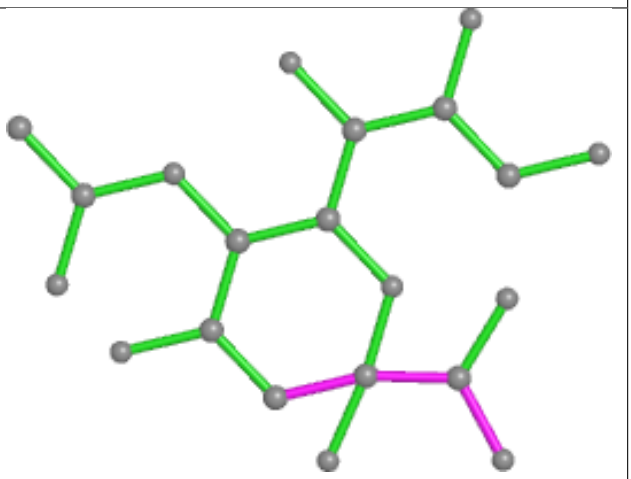
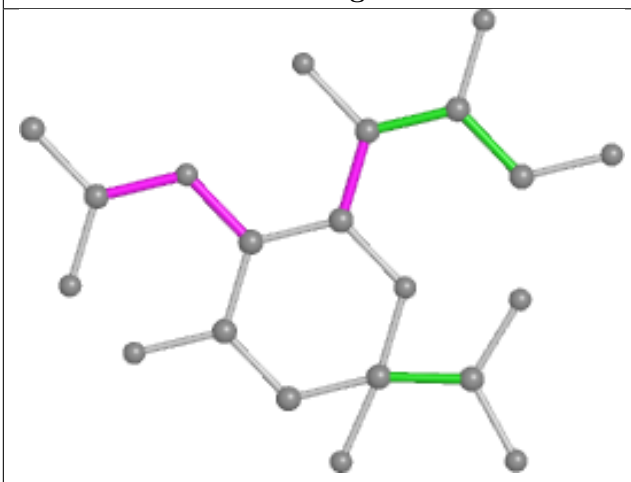


Bond angles



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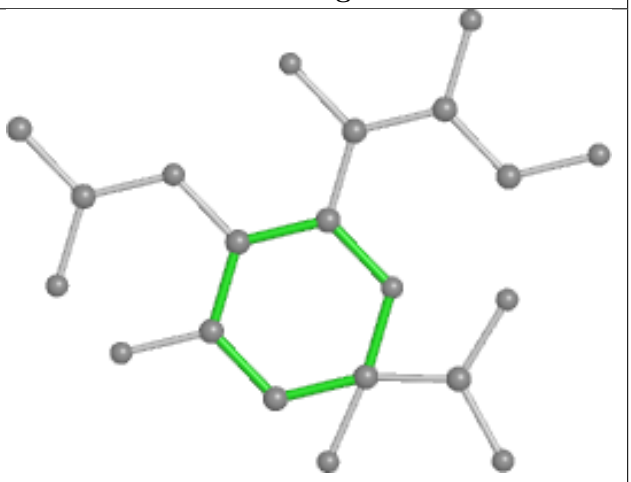
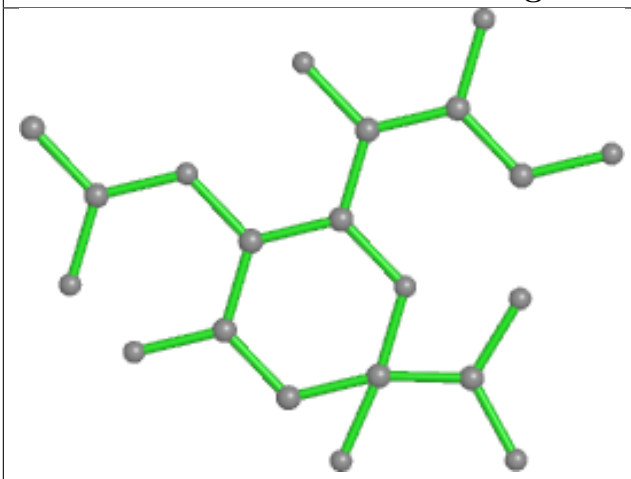


Rings

Ligand SIA L 1282



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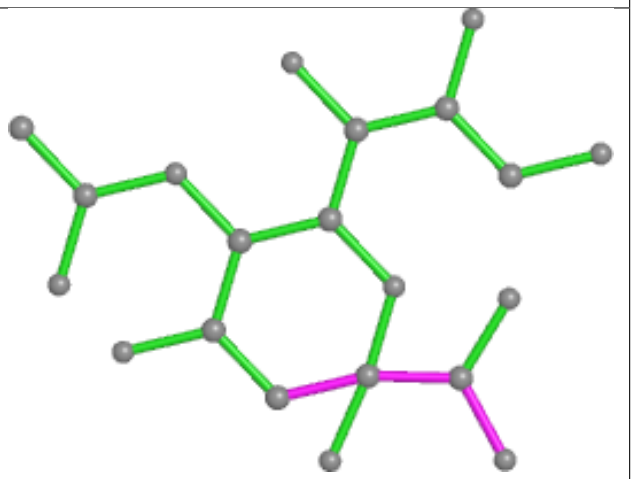

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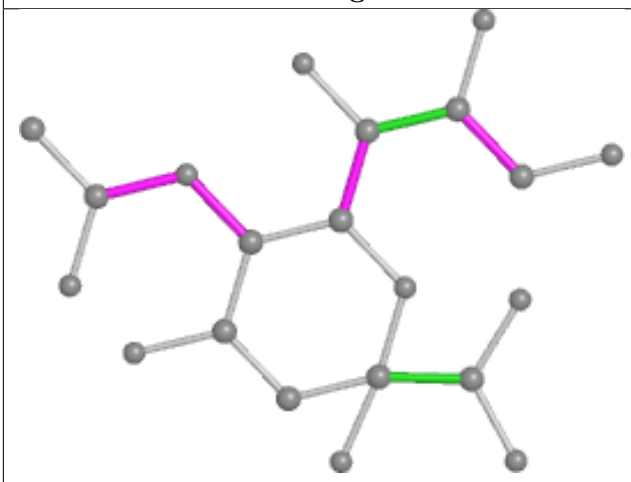
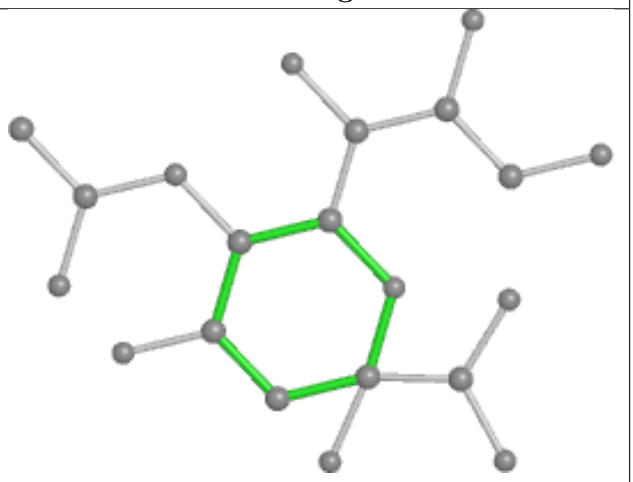
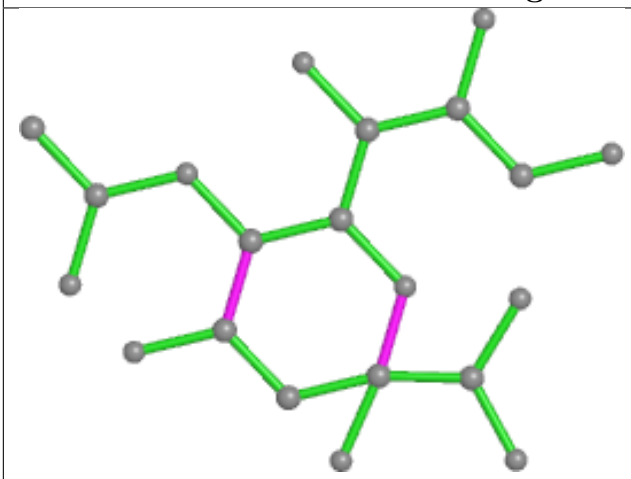


Torsions



Rings

Ligand SIA J 1082



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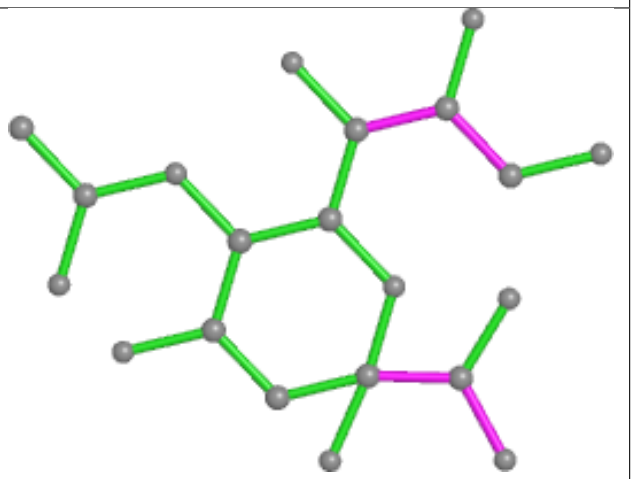
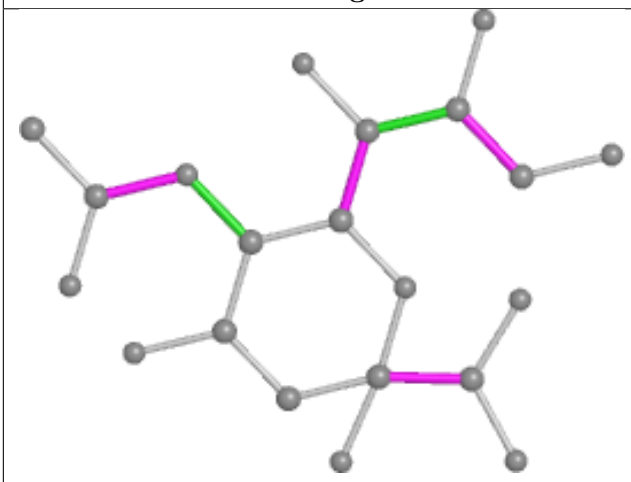


Bond angles



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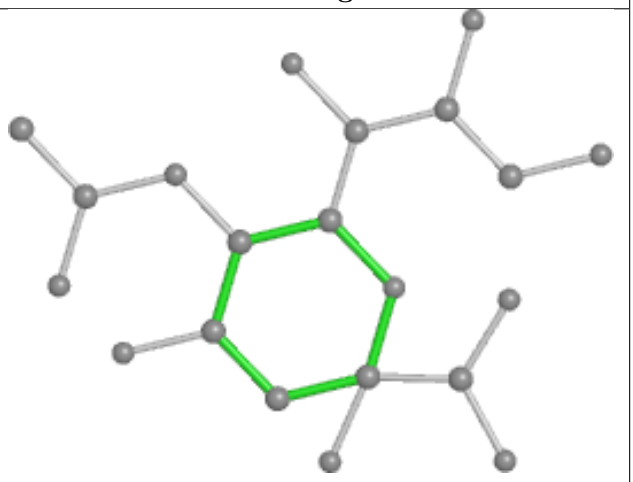
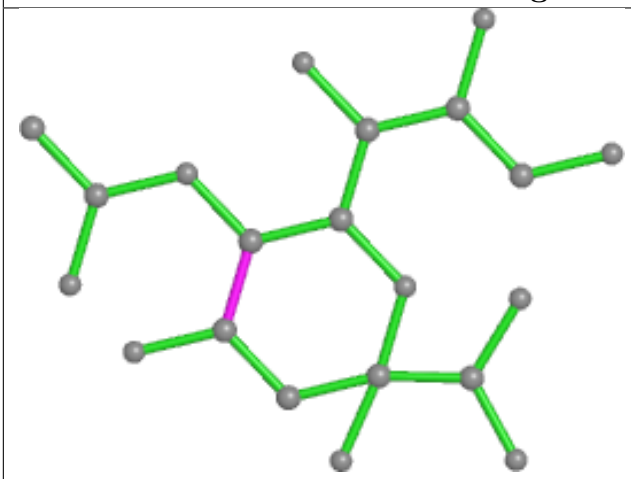


Rings

Ligand SIA G 782



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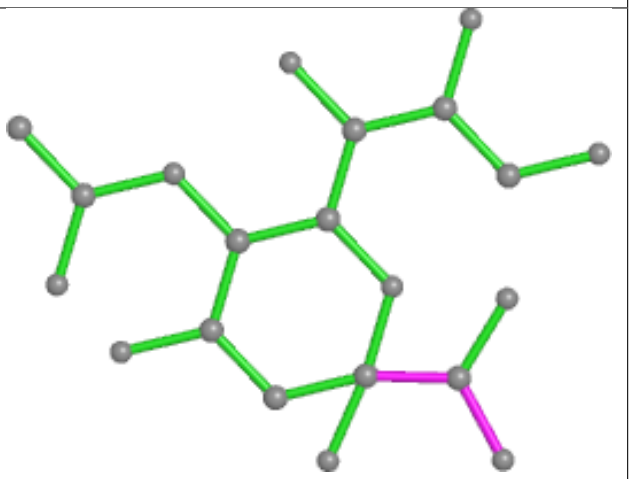

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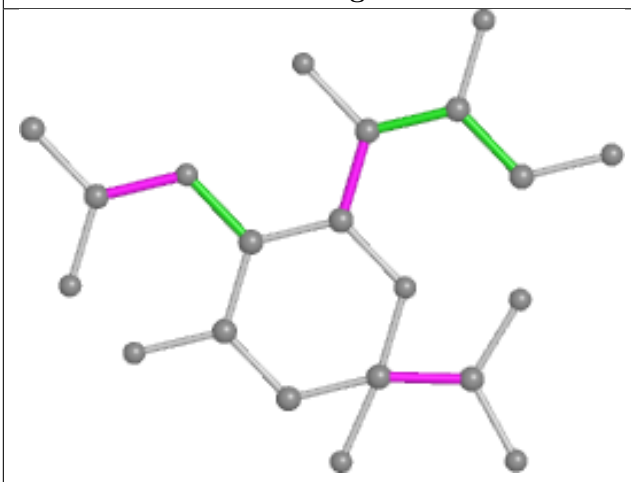

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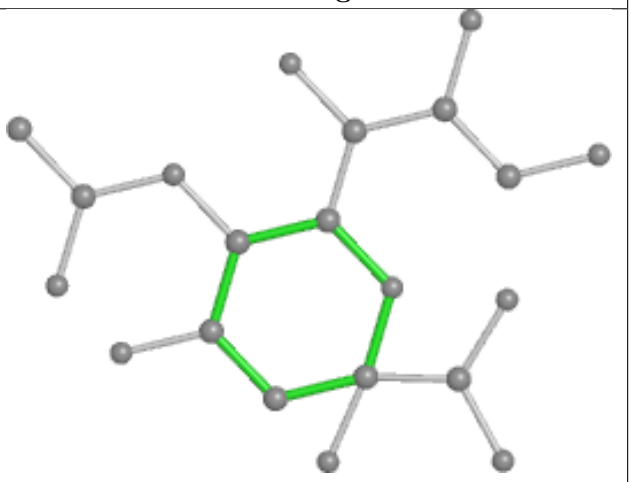
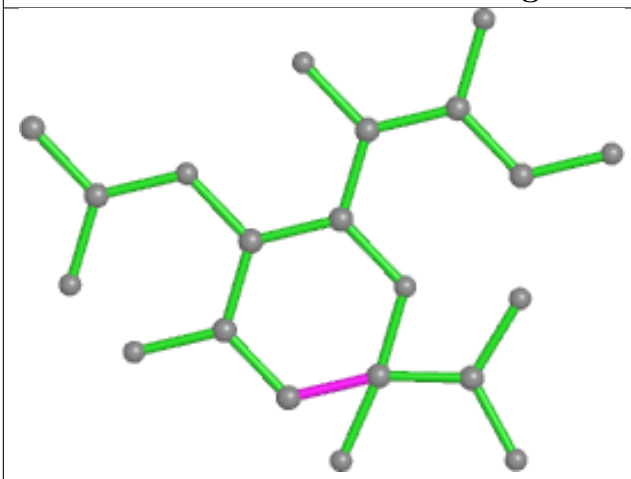


Rings

Ligand SIA A 1180



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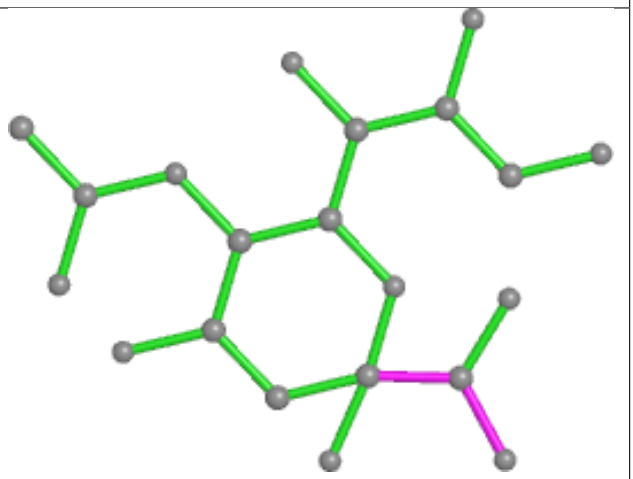

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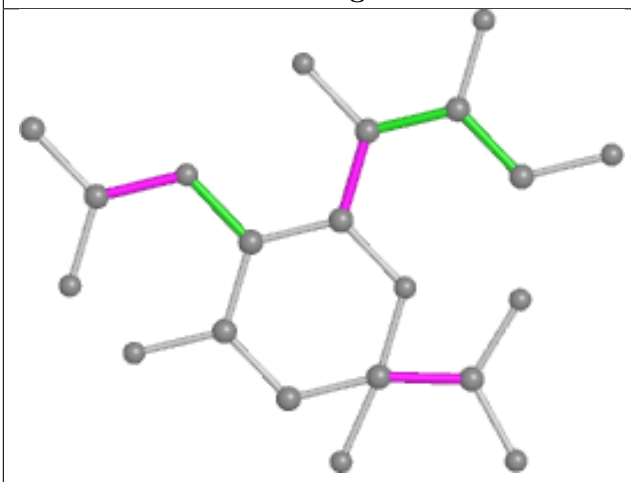

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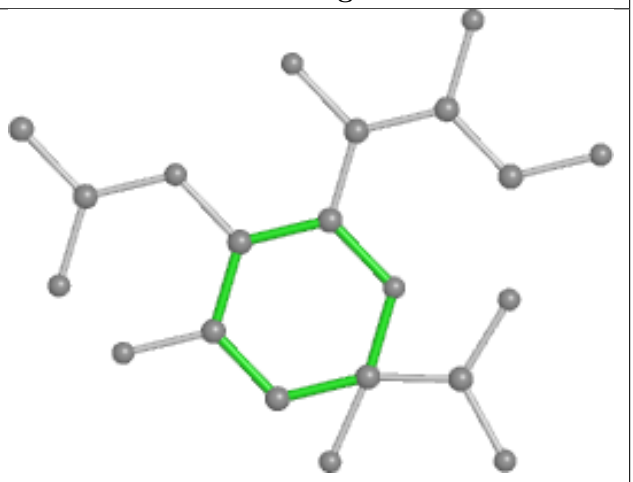
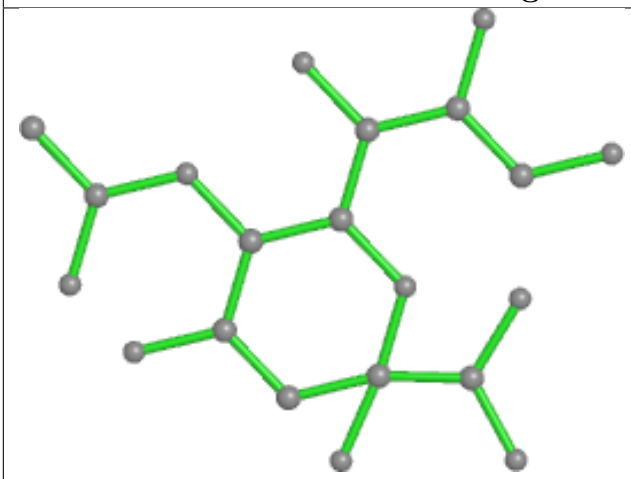
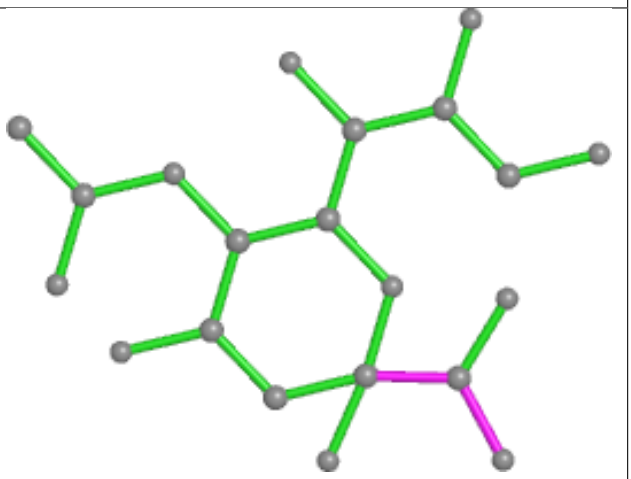


Rings

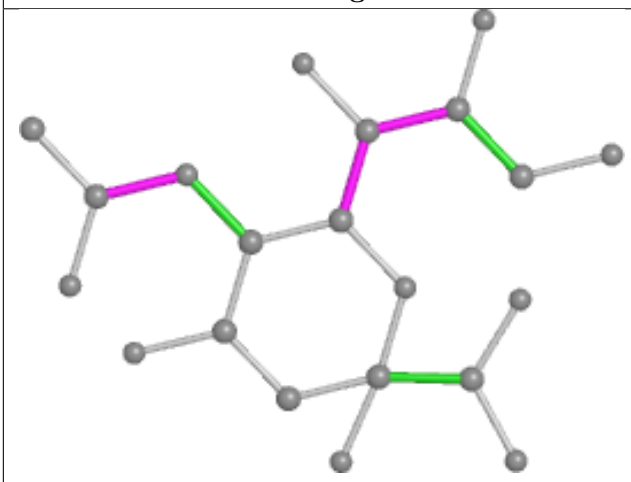
Ligand SIA D 2180



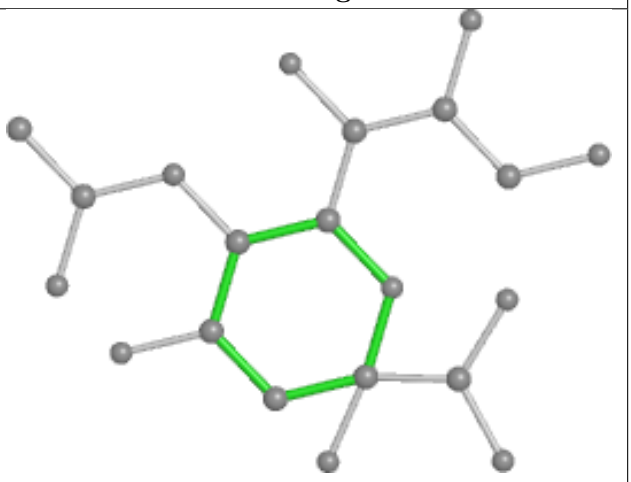
Bond lengths



Bond angles

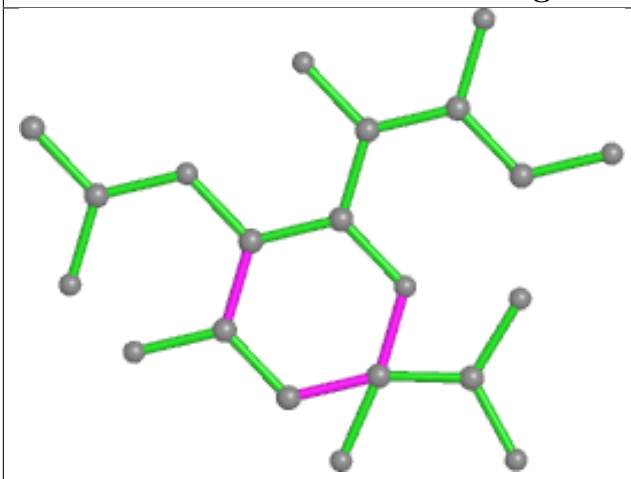


Torsions

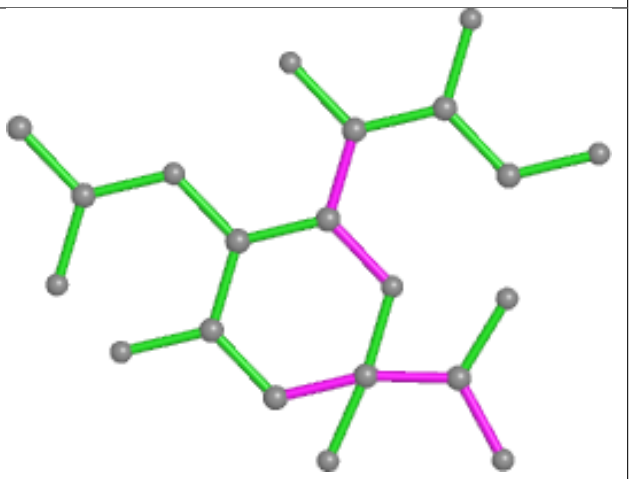


Rings

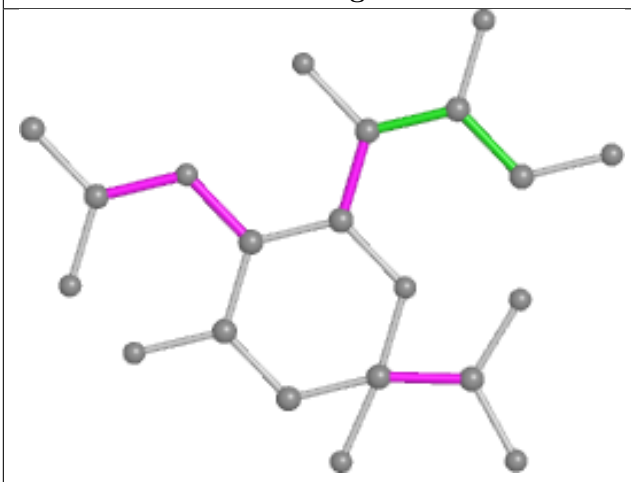
Ligand SIA F 682



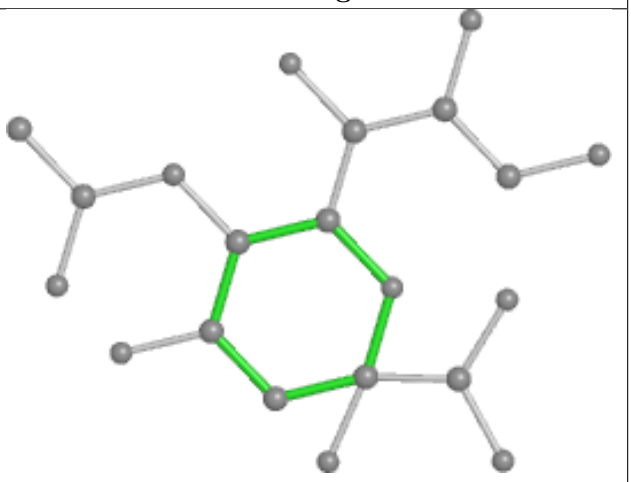
Bond lengths



Bond angles

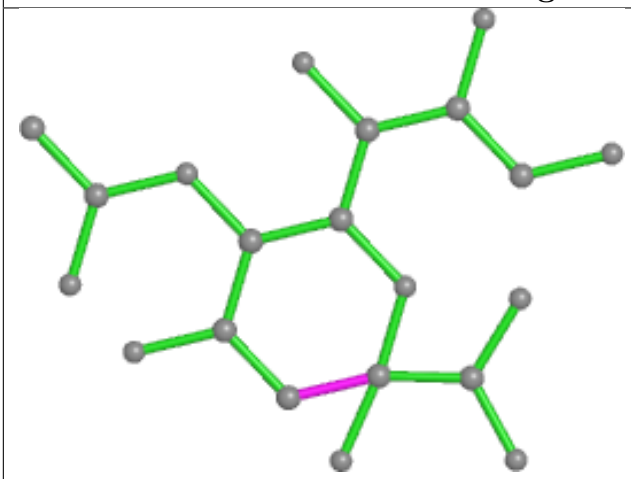


Torsions

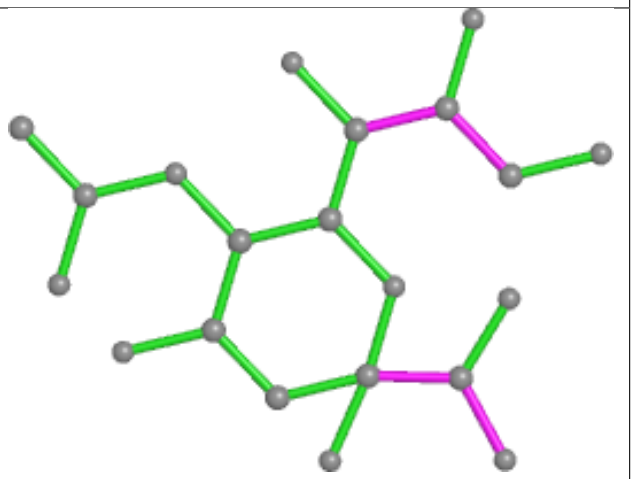


Rings

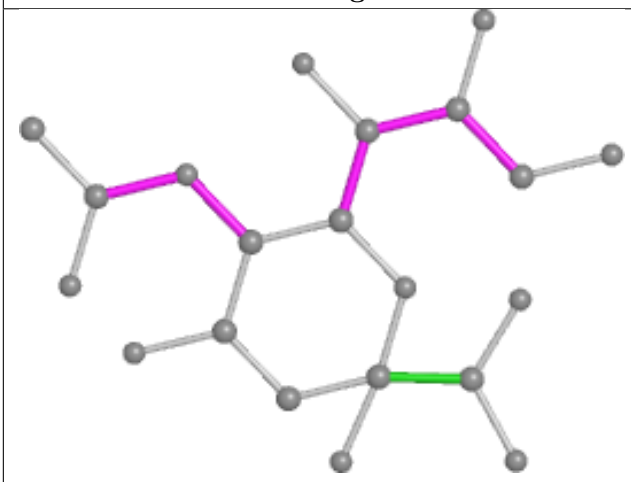
Ligand SIA I 982



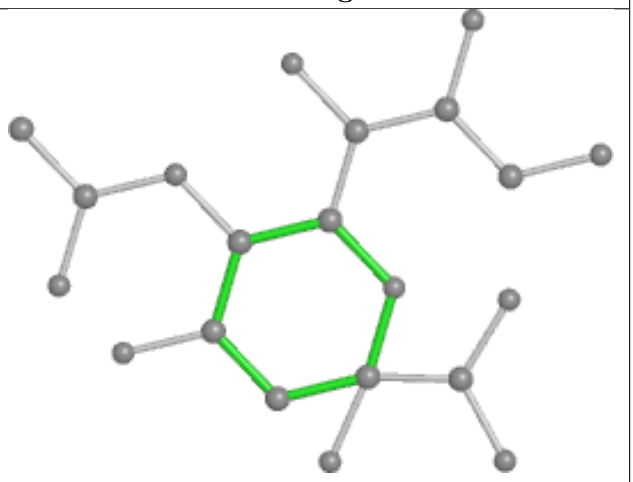
Bond lengths



Bond angles

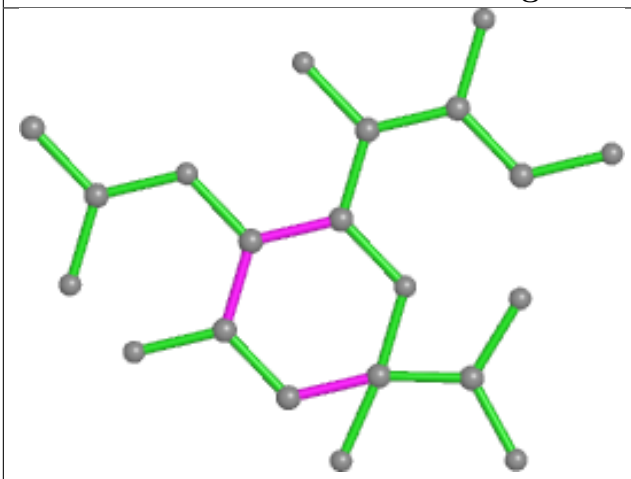


Torsions

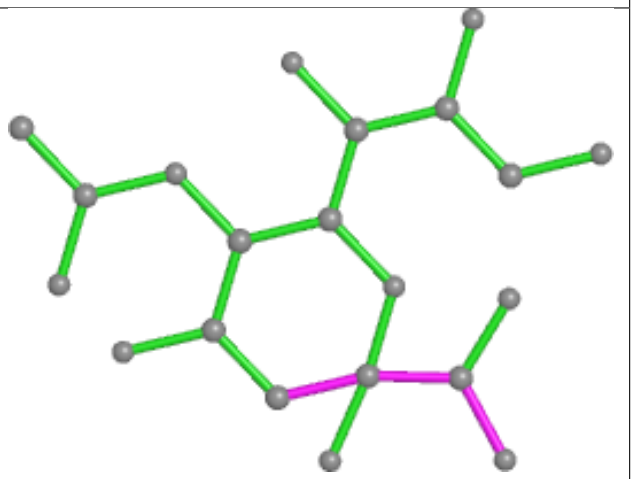


Rings

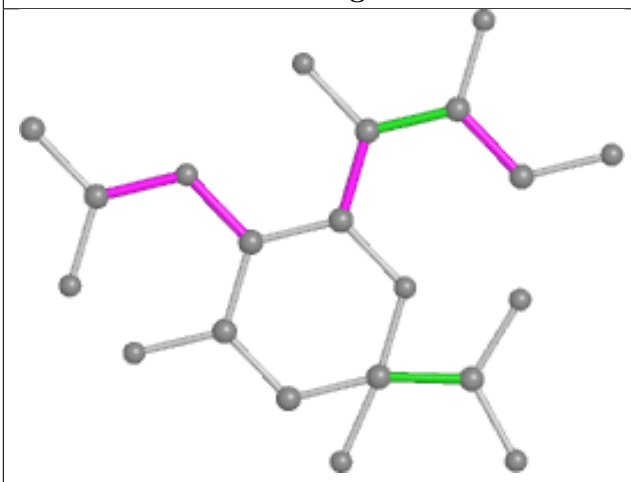
Ligand SIA A 1181



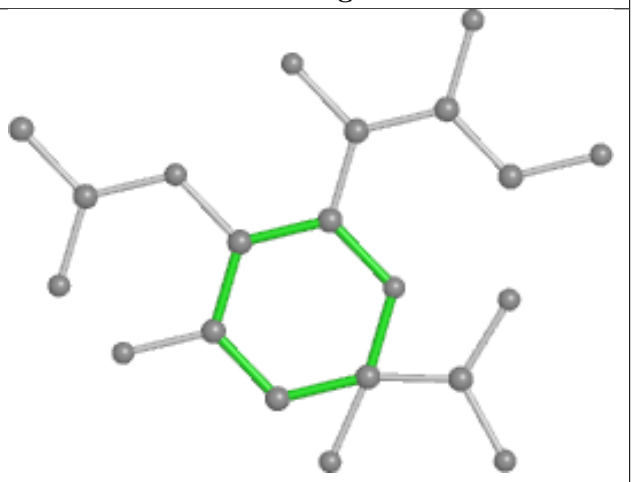
Bond lengths



Bond angles

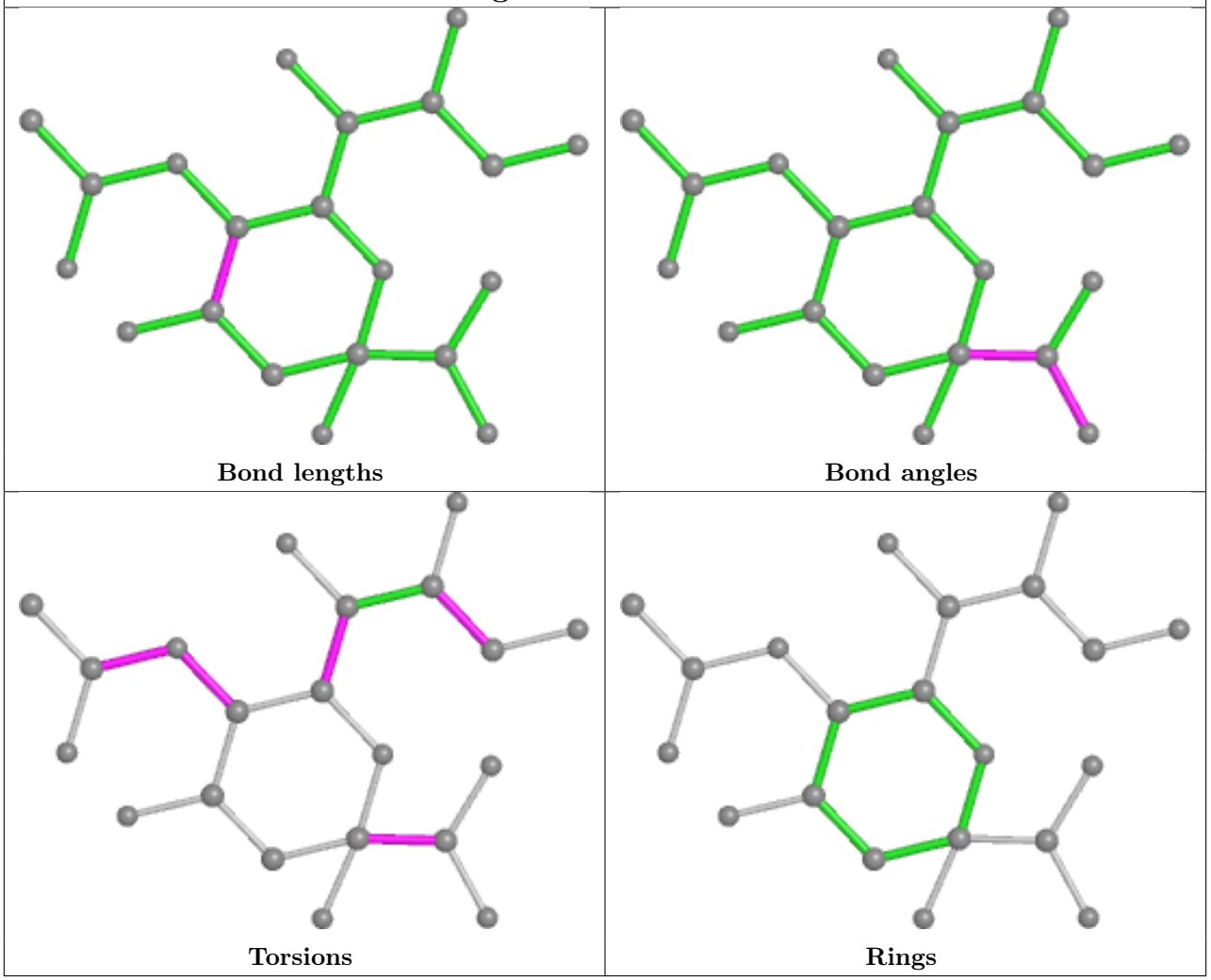


Torsions



Rings

Ligand SIA K 1182



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	532/532 (100%)	-0.06	1 (0%)	95	94	2, 25, 69, 83	0
1	B	532/532 (100%)	0.01	5 (0%)	84	75	4, 29, 74, 86	0
1	C	532/532 (100%)	-0.03	3 (0%)	89	83	2, 26, 64, 85	0
1	D	532/532 (100%)	-0.05	3 (0%)	89	83	2, 25, 70, 84	0
1	E	532/532 (100%)	0.01	5 (0%)	84	75	4, 30, 73, 86	0
1	F	532/532 (100%)	-0.05	5 (0%)	84	75	3, 26, 65, 81	0
1	G	532/532 (100%)	-0.08	0	100	100	3, 26, 67, 85	0
1	H	532/532 (100%)	-0.02	3 (0%)	89	83	2, 27, 71, 84	0
1	I	532/532 (100%)	0.05	8 (1%)	73	61	3, 31, 74, 85	0
1	J	532/532 (100%)	-0.04	2 (0%)	92	89	2, 26, 64, 83	0
1	K	532/532 (100%)	-0.01	3 (0%)	89	83	3, 27, 71, 85	0
1	L	532/532 (100%)	0.02	2 (0%)	92	89	2, 31, 73, 83	0
All	All	6384/6384 (100%)	-0.02	40 (0%)	89	83	2, 27, 70, 86	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	306	LEU	4.5
1	E	307	ASP	3.9
1	H	400	THR	3.7
1	A	315	SER	3.4
1	I	318	LEU	3.2

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

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 (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	1179	14/15	0.76	0.53	70,76,78,78	0
2	NAG	H	3279	14/15	0.83	0.28	63,66,69,69	0
4	SO4	A	1384	5/5	0.84	0.38	76,76,77,77	0
5	BEZ	H	3387	9/9	0.84	0.21	41,43,45,46	0
4	SO4	C	1185	5/5	0.85	0.28	100,100,101,101	0
4	SO4	K	4385	5/5	0.85	0.44	97,98,98,99	0
5	BEZ	B	1386	9/9	0.85	0.23	54,55,56,56	0
2	NAG	K	4279	14/15	0.85	0.23	63,67,71,71	0
5	BEZ	L	4380	9/9	0.85	0.55	59,59,60,60	0
4	SO4	H	3385	5/5	0.86	0.28	97,97,97,97	0
3	SIA	B	1280	21/21	0.86	0.28	45,61,66,67	0
2	NAG	D	2179	14/15	0.86	0.45	70,76,78,79	0
2	NAG	G	3179	14/15	0.86	0.24	67,72,75,75	0
4	SO4	F	2185	5/5	0.86	0.28	106,106,106,106	0
4	SO4	D	2184	5/5	0.87	0.38	100,100,101,101	0
4	SO4	J	4185	5/5	0.87	0.25	96,96,97,97	0
5	BEZ	K	4386	9/9	0.87	0.54	48,49,50,50	0
2	NAG	J	4179	14/15	0.87	0.36	69,75,78,78	0
3	SIA	A	1180	21/21	0.88	0.25	64,71,74,75	0
3	SIA	J	1082	21/21	0.88	0.28	59,71,76,77	0
5	BEZ	B	12	9/9	0.88	0.41	52,53,54,55	0
5	BEZ	L	4381	9/9	0.88	0.20	54,55,55,55	0
2	NAG	C	1379	14/15	0.89	0.23	59,64,68,68	0
3	SIA	E	582	21/21	0.89	0.24	42,60,70,70	0
5	BEZ	C	5014	9/9	0.89	0.20	36,40,40,41	0
5	BEZ	G	3385	9/9	0.89	0.32	58,59,60,60	0
4	SO4	I	3185	5/5	0.89	0.27	95,95,96,96	0
3	SIA	H	882	21/21	0.89	0.23	52,66,69,70	0
3	SIA	I	982	21/21	0.89	0.29	51,60,64,65	0
5	BEZ	A	1385	9/9	0.89	0.19	49,50,52,52	0
3	SIA	G	782	21/21	0.90	0.27	61,69,73,74	0
5	BEZ	G	3386	9/9	0.90	0.20	45,47,48,49	0

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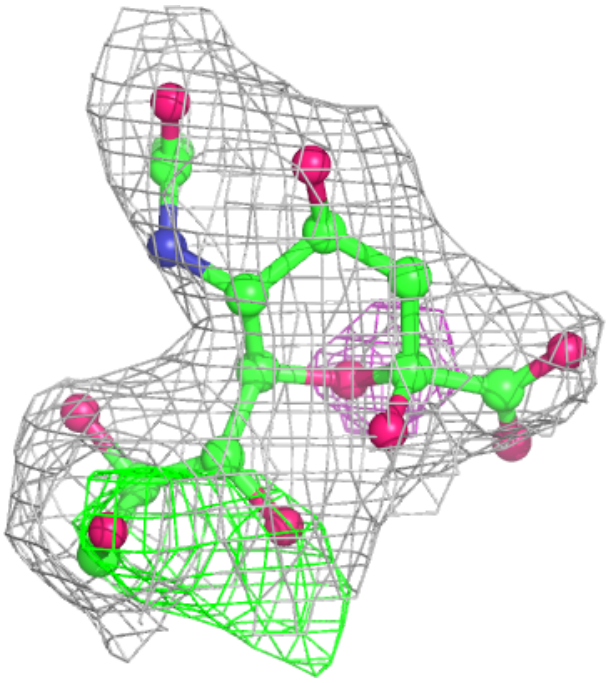
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2379	14/15	0.90	0.16	59,64,66,66	0
5	BEZ	I	3381	9/9	0.90	0.19	52,52,53,54	0
3	SIA	D	2180	21/21	0.90	0.27	57,69,72,73	0
5	BEZ	K	4387	9/9	0.90	0.26	36,39,40,41	0
3	SIA	A	1181	21/21	0.90	0.20	44,57,67,68	0
5	BEZ	D	2385	9/9	0.90	0.44	51,51,53,53	0
2	NAG	L	4379	14/15	0.91	0.23	56,59,62,63	0
5	BEZ	F	5024	9/9	0.91	0.23	42,44,46,46	0
5	BEZ	I	3380	9/9	0.91	0.33	53,53,54,55	0
2	NAG	I	3379	14/15	0.91	0.32	57,61,62,63	0
3	SIA	F	682	21/21	0.92	0.25	52,56,62,62	0
4	SO4	D	2384	5/5	0.92	0.34	76,77,77,77	0
3	SIA	L	1282	21/21	0.92	0.24	50,55,63,65	0
5	BEZ	E	2386	9/9	0.92	0.15	47,47,49,50	0
5	BEZ	E	2387	9/9	0.92	0.22	42,43,43,44	0
4	SO4	F	2285	5/5	0.93	0.24	80,80,81,81	0
3	SIA	K	1182	21/21	0.93	0.23	60,63,67,69	0
5	BEZ	D	2386	9/9	0.93	0.16	44,45,46,46	0
4	SO4	B	1385	5/5	0.93	0.16	96,97,97,98	0
2	NAG	B	1279	14/15	0.93	0.30	59,64,68,70	0
4	SO4	E	2385	5/5	0.94	0.17	94,94,94,95	0
5	BEZ	H	3386	9/9	0.94	0.26	49,51,51,51	0
4	SO4	J	4184	5/5	0.94	0.22	94,94,95,95	0
2	NAG	E	2279	14/15	0.94	0.29	57,60,62,63	0
4	SO4	J	4384	5/5	0.94	0.19	84,85,85,86	0
4	SO4	B	1284	5/5	0.94	0.23	80,80,81,81	0
5	BEZ	A	11	9/9	0.94	0.43	49,51,52,52	0
4	SO4	H	3284	5/5	0.94	0.33	84,84,85,85	0
4	SO4	E	2284	5/5	0.94	0.16	85,86,86,86	0
4	SO4	K	4284	5/5	0.95	0.29	85,85,86,86	0
4	SO4	I	3285	5/5	0.95	0.23	79,79,79,80	0
4	SO4	G	3384	5/5	0.95	0.33	81,81,81,81	0
5	BEZ	J	5042	9/9	0.95	0.16	44,45,46,46	0
5	BEZ	J	5041	8/9	0.96	0.35	41,45,45,46	0
4	SO4	L	4285	5/5	0.96	0.25	74,74,75,75	0
4	SO4	C	1285	5/5	0.96	0.19	76,76,77,77	0
5	BEZ	F	5023	8/9	0.96	0.24	46,49,50,51	0
4	SO4	G	3184	5/5	0.96	0.27	86,86,87,88	0
4	SO4	A	1184	5/5	0.96	0.28	94,94,94,95	0
5	BEZ	C	5013	8/9	0.97	0.20	40,44,46,46	0

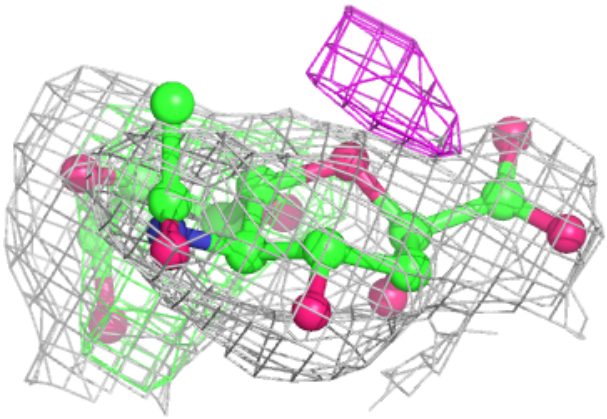
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

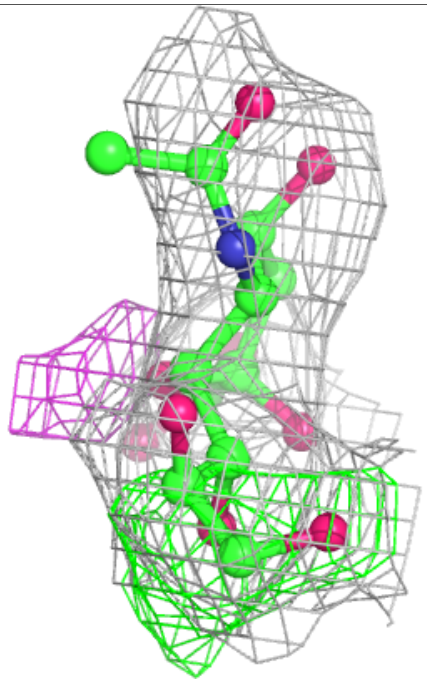
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

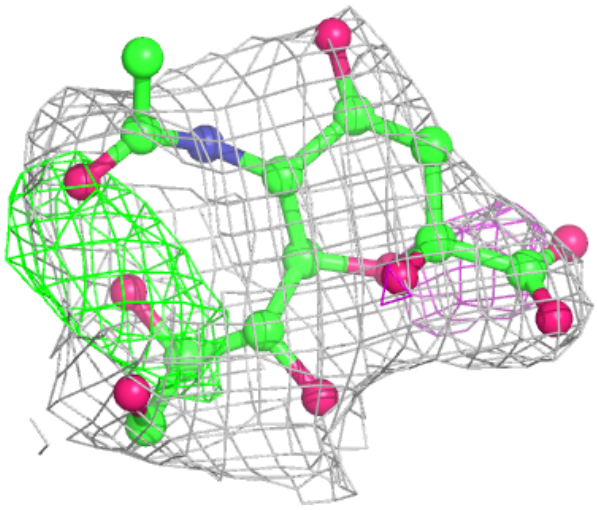


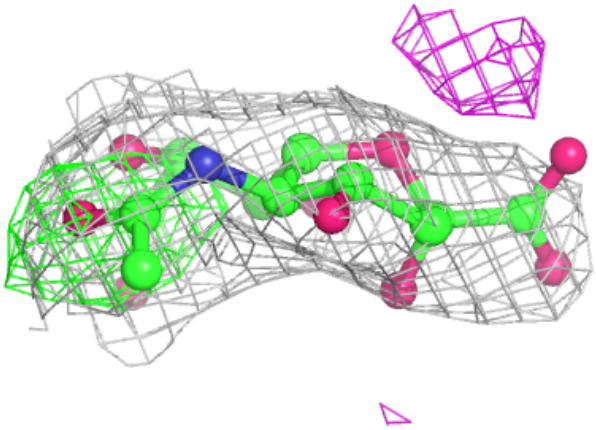


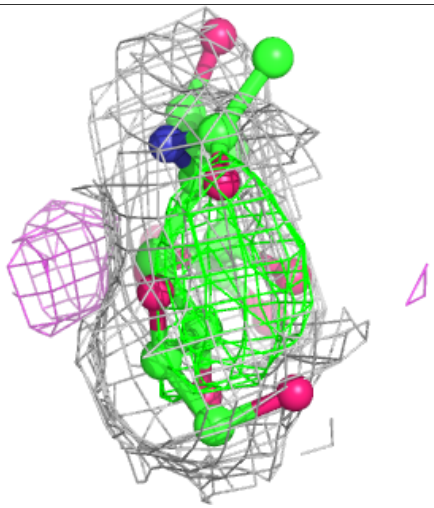


Electron density around SIA A 1180:

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

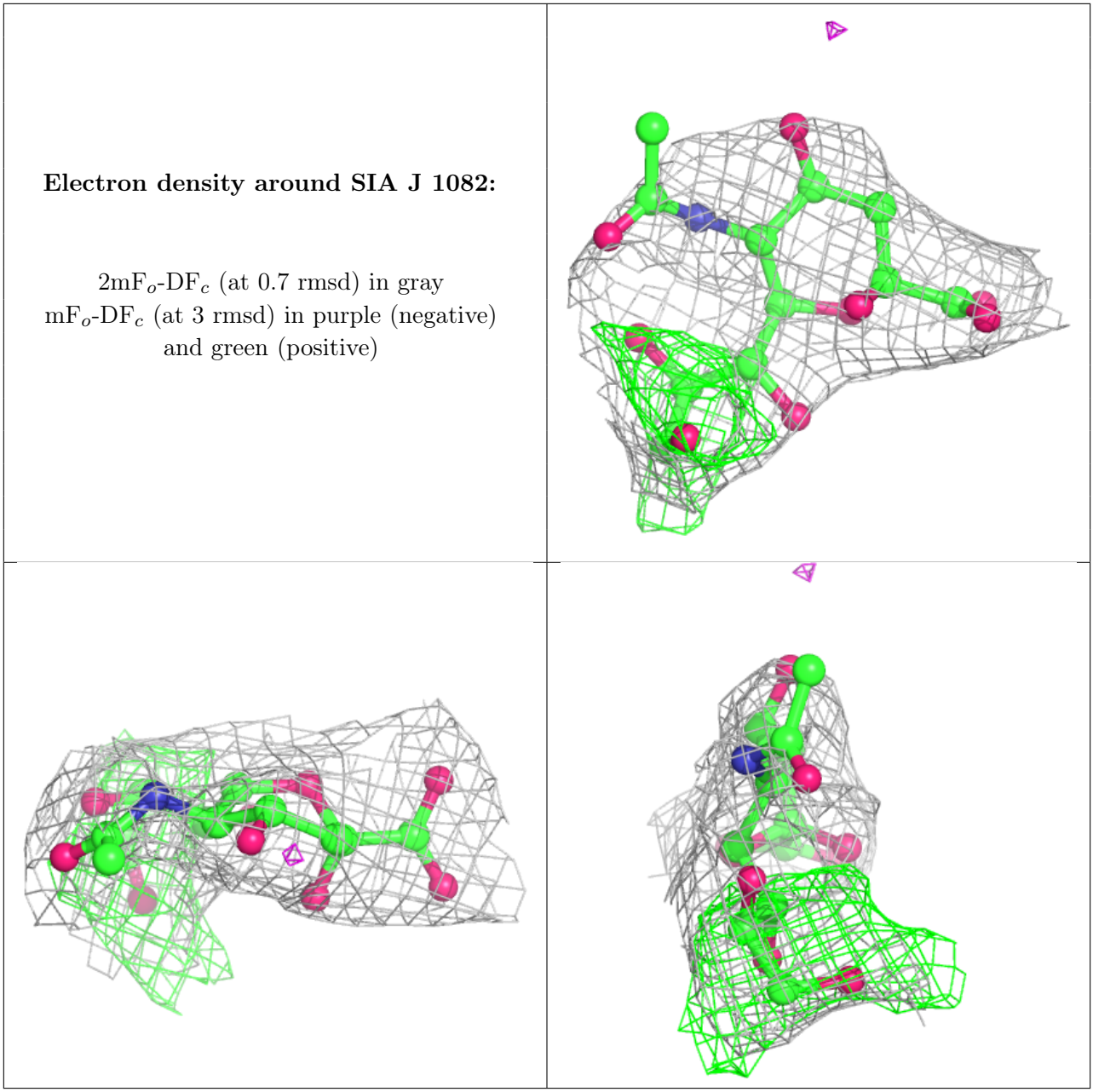






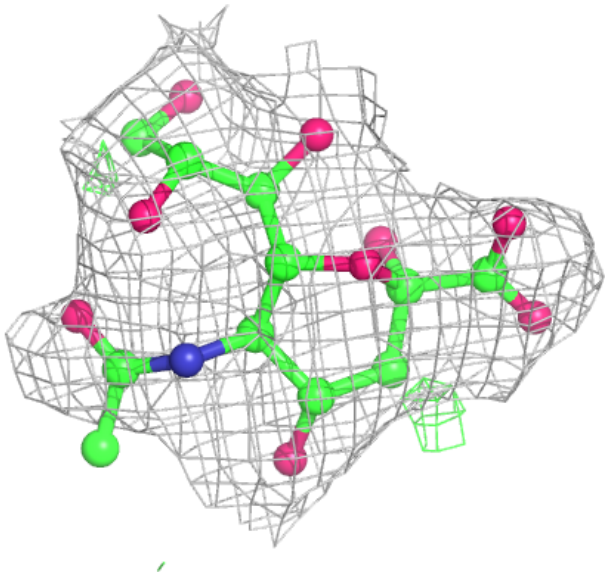
Electron density around SIA J 1082:

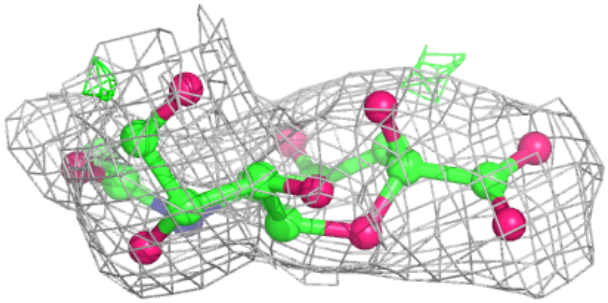
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

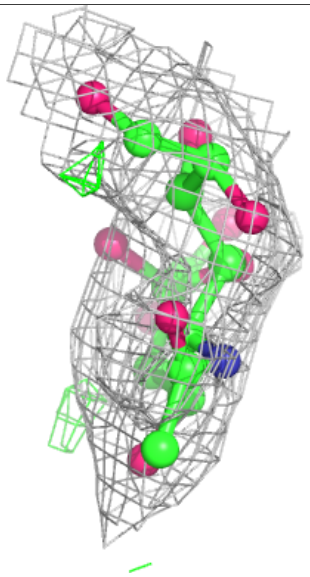


Electron density around SIA E 582:

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

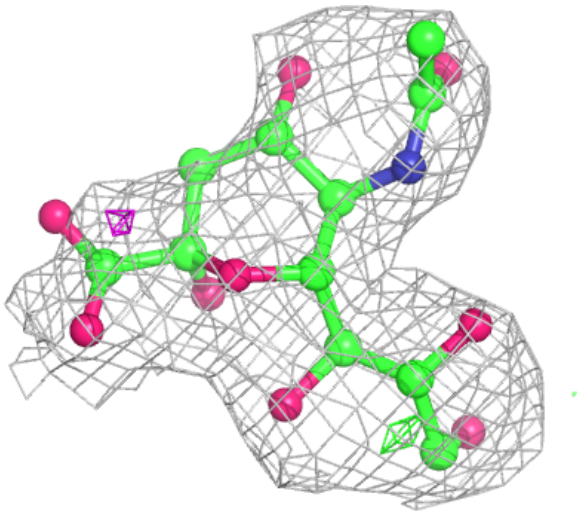


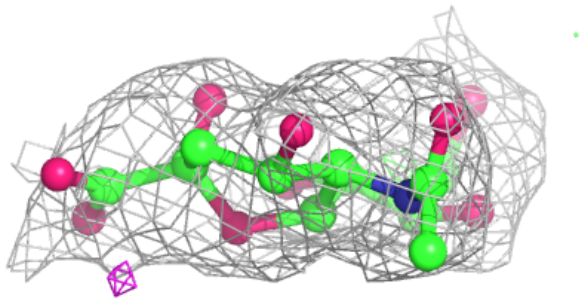


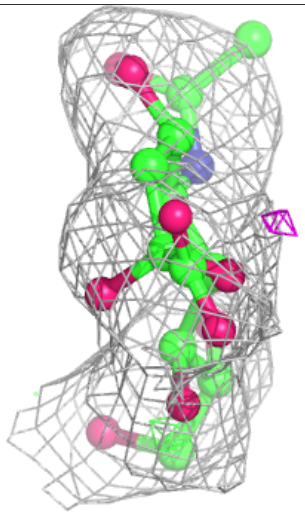


Electron density around SIA H 882:

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

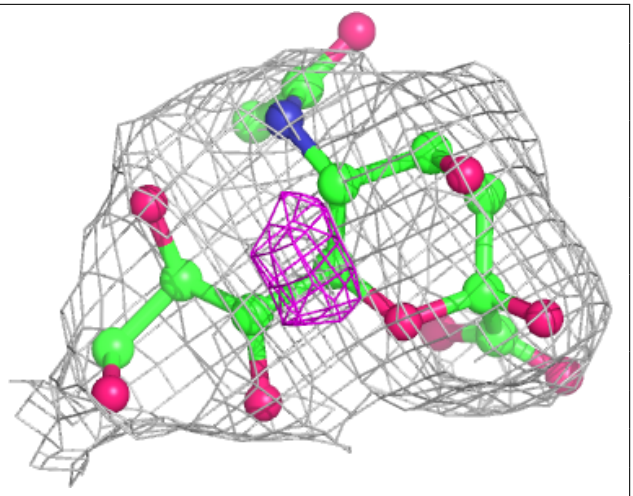


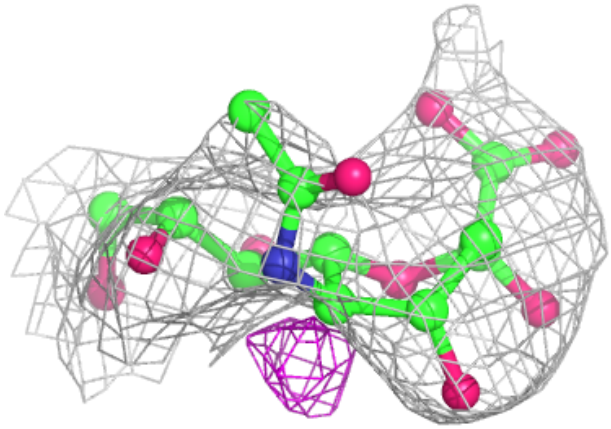


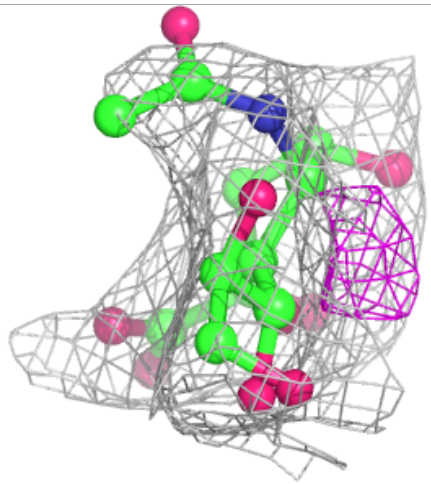


Electron density around SIA I 982:

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

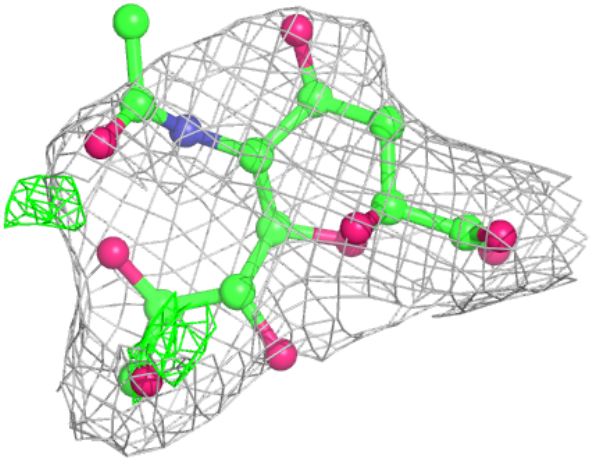


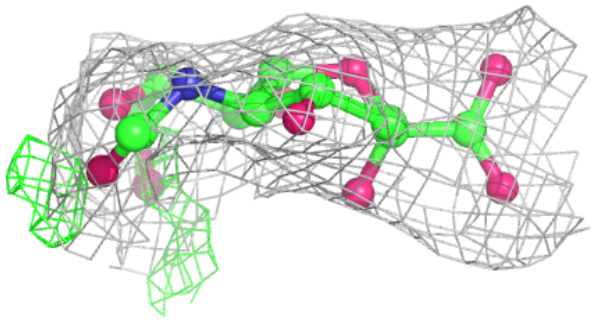


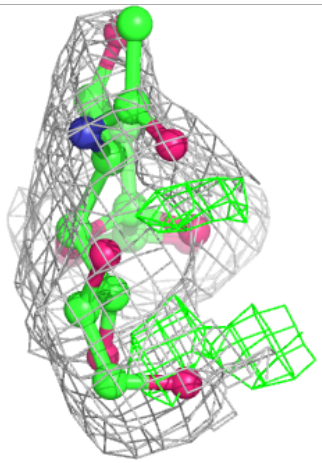


Electron density around SIA G 782:

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

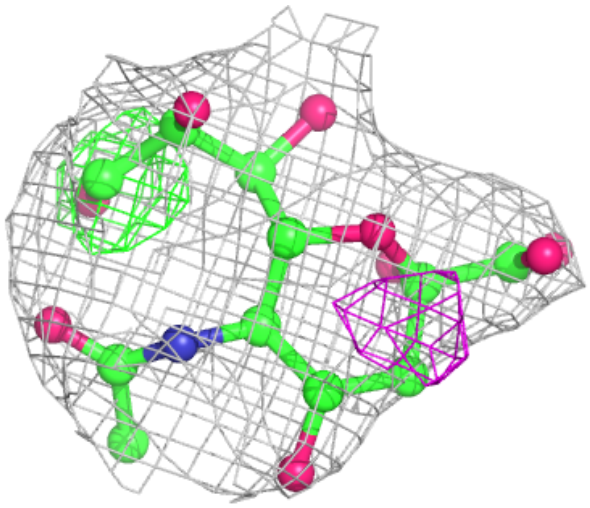


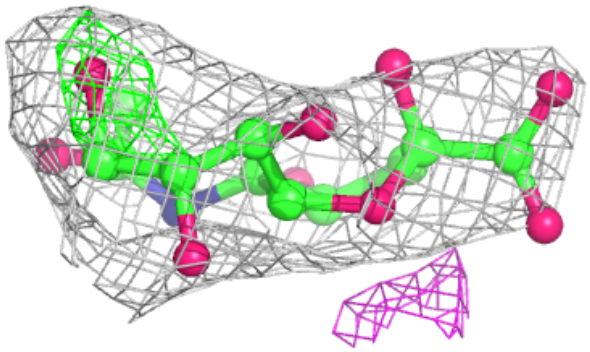


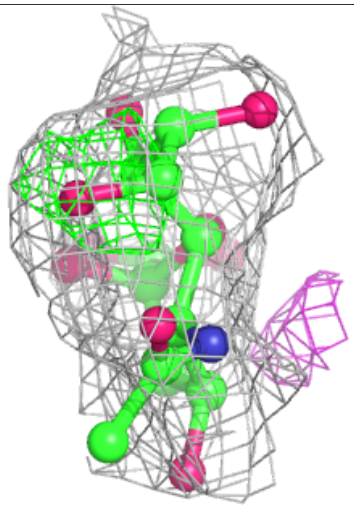


Electron density around SIA D 2180:

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

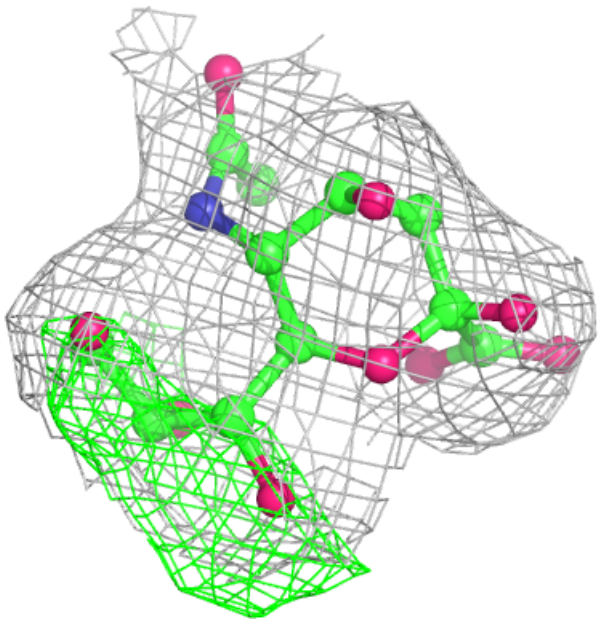


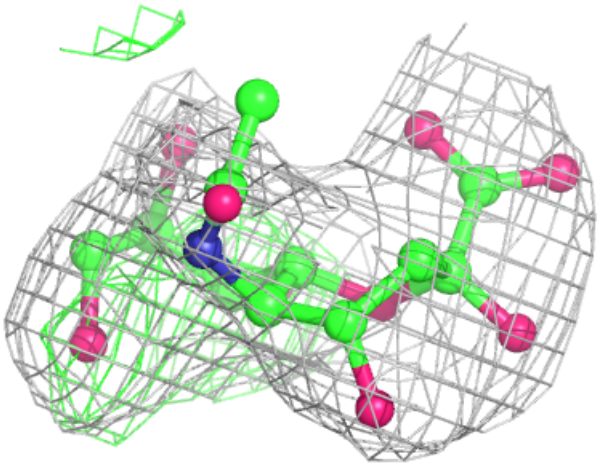


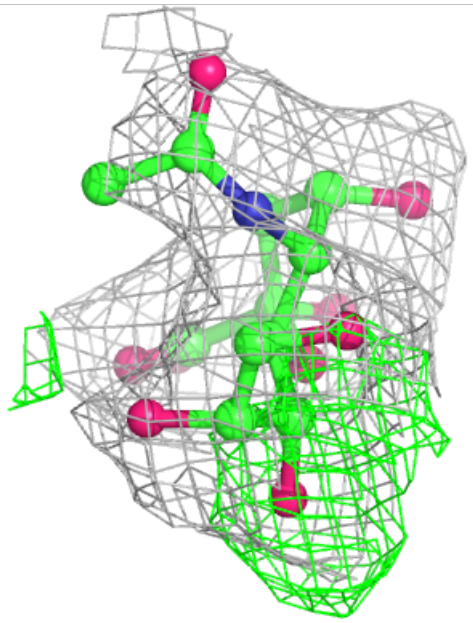


Electron density around SIA A 1181:

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

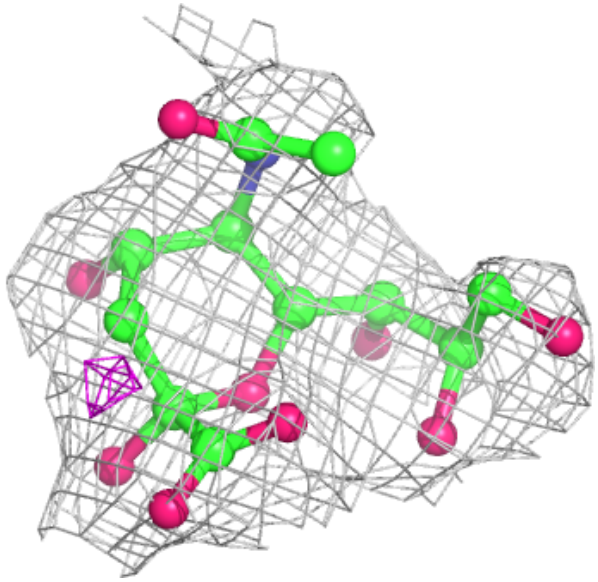


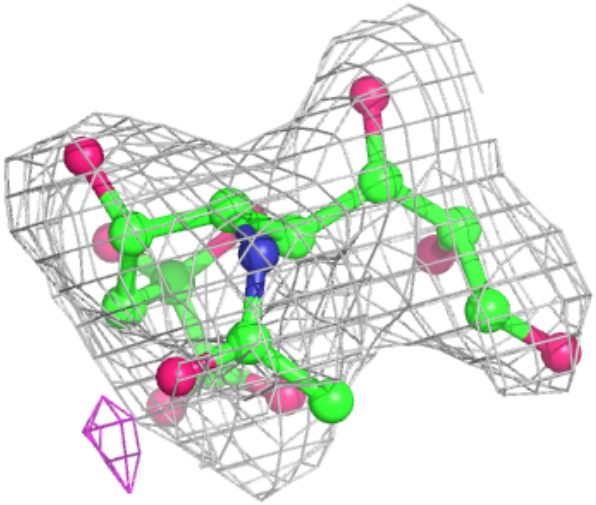


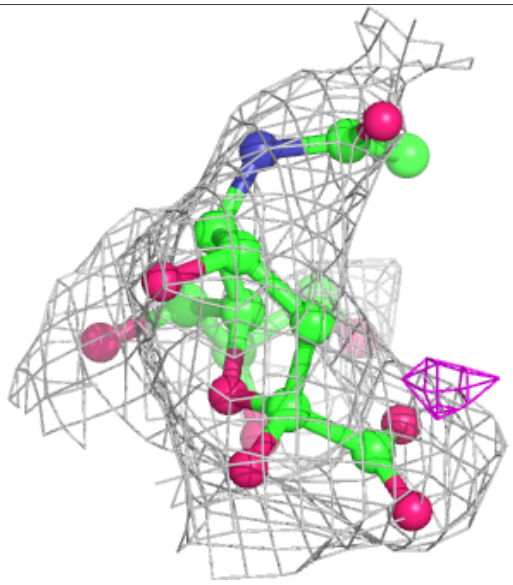


Electron density around SIA F 682:

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

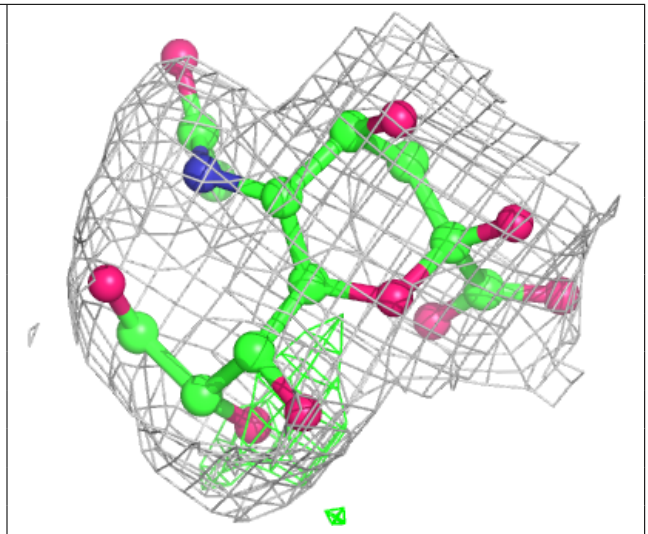


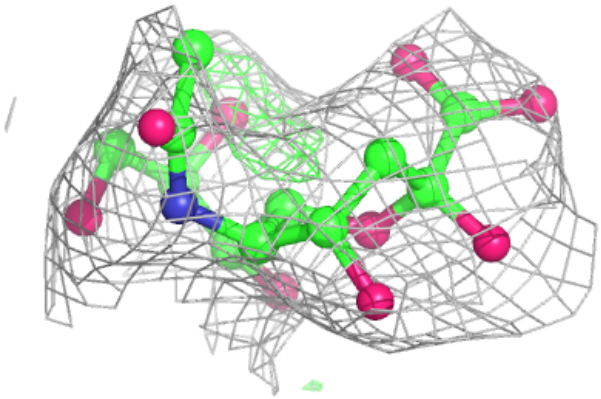


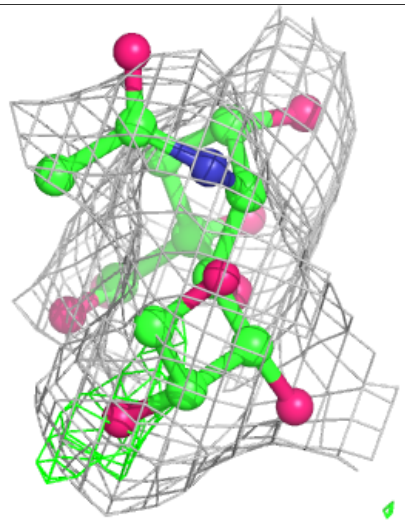


Electron density around SIA L 1282:

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

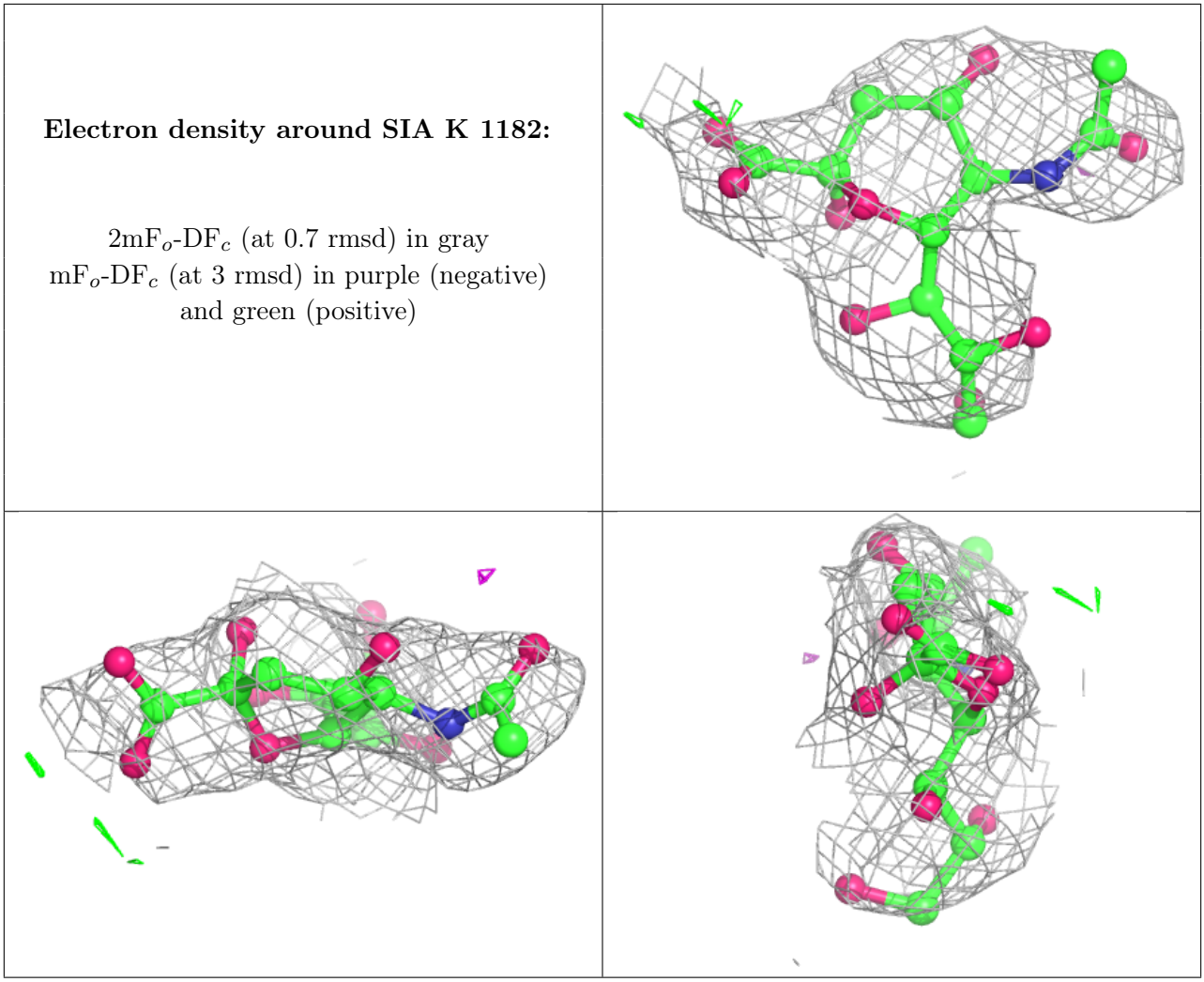






Electron density around SIA K 1182:

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



6.5 Other polymers

There are no such residues in this entry.