



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 8, 2023 – 12:17 am GMT

PDB ID : 2VCV  
Title : Glutathione transferase A3-3 in complex with glutathione and delta-4- androstene-3-17-dione  
Authors : Tars, K.; Olin, B.; Mannervik, B.  
Deposited on : 2007-09-27  
Resolution : 1.80 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

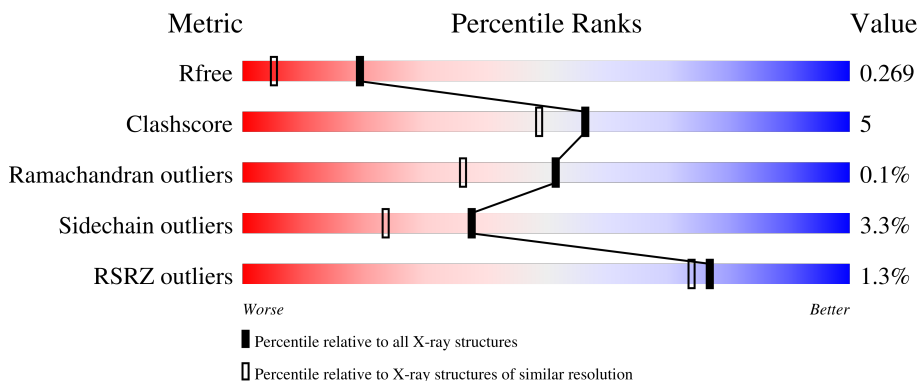
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	222	89% 9% ..
1	B	222	85% 13% ..
1	C	222	5% 82% 15% ..
1	D	222	90% 7% ..
1	E	222	2% 89% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	222	 88% 10% .
1	G	222	 91% 8% .
1	H	222	 84% 13% ..
1	I	222	 87% 11% ..
1	J	222	 83% 14% ..
1	K	222	 90% 8% ..
1	L	222	 87% 11% .
1	M	222	 85% 13% ..
1	N	222	 84% 14% ..
1	O	222	 86% 11% ..
1	P	222	 84% 14% ..

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	GSH	A	1223	X	-	-	-
2	GSH	B	1223	X	-	-	-
2	GSH	C	1223	X	-	-	-
2	GSH	D	1223	X	-	-	-
2	GSH	E	1223	X	-	-	-
2	GSH	F	1223	X	-	-	-
2	GSH	G	1223	X	-	-	-
2	GSH	H	1223	X	-	-	-
2	GSH	I	1223	X	-	-	-
2	GSH	J	1223	X	-	-	-
2	GSH	K	1223	X	-	-	-
2	GSH	L	1223	X	-	-	-
2	GSH	M	1223	X	-	-	-
2	GSH	N	1223	X	-	-	-
2	GSH	O	1223	X	-	-	-
2	GSH	P	1223	X	-	-	-

## 2 Entry composition [i](#)

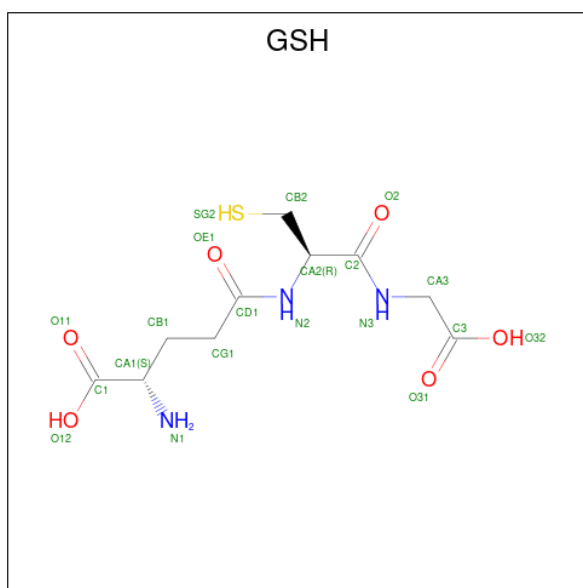
There are 4 unique types of molecules in this entry. The entry contains 32159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE S-TRANSFERASE A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	Total 1768	C 1142	N 299	O 319	S 8	0	2	0
1	B	219	Total 1771	C 1145	N 299	O 319	S 8	0	3	0
1	C	219	Total 1771	C 1145	N 299	O 319	S 8	0	3	0
1	D	219	Total 1768	C 1141	N 300	O 319	S 8	0	2	0
1	E	219	Total 1768	C 1141	N 300	O 319	S 8	0	2	0
1	F	219	Total 1771	C 1144	N 300	O 319	S 8	0	3	0
1	G	219	Total 1771	C 1144	N 299	O 319	S 9	0	3	0
1	H	219	Total 1771	C 1145	N 299	O 319	S 8	0	3	0
1	I	219	Total 1771	C 1144	N 300	O 319	S 8	0	3	0
1	J	219	Total 1768	C 1142	N 299	O 319	S 8	0	2	0
1	K	219	Total 1774	C 1147	N 300	O 319	S 8	0	4	0
1	L	219	Total 1777	C 1148	N 301	O 319	S 9	0	5	0
1	M	219	Total 1765	C 1139	N 299	O 319	S 8	0	1	0
1	N	219	Total 1779	C 1150	N 301	O 320	S 8	0	5	0
1	O	219	Total 1777	C 1148	N 300	O 321	S 8	0	4	0
1	P	219	Total 1775	C 1146	N 302	O 319	S 8	0	3	0

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



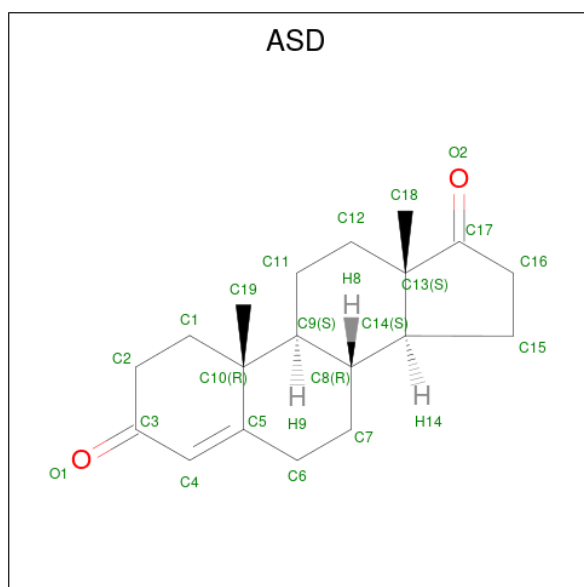
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	I	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	J	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	K	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	L	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	M	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	N	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	O	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	P	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is 4-ANDROSTENE-3-17-DIONE (three-letter code: ASD) (formula: C<sub>19</sub>H<sub>26</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		
3	E	1	Total	C	O	0	0
			21	19	2		
3	F	1	Total	C	O	0	0
			21	19	2		
3	G	1	Total	C	O	0	0
			21	19	2		
3	H	1	Total	C	O	0	0
			21	19	2		
3	I	1	Total	C	O	0	0
			21	19	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			21	19	2		
3	L	1	Total	C	O	0	0
			21	19	2		
3	P	1	Total	C	O	0	0
			21	19	2		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		
4	B	215	Total	O	0	0
			215	215		
4	C	171	Total	O	0	0
			171	171		
4	D	179	Total	O	0	0
			179	179		
4	E	188	Total	O	0	0
			188	188		
4	F	215	Total	O	0	0
			215	215		
4	G	230	Total	O	0	0
			230	230		
4	H	194	Total	O	0	0
			194	194		
4	I	209	Total	O	0	0
			209	209		
4	J	187	Total	O	0	0
			187	187		
4	K	199	Total	O	0	0
			199	199		
4	L	228	Total	O	0	0
			228	228		
4	M	224	Total	O	0	0
			224	224		
4	N	213	Total	O	0	0
			213	213		
4	O	199	Total	O	0	0
			199	199		
4	P	204	Total	O	0	0
			204	204		

### 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.

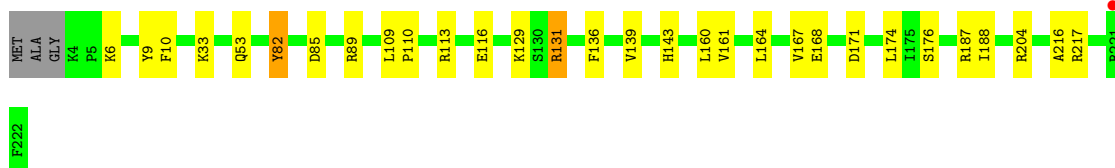
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain A: 




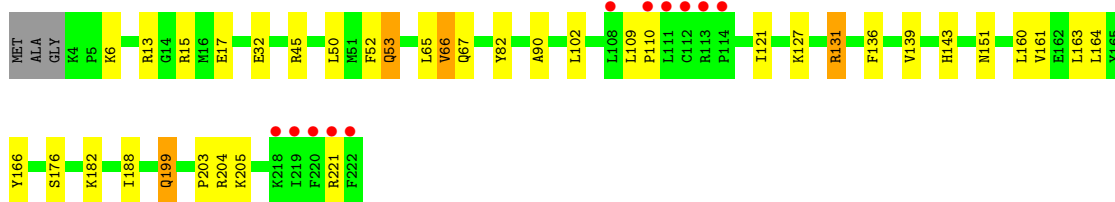
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain B: 




- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain C: 




- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain D: 



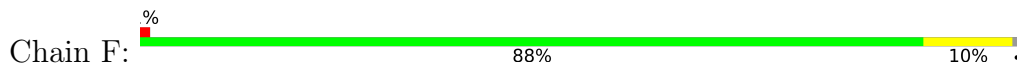
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain E: 

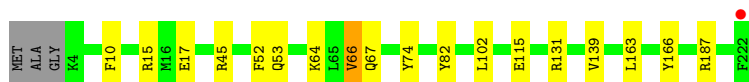




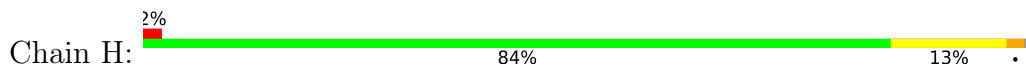
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3



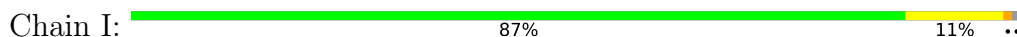
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3



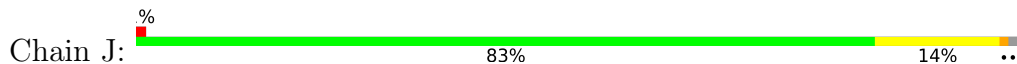
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3



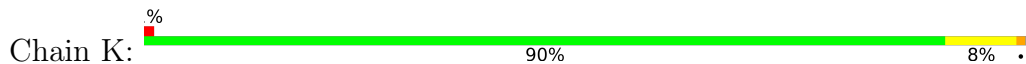
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3



- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

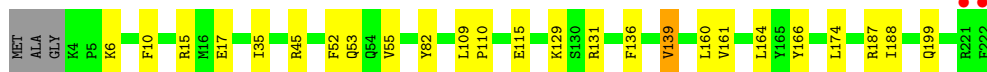
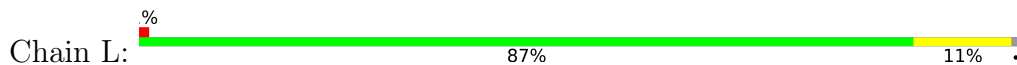


- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

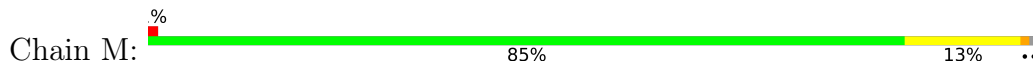




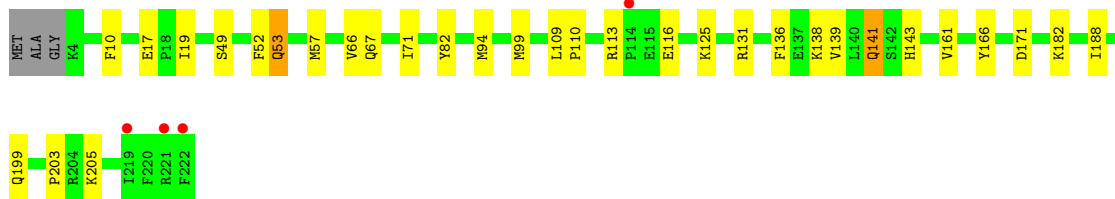
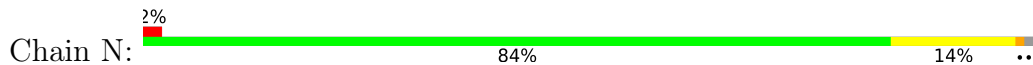
● Molecule 1: GLUTATHIONE S-TRANSFERASE A3



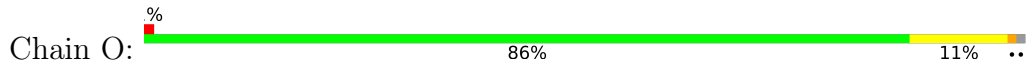
● Molecule 1: GLUTATHIONE S-TRANSFERASE A3



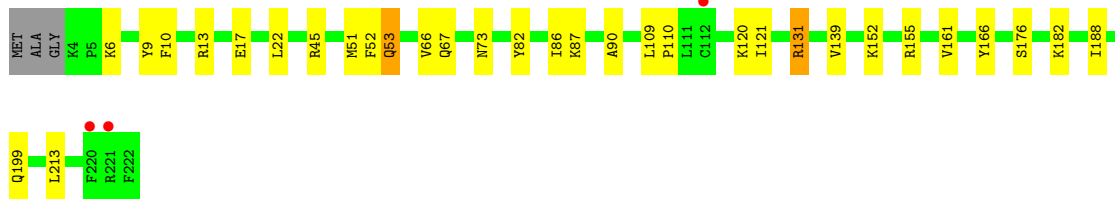
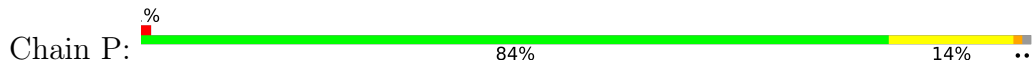
● Molecule 1: GLUTATHIONE S-TRANSFERASE A3



● Molecule 1: GLUTATHIONE S-TRANSFERASE A3



● Molecule 1: GLUTATHIONE S-TRANSFERASE A3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.18Å 92.06Å 113.54Å 89.76° 89.72° 89.73°	Depositor
Resolution (Å)	20.00 – 1.80 19.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-1.80) 93.1 (19.99-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.267 0.225 , 0.269	Depositor DCC
$R_{free}$ test set	16208 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 26.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.387 for h,-k,-l 0.158 for -h,k,-l 0.149 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2348e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, ASD

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	0.47	1/1811 (0.1%)	0.60	0/2433
1	B	0.46	0/1818	0.60	0/2443
1	C	0.44	0/1818	0.57	0/2443
1	D	0.46	0/1812	0.58	0/2433
1	E	0.45	0/1812	0.70	1/2433 (0.0%)
1	F	0.45	0/1820	0.59	0/2444
1	G	0.48	0/1819	0.60	0/2443
1	H	0.45	0/1818	0.60	0/2443
1	I	0.46	0/1820	0.60	0/2444
1	J	0.44	0/1811	0.59	0/2433
1	K	0.46	0/1827	0.61	0/2454
1	L	0.46	0/1837	0.59	0/2465
1	M	0.47	0/1803	0.60	0/2422
1	N	0.47	0/1836	0.60	0/2466
1	O	0.46	0/1829	0.61	0/2456
1	P	0.47	0/1822	0.61	0/2447
All	All	0.46	1/29113 (0.0%)	0.60	1/39102 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	CYS	CB-SG	5.90	1.92	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	PHE	CA-C-O	-17.36	83.64	120.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1768	0	1838	14	0
1	B	1771	0	1843	25	0
1	C	1771	0	1843	23	0
1	D	1768	0	1836	13	0
1	E	1768	0	1836	19	0
1	F	1771	0	1843	22	0
1	G	1771	0	1843	11	0
1	H	1771	0	1843	27	0
1	I	1771	0	1843	25	0
1	J	1768	0	1838	30	0
1	K	1774	0	1848	17	0
1	L	1777	0	1853	12	0
1	M	1765	0	1831	26	0
1	N	1779	0	1852	27	0
1	O	1777	0	1849	22	0
1	P	1775	0	1847	32	0
2	A	20	0	15	2	0
2	B	20	0	15	0	0
2	C	20	0	15	1	0
2	D	20	0	15	1	0
2	E	20	0	15	0	0
2	F	20	0	15	3	0
2	G	20	0	15	2	0
2	H	20	0	15	0	0
2	I	20	0	15	1	0
2	J	20	0	15	1	0
2	K	20	0	15	1	0
2	L	20	0	15	1	0
2	M	20	0	15	1	0
2	N	20	0	15	1	0
2	O	20	0	15	0	0
2	P	20	0	15	0	0
3	A	21	0	26	1	0
3	B	21	0	26	4	0
3	D	21	0	26	1	0
3	E	21	0	26	0	0
3	F	21	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	21	0	26	0	0
3	H	21	0	26	1	0
3	I	21	0	26	0	0
3	K	21	0	26	0	0
3	L	21	0	26	0	0
3	P	21	0	26	1	0
4	A	208	0	0	2	0
4	B	215	0	0	4	0
4	C	171	0	0	1	0
4	D	179	0	0	2	0
4	E	188	0	0	4	0
4	F	215	0	0	3	0
4	G	230	0	0	1	0
4	H	194	0	0	9	0
4	I	209	0	0	1	0
4	J	187	0	0	3	0
4	K	199	0	0	7	0
4	L	228	0	0	2	0
4	M	224	0	0	4	0
4	N	213	0	0	4	0
4	O	199	0	0	4	0
4	P	204	0	0	6	0
All	All	32159	0	30012	293	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 5.

The worst 5 of 293 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:MET:CE	1:J:66:VAL:HG22	1.72	1.20
1:I:94:MET:HE2	1:J:66:VAL:HG22	1.16	1.10
1:G:64:LYS:HE3	1:J:46:ASN:HD21	1.20	1.04
1:I:94:MET:HE2	1:J:66:VAL:CG2	1.99	0.93
1:E:187:ARG:HD2	4:E:2127:HOH:O	1.70	0.92

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	219/222 (99%)	215 (98%)	4 (2%)	0	100	100
1	B	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
1	C	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	29	15
1	D	219/222 (99%)	213 (97%)	6 (3%)	0	100	100
1	E	219/222 (99%)	213 (97%)	6 (3%)	0	100	100
1	F	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
1	G	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
1	H	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
1	I	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
1	J	219/222 (99%)	214 (98%)	5 (2%)	0	100	100
1	K	221/222 (100%)	216 (98%)	5 (2%)	0	100	100
1	L	222/222 (100%)	218 (98%)	4 (2%)	0	100	100
1	M	218/222 (98%)	214 (98%)	4 (2%)	0	100	100
1	N	222/222 (100%)	214 (96%)	8 (4%)	0	100	100
1	O	221/222 (100%)	215 (97%)	5 (2%)	1 (0%)	29	15
1	P	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	15
All	All	3520/3552 (99%)	3428 (97%)	89 (2%)	3 (0%)	51	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	13	ARG
1	C	13	ARG
1	P	13	ARG

### 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	192/191 (100%)	183 (95%)	9 (5%)	26	12
1	B	193/191 (101%)	189 (98%)	4 (2%)	53	42
1	C	193/191 (101%)	184 (95%)	9 (5%)	26	12
1	D	192/191 (100%)	186 (97%)	6 (3%)	40	25
1	E	192/191 (100%)	186 (97%)	6 (3%)	40	25
1	F	193/191 (101%)	188 (97%)	5 (3%)	46	32
1	G	193/191 (101%)	187 (97%)	6 (3%)	40	25
1	H	193/191 (101%)	188 (97%)	5 (3%)	46	32
1	I	193/191 (101%)	188 (97%)	5 (3%)	46	32
1	J	192/191 (100%)	188 (98%)	4 (2%)	53	42
1	K	194/191 (102%)	189 (97%)	5 (3%)	46	32
1	L	195/191 (102%)	188 (96%)	7 (4%)	35	20
1	M	191/191 (100%)	183 (96%)	8 (4%)	30	15
1	N	195/191 (102%)	187 (96%)	8 (4%)	30	16
1	O	194/191 (102%)	186 (96%)	8 (4%)	30	16
1	P	193/191 (101%)	187 (97%)	6 (3%)	40	25
All	All	3088/3056 (101%)	2987 (97%)	101 (3%)	38	23

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	131	ARG
1	M	11	ASN
1	P	131	ARG
1	K	6	LYS
1	L	10	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:



Mol	Chain	Res	Type
1	H	145	GLN
1	J	80	ASN
1	H	151	ASN
1	I	80	ASN
1	J	199	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ASD	L	1224	-	24,24,24	0.60	0	39,39,39	1.44	7 (17%)
2	GSH	E	1223	-	18,19,19	3.10	2 (11%)	23,24,24	1.11	3 (13%)
3	ASD	D	1224	-	24,24,24	1.59	3 (12%)	39,39,39	1.95	7 (17%)
3	ASD	G	1224	-	24,24,24	0.70	0	39,39,39	1.60	7 (17%)
2	GSH	D	1223	-	18,19,19	3.09	2 (11%)	23,24,24	1.08	2 (8%)
2	GSH	B	1223	-	18,19,19	3.19	2 (11%)	23,24,24	1.26	2 (8%)
3	ASD	B	1224	-	24,24,24	0.57	0	39,39,39	1.61	7 (17%)
3	ASD	F	1224	-	24,24,24	1.02	1 (4%)	39,39,39	1.87	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ASD	A	1224	-	24,24,24	0.58	0	39,39,39	1.52	7 (17%)
2	GSH	N	1223	-	18,19,19	3.13	2 (11%)	23,24,24	1.23	4 (17%)
2	GSH	L	1223	-	18,19,19	3.11	2 (11%)	23,24,24	1.42	3 (13%)
2	GSH	F	1223	-	18,19,19	2.96	2 (11%)	23,24,24	1.35	4 (17%)
2	GSH	P	1223	-	18,19,19	3.07	2 (11%)	23,24,24	1.33	4 (17%)
2	GSH	K	1223	-	18,19,19	3.00	2 (11%)	23,24,24	1.28	3 (13%)
3	ASD	P	1224	-	24,24,24	0.90	1 (4%)	39,39,39	1.57	3 (7%)
2	GSH	M	1223	-	18,19,19	3.14	2 (11%)	23,24,24	1.39	3 (13%)
2	GSH	O	1223	-	18,19,19	3.10	2 (11%)	23,24,24	1.39	4 (17%)
3	ASD	I	1224	-	24,24,24	0.58	0	39,39,39	1.53	7 (17%)
2	GSH	H	1223	-	18,19,19	3.07	2 (11%)	23,24,24	1.36	3 (13%)
2	GSH	C	1223	-	18,19,19	3.13	2 (11%)	23,24,24	1.37	5 (21%)
2	GSH	G	1223	-	18,19,19	3.02	2 (11%)	23,24,24	1.43	4 (17%)
3	ASD	H	1224	-	24,24,24	0.62	0	39,39,39	1.55	7 (17%)
2	GSH	I	1223	-	18,19,19	3.09	2 (11%)	23,24,24	1.29	4 (17%)
3	ASD	K	1224	-	24,24,24	0.62	0	39,39,39	1.49	7 (17%)
2	GSH	A	1223	-	18,19,19	3.03	2 (11%)	23,24,24	1.39	3 (13%)
2	GSH	J	1223	-	18,19,19	3.16	2 (11%)	23,24,24	1.31	4 (17%)
3	ASD	E	1224	-	24,24,24	0.99	1 (4%)	39,39,39	1.83	5 (12%)

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
3	ASD	L	1224	-	-	-	0/4/4/4
2	GSH	E	1223	-	1/1/6/8	2/24/24/24	-
3	ASD	D	1224	-	-	-	0/4/4/4
3	ASD	G	1224	-	-	-	0/4/4/4
2	GSH	D	1223	-	1/1/6/8	6/24/24/24	-
2	GSH	B	1223	-	1/1/6/8	5/24/24/24	-
3	ASD	B	1224	-	-	-	0/4/4/4
3	ASD	F	1224	-	-	-	0/4/4/4
3	ASD	A	1224	-	-	-	0/4/4/4
2	GSH	N	1223	-	1/1/6/8	6/24/24/24	-
2	GSH	L	1223	-	1/1/6/8	7/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	F	1223	-	1/1/6/8	7/24/24/24	-
2	GSH	P	1223	-	1/1/6/8	2/24/24/24	-
2	GSH	K	1223	-	1/1/6/8	8/24/24/24	-
3	ASD	P	1224	-	-	-	0/4/4/4
2	GSH	M	1223	-	1/1/6/8	7/24/24/24	-
2	GSH	O	1223	-	1/1/6/8	8/24/24/24	-
3	ASD	I	1224	-	-	-	0/4/4/4
2	GSH	H	1223	-	1/1/6/8	2/24/24/24	-
2	GSH	C	1223	-	1/1/6/8	7/24/24/24	-
2	GSH	G	1223	-	1/1/6/8	8/24/24/24	-
3	ASD	H	1224	-	-	-	0/4/4/4
2	GSH	I	1223	-	1/1/6/8	9/24/24/24	-
3	ASD	K	1224	-	-	-	0/4/4/4
2	GSH	A	1223	-	1/1/6/8	7/24/24/24	-
2	GSH	J	1223	-	1/1/6/8	7/24/24/24	-
3	ASD	E	1224	-	-	-	0/4/4/4

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1223	GSH	O2-C2	9.58	1.42	1.23
2	J	1223	GSH	O2-C2	9.51	1.42	1.23
2	L	1223	GSH	O2-C2	9.39	1.42	1.23
2	C	1223	GSH	O2-C2	9.38	1.42	1.23
2	N	1223	GSH	O2-C2	9.29	1.41	1.23

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1224	ASD	C15-C16-C17	-8.42	97.22	105.70
3	E	1224	ASD	C15-C14-C13	5.84	109.31	104.08
3	F	1224	ASD	C15-C14-C13	5.63	109.12	104.08
3	D	1224	ASD	C16-C17-C13	5.31	113.83	108.59
3	P	1224	ASD	C15-C16-C17	-4.96	100.71	105.70

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1223	GSH	CA1

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Mol	Chain	Res	Type	Atom
2	B	1223	GSH	CA1
2	C	1223	GSH	CA1
2	D	1223	GSH	CA1
2	E	1223	GSH	CA1

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1223	GSH	O11-C1-CA1-N1
2	A	1223	GSH	CG1-CD1-N2-CA2
2	D	1223	GSH	O11-C1-CA1-N1
2	E	1223	GSH	O11-C1-CA1-N1
2	F	1223	GSH	O11-C1-CA1-N1

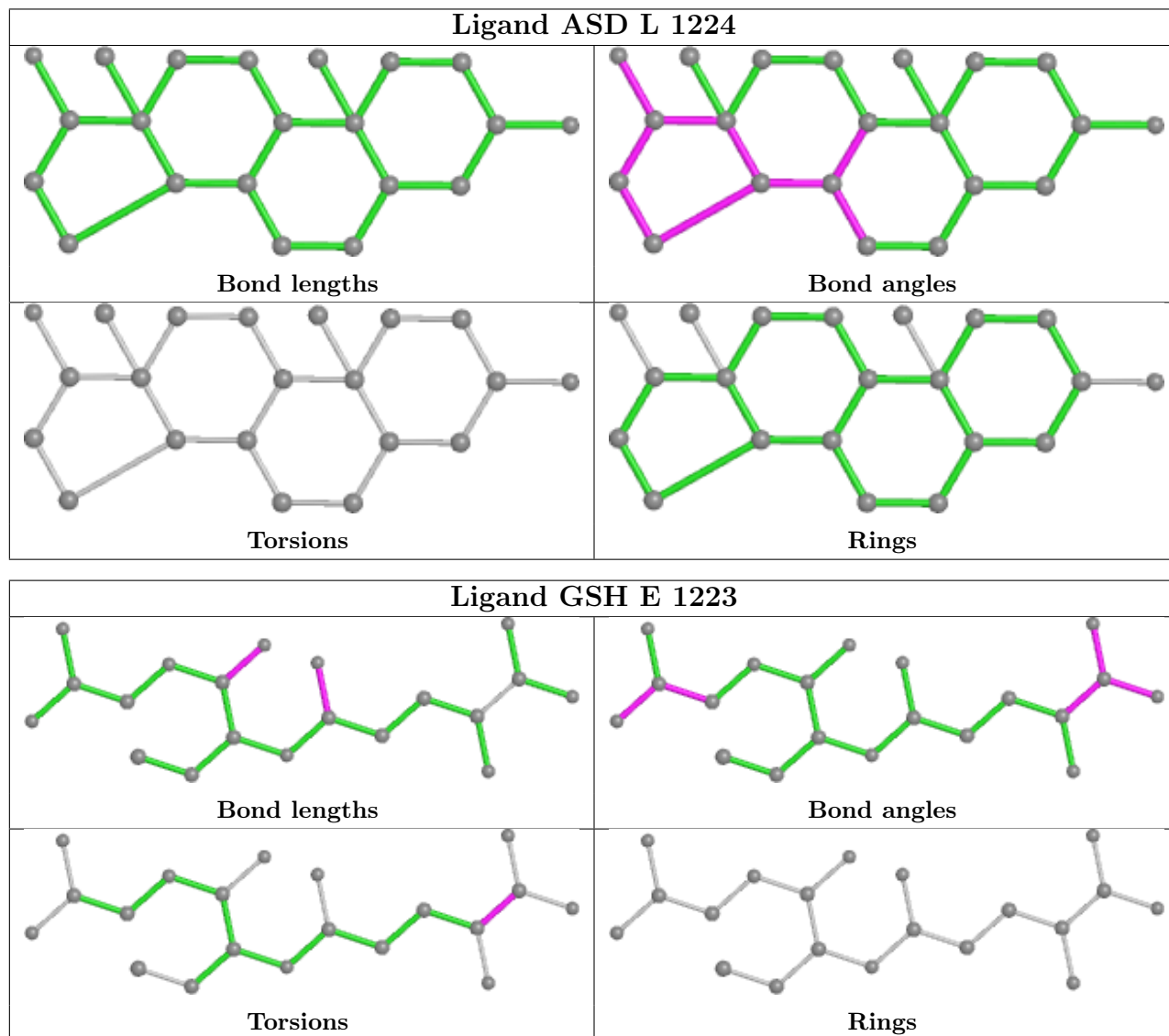
There are no ring outliers.

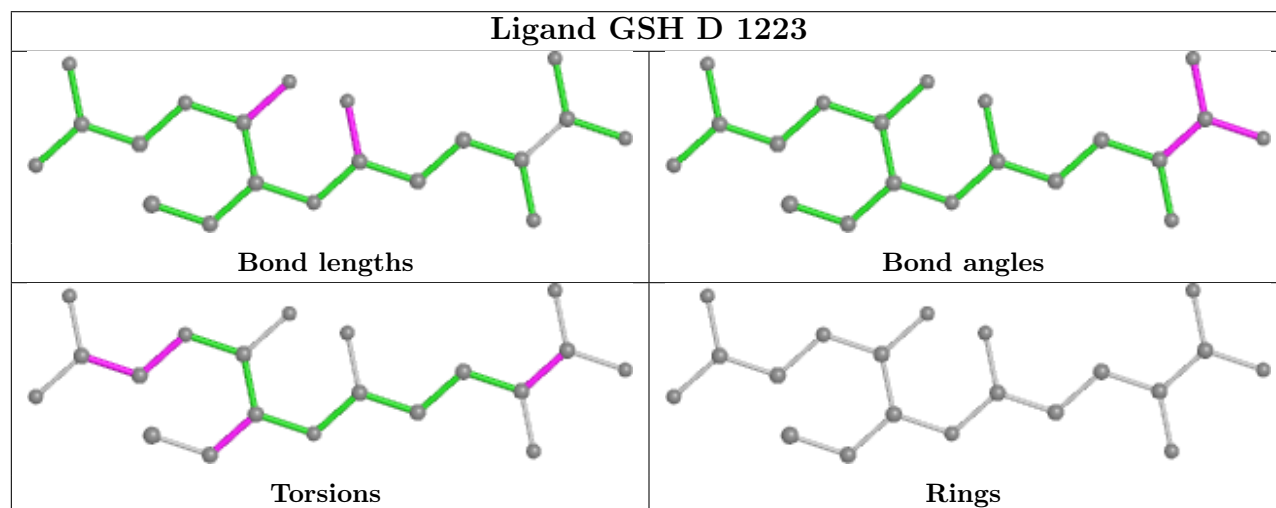
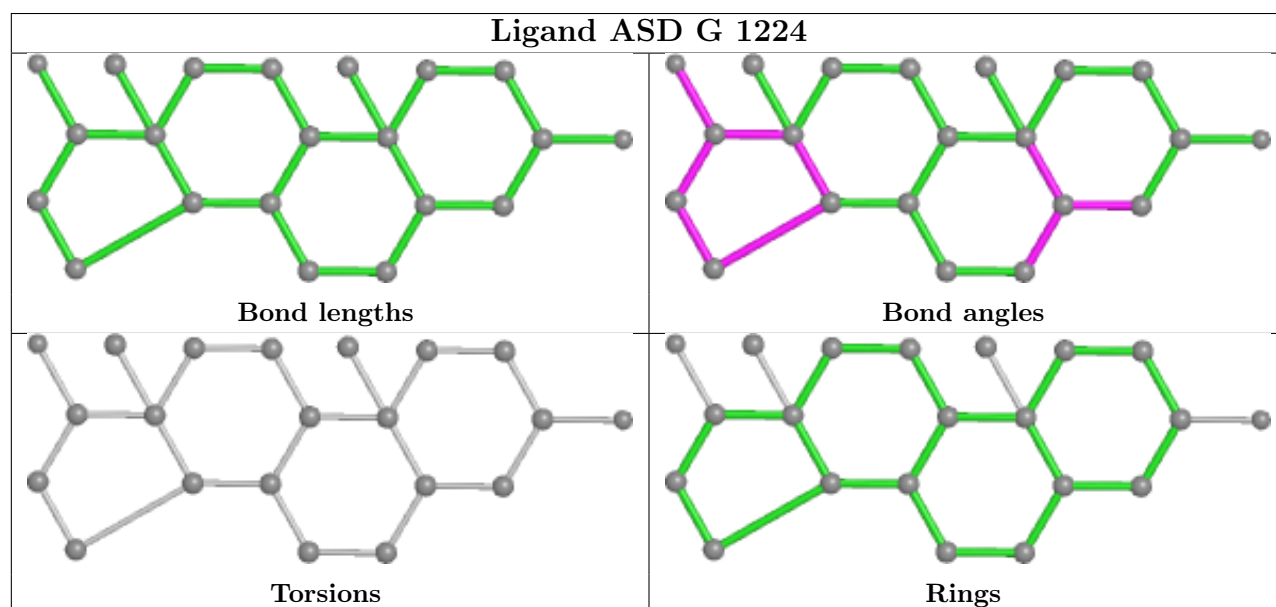
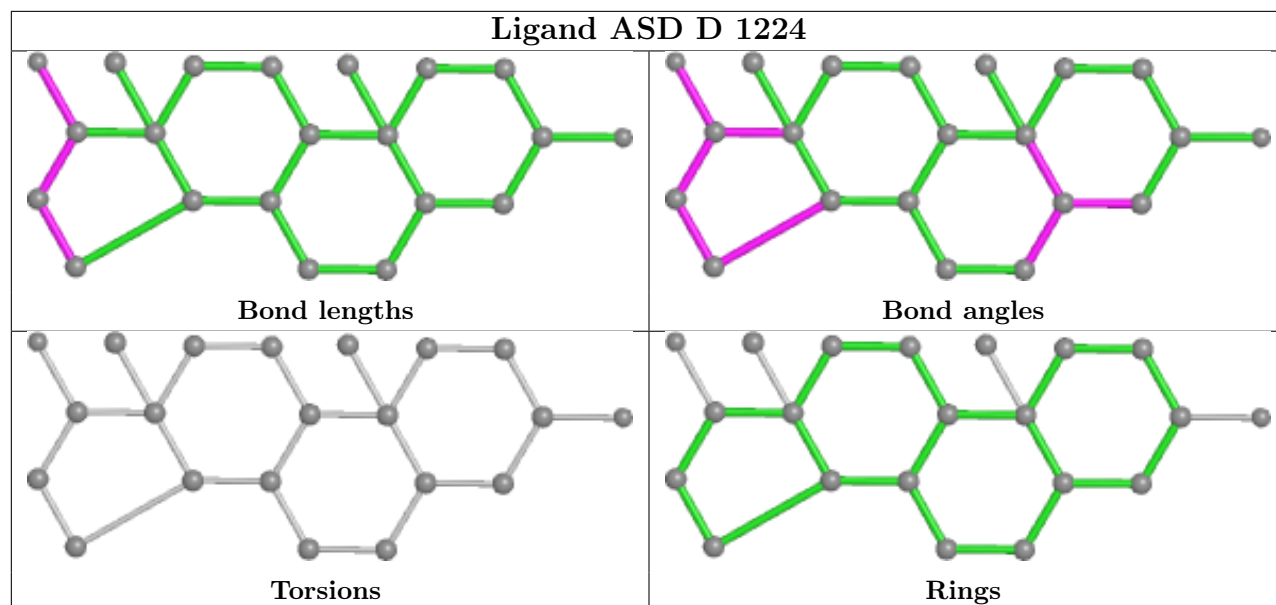
17 monomers are involved in 21 short contacts:

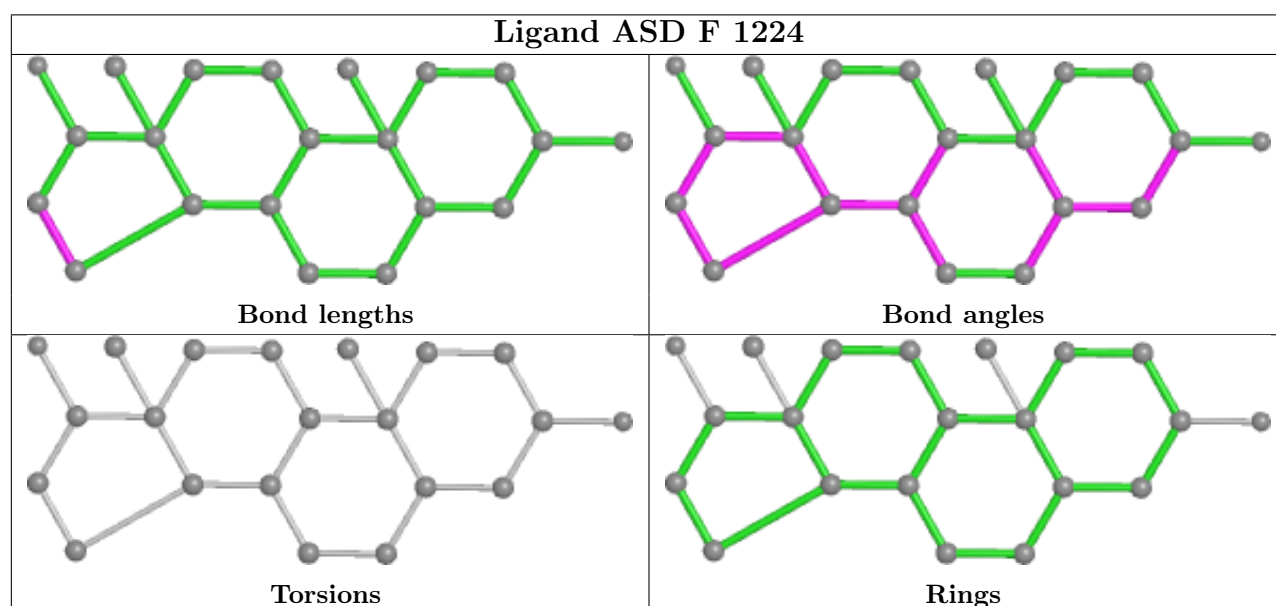
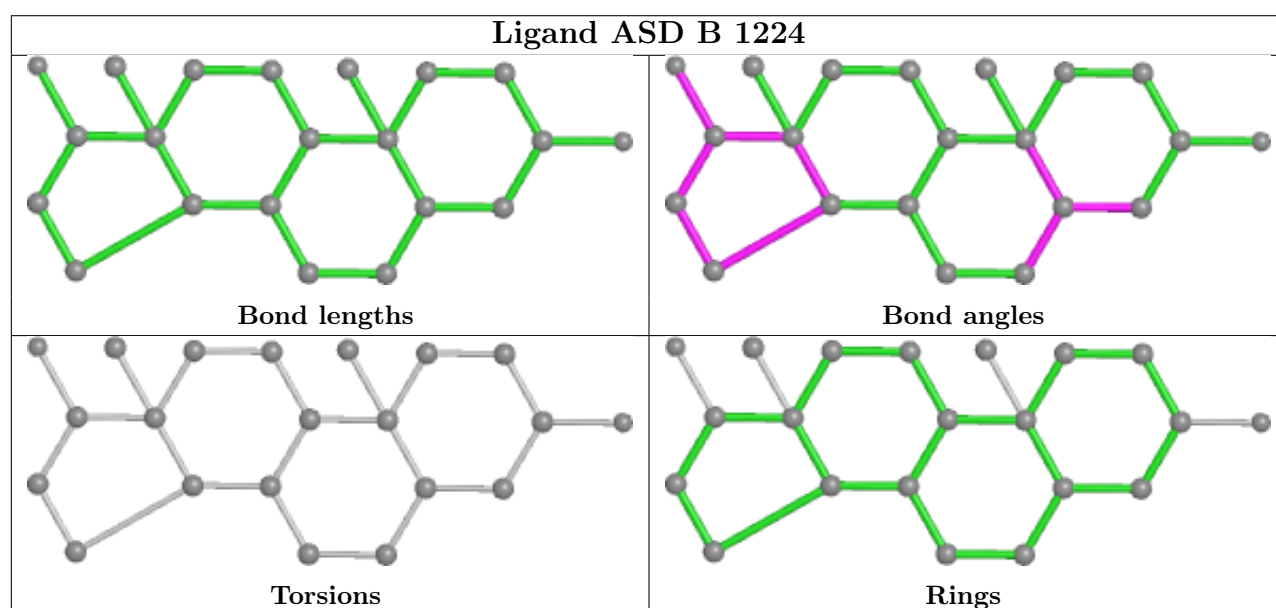
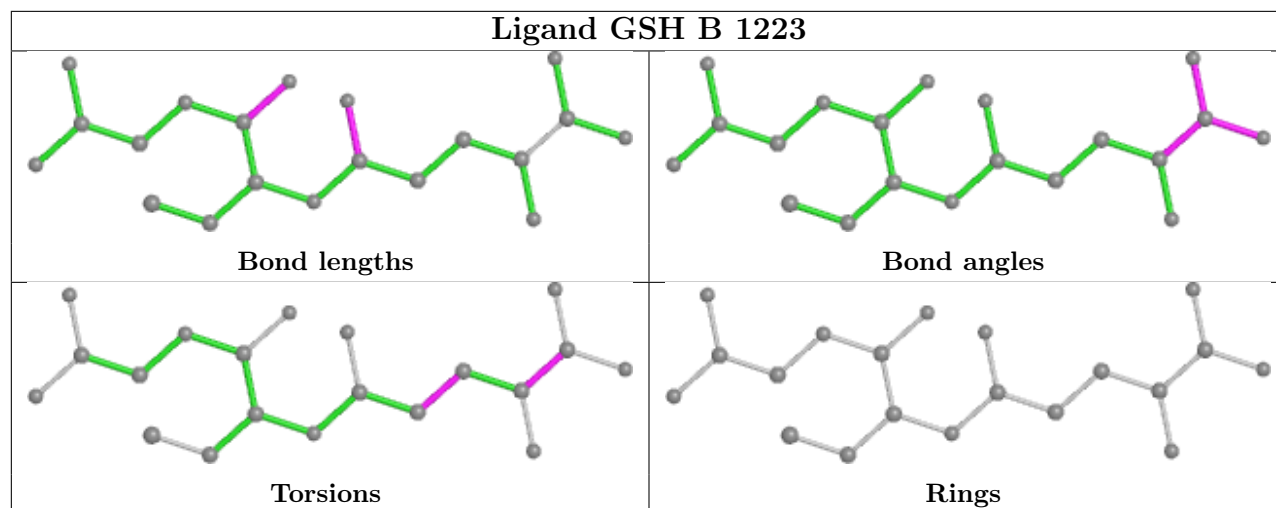
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1224	ASD	1	0
2	D	1223	GSH	1	0
3	B	1224	ASD	4	0
3	F	1224	ASD	2	0
3	A	1224	ASD	1	0
2	N	1223	GSH	1	0
2	L	1223	GSH	1	0
2	F	1223	GSH	3	0
2	K	1223	GSH	1	0
3	P	1224	ASD	1	0
2	M	1223	GSH	1	0
2	C	1223	GSH	1	0
2	G	1223	GSH	2	0
3	H	1224	ASD	1	0
2	I	1223	GSH	1	0
2	A	1223	GSH	2	0
2	J	1223	GSH	1	0

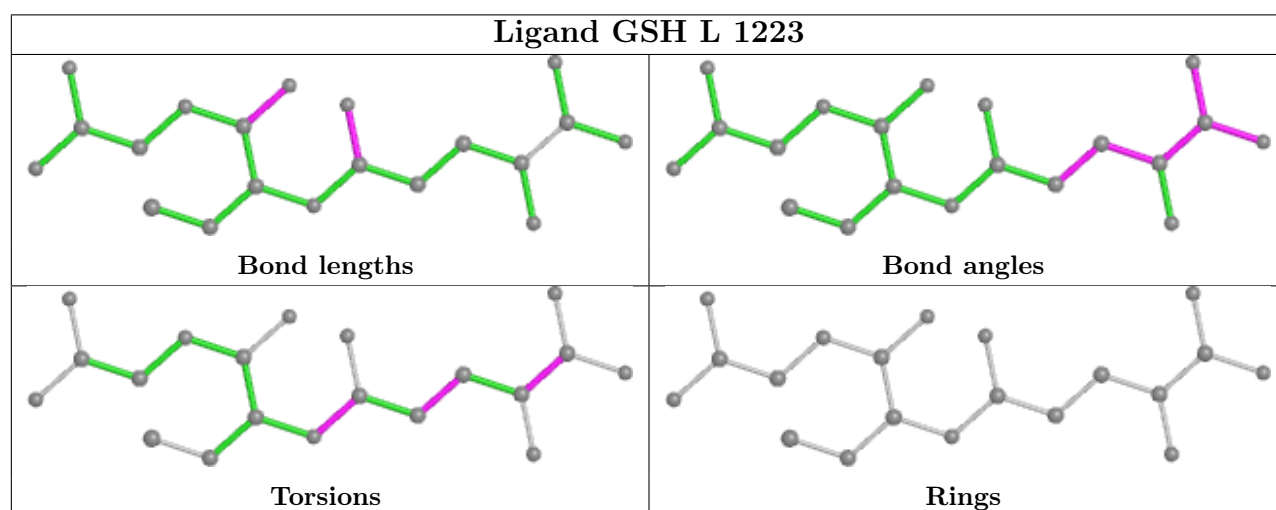
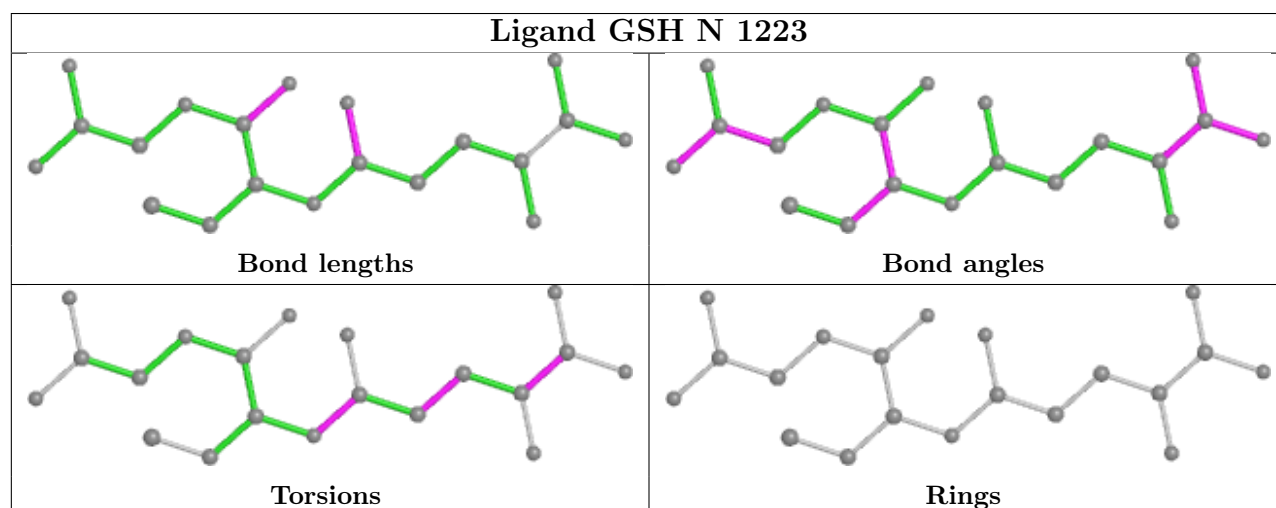
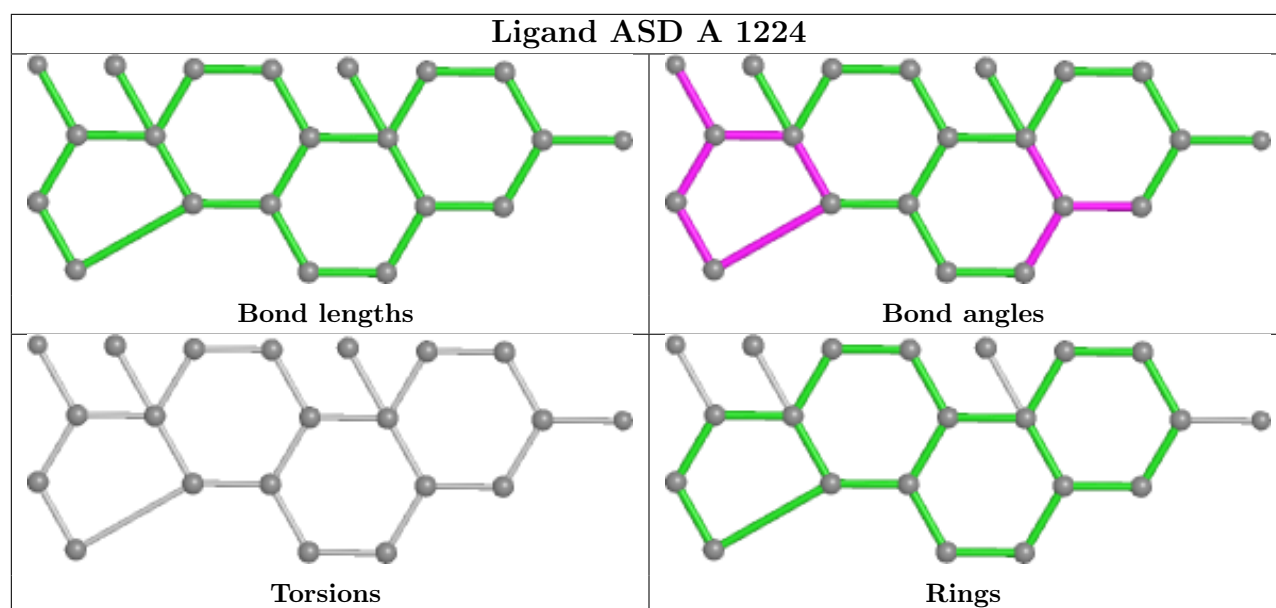
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

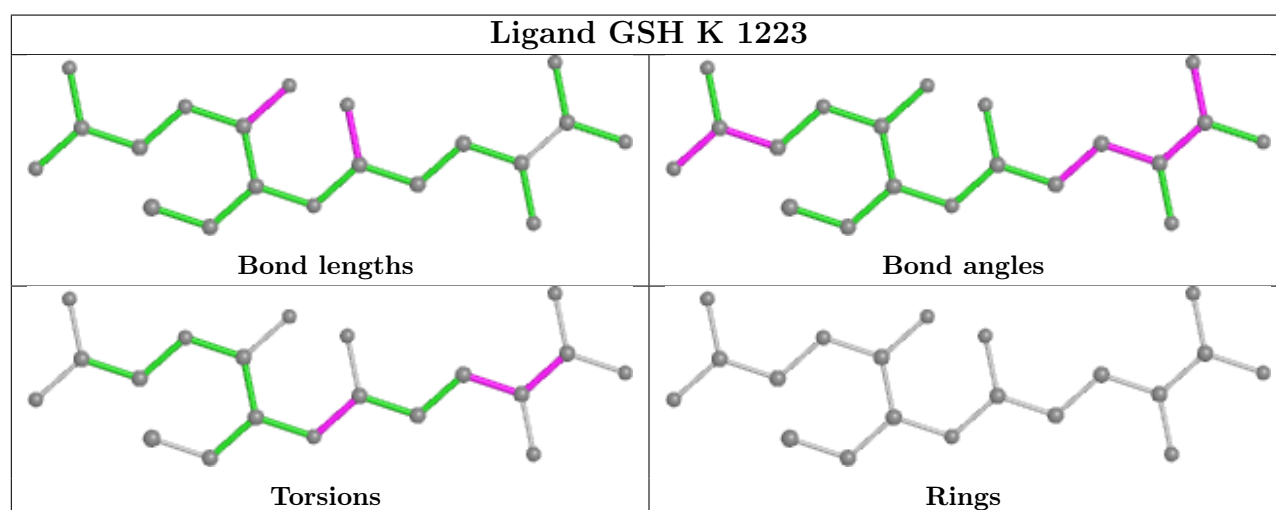
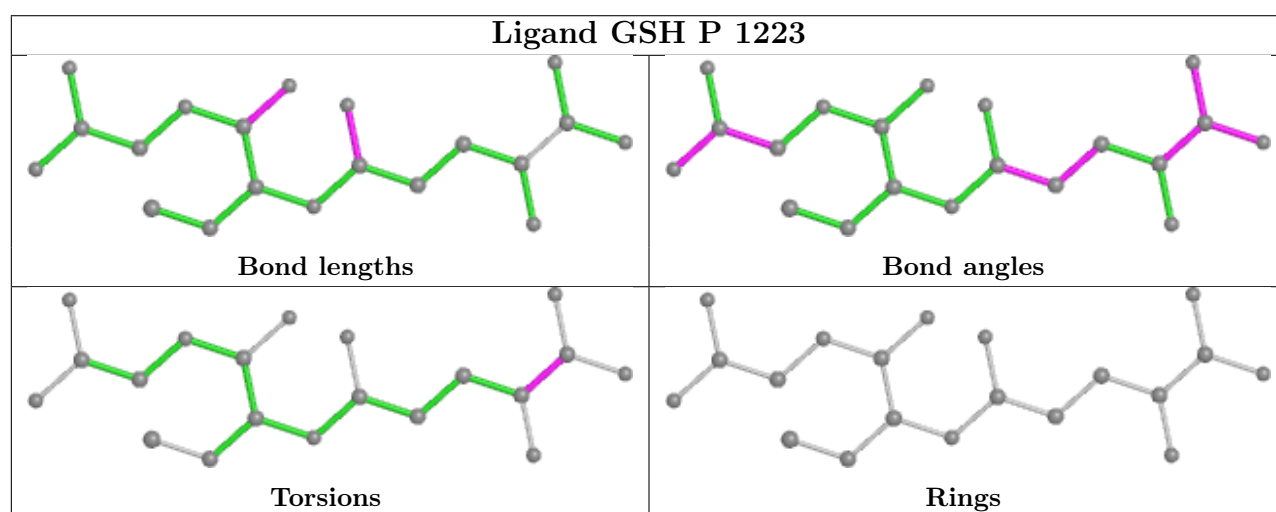
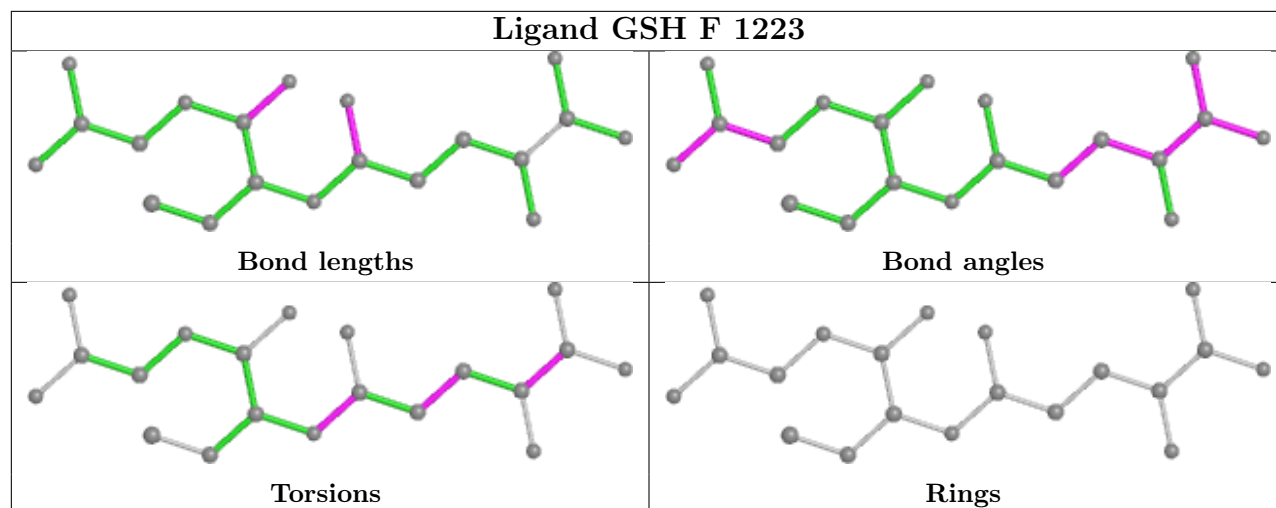


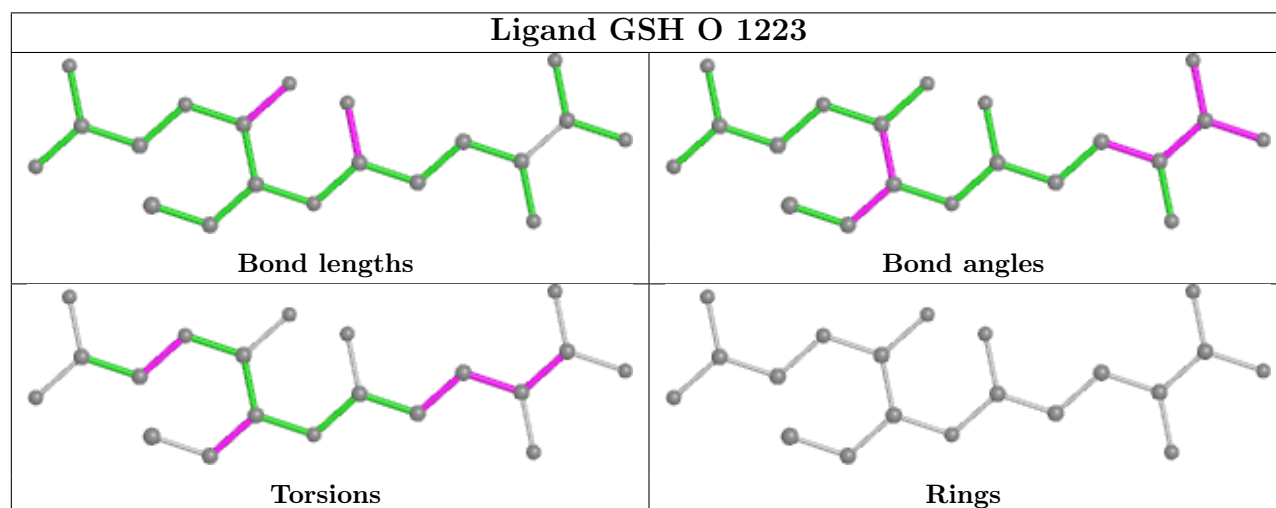
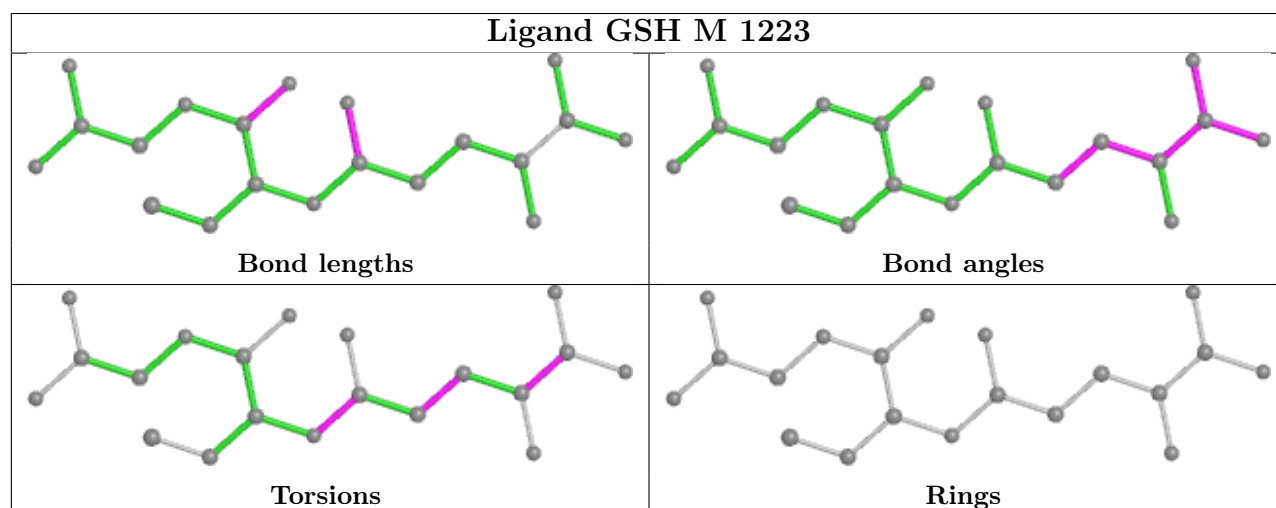
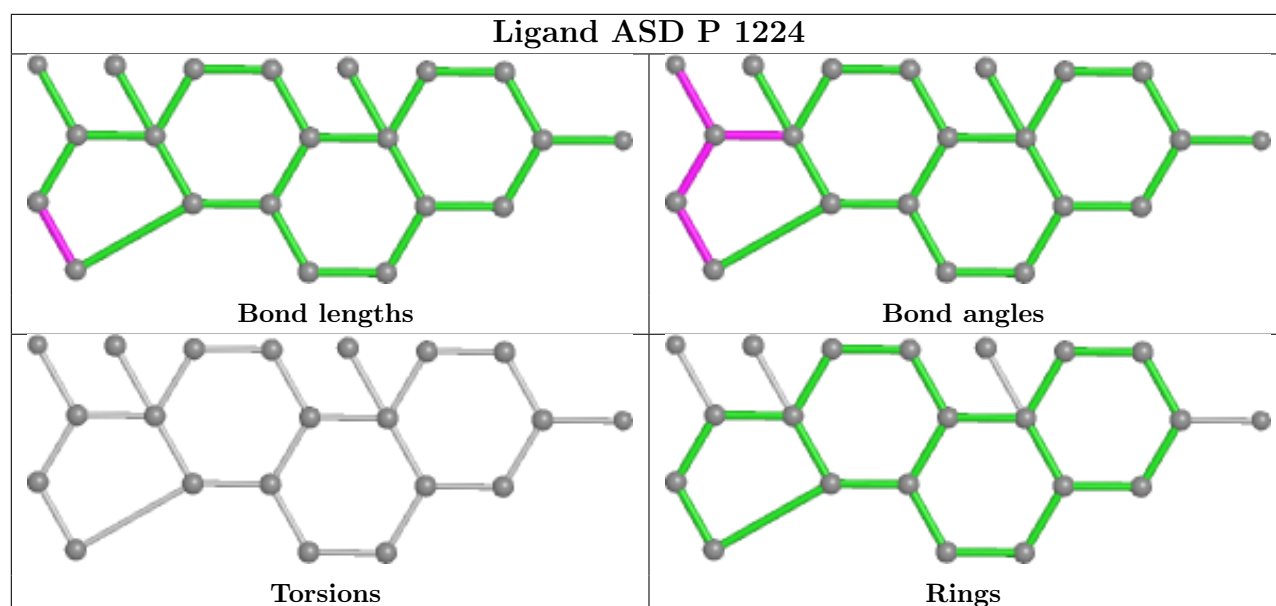


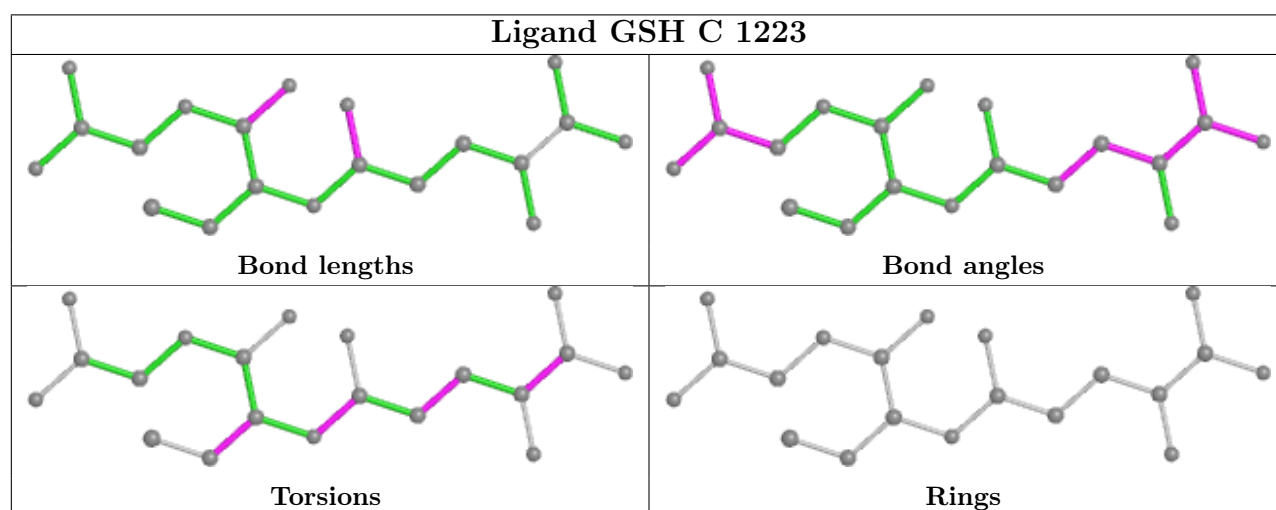
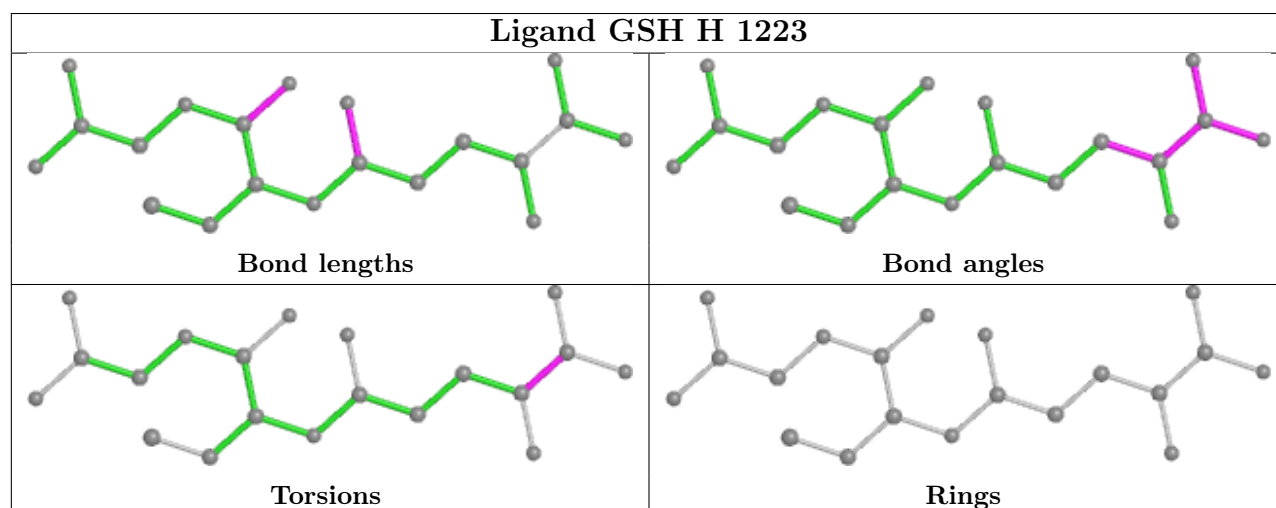
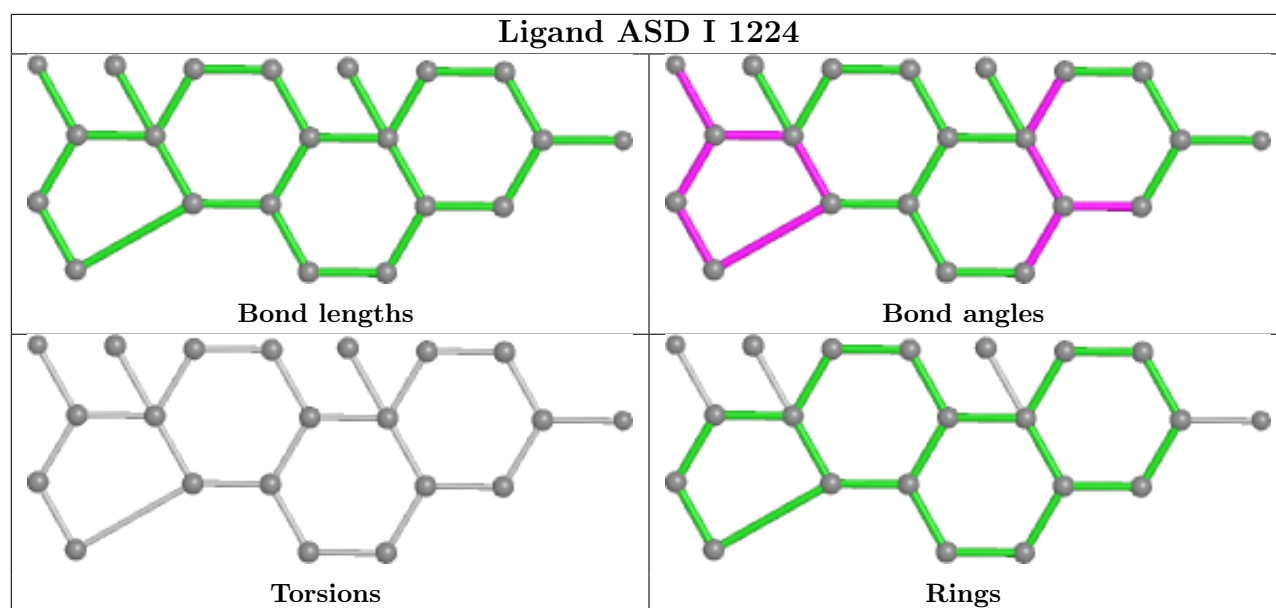


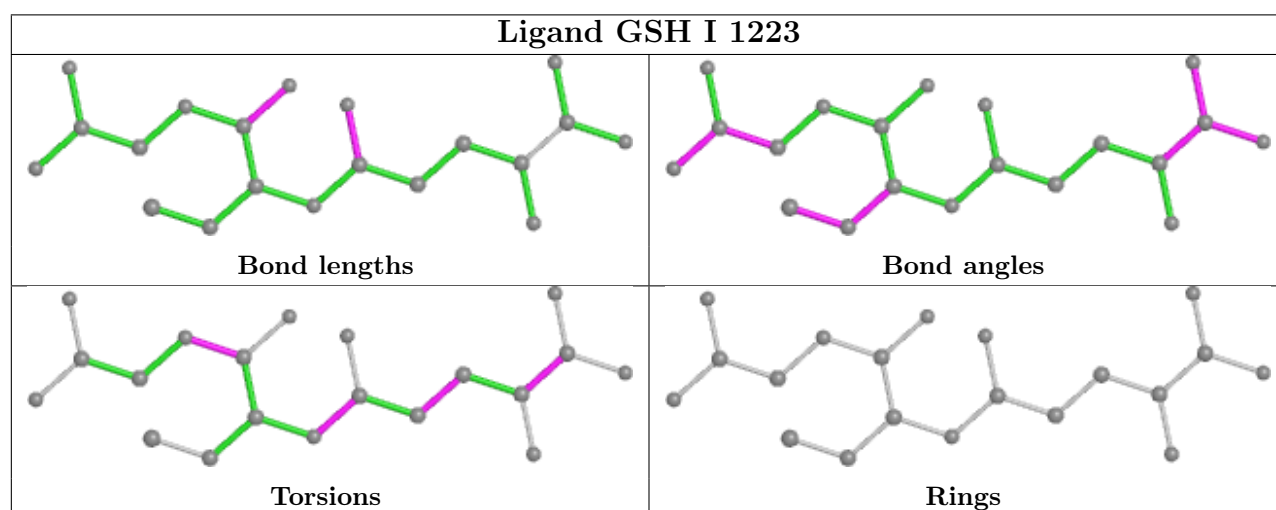
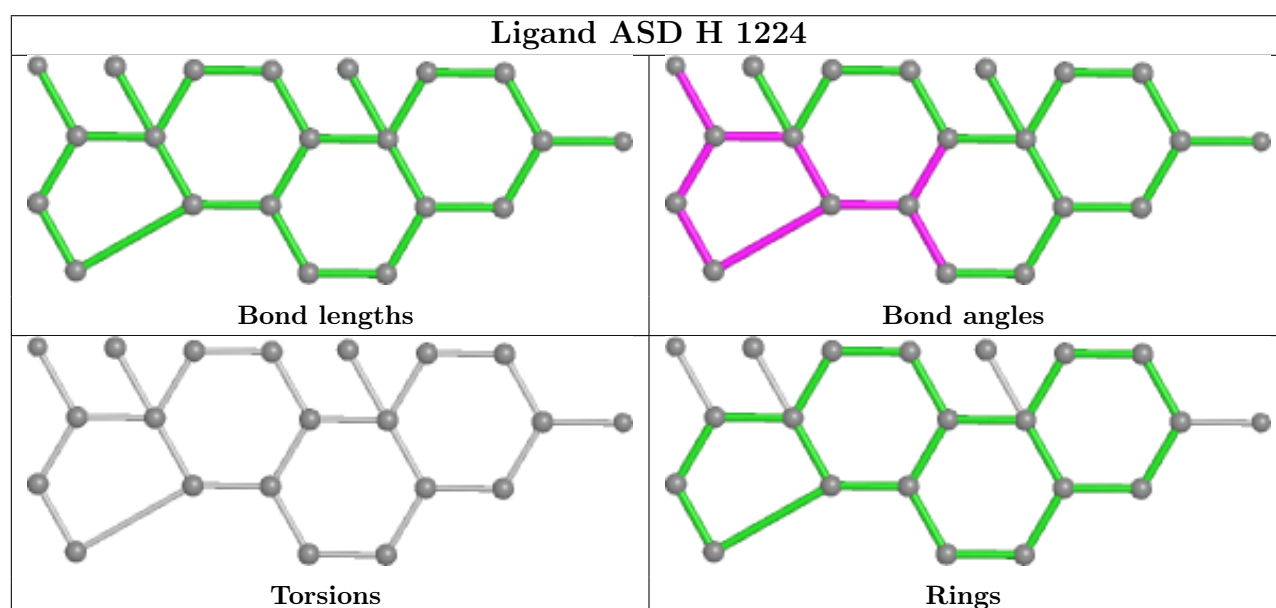
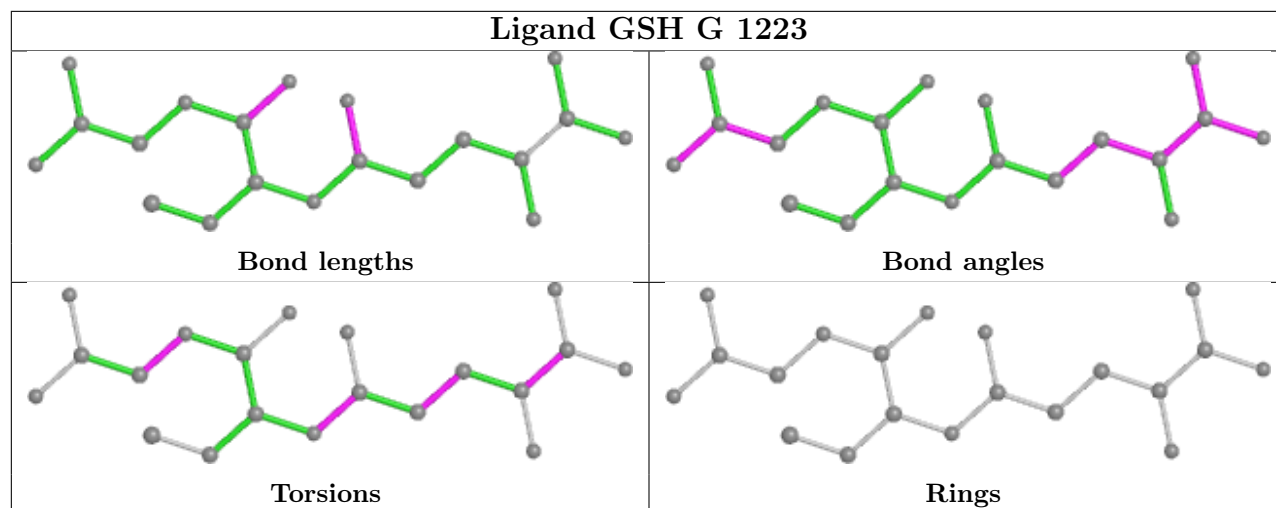


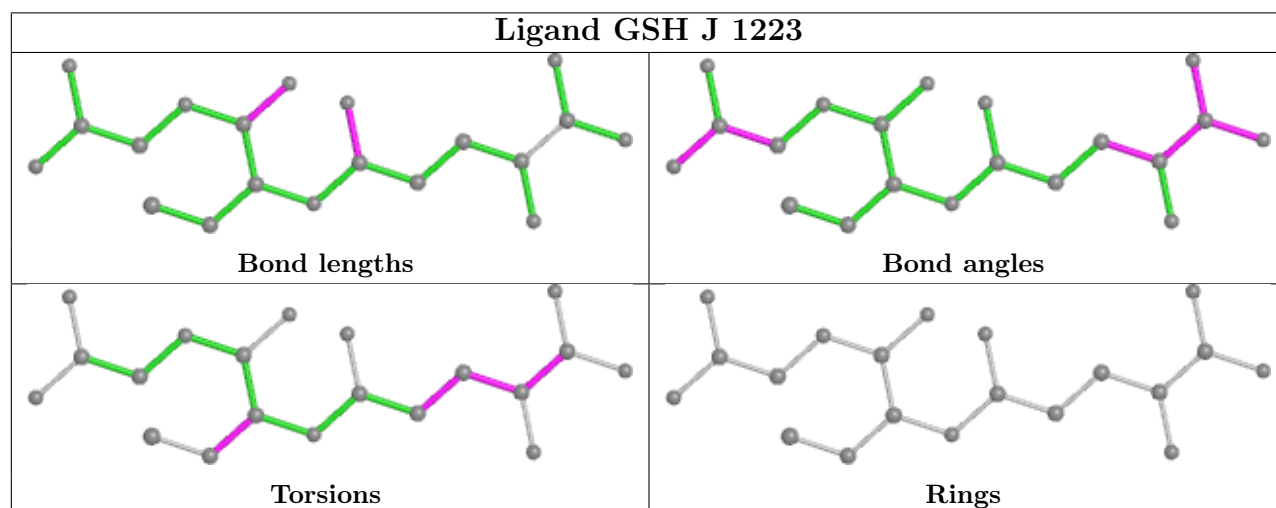
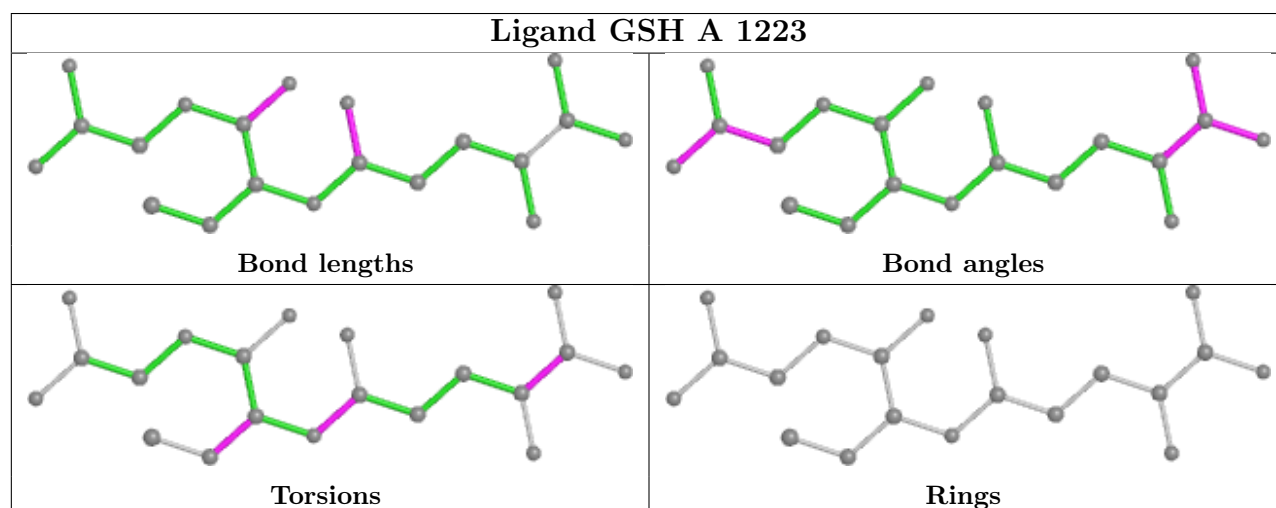
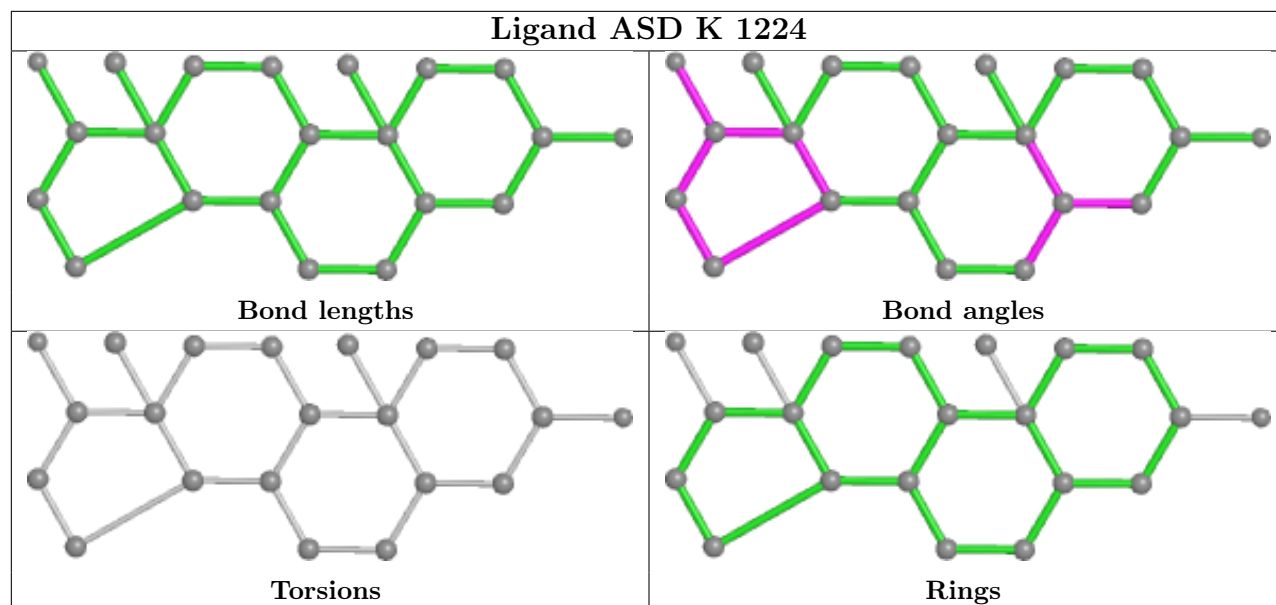


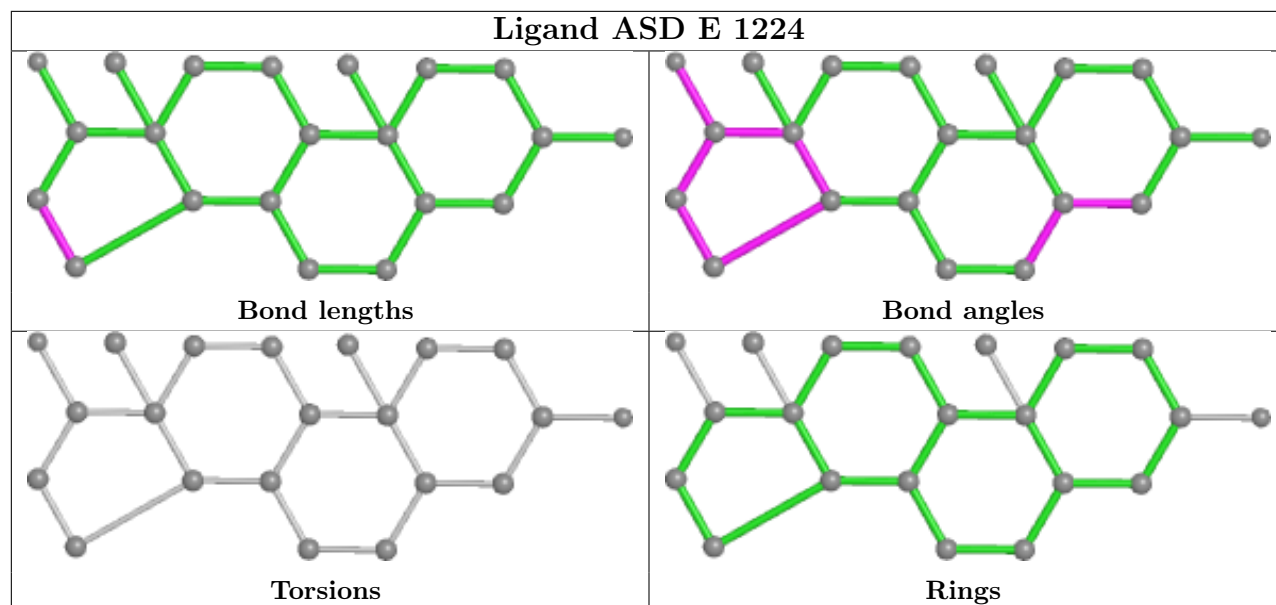












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	219/222 (98%)	-0.19	0 <b>100</b> <b>100</b>	8, 18, 32, 45	0
1	B	219/222 (98%)	-0.28	1 (0%) <b>91</b> <b>89</b>	8, 16, 35, 45	0
1	C	219/222 (98%)	0.32	11 (5%) <b>28</b> <b>23</b>	11, 20, 50, 62	0
1	D	219/222 (98%)	-0.16	1 (0%) <b>91</b> <b>89</b>	10, 19, 35, 48	0
1	E	219/222 (98%)	0.02	5 (2%) <b>60</b> <b>56</b>	11, 20, 44, 54	0
1	F	219/222 (98%)	-0.18	2 (0%) <b>84</b> <b>82</b>	10, 18, 29, 47	0
1	G	219/222 (98%)	-0.23	1 (0%) <b>91</b> <b>89</b>	8, 16, 29, 45	0
1	H	219/222 (98%)	-0.07	5 (2%) <b>60</b> <b>56</b>	7, 19, 43, 56	0
1	I	219/222 (98%)	-0.24	0 <b>100</b> <b>100</b>	9, 17, 33, 38	0
1	J	219/222 (98%)	-0.02	3 (1%) <b>75</b> <b>72</b>	10, 17, 38, 53	0
1	K	219/222 (98%)	-0.17	2 (0%) <b>84</b> <b>82</b>	9, 19, 32, 48	0
1	L	219/222 (98%)	-0.28	2 (0%) <b>84</b> <b>82</b>	7, 16, 33, 42	0
1	M	219/222 (98%)	-0.20	3 (1%) <b>75</b> <b>72</b>	8, 17, 33, 51	0
1	N	219/222 (98%)	-0.09	4 (1%) <b>68</b> <b>64</b>	7, 17, 41, 54	0
1	O	219/222 (98%)	-0.14	2 (0%) <b>84</b> <b>82</b>	6, 17, 35, 53	0
1	P	219/222 (98%)	-0.14	3 (1%) <b>75</b> <b>72</b>	8, 17, 40, 57	0
All	All	3504/3552 (98%)	-0.13	45 (1%) <b>77</b> <b>74</b>	6, 18, 37, 62	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	LEU	4.3
1	P	221	ARG	4.1
1	C	220	PHE	4.1
1	C	110	PRO	4.0
1	C	219	ILE	3.7

## 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.

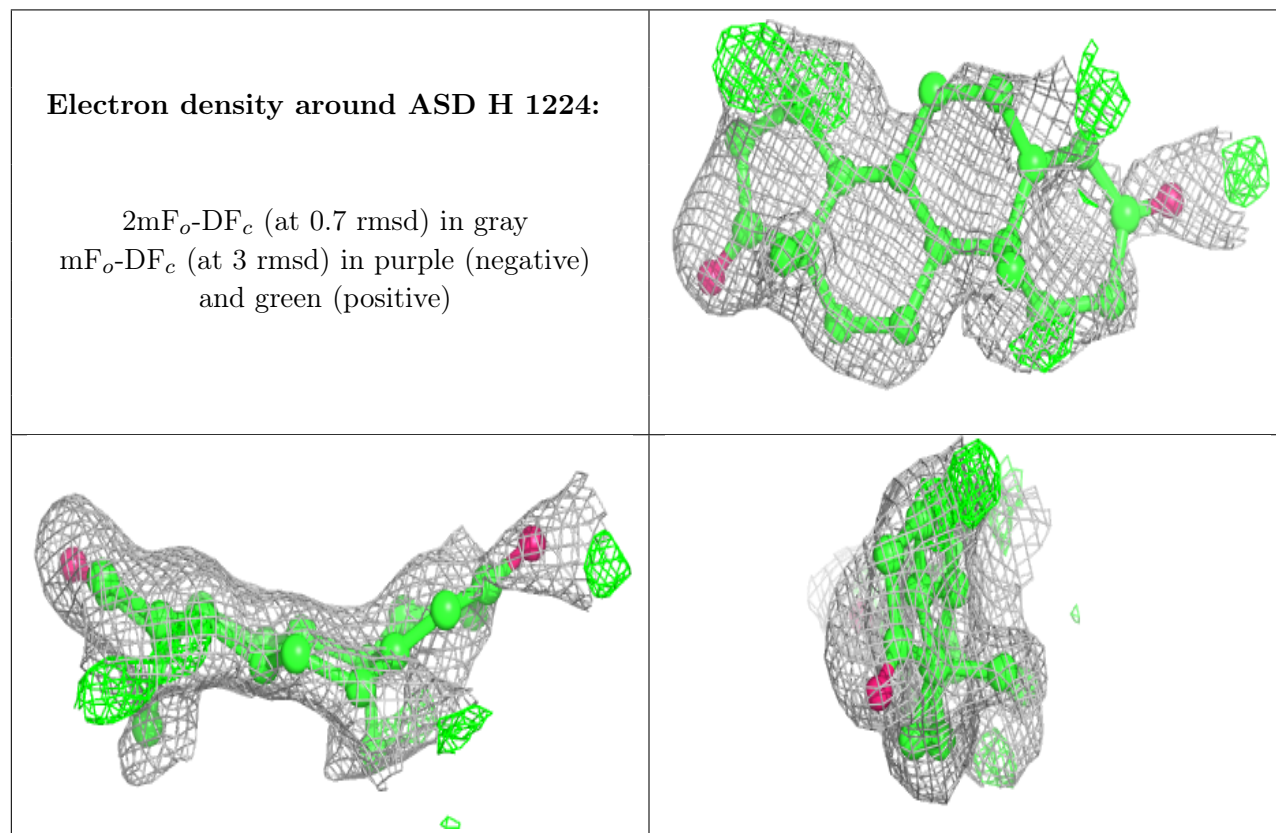
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ASD	H	1224	21/21	0.68	0.20	49,51,53,53	0
3	ASD	D	1224	21/21	0.72	0.22	57,58,59,59	0
3	ASD	E	1224	21/21	0.75	0.18	50,51,52,53	0
2	GSH	I	1223	20/20	0.75	0.18	32,37,38,39	0
2	GSH	B	1223	20/20	0.79	0.17	30,33,35,36	0
3	ASD	A	1224	21/21	0.80	0.16	34,35,36,37	0
3	ASD	F	1224	21/21	0.80	0.16	39,41,42,42	0
3	ASD	G	1224	21/21	0.80	0.19	40,42,44,45	0
2	GSH	O	1223	20/20	0.80	0.14	28,32,38,38	0
3	ASD	P	1224	21/21	0.80	0.16	43,46,48,48	0
3	ASD	K	1224	21/21	0.81	0.17	38,39,40,41	0
2	GSH	D	1223	20/20	0.81	0.16	30,34,39,39	0
3	ASD	I	1224	21/21	0.82	0.16	38,39,39,40	0
3	ASD	B	1224	21/21	0.82	0.16	31,33,35,36	0
2	GSH	H	1223	20/20	0.82	0.15	28,32,36,37	0
2	GSH	C	1223	20/20	0.85	0.13	23,32,35,39	0
2	GSH	M	1223	20/20	0.86	0.14	22,25,33,33	0
2	GSH	E	1223	20/20	0.86	0.13	33,35,36,37	0
2	GSH	J	1223	20/20	0.86	0.12	21,27,31,33	0
3	ASD	L	1224	21/21	0.86	0.14	32,34,36,36	0
2	GSH	L	1223	20/20	0.86	0.17	23,28,29,31	0
2	GSH	G	1223	20/20	0.88	0.17	16,24,32,33	0
2	GSH	P	1223	20/20	0.89	0.14	21,26,35,35	0
2	GSH	N	1223	20/20	0.89	0.13	22,26,33,33	0
2	GSH	F	1223	20/20	0.89	0.13	25,27,33,33	0
2	GSH	A	1223	20/20	0.90	0.14	22,28,30,30	0
2	GSH	K	1223	20/20	0.90	0.13	18,27,31,31	0

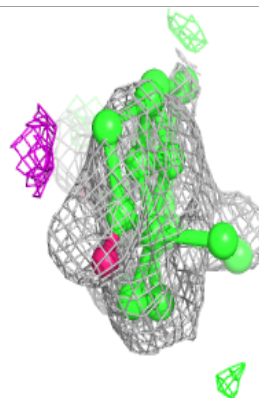
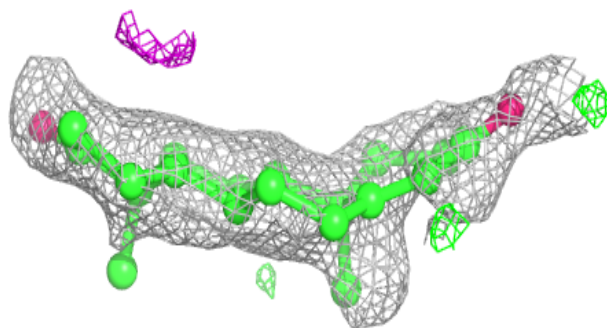
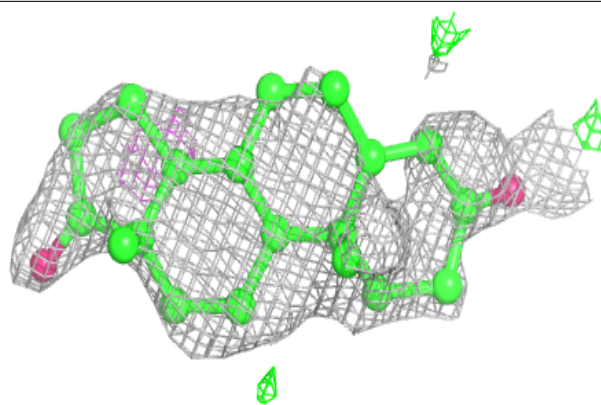


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

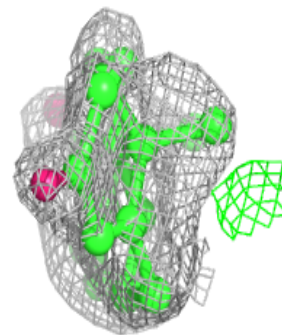
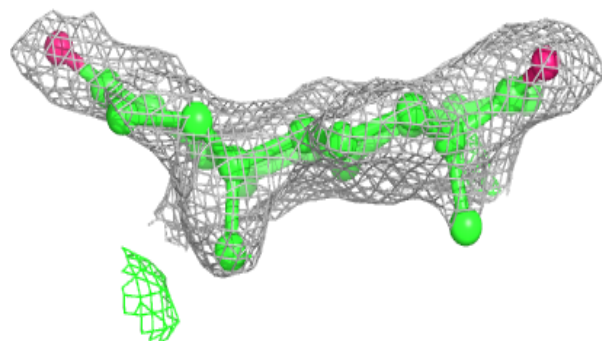
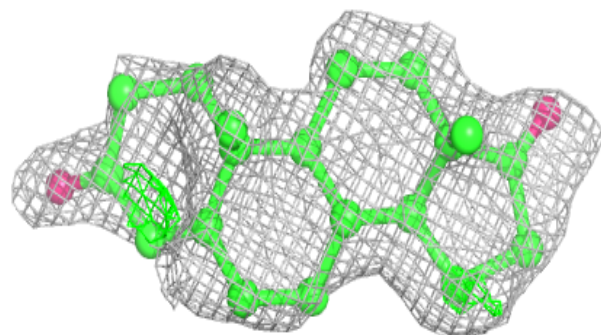


**Electron density around ASD D 1224:**

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

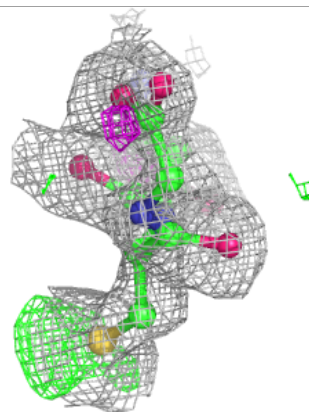
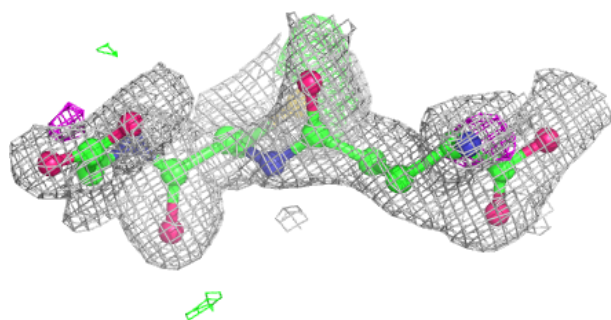
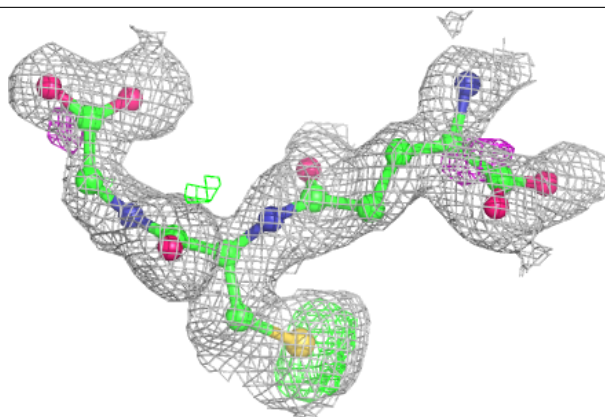
**Electron density around ASD E 1224:**

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and green (positive)

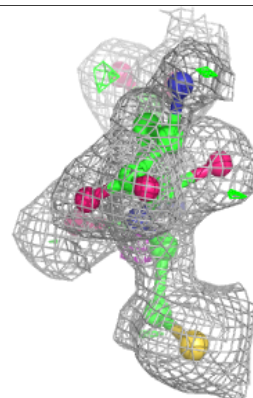
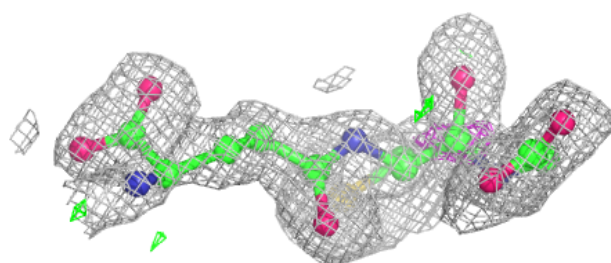
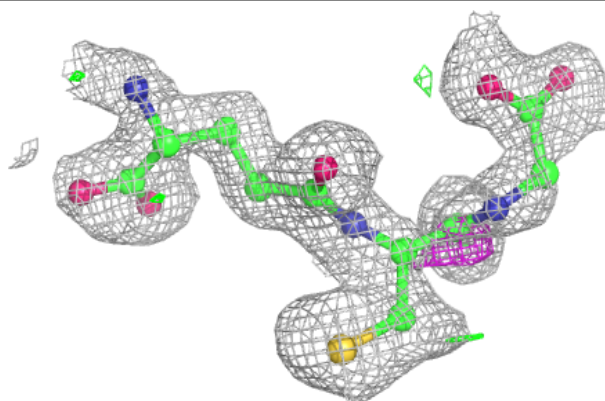


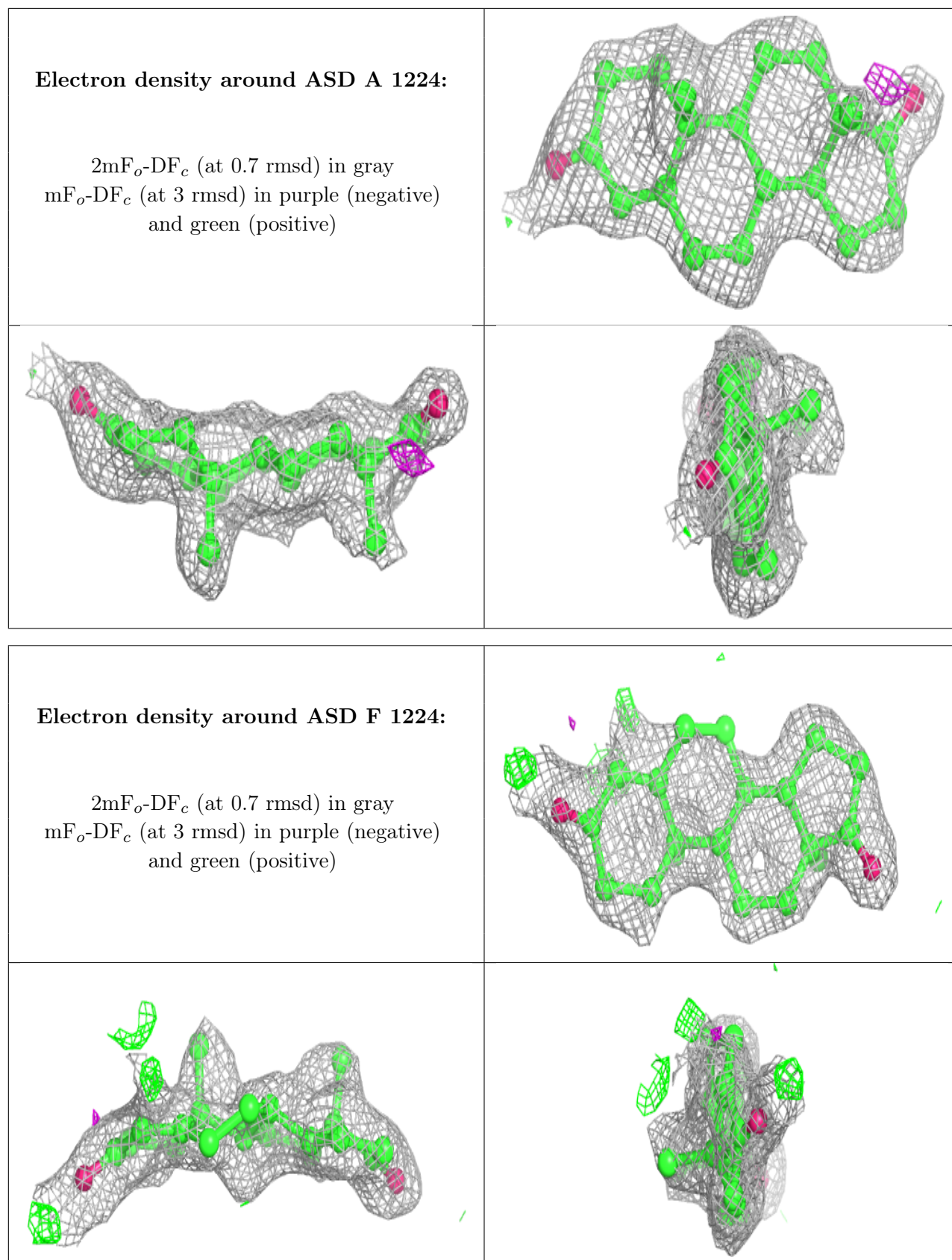
**Electron density around GSH I 1223:**

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and green (positive)

**Electron density around GSH B 1223:**

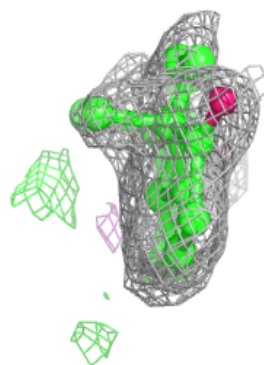
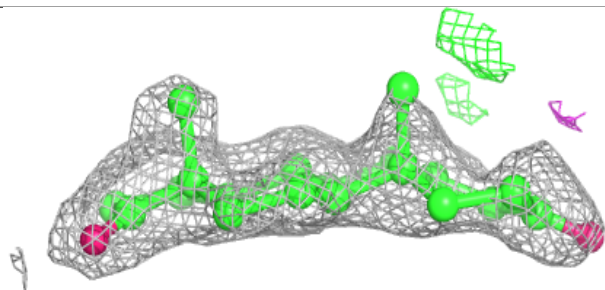
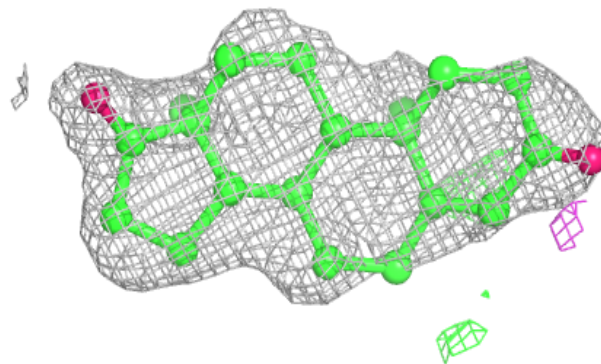
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and green (positive)



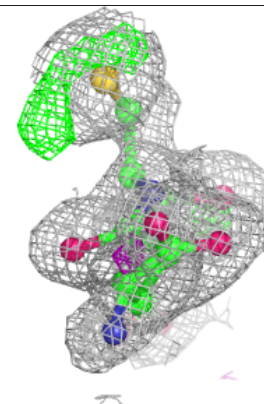
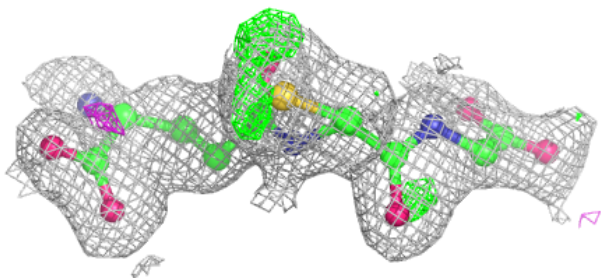
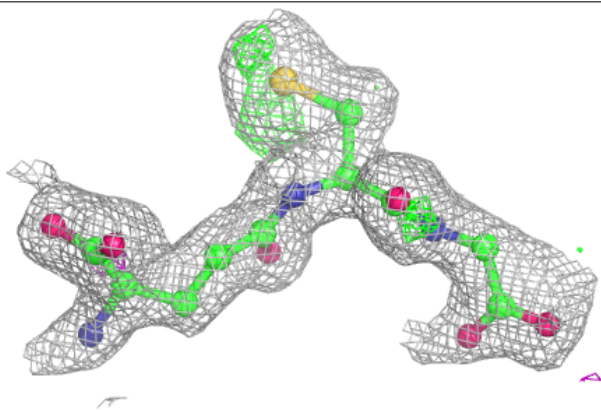


**Electron density around ASD G 1224:**

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

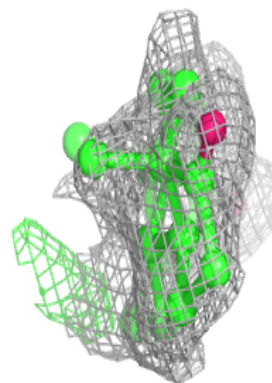
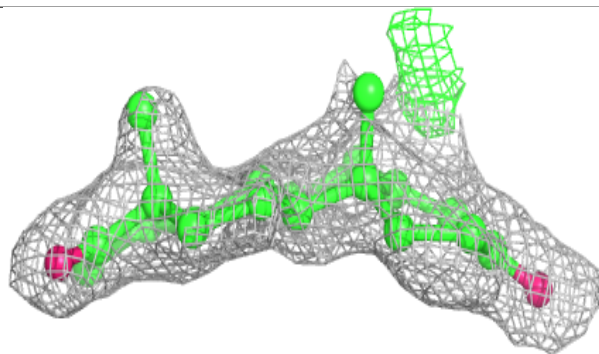
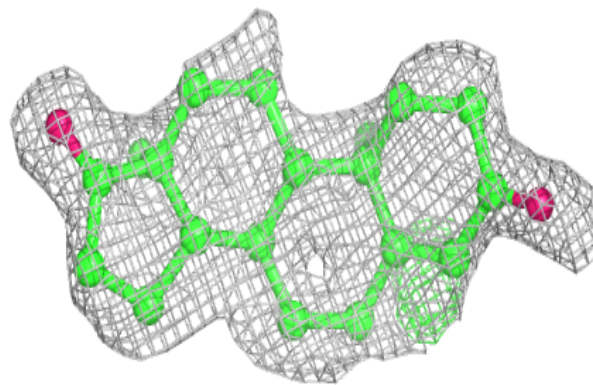
**Electron density around GSH O 1223:**

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and green (positive)

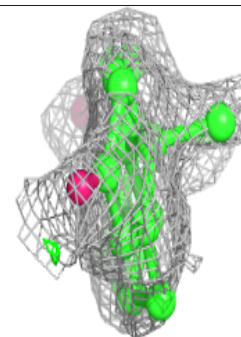
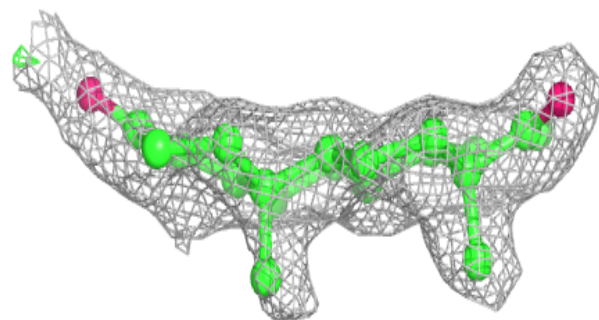
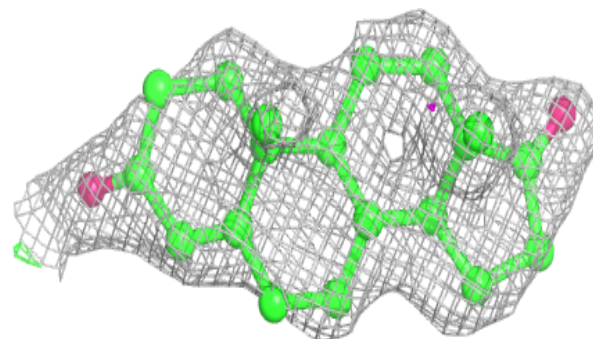


**Electron density around ASD P 1224:**

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and green (positive)

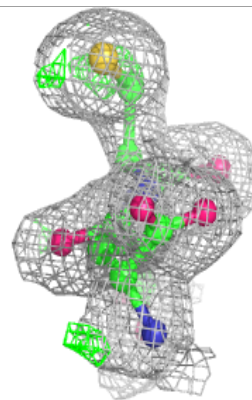
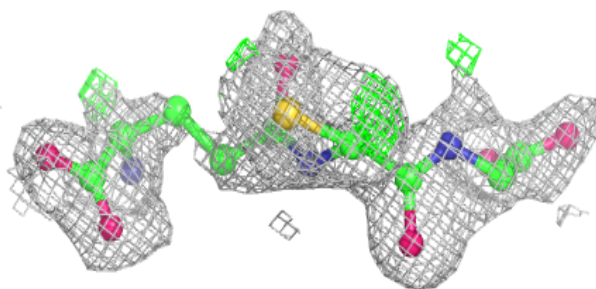
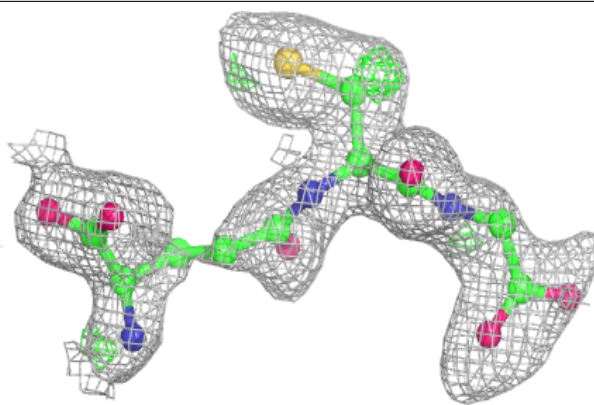
**Electron density around ASD K 1224:**

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and green (positive)

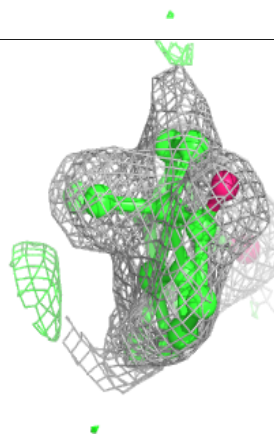
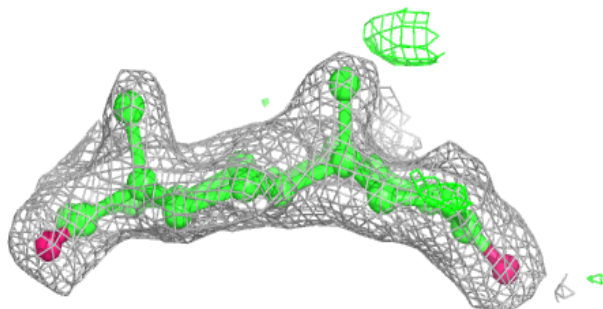
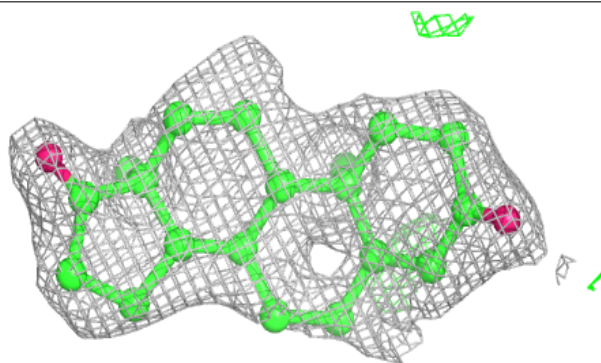


**Electron density around GSH D 1223:**

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

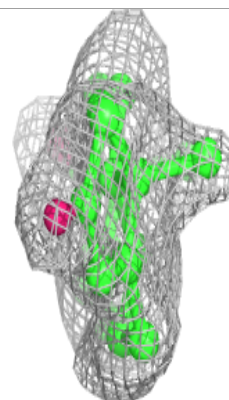
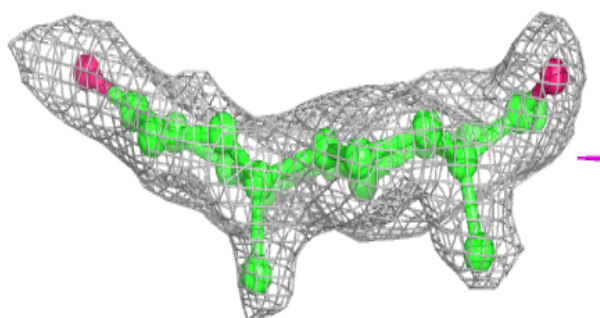
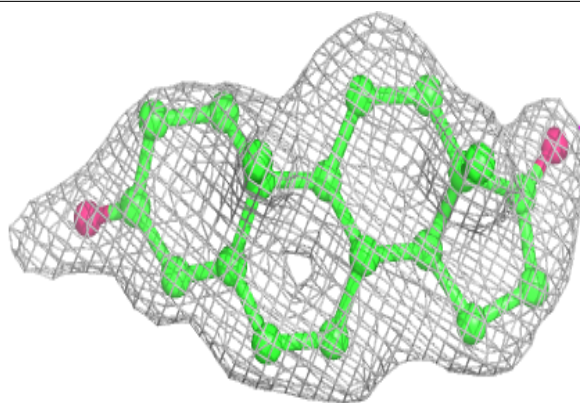
**Electron density around ASD I 1224:**

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and green (positive)

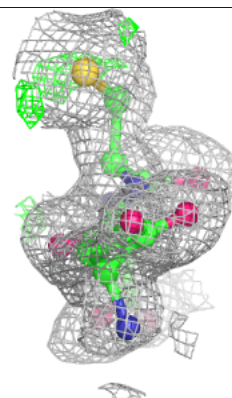
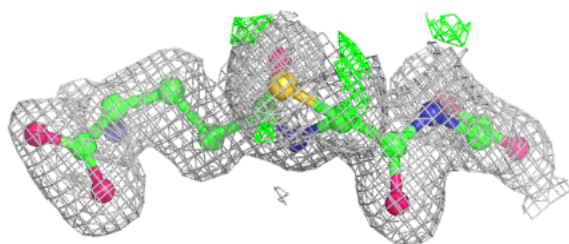
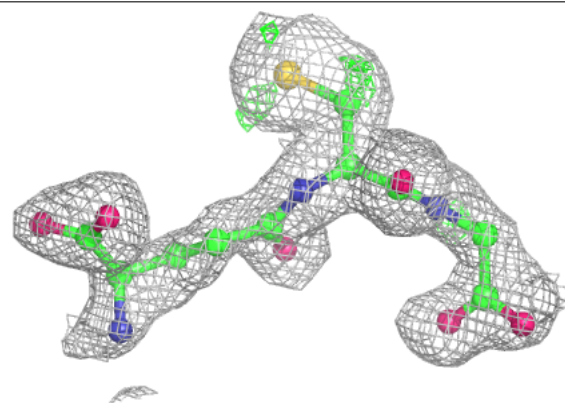


**Electron density around ASD B 1224:**

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and green (positive)

**Electron density around GSH H 1223:**

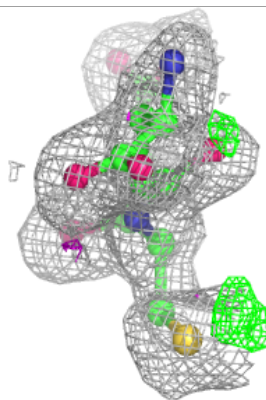
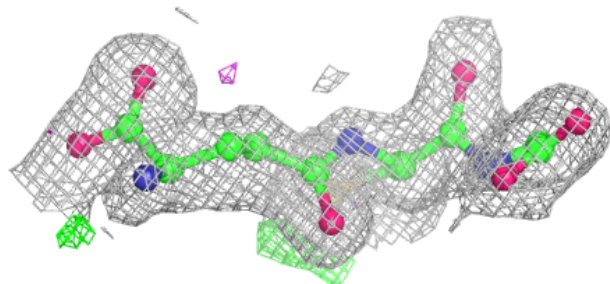
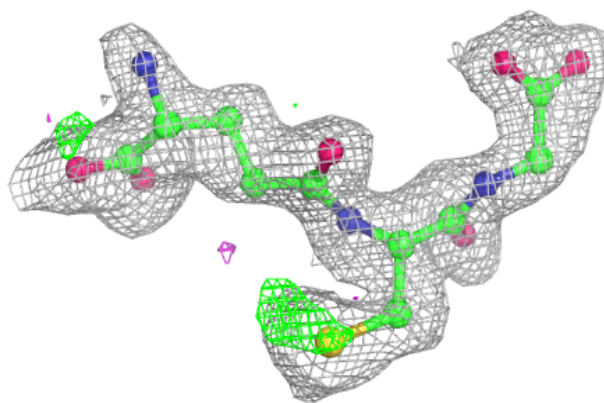
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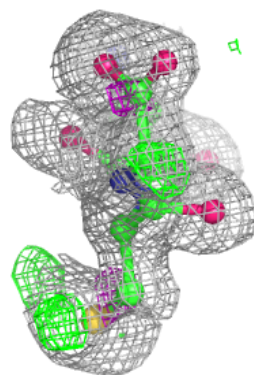
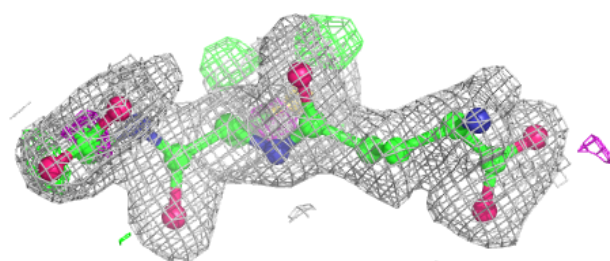
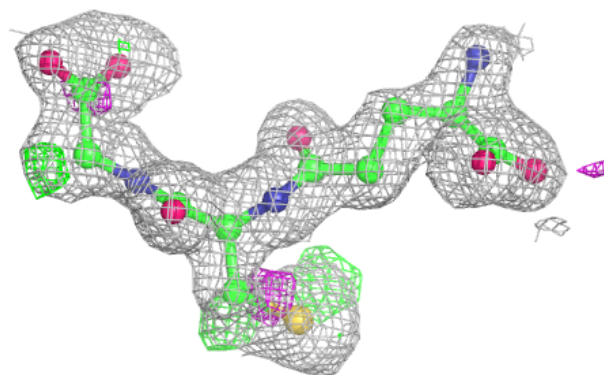


**Electron density around GSH C 1223:**

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

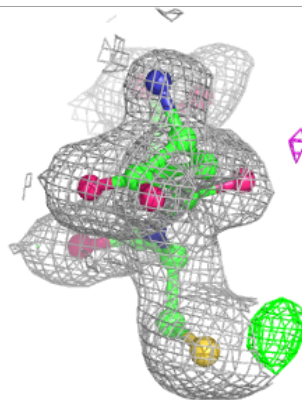
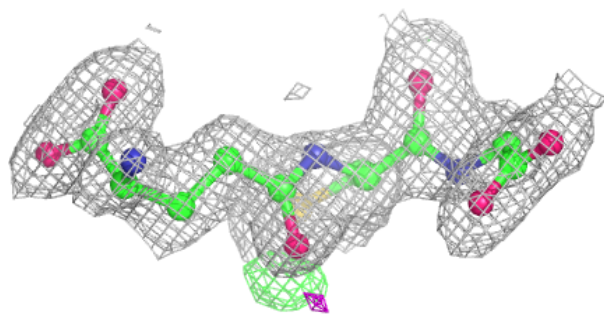
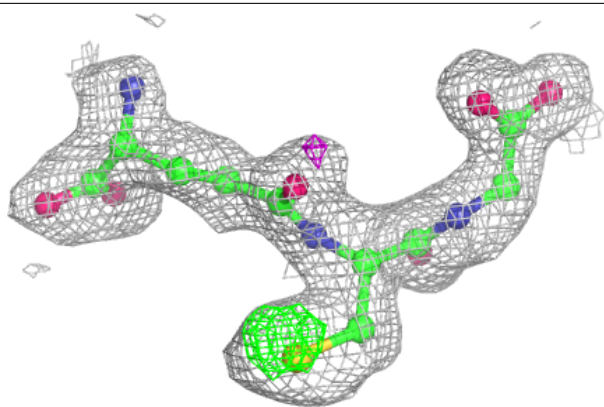
**Electron density around GSH M 1223:**

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and green (positive)

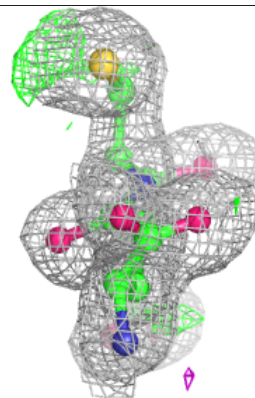
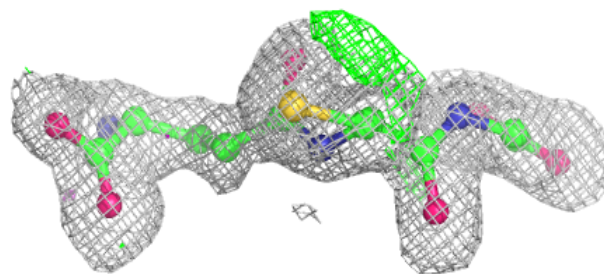
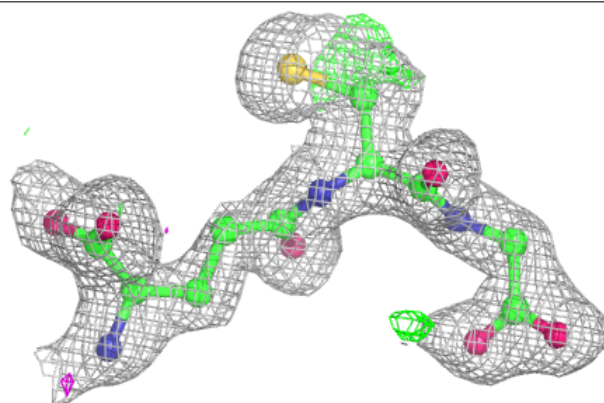


**Electron density around GSH E 1223:**

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and green (positive)

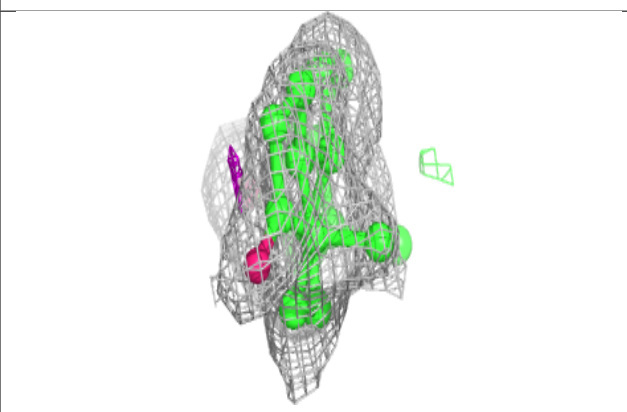
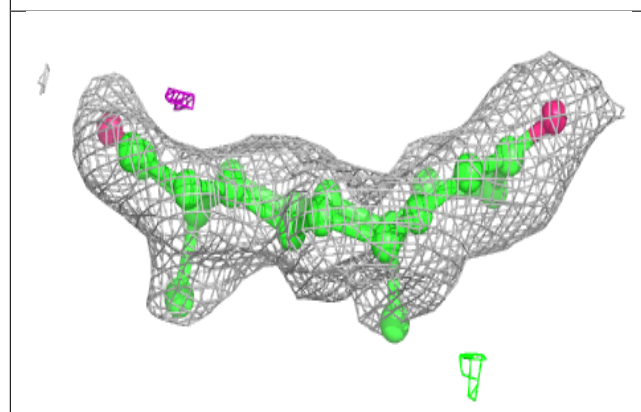
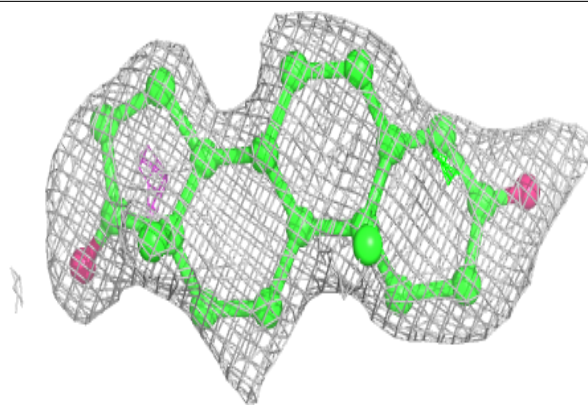
**Electron density around GSH J 1223:**

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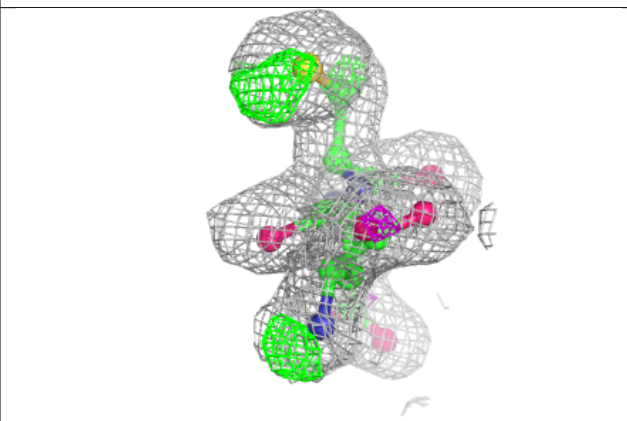
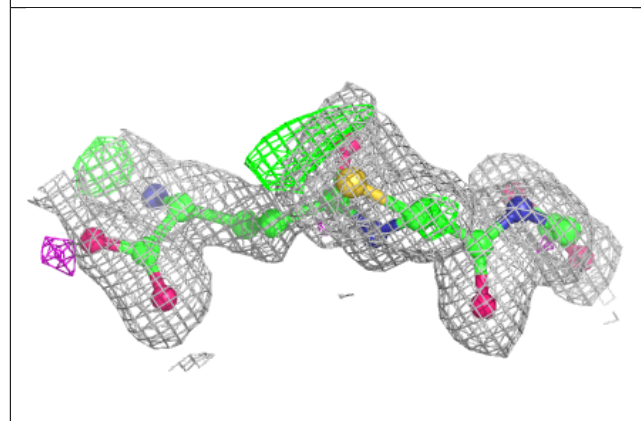
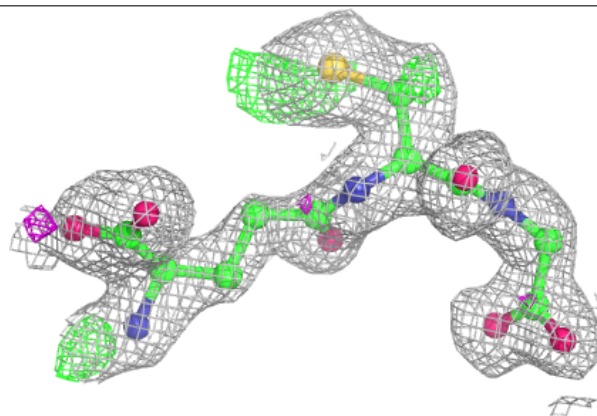


**Electron density around ASD L 1224:**

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and green (positive)

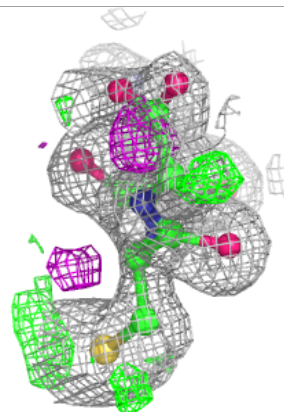
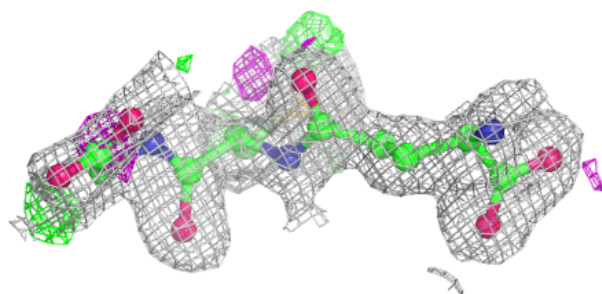
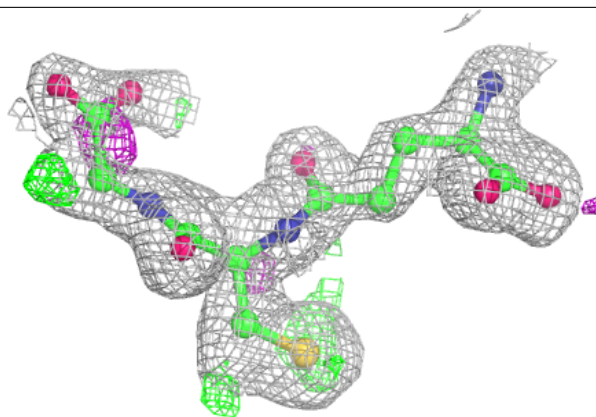
**Electron density around GSH L 1223:**

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

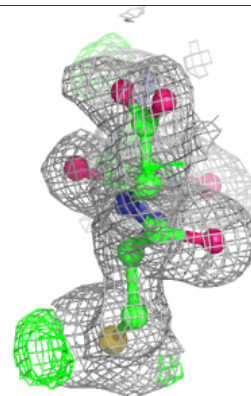
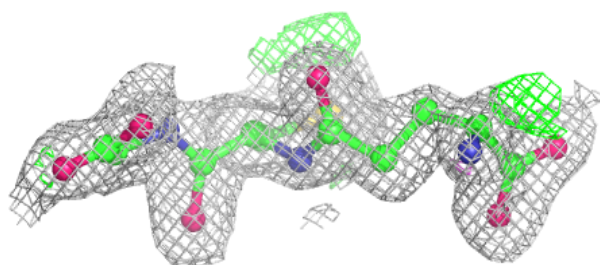
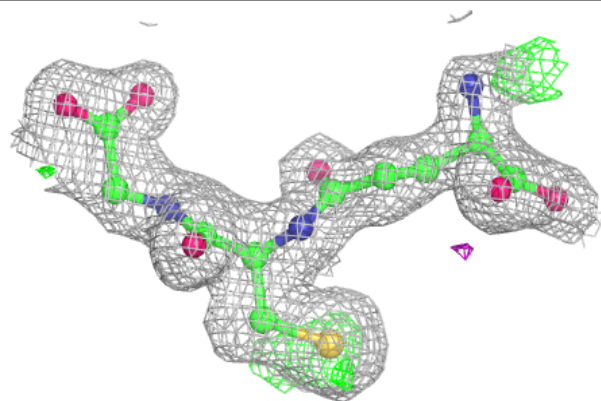


**Electron density around GSH G 1223:**

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

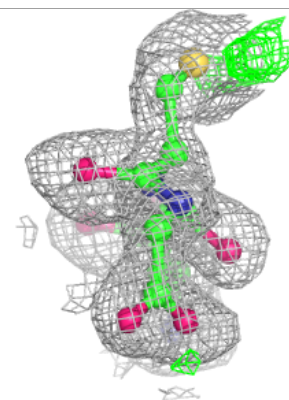
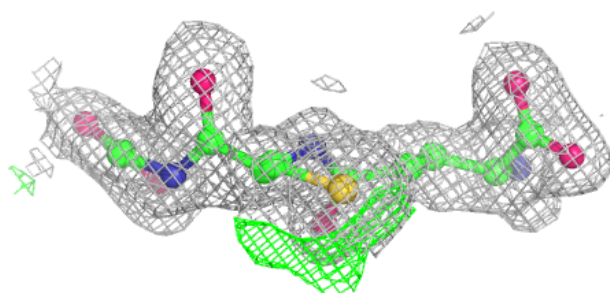
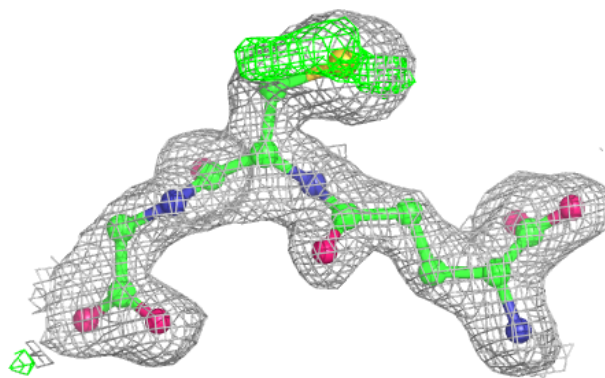
**Electron density around GSH P 1223:**

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

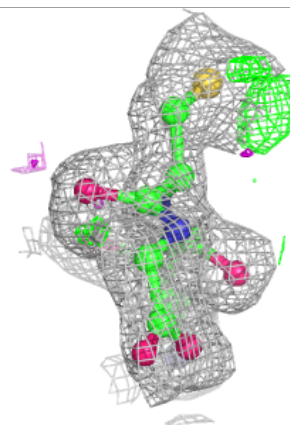
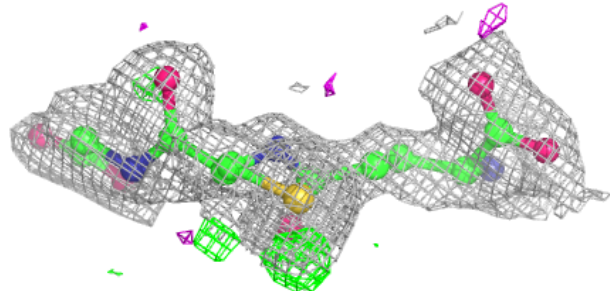
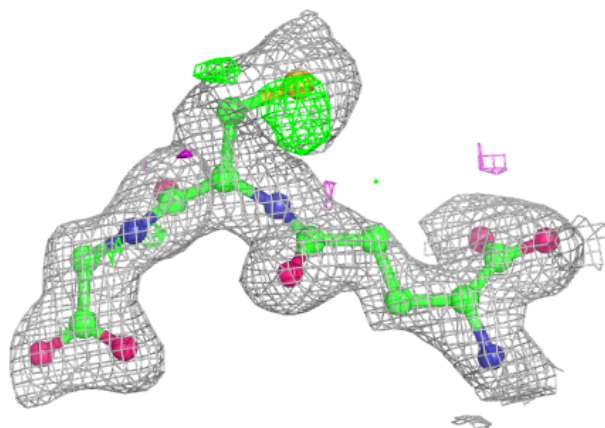


**Electron density around GSH N 1223:**

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

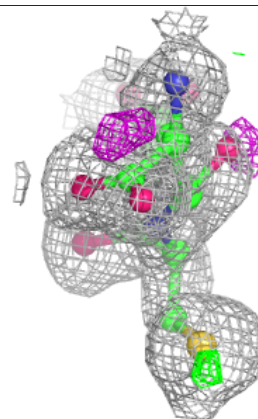
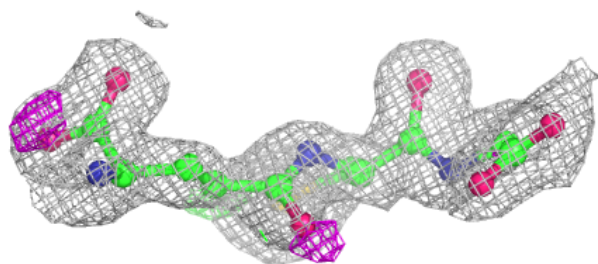
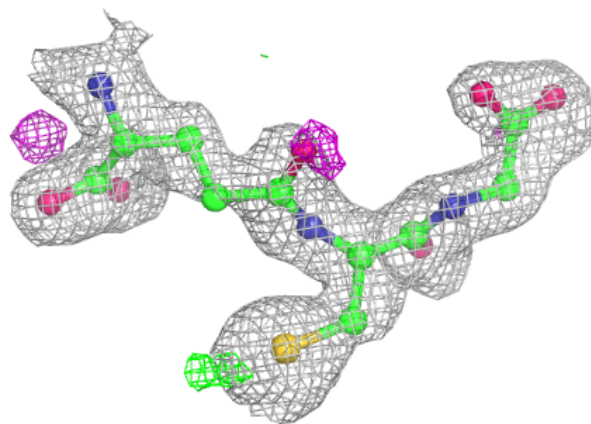
**Electron density around GSH F 1223:**

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

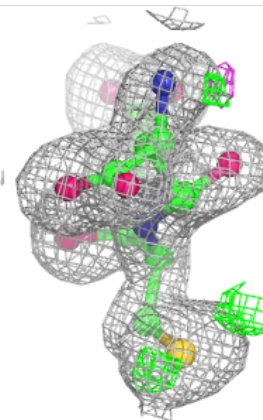
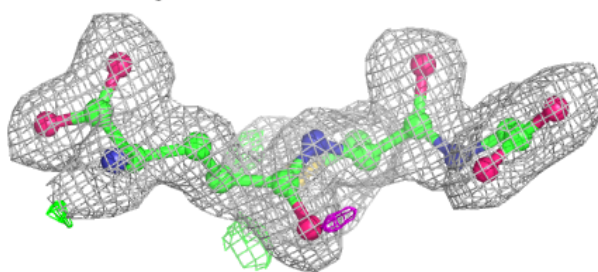
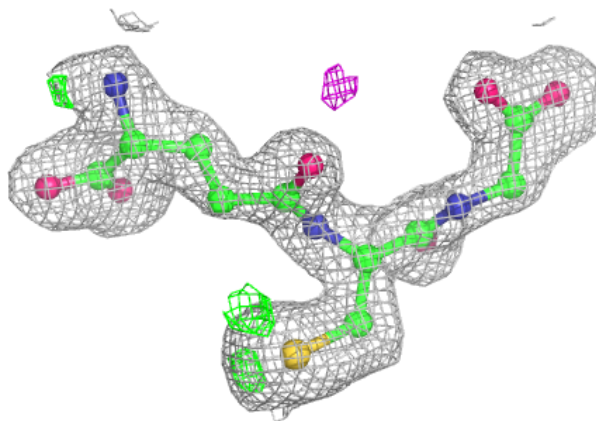


**Electron density around GSH A 1223:**

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

**Electron density around GSH K 1223:**

$2mF_o-DF_c$  (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.