



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:33 AM UTC

PDB ID : 2VCV / pdb_00002vcv
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

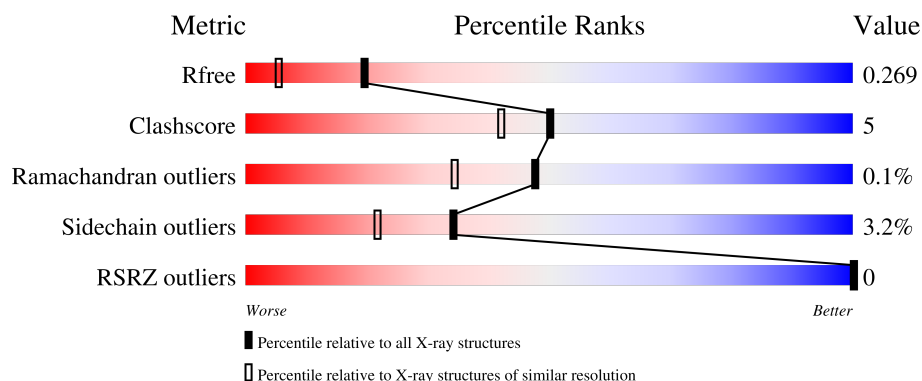
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 ≥ 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	 90% 8% ..
1	B	222	 83% 14% ..
1	C	222	 83% 14% ..
1	D	222	 90% 8% ..
1	E	222	 89% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	222	 88% 10% ..
1	G	222	 89% 9% ..
1	H	222	 82% 14% ..
1	I	222	 86% 10% ..
1	J	222	 83% 15% ..
1	K	222	 87% 10% ..
1	L	222	 84% 14% ..
1	M	222	 85% 13% ..
1	N	222	 84% 14% ..
1	O	222	 86% 12% ..
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

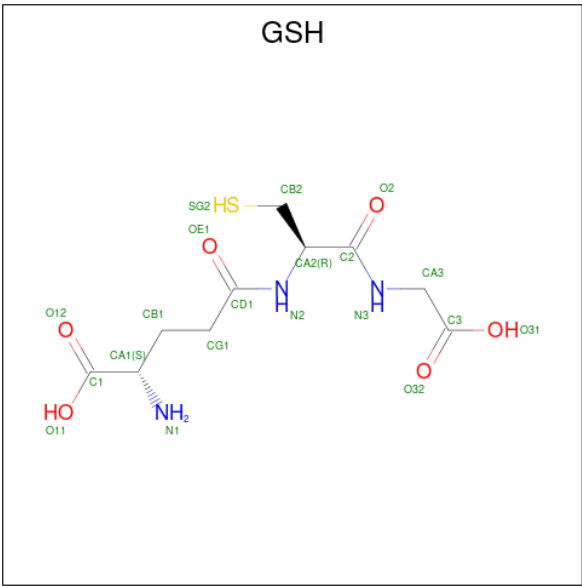
There are 4 unique types of molecules in this entry. The entry contains 32159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



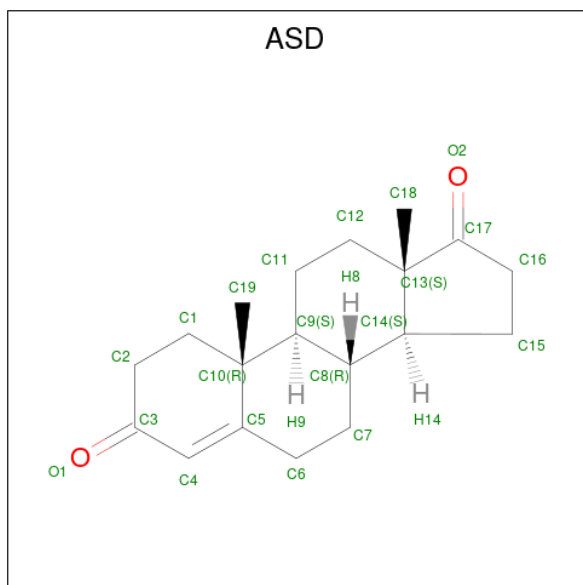
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total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

Continued on next page...

Continued from previous page...

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 (CCD ID: ASD) (formula: C₁₉H₂₆O₂).



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		

Continued on next page...

Continued from previous page...

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.

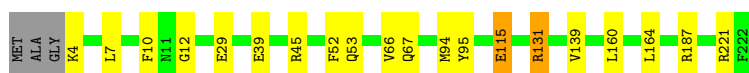
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		
4	B	215	Total	O	0	0
			215	215		
4	C	171	Total	O	0	0
			171	171		
4	D	179	Total	O	0	0
			179	179		
4	E	188	Total	O	0	0
			188	188		
4	F	215	Total	O	0	0
			215	215		
4	G	230	Total	O	0	0
			230	230		
4	H	194	Total	O	0	0
			194	194		
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.

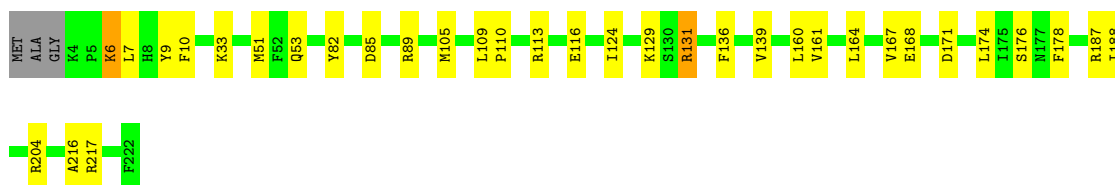
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain A: 



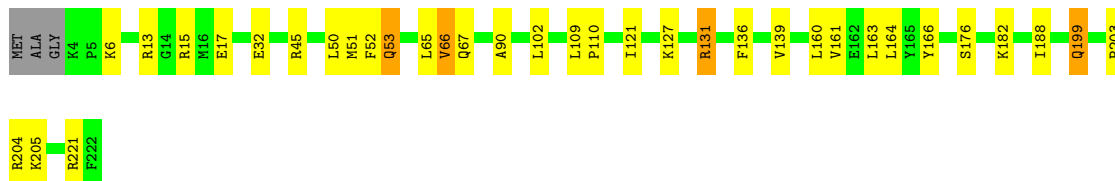
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

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

Chain F: 88% 10% .



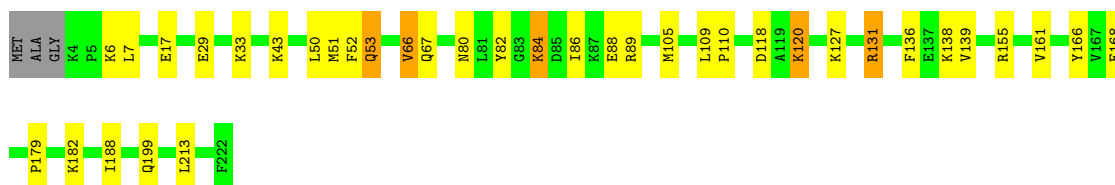
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain G: 89% 9% .



- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain H: 82% 14% ..



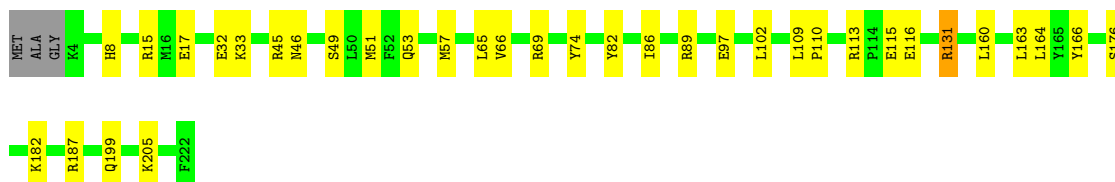
- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain I: 86% 10% ..



- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

Chain J: 83% 15% .

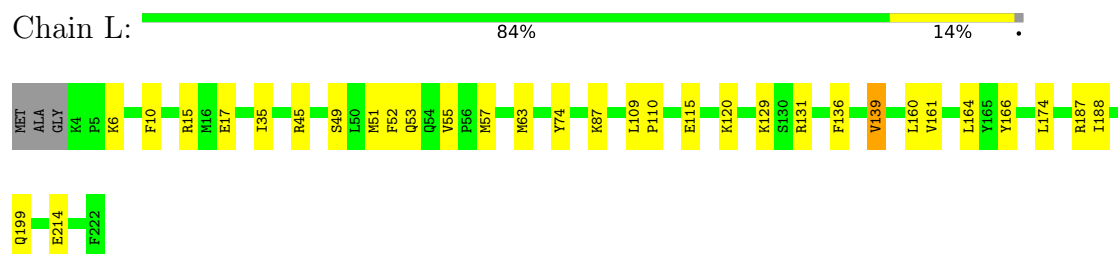


- Molecule 1: GLUTATHIONE S-TRANSFERASE A3

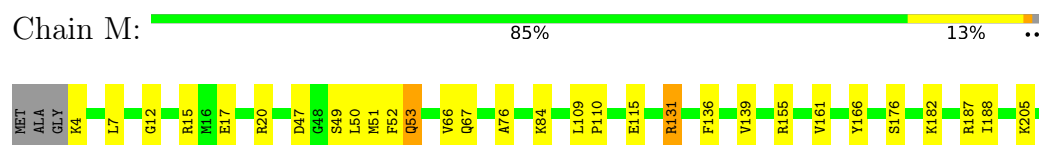
Chain K: 87% 10% ..



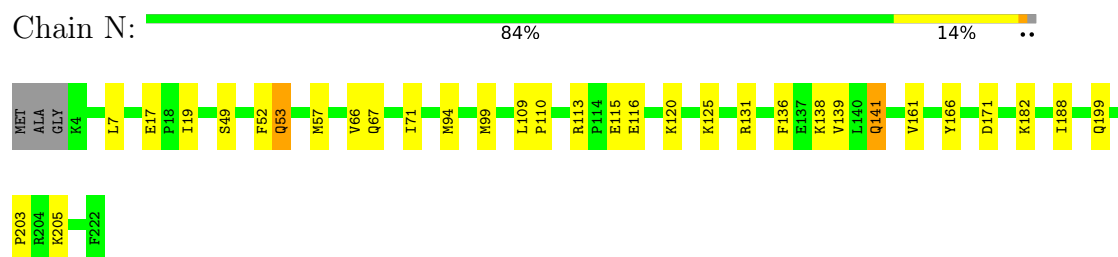
• Molecule 1: GLUTATHIONE S-TRANSFERASE A3



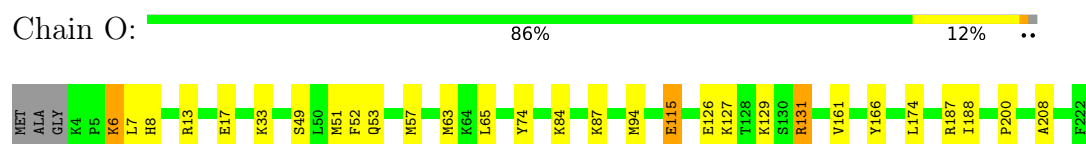
• Molecule 1: GLUTATHIONE S-TRANSFERASE A3



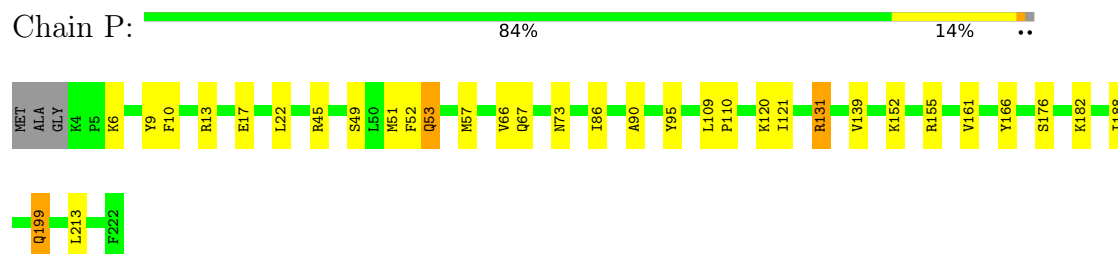
• Molecule 1: GLUTATHIONE S-TRANSFERASE A3



• Molecule 1: GLUTATHIONE S-TRANSFERASE A3



• Molecule 1: GLUTATHIONE S-TRANSFERASE A3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.18Å 92.06Å 113.54Å 89.76° 89.72° 89.73°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-1.80) 93.1 (20.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.80Å)	Xtriage
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 (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
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	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32159	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/1811	0.86	0/2433
1	B	0.57	0/1818	0.86	2/2443 (0.1%)
1	C	0.55	0/1818	0.85	0/2443
1	D	0.57	0/1812	0.85	0/2433
1	E	0.56	0/1812	0.90	1/2433 (0.0%)
1	F	0.56	0/1820	0.87	0/2444
1	G	0.59	0/1819	0.86	0/2443
1	H	0.56	0/1818	0.86	0/2443
1	I	0.58	0/1820	0.85	0/2444
1	J	0.56	0/1811	0.85	0/2433
1	K	0.56	0/1827	0.86	0/2454
1	L	0.57	0/1837	0.86	0/2465
1	M	0.58	0/1803	0.85	0/2422
1	N	0.58	0/1836	0.86	0/2466
1	O	0.58	0/1829	0.85	0/2456
1	P	0.58	0/1822	0.85	0/2447
All	All	0.57	0/29113	0.86	3/39102 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	PHE	CA-C-O	-12.45	83.64	121.00
1	B	178	PHE	CA-C-N	5.69	125.16	119.24
1	B	178	PHE	C-N-CA	5.69	125.16	119.24

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	18	0
1	B	1771	0	1843	29	0
1	C	1771	0	1843	24	0
1	D	1768	0	1836	14	0
1	E	1768	0	1836	19	0
1	F	1771	0	1843	23	0
1	G	1771	0	1843	13	0
1	H	1771	0	1843	29	0
1	I	1771	0	1843	27	0
1	J	1768	0	1838	33	0
1	K	1774	0	1848	21	0
1	L	1777	0	1853	17	0
1	M	1765	0	1831	26	0
1	N	1779	0	1852	27	0
1	O	1777	0	1849	24	0
1	P	1775	0	1847	34	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

Continued on next page...

Continued from previous page...

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	10	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	315	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.

All (315) 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:G:64:LYS:HE3	1:J:46:ASN:HD21	1.20	1.04
1:I:94:MET:HE3	1:J:66:VAL:CG2	1.91	0.98
1:I:94:MET:HE3	1:J:66:VAL:HG22	0.96	0.95
1:E:187:ARG:HD2	4:E:2127:HOH:O	1.70	0.92
1:O:94:MET:HE3	1:P:66:VAL:HB	1.52	0.89
1:M:187:ARG:HD2	4:M:2148:HOH:O	1.80	0.80
1:G:64:LYS:HE3	1:J:46:ASN:ND2	1.98	0.78
1:K:95:TYR:CD1	1:L:51:MET:HE1	2.21	0.76
1:C:17:GLU:HG2	1:C:166:TYR:OH	1.87	0.74
1:L:45:ARG:HD2	4:L:2056:HOH:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:131:ARG:HD3	1:L:53:GLN:OE1	1.89	0.73
1:M:131:ARG:HD2	1:N:53:GLN:HG2	1.74	0.69
1:L:187:ARG:HD2	4:L:2148:HOH:O	1.90	0.69
1:M:51:MET:HB2	1:N:94:MET:HE3	1.74	0.68
1:N:17:GLU:HG2	1:N:166:TYR:OH	1.93	0.68
1:O:94:MET:HE2	1:P:51:MET:CB	2.24	0.68
1:B:187:ARG:HD2	4:B:2140:HOH:O	1.94	0.66
1:F:187:ARG:HD2	4:F:2143:HOH:O	1.96	0.65
1:B:136:PHE:HA	1:B:139[A]:VAL:HG12	1.78	0.64
1:N:66[B]:VAL:HG11	4:N:2050:HOH:O	1.98	0.64
1:A:39:GLU:HG3	1:O:87:LYS:HD3	1.80	0.63
1:E:51:MET:HB2	1:F:94:MET:HE3	1.80	0.63
1:O:94:MET:HE2	1:P:51:MET:HB3	1.80	0.63
1:P:66:VAL:HG12	1:P:67:GLN:N	2.12	0.63
1:O:131:ARG:HD2	1:P:52:PHE:O	1.99	0.62
1:P:45:ARG:HD3	1:P:53:GLN:HB2	1.81	0.62
1:I:15:ARG:HD2	2:I:1223:GSH:HG13	1.82	0.62
1:M:131:ARG:HH11	1:N:53:GLN:HG3	1.65	0.62
1:M:51:MET:CB	1:N:94:MET:HE3	2.29	0.61
1:E:187:ARG:CD	4:E:2127:HOH:O	2.39	0.61
1:M:176:SER:HA	1:M:182:LYS:HE3	1.83	0.61
1:M:52:PHE:O	1:N:131:ARG:HD2	2.01	0.61
1:O:6:LYS:HE2	1:O:8:HIS:CE1	2.36	0.61
1:H:109:LEU:N	1:H:110:PRO:HD2	2.16	0.60
1:O:53:GLN:OE1	1:P:131:ARG:HD3	2.00	0.60
1:P:66:VAL:HG13	4:P:2050:HOH:O	2.01	0.60
1:J:17:GLU:HG2	1:J:166:TYR:OH	2.00	0.60
1:D:145:GLN:HG2	4:D:2116:HOH:O	2.00	0.60
1:H:155:ARG:HD3	4:H:2144:HOH:O	2.01	0.60
1:A:95:TYR:CD1	1:B:51:MET:HE1	2.37	0.60
1:P:109:LEU:HD21	1:P:121:ILE:HG12	1.84	0.60
1:I:94:MET:HE2	1:J:51:MET:CB	2.32	0.59
1:O:49:SER:HB3	1:O:57:MET:HE2	1.84	0.58
1:A:52:PHE:O	1:B:131:ARG:HD2	2.03	0.58
1:L:109:LEU:N	1:L:110:PRO:HD2	2.17	0.58
1:P:199:GLN:NE2	4:P:2189:HOH:O	2.36	0.58
1:G:17:GLU:HG2	1:G:166:TYR:OH	2.04	0.58
1:G:187:ARG:HD2	4:G:2158:HOH:O	2.04	0.57
1:A:53:GLN:OE1	1:B:131:ARG:HD3	2.05	0.57
1:E:109:LEU:N	1:E:110:PRO:HD2	2.19	0.57
1:D:136:PHE:HA	1:D:139:VAL:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:GLU:HG2	1:F:166:TYR:OH	2.06	0.56
1:K:66[B]:VAL:CG1	4:K:2071:HOH:O	2.54	0.56
1:K:66[B]:VAL:HG12	1:K:67:GLN:N	2.21	0.55
1:P:66:VAL:HG12	1:P:67:GLN:H	1.71	0.55
1:E:51:MET:CB	1:F:94:MET:HE3	2.37	0.55
1:E:131:ARG:HD3	1:F:53:GLN:OE1	2.06	0.55
1:I:136:PHE:HA	1:I:139:VAL:HG12	1.88	0.55
1:C:136:PHE:HA	1:C:139[A]:VAL:HG12	1.89	0.54
1:A:53:GLN:HG2	1:B:131:ARG:HD2	1.88	0.54
1:P:66:VAL:HG11	4:P:2043:HOH:O	2.06	0.54
1:P:17:GLU:HG2	1:P:166:TYR:OH	2.07	0.54
1:F:12:GLY:C	1:F:205:LYS:HG2	2.33	0.54
1:H:213:LEU:HA	3:H:1224:ASD:H161	1.90	0.54
1:I:90:ALA:HB1	1:J:65:LEU:HD21	1.90	0.53
1:O:17:GLU:HG2	1:O:166:TYR:OH	2.07	0.53
1:H:136:PHE:HA	1:H:139[B]:VAL:HG22	1.90	0.53
1:A:95:TYR:CE1	1:B:51:MET:HE1	2.43	0.53
1:J:187:ARG:HD2	4:J:2125:HOH:O	2.08	0.53
1:C:50:LEU:HB2	1:C:53:GLN:HA	1.91	0.53
1:P:109:LEU:N	1:P:110:PRO:HD2	2.24	0.53
1:J:109:LEU:N	1:J:110:PRO:HD2	2.23	0.53
1:I:94:MET:HE2	1:J:51:MET:HB2	1.91	0.53
1:E:17:GLU:HG2	1:E:166:TYR:OH	2.09	0.52
2:F:1223:GSH:HB22	3:F:1224:ASD:H4	1.92	0.52
1:E:52:PHE:O	1:F:131:ARG:HD2	2.08	0.52
1:E:131:ARG:HH11	1:F:53:GLN:HG3	1.74	0.52
1:H:80:ASN:ND2	4:H:2079:HOH:O	2.41	0.52
1:K:17:GLU:HG2	1:K:166:TYR:OH	2.09	0.52
1:N:66[B]:VAL:HG12	1:N:67:GLN:N	2.24	0.52
1:A:45:ARG:HD2	4:A:2045:HOH:O	2.09	0.52
1:H:53:GLN:HB3	4:H:2047:HOH:O	2.08	0.52
1:P:73:ASN:HA	1:P:155[A]:ARG:HH12	1.74	0.52
1:P:66:VAL:CG1	1:P:67:GLN:H	2.23	0.51
1:H:43:LYS:HD3	4:H:2041:HOH:O	2.11	0.51
1:L:161:VAL:HG21	1:L:188:ILE:HB	1.93	0.51
1:C:203:PRO:O	1:C:205:LYS:HD2	2.11	0.51
1:E:86:ILE:HG12	1:F:74:TYR:CD1	2.45	0.51
1:I:95:TYR:CD1	1:J:51:MET:HE1	2.45	0.51
1:C:51:MET:HE1	1:D:95:TYR:CD1	2.46	0.51
1:M:15:ARG:HD2	2:M:1223:GSH:HG13	1.92	0.51
1:M:50:LEU:HB2	1:M:53:GLN:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:LEU:O	1:J:164:LEU:HG	2.11	0.51
1:N:52:PHE:C	1:N:53:GLN:HG2	2.36	0.51
1:C:127:LYS:O	1:C:131:ARG:HB3	2.11	0.51
1:E:131:ARG:HH11	1:F:53:GLN:CG	2.23	0.51
1:K:66[B]:VAL:HG11	4:K:2059:HOH:O	2.10	0.51
1:I:53:GLN:HG2	1:J:131:ARG:HD2	1.92	0.51
1:C:15:ARG:HD2	2:C:1223:GSH:HG13	1.94	0.50
1:I:52:PHE:O	1:I:53:GLN:HG2	2.11	0.50
1:H:66:VAL:O	1:H:67:GLN:HB2	2.11	0.50
1:G:95:TYR:CD1	1:H:51:MET:HE1	2.47	0.50
1:C:109:LEU:N	1:C:110:PRO:HD2	2.26	0.50
1:M:161:VAL:HG21	1:M:188:ILE:HB	1.94	0.50
1:P:52:PHE:O	1:P:53:GLN:HG2	2.12	0.50
1:K:95:TYR:CE1	1:L:51:MET:HE1	2.45	0.50
1:H:138:LYS:CD	4:H:2124:HOH:O	2.60	0.50
1:P:66:VAL:CG1	1:P:67:GLN:N	2.74	0.50
1:F:52:PHE:O	1:F:53:GLN:HG2	2.12	0.49
1:O:161:VAL:HG21	1:O:188:ILE:HB	1.94	0.49
1:I:69:ARG:HE	1:J:69:ARG:NE	2.11	0.49
1:D:145:GLN:HE22	1:D:151:ASN:HB2	1.76	0.49
1:L:17:GLU:HG2	1:L:166:TYR:OH	2.12	0.49
1:L:15:ARG:HD2	2:L:1223:GSH:HG13	1.93	0.49
1:P:22:LEU:HD22	1:P:155[B]:ARG:HG3	1.94	0.49
2:A:1223:GSH:HB22	3:A:1224:ASD:H4	1.94	0.49
1:H:50:LEU:HB2	1:H:53:GLN:HA	1.94	0.49
1:I:52:PHE:C	1:I:53:GLN:HG2	2.37	0.49
1:L:129:LYS:HD2	1:L:174:LEU:HD22	1.95	0.49
1:O:187:ARG:HD2	4:O:2125:HOH:O	2.13	0.49
1:C:52:PHE:O	1:C:53:GLN:HG2	2.13	0.49
1:L:136:PHE:HA	1:L:139:VAL:CG1	2.43	0.49
1:M:136:PHE:O	1:M:139:VAL:HG12	2.13	0.49
1:C:52:PHE:O	1:D:131:ARG:HD2	2.13	0.49
1:C:199:GLN:NE2	4:C:2156:HOH:O	2.44	0.49
1:N:125:LYS:HE2	1:N:171:ASP:HB2	1.94	0.49
1:A:131:ARG:HD3	1:B:53:GLN:OE1	2.13	0.48
1:I:17:GLU:HG2	1:I:166:TYR:OH	2.12	0.48
1:A:45:ARG:NH2	2:A:1223:GSH:O31	2.46	0.48
1:H:127:LYS:O	1:H:131:ARG:HB3	2.13	0.48
1:I:53:GLN:HG3	1:J:131:ARG:HH11	1.78	0.48
1:K:66[B]:VAL:HG12	4:K:2071:HOH:O	2.13	0.48
1:C:160:LEU:O	1:C:164:LEU:HG	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:CZ	1:A:12:GLY:HA3	2.49	0.48
1:H:105:MET:HE2	4:H:2038:HOH:O	2.14	0.48
1:I:94:MET:HE2	1:J:51:MET:HB3	1.95	0.47
1:P:66:VAL:CG1	4:P:2044:HOH:O	2.62	0.47
1:A:187:ARG:NH2	4:A:2179:HOH:O	2.44	0.47
1:B:109:LEU:N	1:B:110:PRO:HD2	2.30	0.47
2:D:1223:GSH:HB22	3:D:1224:ASD:H4	1.95	0.47
1:O:94:MET:HE2	1:P:51:MET:HB2	1.95	0.47
2:N:1223:GSH:HA1	4:N:2011:HOH:O	2.14	0.47
1:M:131:ARG:HD2	1:N:53:GLN:CG	2.44	0.47
1:N:94:MET:HE2	4:N:2039:HOH:O	2.14	0.47
1:B:10:PHE:CZ	3:B:1224:ASD:H152	2.50	0.47
1:K:4:LYS:HE2	1:K:29:GLU:HB3	1.96	0.47
1:A:160:LEU:O	1:A:164:LEU:HG	2.15	0.47
1:E:86:ILE:HG12	1:F:74:TYR:CE1	2.49	0.47
1:I:131:ARG:HD3	1:J:53:GLN:OE1	2.15	0.47
1:D:145:GLN:NE2	1:D:151:ASN:HB2	2.29	0.47
1:N:109:LEU:N	1:N:110:PRO:HD2	2.30	0.46
1:O:51:MET:HE1	1:P:95:TYR:CD1	2.50	0.46
1:P:161:VAL:HG21	1:P:188:ILE:HB	1.97	0.46
1:J:45:ARG:HD2	4:J:2035:HOH:O	2.15	0.46
1:M:12:GLY:C	1:M:205:LYS:HG2	2.41	0.46
1:H:6:LYS:HE2	1:H:33:LYS:HB2	1.98	0.46
1:J:32:GLU:OE2	1:J:205:LYS:NZ	2.48	0.46
1:G:53:GLN:OE1	1:H:131:ARG:HD3	2.16	0.46
1:G:66:VAL:O	1:G:67:GLN:HB2	2.15	0.46
1:I:13:ARG:HD3	1:I:206:PRO:O	2.16	0.46
1:I:94:MET:HE3	1:J:66:VAL:H	1.81	0.46
1:L:160:LEU:O	1:L:164:LEU:HG	2.15	0.46
1:N:161:VAL:HG21	1:N:188:ILE:HB	1.97	0.46
1:K:110:PRO:HG3	4:K:2193:HOH:O	2.16	0.46
1:P:49:SER:HB3	1:P:57:MET:HE2	1.97	0.46
1:E:66:VAL:O	1:E:67:GLN:HB2	2.16	0.46
1:J:102:LEU:HD23	1:J:163:LEU:HD21	1.97	0.46
1:K:63:MET:HE1	1:K:74:TYR:CE1	2.50	0.46
1:F:161:VAL:HG21	1:F:188:ILE:HB	1.98	0.46
1:M:136:PHE:O	1:M:139:VAL:CG1	2.64	0.46
1:O:6:LYS:HE2	1:O:8:HIS:HE1	1.78	0.46
1:O:52:PHE:O	1:P:131:ARG:HD2	2.16	0.46
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.98	0.45
1:K:131:ARG:HD2	1:L:52:PHE:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:O	1:A:67:GLN:HB2	2.15	0.45
1:D:11:ASN:C	1:D:11:ASN:HD22	2.23	0.45
1:D:76:ALA:CB	1:D:155:ARG:HD2	2.46	0.45
1:I:74:TYR:CD1	1:J:86:ILE:HG12	2.51	0.45
1:J:82:TYR:O	1:J:89:ARG:HG2	2.16	0.45
1:P:52:PHE:C	1:P:53:GLN:HG2	2.42	0.45
1:B:216:ALA:HB2	3:B:1224:ASD:H151	1.97	0.45
1:C:176:SER:HA	1:C:182:LYS:HE3	1.98	0.45
1:J:69:ARG:NH1	1:J:97:GLU:OE2	2.49	0.45
1:N:182:LYS:HE2	4:N:2174:HOH:O	2.16	0.45
1:P:66:VAL:CG1	4:P:2050:HOH:O	2.61	0.45
1:D:109:LEU:N	1:D:110:PRO:HD2	2.32	0.45
1:E:131:ARG:HD2	1:F:52:PHE:O	2.17	0.45
2:F:1223:GSH:CB2	3:F:1224:ASD:H4	2.47	0.45
1:H:17:GLU:HG2	1:H:166:TYR:OH	2.16	0.45
1:M:53:GLN:HB3	4:M:2050:HOH:O	2.16	0.45
1:C:66:VAL:O	1:C:67:GLN:HB2	2.16	0.45
1:J:115:GLU:HB2	4:J:2104:HOH:O	2.17	0.45
1:K:20:ARG:CZ	1:K:205:LYS:HD3	2.47	0.45
1:M:131:ARG:HD2	1:N:52:PHE:O	2.17	0.45
1:P:213:LEU:HA	3:P:1224:ASD:H161	1.99	0.45
1:C:109:LEU:HD11	1:C:121:ILE:HG13	1.99	0.45
1:J:176:SER:HA	1:J:182:LYS:HE2	1.98	0.45
1:K:45:ARG:HB3	4:K:2058:HOH:O	2.17	0.45
1:E:161:VAL:HG21	1:E:188:ILE:HB	1.98	0.44
1:L:63:MET:HE1	1:L:74:TYR:CE1	2.52	0.44
1:O:63:MET:HE1	1:O:74:TYR:CZ	2.53	0.44
1:B:105:MET:HE2	1:B:124:ILE:HG12	2.00	0.44
1:E:127:LYS:O	1:E:131:ARG:HB3	2.17	0.44
1:H:84:LYS:HE3	1:H:88:GLU:OE2	2.18	0.44
1:I:102:LEU:HD23	1:I:163:LEU:HD21	1.99	0.44
1:O:65:LEU:HD21	1:P:90:ALA:HB1	2.00	0.44
1:H:52:PHE:O	1:H:53:GLN:HG2	2.17	0.44
1:B:6:LYS:HD2	1:B:33:LYS:HB2	1.99	0.44
1:F:129:LYS:HD2	1:F:174:LEU:CD2	2.48	0.44
1:K:66[B]:VAL:CG1	1:K:67:GLN:N	2.79	0.44
1:N:99:MET:HG3	1:N:136:PHE:CZ	2.53	0.44
1:G:45:ARG:NH2	2:G:1223:GSH:O32	2.50	0.44
1:H:155:ARG:CD	4:H:2144:HOH:O	2.64	0.44
1:O:127:LYS:HD3	4:O:2111:HOH:O	2.16	0.44
1:A:115:GLU:CD	1:A:115:GLU:H	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:LEU:HD23	1:F:163:LEU:HD21	2.00	0.44
1:N:19:ILE:HD13	1:N:71:ILE:HG21	2.00	0.44
1:O:33:LYS:HE3	4:O:2025:HOH:O	2.18	0.44
1:C:32:GLU:OE2	1:C:205:LYS:NZ	2.50	0.44
1:H:161:VAL:HG21	1:H:188:ILE:HB	2.00	0.44
1:N:203:PRO:O	1:N:205:LYS:HD2	2.18	0.44
1:M:17:GLU:HG2	1:M:166:TYR:OH	2.17	0.44
1:G:84:LYS:HG2	1:G:88:GLU:CD	2.43	0.43
1:H:82:TYR:O	1:H:89:ARG:HG2	2.17	0.43
1:K:163:LEU:O	1:K:167:VAL:HG23	2.18	0.43
1:B:10:PHE:CE1	3:B:1224:ASD:H72	2.54	0.43
1:B:168:GLU:HG3	4:B:2167:HOH:O	2.17	0.43
1:P:73:ASN:HA	1:P:155[A]:ARG:NH1	2.34	0.43
1:C:45:ARG:HG2	1:C:53:GLN:HB2	2.01	0.43
1:C:50:LEU:CB	1:C:53:GLN:HA	2.47	0.43
1:D:115:GLU:H	1:D:115:GLU:HG3	1.28	0.43
1:G:74:TYR:CD1	1:H:86:ILE:HG12	2.53	0.43
1:A:131:ARG:CD	1:B:53:GLN:OE1	2.66	0.43
1:G:102:LEU:HD23	1:G:163:LEU:HD21	1.99	0.43
1:F:67:GLN:OE1	2:F:1223:GSH:N1	2.47	0.43
1:A:94:MET:HE2	1:B:51:MET:SD	2.58	0.43
1:B:160:LEU:O	1:B:164:LEU:HG	2.18	0.43
1:H:168:GLU:HG3	4:H:2157:HOH:O	2.19	0.43
1:I:21:TRP:NE1	1:I:162:GLU:HG3	2.33	0.43
1:N:49:SER:HB3	1:N:57:MET:HE2	2.00	0.43
1:K:160:LEU:O	1:K:164:LEU:HG	2.18	0.43
1:M:4:LYS:N	4:M:2001:HOH:O	2.51	0.43
1:C:161:VAL:HG21	1:C:188:ILE:HB	2.01	0.43
1:K:45:ARG:NH2	2:K:1223:GSH:O32	2.52	0.43
1:B:113:ARG:O	1:B:116:GLU:HG2	2.18	0.42
1:B:204:ARG:NH2	4:B:2200:HOH:O	2.35	0.42
1:E:53:GLN:HG2	4:E:2047:HOH:O	2.18	0.42
1:C:204:ARG:CZ	1:O:200:PRO:HG3	2.48	0.42
1:F:53:GLN:HB3	4:F:2053:HOH:O	2.19	0.42
1:O:129:LYS:HD2	1:O:174:LEU:HD23	2.00	0.42
1:A:52:PHE:O	1:A:53:GLN:HG2	2.18	0.42
1:E:155:ARG:HB2	4:E:2140:HOH:O	2.20	0.42
1:M:109:LEU:N	1:M:110:PRO:HD2	2.34	0.42
1:N:66[B]:VAL:HG12	1:N:67:GLN:H	1.83	0.42
1:H:29:GLU:HG2	4:H:2009:HOH:O	2.18	0.42
1:M:20:ARG:CZ	1:M:205:LYS:HD3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:53:GLN:HE21	1:N:53:GLN:HB3	1.68	0.42
1:B:216:ALA:CB	3:B:1224:ASD:H151	2.50	0.42
1:J:49:SER:HB3	1:J:57:MET:HE2	2.02	0.42
1:M:52:PHE:O	1:M:53:GLN:HG2	2.19	0.42
1:D:17:GLU:HG2	1:D:166:TYR:OH	2.20	0.42
1:H:84:LYS:NZ	4:H:2083:HOH:O	2.53	0.42
1:M:53:GLN:HB3	1:M:53:GLN:HE21	1.59	0.42
1:B:9:TYR:CE2	1:B:10:PHE:CE1	3.08	0.41
1:B:171:ASP:HB3	1:B:174:LEU:HG	2.01	0.41
1:H:179:PRO:HA	1:H:182:LYS:HD2	2.01	0.41
1:J:113:ARG:HB2	1:J:116:GLU:HG2	2.03	0.41
1:K:66[B]:VAL:HG13	4:K:2061:HOH:O	2.19	0.41
1:B:161:VAL:HG21	1:B:188:ILE:HB	2.01	0.41
1:B:167:VAL:HG13	1:B:174:LEU:HD12	2.02	0.41
1:F:50:LEU:HB2	1:F:53:GLN:HA	2.03	0.41
1:H:53:GLN:HB3	1:H:53:GLN:HE21	1.58	0.41
1:J:8:HIS:CE1	1:J:33:LYS:HD3	2.55	0.41
1:P:176:SER:HA	1:P:182:LYS:HE3	2.01	0.41
1:D:4:LYS:HE2	1:D:29:GLU:HB3	2.02	0.41
1:I:74:TYR:CE1	1:J:86:ILE:HG12	2.55	0.41
1:E:51:MET:SD	1:F:94:MET:HE2	2.60	0.41
1:F:52:PHE:C	1:F:53:GLN:HG2	2.45	0.41
1:O:208:ALA:HB3	4:O:2187:HOH:O	2.21	0.41
1:H:120:LYS:HA	1:H:120:LYS:HD3	1.84	0.41
1:I:86:ILE:HG12	1:J:74:TYR:CD1	2.56	0.41
1:L:35:ILE:HD11	1:L:55:VAL:HG11	2.02	0.41
1:M:66:VAL:O	1:M:67:GLN:HB2	2.20	0.41
1:C:53:GLN:NE2	1:D:131:ARG:HD3	2.35	0.41
1:C:65:LEU:HD21	1:D:90:ALA:HB1	2.02	0.41
1:I:187:ARG:HD2	4:I:2143:HOH:O	2.20	0.41
1:B:82:TYR:O	1:B:89:ARG:HG2	2.20	0.41
1:G:15:ARG:HD2	2:G:1223:GSH:HG13	2.02	0.41
1:I:10:PHE:CE2	1:I:12:GLY:HA3	2.55	0.41
1:B:217:ARG:NH2	4:B:2211:HOH:O	2.54	0.41
1:F:17:GLU:OE1	1:F:205:LYS:HB2	2.21	0.41
1:B:129:LYS:HD2	1:B:174:LEU:HD22	2.03	0.41
1:F:18:PRO:HB3	4:F:2156:HOH:O	2.21	0.41
1:N:138:LYS:HA	1:N:141[B]:GLN:HG2	2.03	0.41
1:O:115:GLU:H	1:O:115:GLU:HG3	1.21	0.41
1:J:15:ARG:HD2	2:J:1223:GSH:HG13	2.03	0.41
1:K:53:GLN:NE2	4:K:2058:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:SER:HB3	1:L:57:MET:HE2	2.03	0.41
1:M:136:PHE:HA	1:M:139:VAL:HG12	2.03	0.41
1:A:4:LYS:HE2	1:A:29:GLU:HB3	2.03	0.40
1:G:52:PHE:O	1:H:131:ARG:HD2	2.21	0.40
1:M:110:PRO:HD3	4:M:2044:HOH:O	2.21	0.40
1:P:152:LYS:HE2	4:P:2144:HOH:O	2.21	0.40
1:B:85:ASP:O	1:B:89:ARG:HG3	2.21	0.40
1:I:9:TYR:CE2	1:I:10:PHE:CE1	3.10	0.40
1:C:90:ALA:HA	4:D:2066:HOH:O	2.22	0.40
1:N:113:ARG:O	1:N:116:GLU:HG2	2.20	0.40
1:P:9:TYR:CE2	1:P:10:PHE:CE1	3.09	0.40
1:K:63:MET:HE2	1:L:87:LYS:HE2	2.03	0.40
1:M:76:ALA:CB	1:M:155:ARG:HD2	2.52	0.40
1:O:74:TYR:CD1	1:P:86:ILE:HG12	2.57	0.40

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%)	24	14
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	14
1	P	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	14
All	All	3520/3552 (99%)	3428 (97%)	89 (2%)	3 (0%)	48	34

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%)	187 (97%)	5 (3%)	40	28
1	B	193/191 (101%)	189 (98%)	4 (2%)	47	36
1	C	193/191 (101%)	187 (97%)	6 (3%)	35	23
1	D	192/191 (100%)	187 (97%)	5 (3%)	40	28
1	E	192/191 (100%)	186 (97%)	6 (3%)	35	23
1	F	193/191 (101%)	188 (97%)	5 (3%)	40	28
1	G	193/191 (101%)	187 (97%)	6 (3%)	35	23
1	H	193/191 (101%)	185 (96%)	8 (4%)	27	15
1	I	193/191 (101%)	186 (96%)	7 (4%)	31	18
1	J	192/191 (100%)	190 (99%)	2 (1%)	68	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	194/191 (102%)	186 (96%)	8 (4%)	27	15
1	L	195/191 (102%)	186 (95%)	9 (5%)	24	12
1	M	191/191 (100%)	183 (96%)	8 (4%)	26	14
1	N	195/191 (102%)	186 (95%)	9 (5%)	24	12
1	O	194/191 (102%)	187 (96%)	7 (4%)	31	18
1	P	193/191 (101%)	187 (97%)	6 (3%)	35	23
All	All	3088/3056 (101%)	2987 (97%)	101 (3%)	34	21

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	115	GLU
1	A	131	ARG
1	A	139	VAL
1	A	221	ARG
1	B	6	LYS
1	B	7	LEU
1	B	131	ARG
1	B	176	SER
1	C	6	LYS
1	C	53	GLN
1	C	66	VAL
1	C	131	ARG
1	C	199	GLN
1	C	221	ARG
1	D	7	LEU
1	D	115	GLU
1	D	131	ARG
1	D	152	LYS
1	D	205	LYS
1	E	6	LYS
1	E	7	LEU
1	E	66	VAL
1	E	115	GLU
1	E	131	ARG
1	E	139	VAL
1	F	6	LYS
1	F	7	LEU
1	F	66	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	115	GLU
1	F	131	ARG
1	G	6	LYS
1	G	7	LEU
1	G	66	VAL
1	G	115	GLU
1	G	131	ARG
1	G	139	VAL
1	H	7	LEU
1	H	53	GLN
1	H	66	VAL
1	H	84	LYS
1	H	118	ASP
1	H	120	LYS
1	H	131	ARG
1	H	199	GLN
1	I	7	LEU
1	I	13	ARG
1	I	53	GLN
1	I	115	GLU
1	I	131	ARG
1	I	139	VAL
1	I	205	LYS
1	J	131	ARG
1	J	199	GLN
1	K	6	LYS
1	K	7	LEU
1	K	84	LYS
1	K	115	GLU
1	K	131	ARG
1	K	139	VAL
1	K	205	LYS
1	K	211	LYS
1	L	6	LYS
1	L	10	PHE
1	L	115	GLU
1	L	120[A]	LYS
1	L	120[B]	LYS
1	L	131	ARG
1	L	139	VAL
1	L	199	GLN
1	L	214	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	7	LEU
1	M	47	ASP
1	M	49	SER
1	M	53	GLN
1	M	84	LYS
1	M	115	GLU
1	M	131	ARG
1	M	214	GLU
1	N	7	LEU
1	N	53	GLN
1	N	115	GLU
1	N	120[A]	LYS
1	N	120[B]	LYS
1	N	139	VAL
1	N	141[A]	GLN
1	N	141[B]	GLN
1	N	199	GLN
1	O	6	LYS
1	O	7	LEU
1	O	84	LYS
1	O	115	GLU
1	O	126[A]	GLU
1	O	126[B]	GLU
1	O	131	ARG
1	P	6	LYS
1	P	53	GLN
1	P	120	LYS
1	P	131	ARG
1	P	139	VAL
1	P	199	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	46	ASN
1	A	54	GLN
1	A	145	GLN
1	B	80	ASN
1	B	141	GLN
1	C	46	ASN
1	C	103	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	151	ASN
1	C	199	GLN
1	D	11	ASN
1	D	46	ASN
1	D	80	ASN
1	D	145	GLN
1	D	151	ASN
1	E	54	GLN
1	E	80	ASN
1	E	145	GLN
1	F	46	ASN
1	F	80	ASN
1	F	145	GLN
1	G	46	ASN
1	G	54	GLN
1	G	145	GLN
1	G	190	ASN
1	H	53	GLN
1	H	54	GLN
1	H	80	ASN
1	H	141	GLN
1	H	145	GLN
1	H	151	ASN
1	H	199	GLN
1	I	46	ASN
1	I	80	ASN
1	I	141	GLN
1	J	46	ASN
1	J	54	GLN
1	J	80	ASN
1	K	46	ASN
1	K	54	GLN
1	K	80	ASN
1	K	141	GLN
1	L	46	ASN
1	M	11	ASN
1	M	46	ASN
1	M	177	ASN
1	M	190	ASN
1	O	46	ASN
1	P	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	GSH	K	1223	-	18,19,19	3.11	2 (11%)	21,24,24	1.14	1 (4%)
2	GSH	I	1223	-	18,19,19	3.18	2 (11%)	21,24,24	1.26	3 (14%)
2	GSH	B	1223	-	18,19,19	3.30	2 (11%)	21,24,24	1.16	2 (9%)
2	GSH	M	1223	-	18,19,19	3.24	2 (11%)	21,24,24	1.33	3 (14%)
3	ASD	G	1224	-	24,24,24	0.71	0	39,39,39	1.64	7 (17%)
2	GSH	D	1223	-	18,19,19	3.20	2 (11%)	21,24,24	1.00	2 (9%)
2	GSH	N	1223	-	18,19,19	3.24	2 (11%)	21,24,24	1.15	3 (14%)
3	ASD	P	1224	-	24,24,24	0.92	1 (4%)	39,39,39	1.61	3 (7%)
2	GSH	F	1223	-	18,19,19	3.08	3 (16%)	21,24,24	1.17	3 (14%)
3	ASD	B	1224	-	24,24,24	0.59	0	39,39,39	1.64	7 (17%)
3	ASD	E	1224	-	24,24,24	1.00	1 (4%)	39,39,39	1.89	7 (17%)
3	ASD	L	1224	-	24,24,24	0.61	0	39,39,39	1.48	8 (20%)
2	GSH	G	1223	-	18,19,19	3.13	3 (16%)	21,24,24	1.35	3 (14%)
2	GSH	E	1223	-	18,19,19	3.21	2 (11%)	21,24,24	0.95	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GSH	P	1223	-	18,19,19	3.16	2 (11%)	21,24,24	1.23	3 (14%)
2	GSH	A	1223	-	18,19,19	3.15	2 (11%)	21,24,24	1.22	2 (9%)
2	GSH	J	1223	-	18,19,19	3.25	2 (11%)	21,24,24	1.16	3 (14%)
2	GSH	O	1223	-	18,19,19	3.21	2 (11%)	21,24,24	1.23	3 (14%)
3	ASD	F	1224	-	24,24,24	1.03	1 (4%)	39,39,39	1.94	9 (23%)
2	GSH	L	1223	-	18,19,19	3.23	3 (16%)	21,24,24	1.29	3 (14%)
3	ASD	H	1224	-	24,24,24	0.63	0	39,39,39	1.59	7 (17%)
3	ASD	K	1224	-	24,24,24	0.64	0	39,39,39	1.53	7 (17%)
3	ASD	A	1224	-	24,24,24	0.60	0	39,39,39	1.56	7 (17%)
2	GSH	C	1223	-	18,19,19	3.23	2 (11%)	21,24,24	1.25	5 (23%)
3	ASD	I	1224	-	24,24,24	0.60	0	39,39,39	1.58	7 (17%)
2	GSH	H	1223	-	18,19,19	3.15	2 (11%)	21,24,24	1.28	3 (14%)
3	ASD	D	1224	-	24,24,24	1.60	3 (12%)	39,39,39	2.01	7 (17%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	O	1223	-	1/1/6/8	8/24/24/24	-
3	ASD	F	1224	-	-	-	0/4/4/4
2	GSH	L	1223	-	1/1/6/8	6/24/24/24	-
3	ASD	H	1224	-	-	-	0/4/4/4
3	ASD	K	1224	-	-	-	0/4/4/4
3	ASD	A	1224	-	-	-	0/4/4/4
2	GSH	C	1223	-	1/1/6/8	7/24/24/24	-
3	ASD	I	1224	-	-	-	0/4/4/4
2	GSH	H	1223	-	1/1/6/8	4/24/24/24	-
3	ASD	D	1224	-	-	-	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1223	GSH	O2-C2	9.92	1.42	1.23
2	J	1223	GSH	O2-C2	9.84	1.42	1.23
2	L	1223	GSH	O2-C2	9.72	1.42	1.23
2	C	1223	GSH	O2-C2	9.72	1.42	1.23
2	N	1223	GSH	O2-C2	9.62	1.41	1.23
2	M	1223	GSH	O2-C2	9.47	1.41	1.23
2	A	1223	GSH	O2-C2	9.42	1.41	1.23
2	E	1223	GSH	O2-C2	9.38	1.41	1.23
2	I	1223	GSH	O2-C2	9.38	1.41	1.23
2	K	1223	GSH	O2-C2	9.37	1.41	1.23
2	D	1223	GSH	O2-C2	9.36	1.41	1.23
2	O	1223	GSH	O2-C2	9.35	1.41	1.23
2	B	1223	GSH	OE1-CD1	9.35	1.41	1.23
2	G	1223	GSH	O2-C2	9.33	1.41	1.23
2	P	1223	GSH	O2-C2	9.32	1.41	1.23
2	E	1223	GSH	OE1-CD1	9.31	1.41	1.23
2	O	1223	GSH	OE1-CD1	9.30	1.41	1.23
2	D	1223	GSH	OE1-CD1	9.28	1.41	1.23
2	M	1223	GSH	OE1-CD1	9.25	1.41	1.23
2	H	1223	GSH	O2-C2	9.21	1.41	1.23
2	H	1223	GSH	OE1-CD1	9.21	1.41	1.23
2	I	1223	GSH	OE1-CD1	9.16	1.41	1.23
2	J	1223	GSH	OE1-CD1	9.13	1.41	1.23
2	C	1223	GSH	OE1-CD1	9.13	1.41	1.23
2	N	1223	GSH	OE1-CD1	9.10	1.41	1.23
2	L	1223	GSH	OE1-CD1	9.09	1.41	1.23
2	P	1223	GSH	OE1-CD1	9.09	1.41	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1223	GSH	O2-C2	8.94	1.40	1.23
2	F	1223	GSH	OE1-CD1	8.83	1.40	1.23
2	G	1223	GSH	OE1-CD1	8.79	1.40	1.23
2	A	1223	GSH	OE1-CD1	8.79	1.40	1.23
2	K	1223	GSH	OE1-CD1	8.65	1.40	1.23
3	D	1224	ASD	C15-C16	5.70	1.66	1.53
3	D	1224	ASD	C16-C17	3.99	1.58	1.51
3	F	1224	ASD	C15-C16	3.55	1.61	1.53
3	E	1224	ASD	C15-C16	3.18	1.60	1.53
3	D	1224	ASD	O2-C17	2.50	1.25	1.21
3	P	1224	ASD	C15-C16	2.48	1.58	1.53
2	F	1223	GSH	O11-C1	-2.14	1.23	1.30
2	L	1223	GSH	O11-C1	-2.12	1.23	1.30
2	G	1223	GSH	O11-C1	-2.09	1.24	1.30

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1224	ASD	C15-C16-C17	-8.79	97.22	105.70
3	E	1224	ASD	C15-C14-C13	6.09	109.31	104.08
3	F	1224	ASD	C15-C14-C13	5.86	109.12	104.08
3	D	1224	ASD	C16-C17-C13	5.30	113.83	108.56
3	P	1224	ASD	C15-C16-C17	-5.17	100.71	105.70
3	E	1224	ASD	C15-C16-C17	-4.93	100.94	105.70
3	G	1224	ASD	C15-C14-C13	4.85	108.25	104.08
3	P	1224	ASD	C16-C17-C13	4.66	113.20	108.56
3	H	1224	ASD	C16-C17-C13	4.50	113.04	108.56
3	B	1224	ASD	C15-C14-C13	4.34	107.81	104.08
3	E	1224	ASD	C16-C17-C13	4.29	112.83	108.56
3	G	1224	ASD	C16-C17-C13	4.12	112.66	108.56
3	B	1224	ASD	C16-C17-C13	4.09	112.63	108.56
3	F	1224	ASD	C15-C16-C17	-4.02	101.82	105.70
3	L	1224	ASD	C16-C17-C13	3.99	112.53	108.56
3	F	1224	ASD	C16-C17-C13	3.83	112.38	108.56
3	I	1224	ASD	C16-C17-C13	3.82	112.37	108.56
3	F	1224	ASD	C7-C8-C9	3.80	115.08	110.52
3	I	1224	ASD	C15-C14-C13	3.75	107.30	104.08
3	A	1224	ASD	C6-C5-C4	-3.75	114.86	120.86
3	K	1224	ASD	C16-C17-C13	3.66	112.20	108.56
3	A	1224	ASD	C16-C17-C13	3.61	112.16	108.56
3	H	1224	ASD	C15-C16-C17	-3.40	102.42	105.70
3	G	1224	ASD	C15-C16-C17	-3.38	102.43	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1224	ASD	C6-C5-C10	3.32	122.61	116.76
3	K	1224	ASD	C6-C5-C4	-3.24	115.69	120.86
2	G	1223	GSH	CG1-CB1-CA1	-3.23	106.45	113.86
3	B	1224	ASD	C14-C13-C17	-3.22	96.83	100.61
3	K	1224	ASD	C15-C14-C13	3.19	106.82	104.08
3	B	1224	ASD	O2-C17-C16	-3.16	121.90	125.75
3	A	1224	ASD	C14-C13-C17	-3.15	96.91	100.61
3	A	1224	ASD	C15-C14-C13	3.13	106.77	104.08
3	H	1224	ASD	C7-C8-C9	3.10	114.23	110.52
2	L	1223	GSH	O11-C1-O12	-3.07	117.12	124.08
2	P	1223	GSH	CB1-CG1-CD1	-2.99	106.39	113.06
3	K	1224	ASD	C14-C13-C17	-2.97	97.12	100.61
3	F	1224	ASD	C6-C5-C10	2.94	121.95	116.76
2	B	1223	GSH	O11-C1-O12	-2.91	117.48	124.08
3	I	1224	ASD	O2-C17-C16	-2.89	122.24	125.75
3	B	1224	ASD	C15-C16-C17	-2.88	102.92	105.70
3	I	1224	ASD	C15-C16-C17	-2.83	102.97	105.70
3	G	1224	ASD	C14-C13-C17	-2.78	97.35	100.61
3	A	1224	ASD	C15-C16-C17	-2.77	103.02	105.70
3	K	1224	ASD	C15-C16-C17	-2.77	103.03	105.70
3	F	1224	ASD	C5-C4-C3	-2.76	119.41	123.67
3	K	1224	ASD	O2-C17-C16	-2.75	122.41	125.75
3	L	1224	ASD	C15-C16-C17	-2.74	103.06	105.70
3	D	1224	ASD	C6-C5-C4	-2.73	116.50	120.86
2	F	1223	GSH	O11-C1-O12	-2.70	117.95	124.08
2	C	1223	GSH	O11-C1-O12	-2.67	118.03	124.08
2	K	1223	GSH	CG1-CB1-CA1	-2.66	107.75	113.86
3	F	1224	ASD	C13-C14-C8	-2.64	110.35	113.13
3	I	1224	ASD	C6-C5-C4	-2.64	116.64	120.86
2	O	1223	GSH	O11-C1-O12	-2.64	118.09	124.08
3	B	1224	ASD	C6-C5-C4	-2.61	116.68	120.86
3	H	1224	ASD	C15-C14-C13	2.60	106.31	104.08
3	G	1224	ASD	C6-C5-C4	-2.59	116.72	120.86
2	A	1223	GSH	O11-C1-O12	-2.58	118.22	124.08
2	M	1223	GSH	O11-C1-O12	-2.57	118.24	124.08
3	H	1224	ASD	C9-C8-C14	-2.55	105.75	109.09
3	H	1224	ASD	O2-C17-C16	-2.55	122.65	125.75
2	I	1223	GSH	CA2-CB2-SG2	2.54	117.02	114.16
3	A	1224	ASD	O2-C17-C16	-2.54	122.66	125.75
2	H	1223	GSH	O31-C3-CA3	2.52	122.40	112.81
3	L	1224	ASD	C15-C14-C13	2.49	106.22	104.08
2	G	1223	GSH	O11-C1-O12	-2.49	118.43	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1223	GSH	CB2-CA2-C2	2.46	114.84	109.50
2	J	1223	GSH	O11-C1-O12	-2.45	118.52	124.08
3	F	1224	ASD	C9-C8-C14	-2.44	105.91	109.09
2	H	1223	GSH	O11-C1-O12	-2.43	118.57	124.08
2	L	1223	GSH	O31-C3-CA3	2.42	122.03	112.81
2	P	1223	GSH	O11-C1-O12	-2.41	118.61	124.08
3	E	1224	ASD	O2-C17-C16	-2.41	122.82	125.75
3	L	1224	ASD	C7-C8-C9	2.38	113.37	110.52
2	H	1223	GSH	CB1-CA1-C1	2.37	116.72	110.45
3	K	1224	ASD	C6-C5-C10	2.37	120.94	116.76
2	I	1223	GSH	O11-C1-O12	-2.37	118.71	124.08
2	M	1223	GSH	O31-C3-CA3	2.36	121.80	112.81
3	L	1224	ASD	C14-C13-C17	-2.36	97.84	100.61
3	L	1224	ASD	O2-C17-C16	-2.36	122.88	125.75
3	G	1224	ASD	C6-C5-C10	2.35	120.90	116.76
2	J	1223	GSH	O31-C3-CA3	2.34	121.71	112.81
2	B	1223	GSH	O31-C3-CA3	2.33	121.67	112.81
3	I	1224	ASD	C1-C10-C5	2.33	112.76	108.74
2	C	1223	GSH	O31-C3-CA3	2.32	121.63	112.81
3	D	1224	ASD	O2-C17-C16	-2.32	122.93	125.75
3	G	1224	ASD	O2-C17-C16	-2.32	122.93	125.75
2	N	1223	GSH	O31-C3-CA3	2.30	121.56	112.81
3	D	1224	ASD	C16-C15-C14	-2.29	99.52	103.00
2	L	1223	GSH	CG1-CB1-CA1	-2.29	108.61	113.86
2	E	1223	GSH	O11-C1-O12	-2.28	118.91	124.08
2	F	1223	GSH	CG1-CB1-CA1	-2.27	108.64	113.86
2	I	1223	GSH	O31-C3-CA3	2.26	121.42	112.81
2	J	1223	GSH	CB1-CA1-C1	2.26	116.44	110.45
3	I	1224	ASD	C14-C13-C17	-2.24	97.98	100.61
2	E	1223	GSH	O31-C3-CA3	2.24	121.33	112.81
2	G	1223	GSH	O31-C3-CA3	2.23	121.29	112.81
2	M	1223	GSH	CG1-CB1-CA1	-2.22	108.78	113.86
2	D	1223	GSH	O11-C1-O12	-2.21	119.06	124.08
3	L	1224	ASD	C9-C8-C14	-2.21	106.20	109.09
3	H	1224	ASD	C14-C13-C17	-2.21	98.02	100.61
2	O	1223	GSH	O31-C3-CA3	2.20	121.17	112.81
2	D	1223	GSH	O31-C3-CA3	2.19	121.14	112.81
2	P	1223	GSH	O31-C3-CA3	2.16	121.02	112.81
3	F	1224	ASD	C6-C5-C4	-2.14	117.44	120.86
3	D	1224	ASD	C6-C5-C10	2.13	120.52	116.76
2	O	1223	GSH	CB2-CA2-C2	2.13	114.14	109.50
3	E	1224	ASD	C9-C10-C5	-2.12	106.56	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1224	ASD	C6-C5-C4	-2.11	117.48	120.86
3	P	1224	ASD	O2-C17-C16	-2.11	123.18	125.75
2	F	1223	GSH	O31-C3-CA3	2.11	120.84	112.81
3	B	1224	ASD	C6-C5-C10	2.10	120.47	116.76
3	D	1224	ASD	O2-C17-C13	-2.10	123.22	125.98
2	C	1223	GSH	O31-C3-O32	-2.07	118.01	123.33
2	C	1223	GSH	CG1-CB1-CA1	-2.05	109.16	113.86
3	E	1224	ASD	C7-C8-C9	2.05	112.97	110.52
3	L	1224	ASD	C6-C5-C4	-2.05	117.59	120.86
2	A	1223	GSH	O31-C3-CA3	2.04	120.56	112.81
2	C	1223	GSH	CB2-CA2-C2	2.00	113.86	109.50
2	N	1223	GSH	O11-C1-O12	-2.00	119.54	124.08

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1223	GSH	CA1
2	B	1223	GSH	CA1
2	C	1223	GSH	CA1
2	D	1223	GSH	CA1
2	E	1223	GSH	CA1
2	F	1223	GSH	CA1
2	G	1223	GSH	CA1
2	H	1223	GSH	CA1
2	I	1223	GSH	CA1
2	J	1223	GSH	CA1
2	K	1223	GSH	CA1
2	L	1223	GSH	CA1
2	M	1223	GSH	CA1
2	N	1223	GSH	CA1
2	O	1223	GSH	CA1
2	P	1223	GSH	CA1

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1223	GSH	O12-C1-CA1-N1
2	A	1223	GSH	CG1-CD1-N2-CA2
2	F	1223	GSH	O12-C1-CA1-N1
2	G	1223	GSH	O12-C1-CA1-N1
2	H	1223	GSH	O12-C1-CA1-N1
2	I	1223	GSH	CG1-CD1-N2-CA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	1223	GSH	OE1-CD1-N2-CA2
2	J	1223	GSH	O12-C1-CA1-N1
2	K	1223	GSH	O12-C1-CA1-N1
2	K	1223	GSH	N1-CA1-CB1-CG1
2	K	1223	GSH	CG1-CD1-N2-CA2
2	M	1223	GSH	O12-C1-CA1-N1
2	N	1223	GSH	O12-C1-CA1-N1
2	N	1223	GSH	CG1-CD1-N2-CA2
2	O	1223	GSH	O12-C1-CA1-N1
2	A	1223	GSH	OE1-CD1-N2-CA2
2	K	1223	GSH	OE1-CD1-N2-CA2
2	N	1223	GSH	OE1-CD1-N2-CA2
2	C	1223	GSH	CA1-CB1-CG1-CD1
2	J	1223	GSH	CA1-CB1-CG1-CD1
2	L	1223	GSH	CA1-CB1-CG1-CD1
2	M	1223	GSH	CA1-CB1-CG1-CD1
2	C	1223	GSH	O11-C1-CA1-N1
2	O	1223	GSH	O11-C1-CA1-N1
2	G	1223	GSH	CG1-CD1-N2-CA2
2	L	1223	GSH	CG1-CD1-N2-CA2
2	G	1223	GSH	OE1-CD1-N2-CA2
2	L	1223	GSH	OE1-CD1-N2-CA2
2	G	1223	GSH	O11-C1-CA1-N1
2	I	1223	GSH	O11-C1-CA1-N1
2	K	1223	GSH	O11-C1-CA1-N1
2	F	1223	GSH	CG1-CD1-N2-CA2
2	F	1223	GSH	OE1-CD1-N2-CA2
2	G	1223	GSH	CA1-CB1-CG1-CD1
2	I	1223	GSH	CA1-CB1-CG1-CD1
2	O	1223	GSH	CA1-CB1-CG1-CD1
2	M	1223	GSH	CG1-CD1-N2-CA2
2	A	1223	GSH	O11-C1-CA1-N1
2	E	1223	GSH	O11-C1-CA1-N1
2	F	1223	GSH	O11-C1-CA1-N1
2	H	1223	GSH	O11-C1-CA1-N1
2	M	1223	GSH	O11-C1-CA1-N1
2	N	1223	GSH	O11-C1-CA1-N1
2	D	1223	GSH	O31-C3-CA3-N3
2	J	1223	GSH	O11-C1-CA1-N1
2	M	1223	GSH	OE1-CD1-N2-CA2
2	B	1223	GSH	CA1-CB1-CG1-CD1
2	D	1223	GSH	O11-C1-CA1-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	P	1223	GSH	O11-C1-CA1-N1
2	D	1223	GSH	O32-C3-CA3-N3
2	L	1223	GSH	O11-C1-CA1-N1
2	B	1223	GSH	O11-C1-CA1-N1
2	D	1223	GSH	O12-C1-CA1-N1
2	E	1223	GSH	O12-C1-CA1-N1
2	P	1223	GSH	O12-C1-CA1-N1
2	N	1223	GSH	O11-C1-CA1-CB1
2	J	1223	GSH	C1-CA1-CB1-CG1
2	K	1223	GSH	C1-CA1-CB1-CG1
2	O	1223	GSH	C1-CA1-CB1-CG1
2	A	1223	GSH	O11-C1-CA1-CB1
2	L	1223	GSH	O12-C1-CA1-CB1
2	J	1223	GSH	N2-CA2-CB2-SG2
2	O	1223	GSH	N2-CA2-CB2-SG2
2	F	1223	GSH	CA1-CB1-CG1-CD1
2	N	1223	GSH	CA1-CB1-CG1-CD1
2	J	1223	GSH	O11-C1-CA1-CB1
2	J	1223	GSH	O12-C1-CA1-CB1
2	N	1223	GSH	O12-C1-CA1-CB1
2	A	1223	GSH	O12-C1-CA1-CB1
2	F	1223	GSH	O11-C1-CA1-CB1
2	M	1223	GSH	O11-C1-CA1-CB1
2	B	1223	GSH	O12-C1-CA1-CB1
2	L	1223	GSH	O11-C1-CA1-CB1
2	I	1223	GSH	O12-C1-CA1-N1
2	B	1223	GSH	O11-C1-CA1-CB1
2	F	1223	GSH	O12-C1-CA1-CB1
2	H	1223	GSH	O11-C1-CA1-CB1
2	M	1223	GSH	O12-C1-CA1-CB1
2	C	1223	GSH	O12-C1-CA1-CB1
2	H	1223	GSH	O12-C1-CA1-CB1
2	I	1223	GSH	O2-C2-N3-CA3
2	G	1223	GSH	O11-C1-CA1-CB1
2	A	1223	GSH	N2-CA2-CB2-SG2
2	C	1223	GSH	N2-CA2-CB2-SG2
2	D	1223	GSH	N2-CA2-CB2-SG2
2	O	1223	GSH	C3-CA3-N3-C2
2	C	1223	GSH	OE1-CD1-N2-CA2
2	C	1223	GSH	O11-C1-CA1-CB1
2	I	1223	GSH	O12-C1-CA1-CB1
2	I	1223	GSH	CA2-C2-N3-CA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1223	GSH	C3-CA3-N3-C2
2	G	1223	GSH	O12-C1-CA1-CB1
2	I	1223	GSH	O11-C1-CA1-CB1
2	K	1223	GSH	O11-C1-CA1-CB1
2	O	1223	GSH	O11-C1-CA1-CB1
2	G	1223	GSH	C3-CA3-N3-C2
2	K	1223	GSH	O12-C1-CA1-CB1
2	O	1223	GSH	O12-C1-CA1-CB1
2	C	1223	GSH	O12-C1-CA1-N1

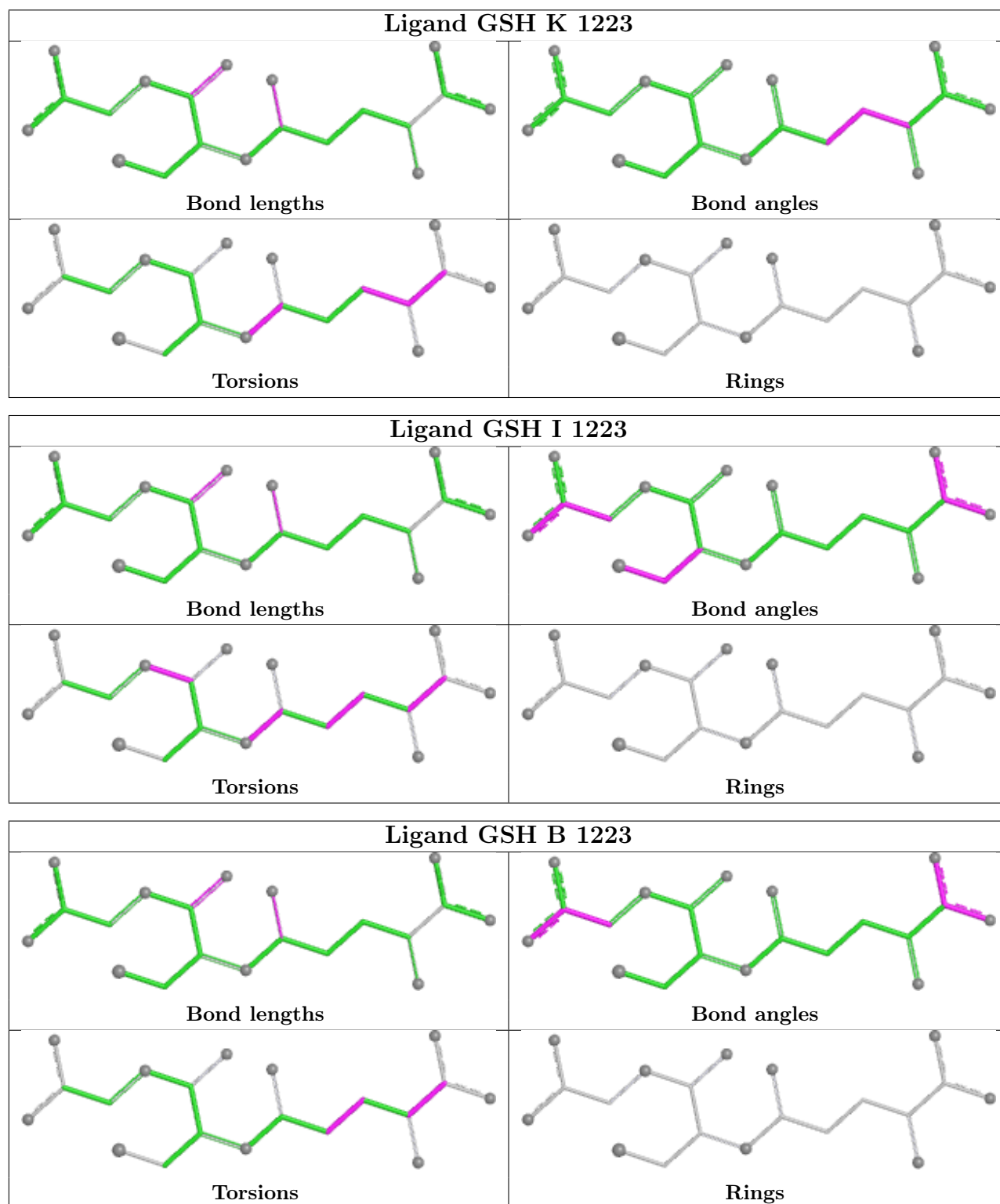
There are no ring outliers.

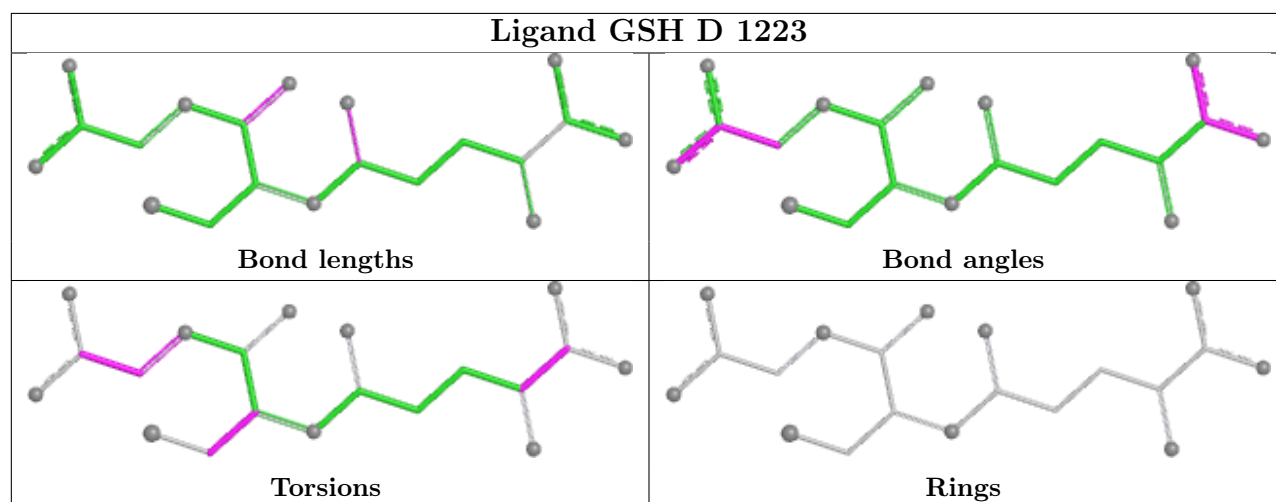
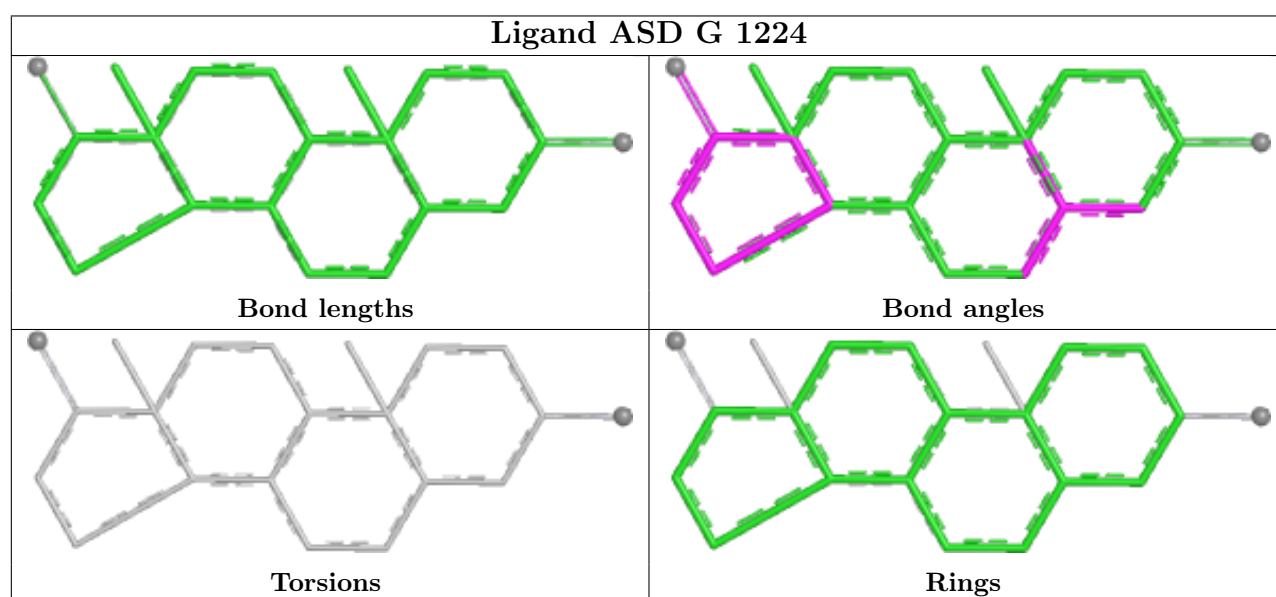
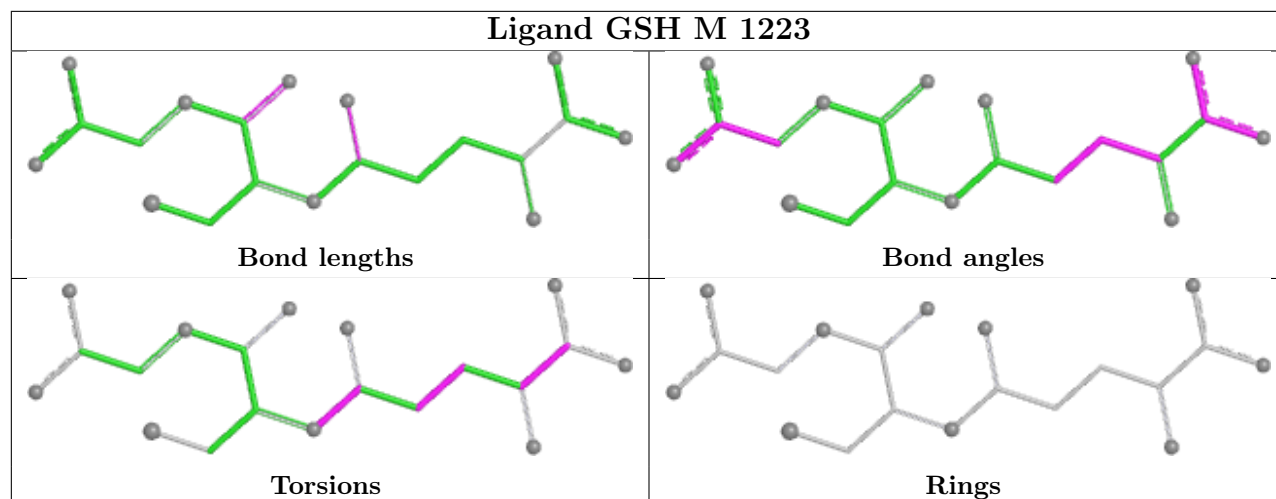
17 monomers are involved in 21 short contacts:

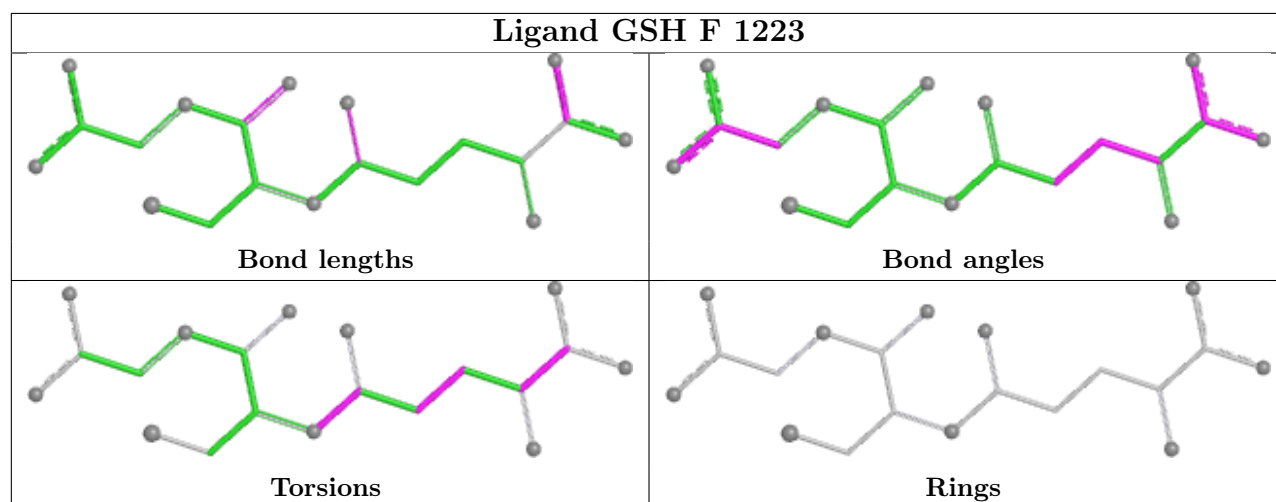
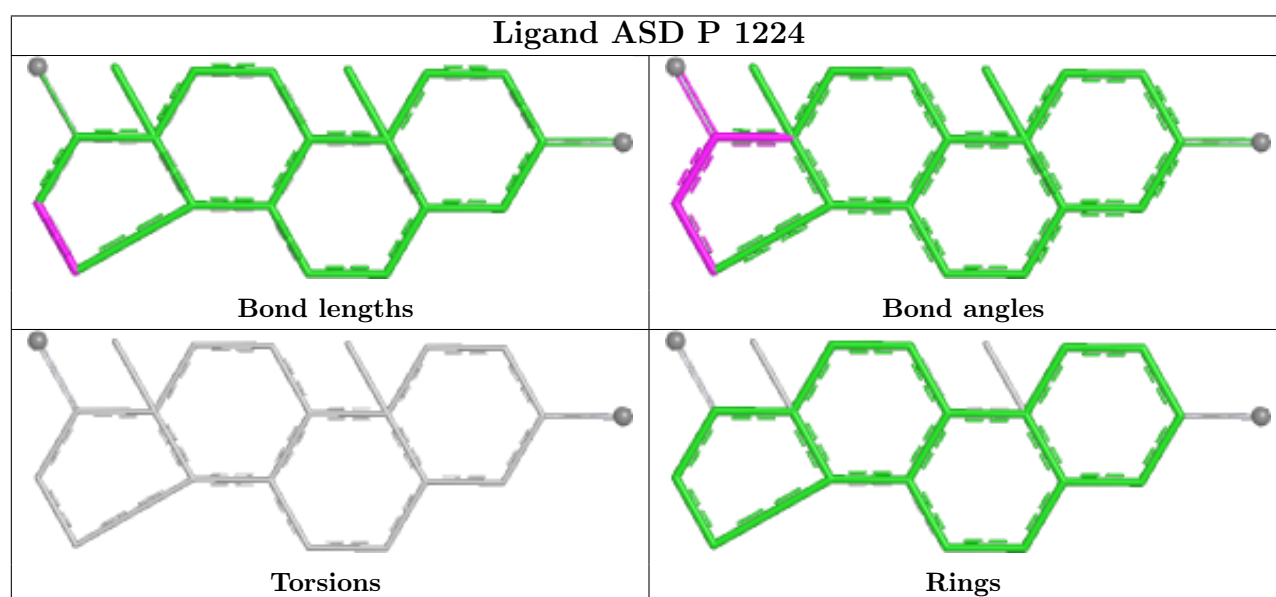
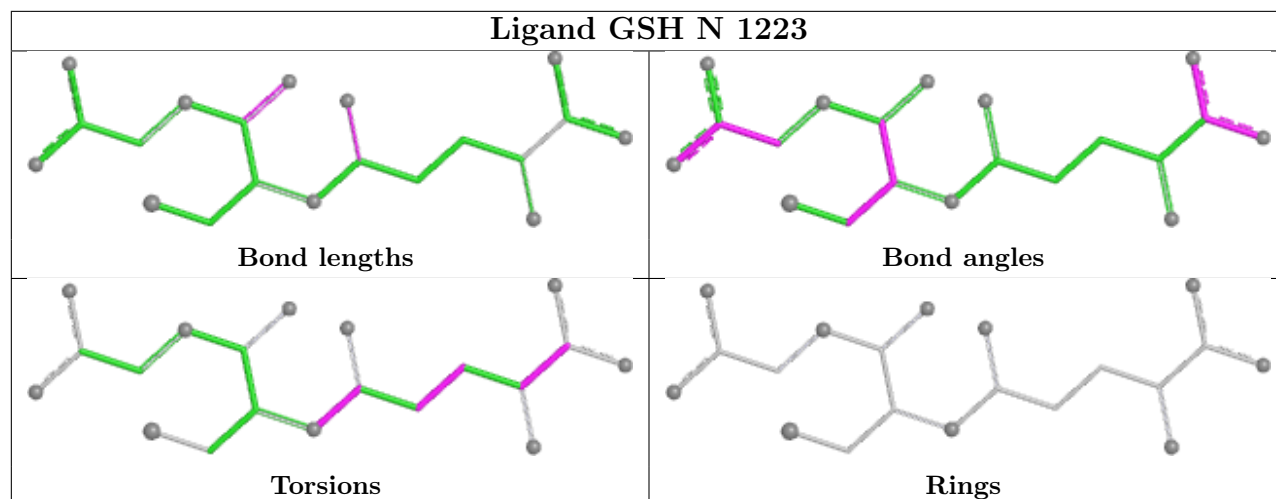
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1223	GSH	1	0
2	I	1223	GSH	1	0
2	M	1223	GSH	1	0
2	D	1223	GSH	1	0
2	N	1223	GSH	1	0
3	P	1224	ASD	1	0
2	F	1223	GSH	3	0
3	B	1224	ASD	4	0
2	G	1223	GSH	2	0
2	A	1223	GSH	2	0
2	J	1223	GSH	1	0
3	F	1224	ASD	2	0
2	L	1223	GSH	1	0
3	H	1224	ASD	1	0
3	A	1224	ASD	1	0
2	C	1223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

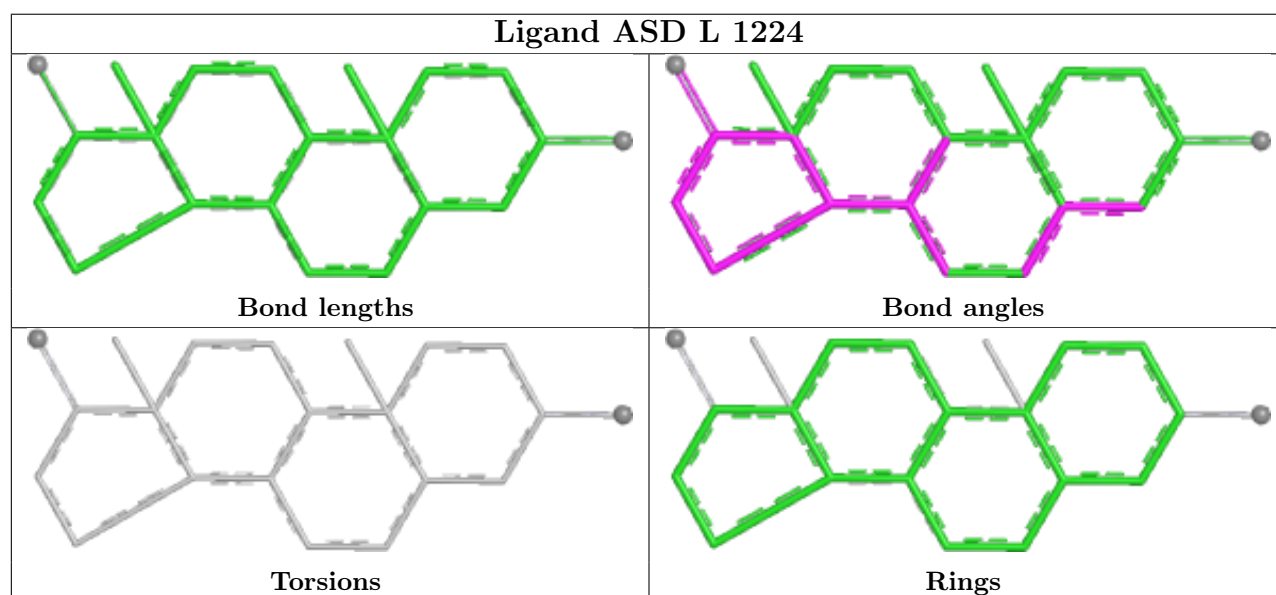
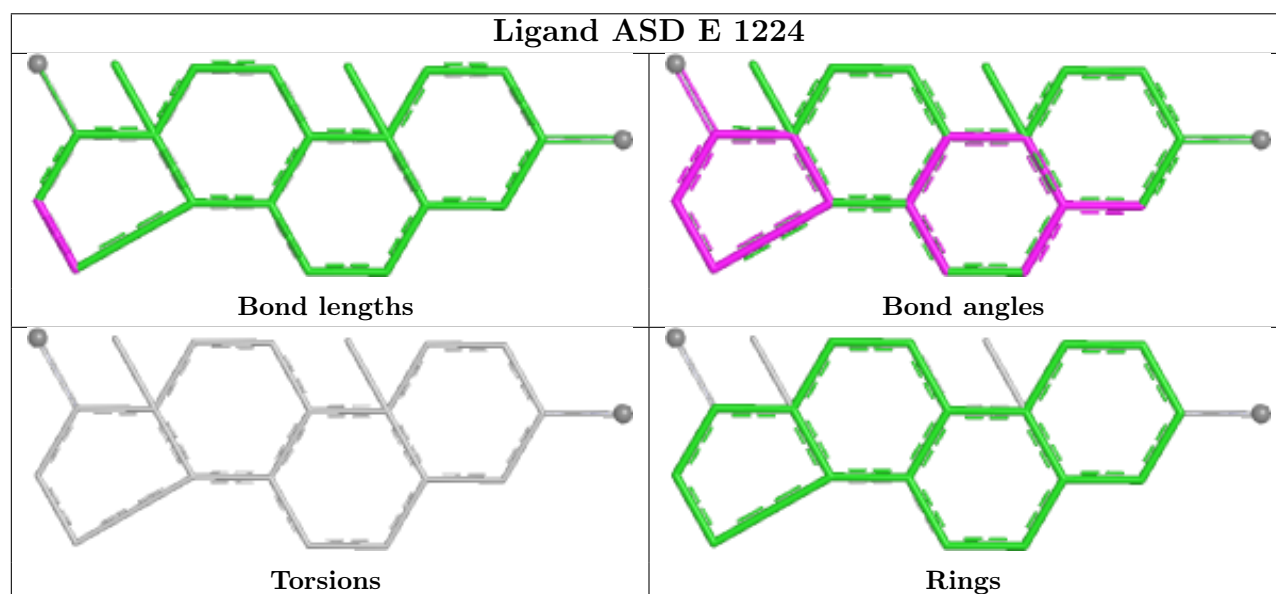
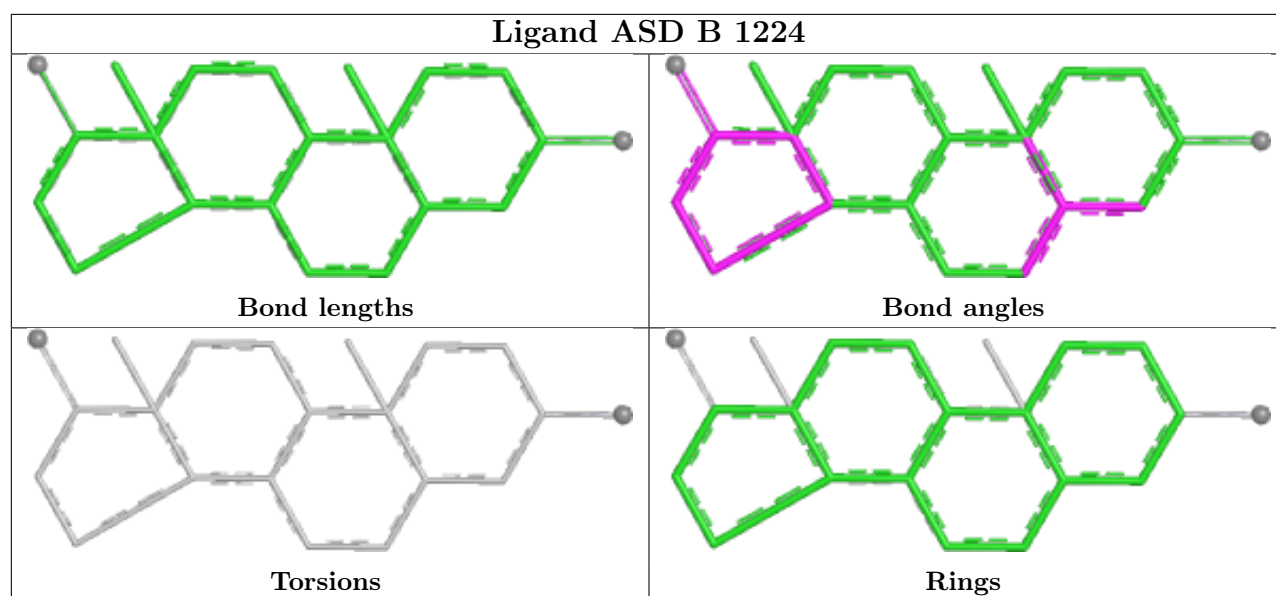
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

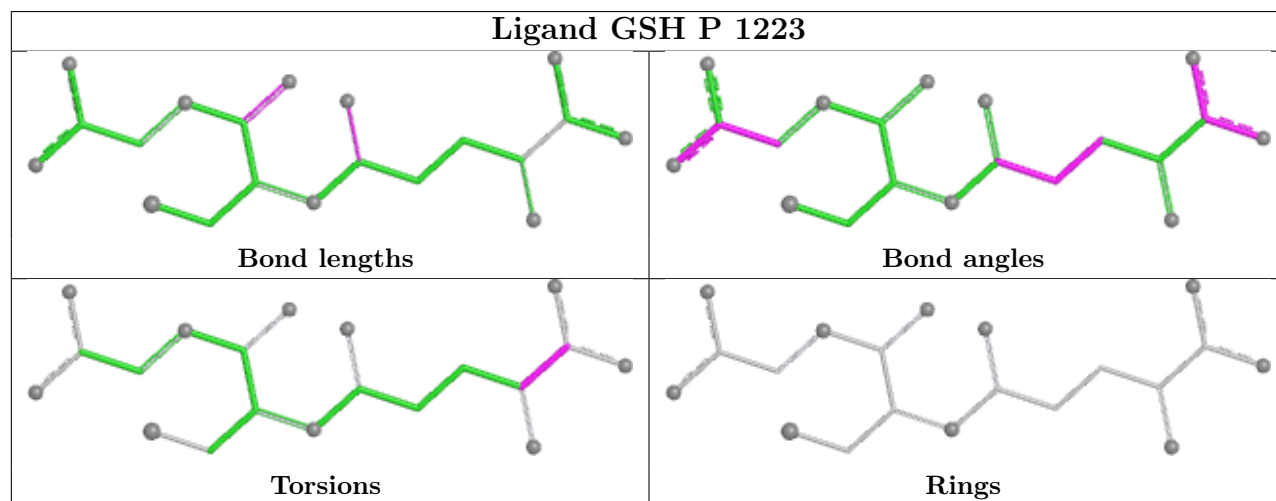
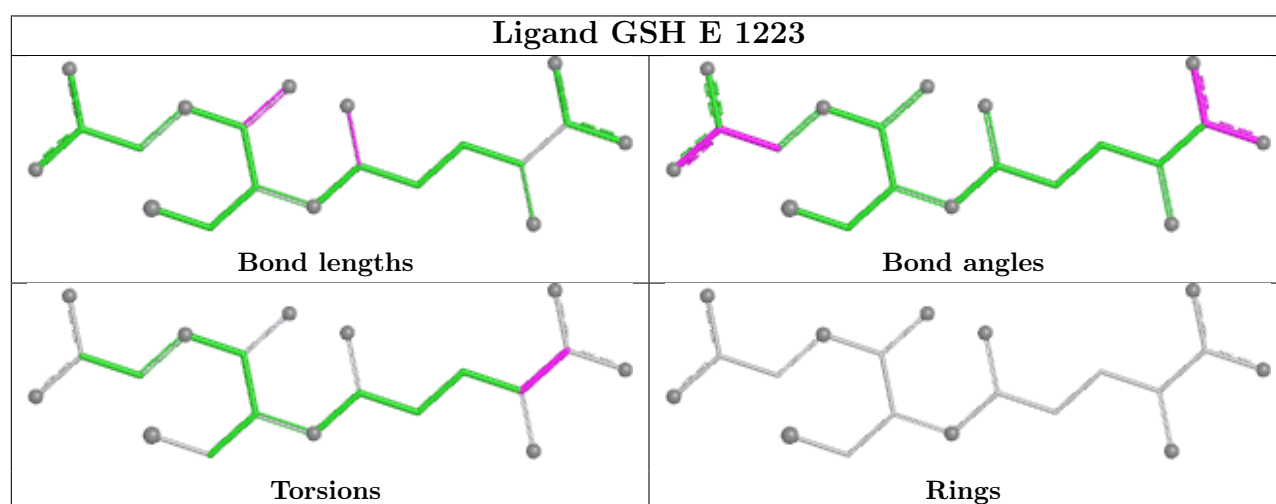
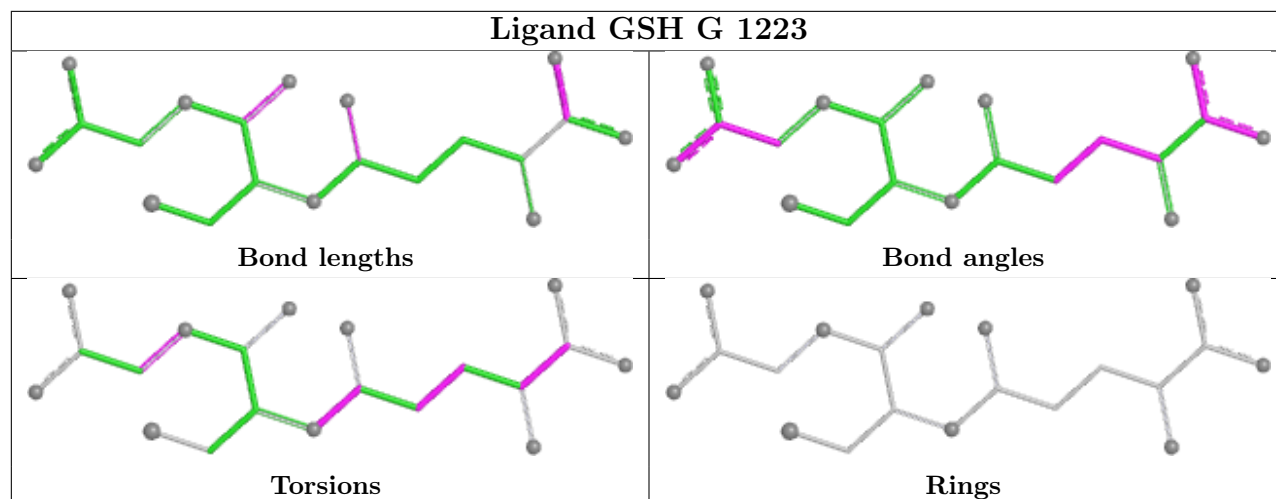
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

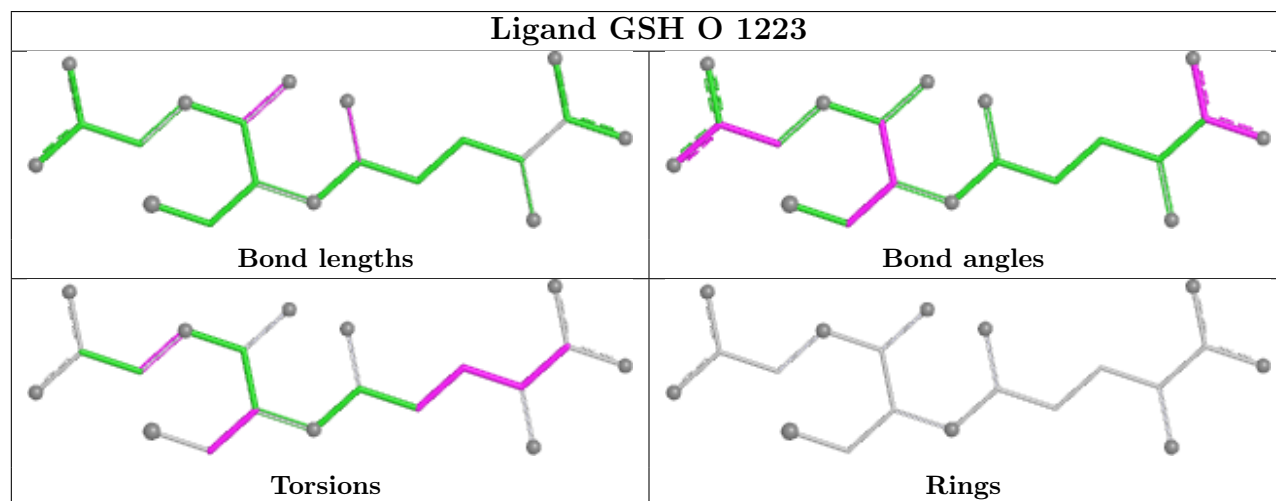
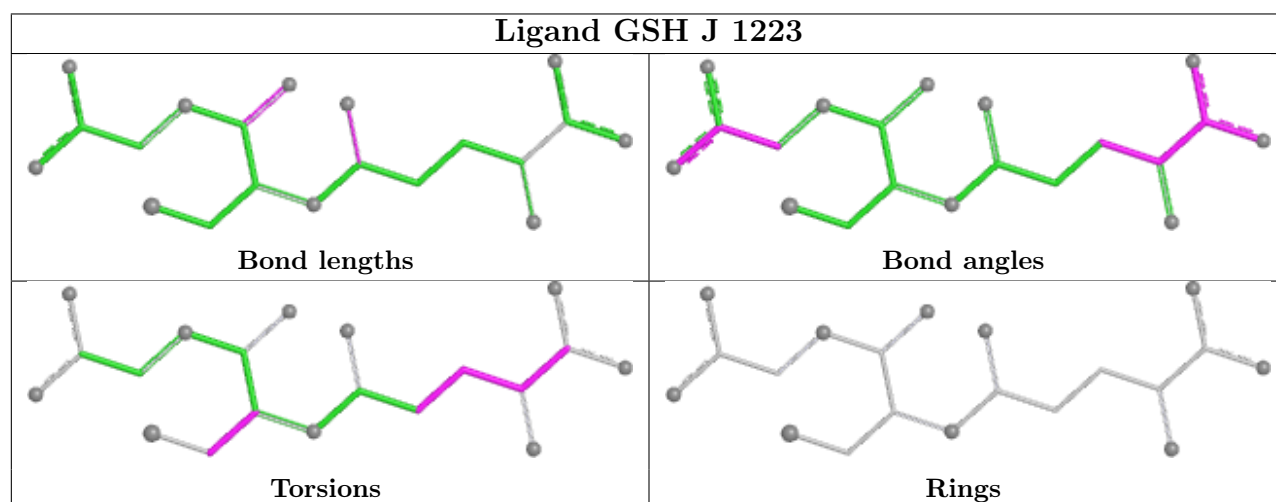
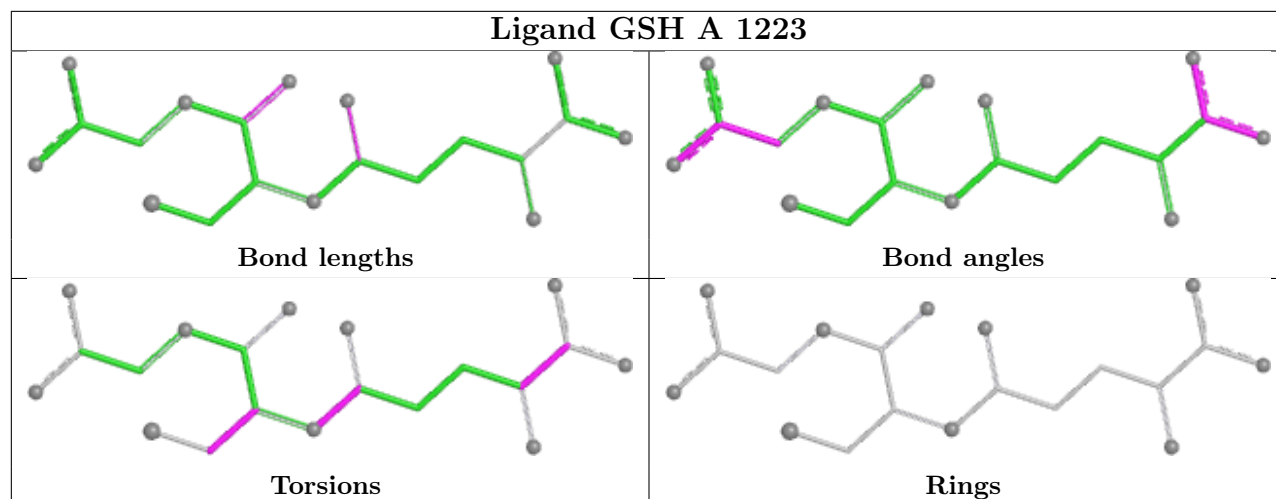


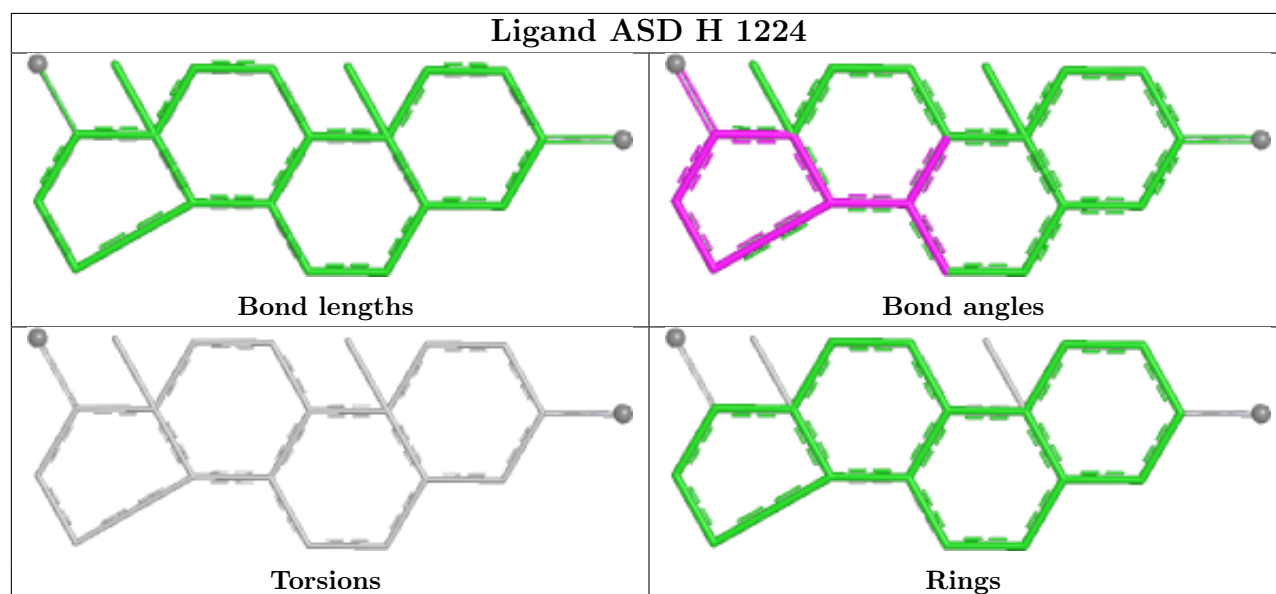
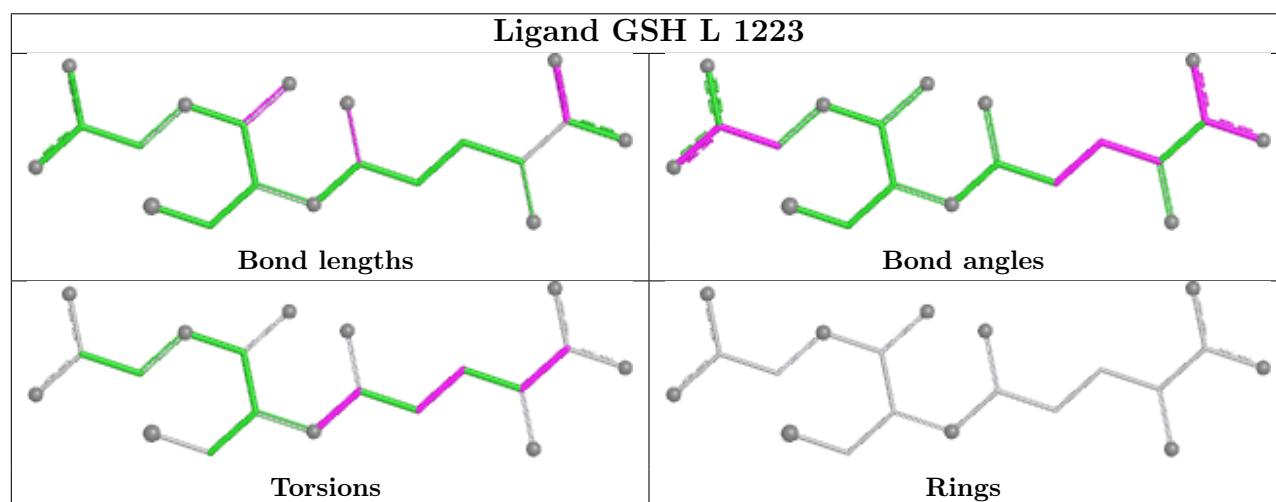
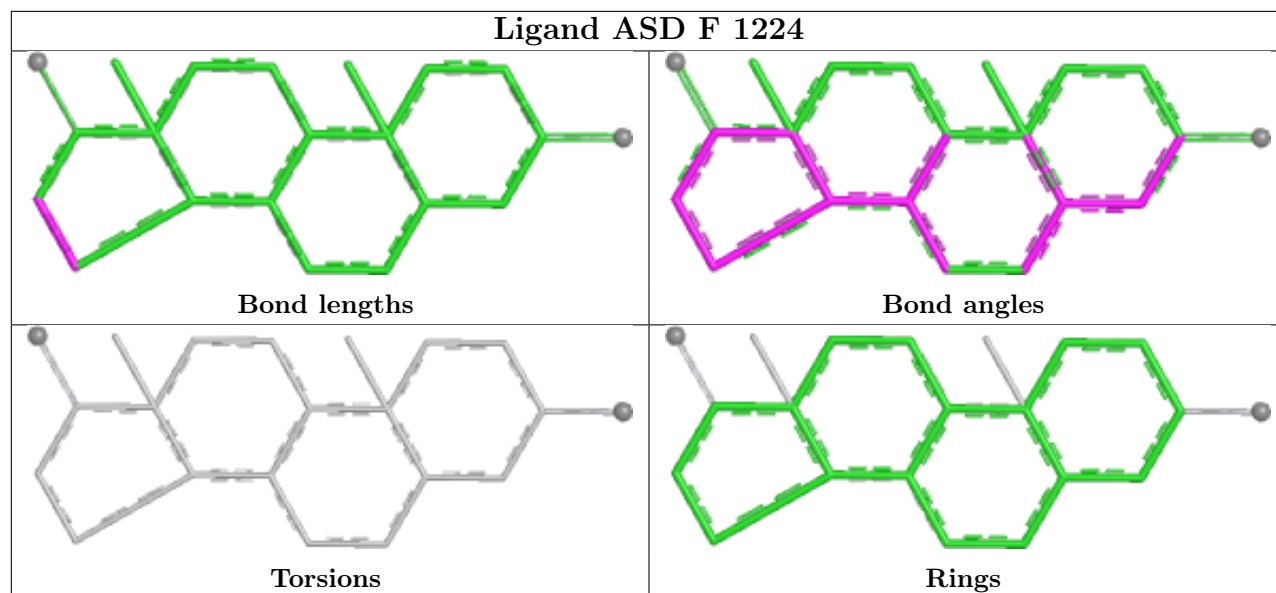


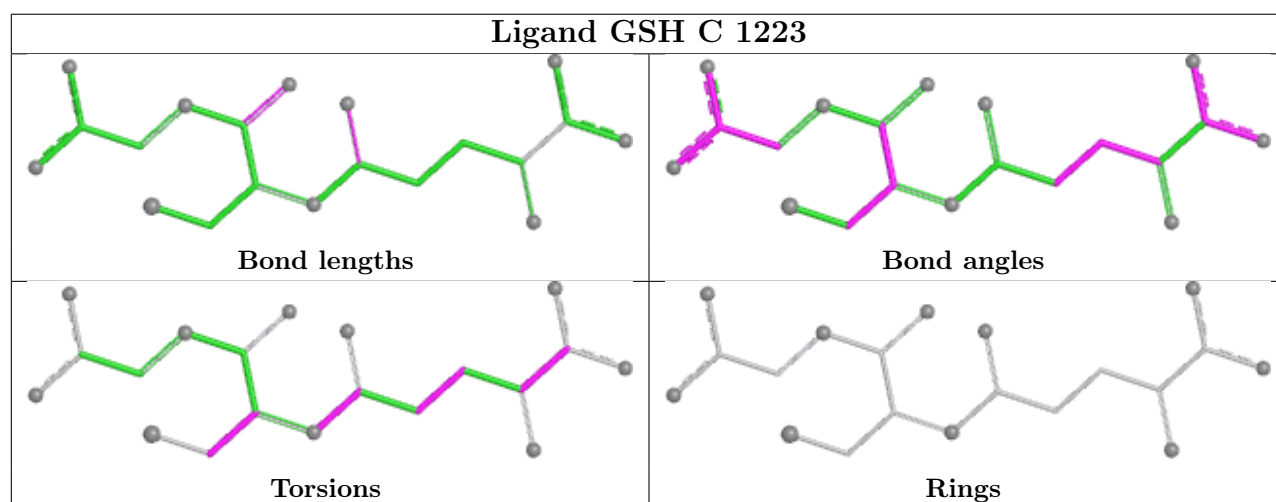
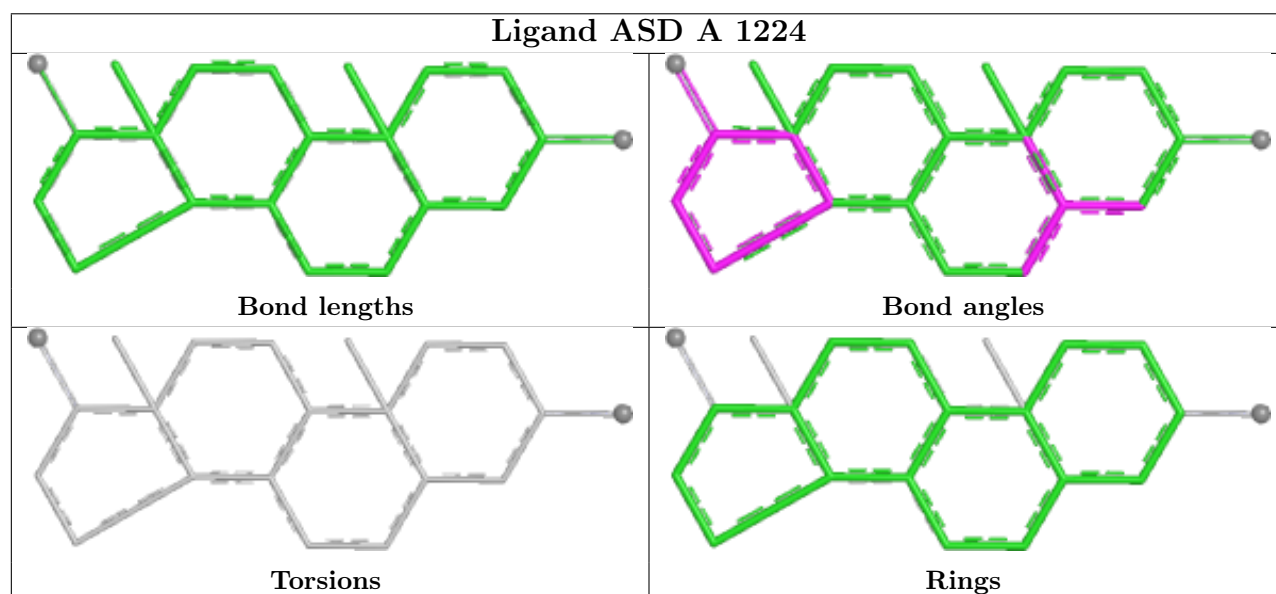
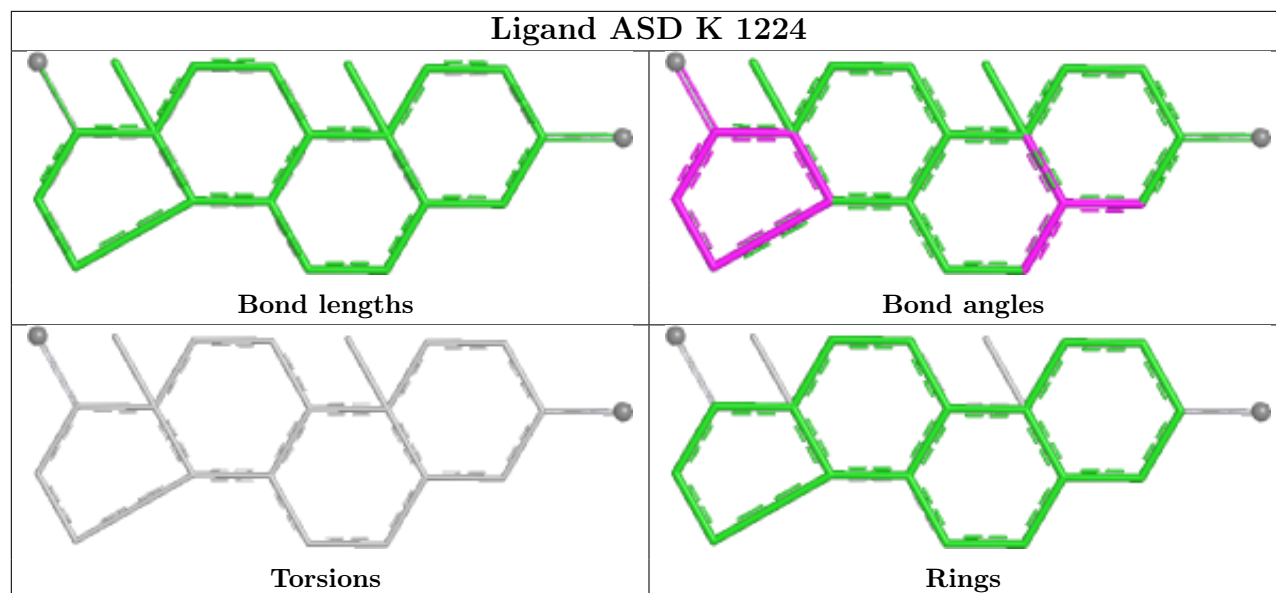


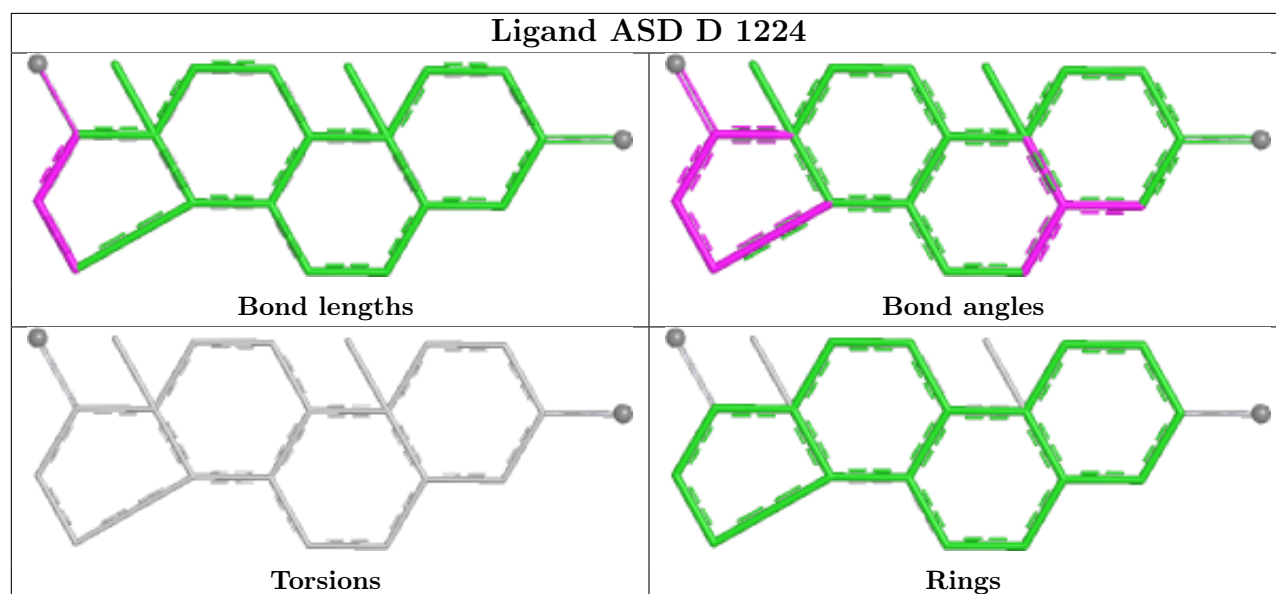
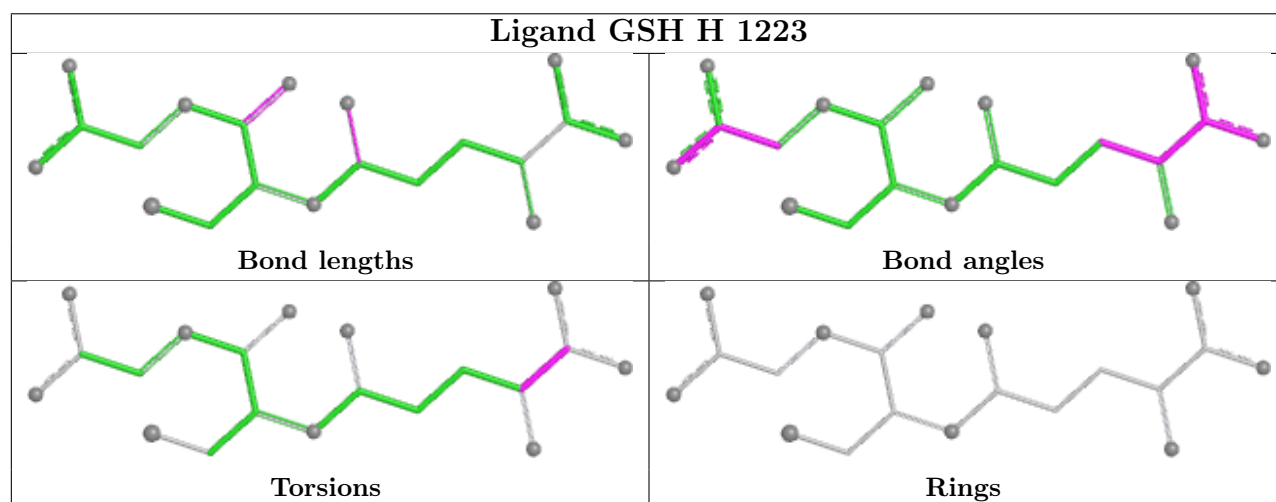
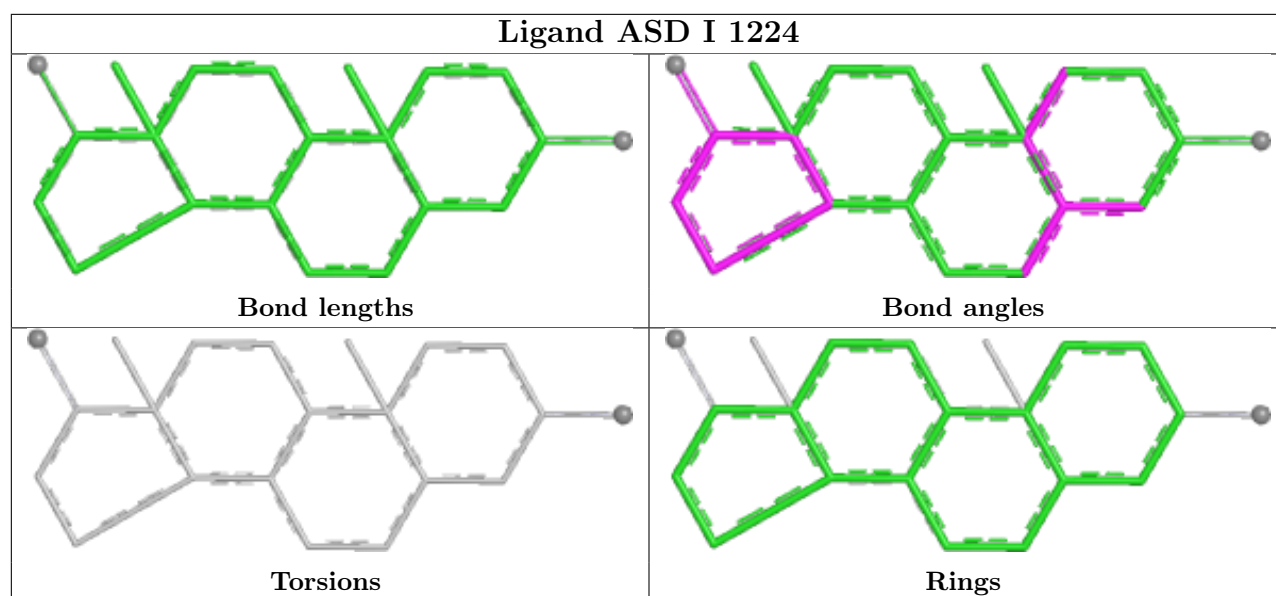












5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/222 (98%)	-1.35	0 100 100	8, 18, 32, 45	2 (0%)
1	B	219/222 (98%)	-1.38	0 100 100	7, 16, 35, 45	3 (1%)
1	C	219/222 (98%)	-1.25	0 100 100	9, 20, 50, 62	3 (1%)
1	D	219/222 (98%)	-1.36	0 100 100	8, 19, 35, 48	2 (0%)
1	E	219/222 (98%)	-1.31	0 100 100	10, 20, 44, 54	2 (0%)
1	F	219/222 (98%)	-1.38	0 100 100	9, 18, 29, 47	3 (1%)
1	G	219/222 (98%)	-1.41	0 100 100	8, 16, 29, 45	3 (1%)
1	H	219/222 (98%)	-1.34	0 100 100	7, 19, 43, 56	3 (1%)
1	I	219/222 (98%)	-1.41	0 100 100	7, 17, 33, 38	3 (1%)
1	J	219/222 (98%)	-1.36	0 100 100	7, 17, 38, 53	2 (0%)
1	K	219/222 (98%)	-1.35	0 100 100	9, 19, 32, 48	4 (1%)
1	L	219/222 (98%)	-1.39	0 100 100	5, 16, 33, 42	5 (2%)
1	M	219/222 (98%)	-1.38	0 100 100	7, 17, 33, 51	1 (0%)
1	N	219/222 (98%)	-1.34	0 100 100	6, 16, 41, 54	5 (2%)
1	O	219/222 (98%)	-1.35	0 100 100	6, 17, 35, 53	4 (1%)
1	P	219/222 (98%)	-1.35	0 100 100	6, 17, 40, 57	3 (1%)
All	All	3504/3552 (98%)	-1.36	0 100 100	5, 18, 37, 62	48 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

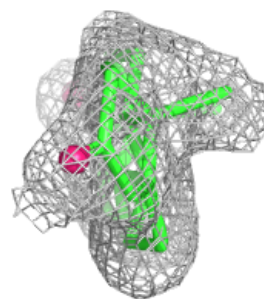
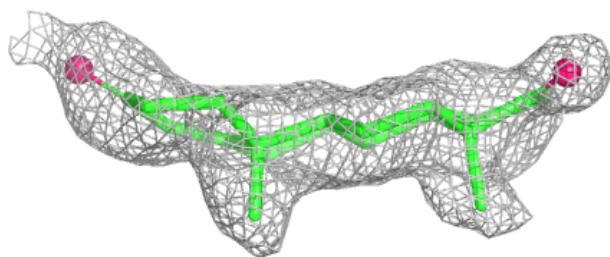
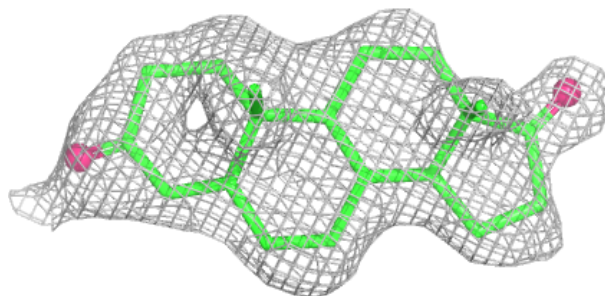
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ASD	A	1224	21/21	0.97	0.04	34,35,36,37	0
2	GSH	L	1223	20/20	0.98	0.04	23,28,29,31	0
2	GSH	O	1223	20/20	0.98	0.04	28,32,38,38	0
2	GSH	P	1223	20/20	0.98	0.04	21,26,35,35	0
2	GSH	C	1223	20/20	0.98	0.04	23,32,35,39	0
3	ASD	B	1224	21/21	0.98	0.04	31,33,35,36	0
3	ASD	D	1224	21/21	0.98	0.06	57,58,59,59	0
3	ASD	E	1224	21/21	0.98	0.04	50,51,52,53	0
3	ASD	F	1224	21/21	0.98	0.05	39,41,42,42	0
3	ASD	G	1224	21/21	0.98	0.04	40,42,44,45	0
3	ASD	H	1224	21/21	0.98	0.05	49,51,53,53	0
3	ASD	I	1224	21/21	0.98	0.04	38,39,39,40	0
3	ASD	L	1224	21/21	0.98	0.04	32,34,36,36	0
3	ASD	P	1224	21/21	0.98	0.05	43,46,48,48	0
2	GSH	A	1223	20/20	0.99	0.04	22,28,30,30	0
2	GSH	D	1223	20/20	0.99	0.04	30,34,39,39	0
2	GSH	E	1223	20/20	0.99	0.04	33,35,36,37	0
2	GSH	F	1223	20/20	0.99	0.04	25,27,33,33	0
2	GSH	G	1223	20/20	0.99	0.04	16,24,32,33	0
2	GSH	H	1223	20/20	0.99	0.04	28,32,36,37	0
2	GSH	I	1223	20/20	0.99	0.05	32,37,38,39	0
2	GSH	J	1223	20/20	0.99	0.04	21,27,31,33	0
2	GSH	K	1223	20/20	0.99	0.04	18,27,31,31	0
2	GSH	B	1223	20/20	0.99	0.04	30,33,35,36	0
3	ASD	K	1224	21/21	0.99	0.04	38,39,40,41	0
2	GSH	M	1223	20/20	0.99	0.03	22,25,33,33	0
2	GSH	N	1223	20/20	0.99	0.04	22,26,33,33	0

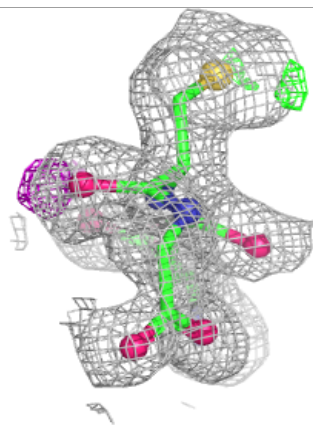
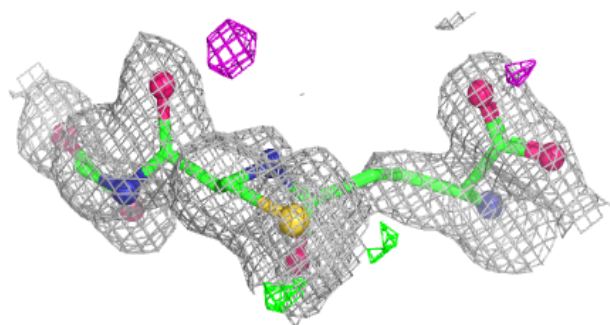
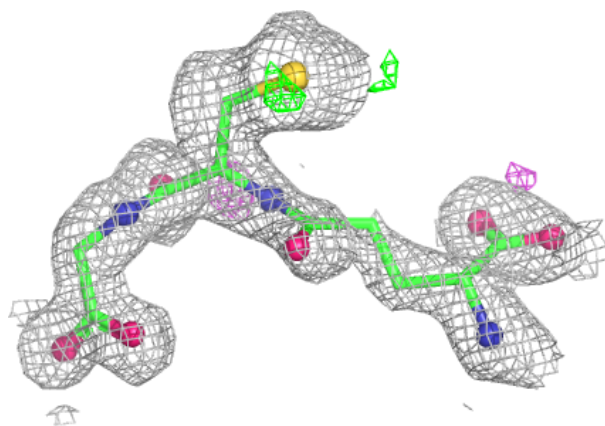
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ASD A 1224:

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

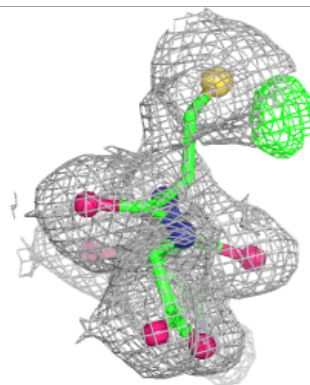
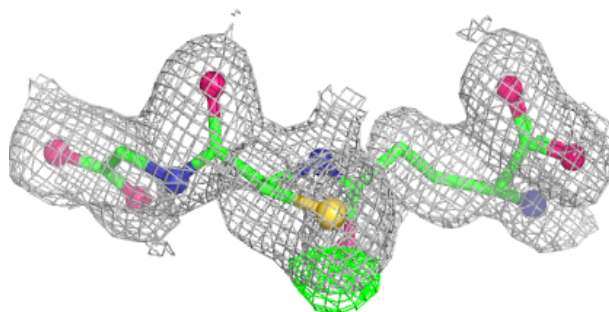
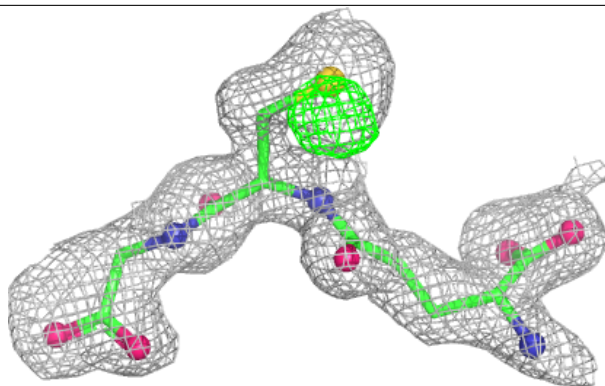
**Electron density around GSH L 1223:**

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

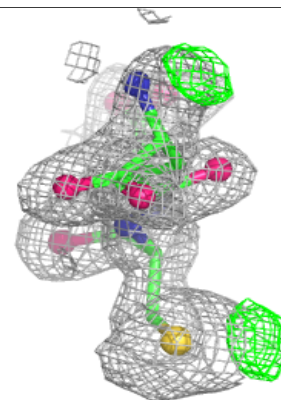
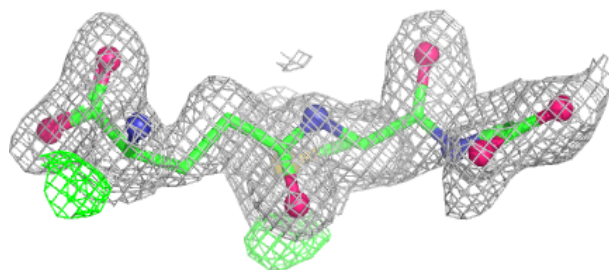
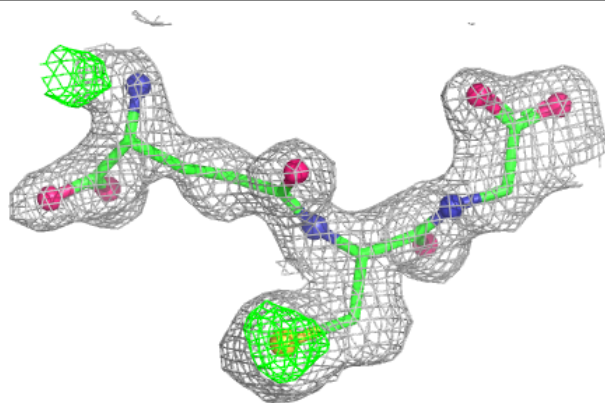


Electron density around GSH O 1223:

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

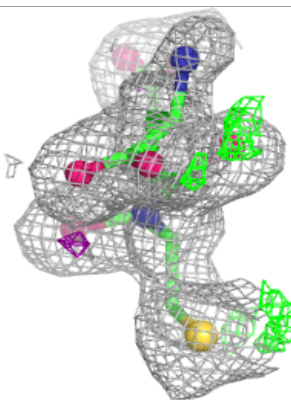
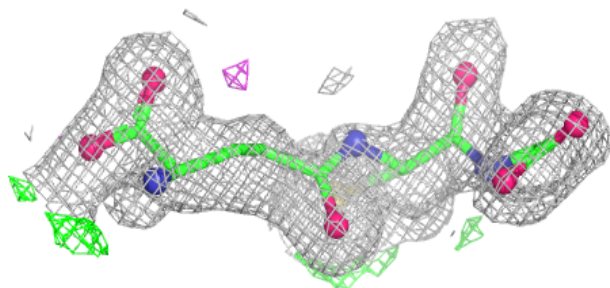
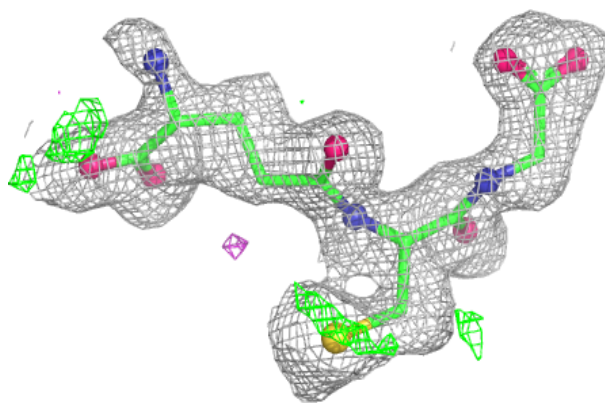
**Electron density around GSH P 1223:**

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

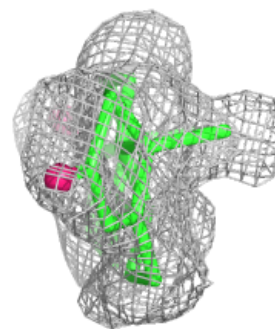
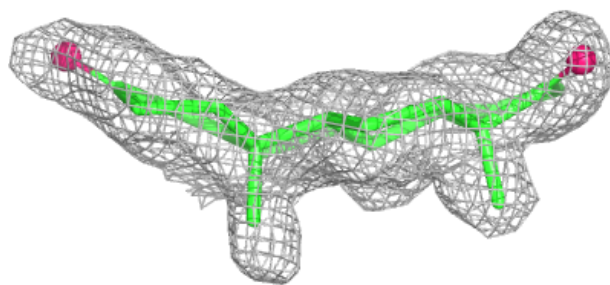
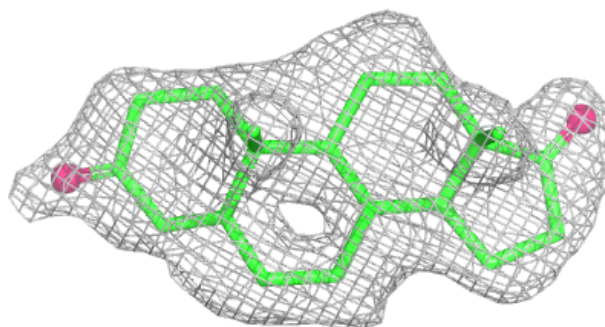


Electron density around GSH C 1223:

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

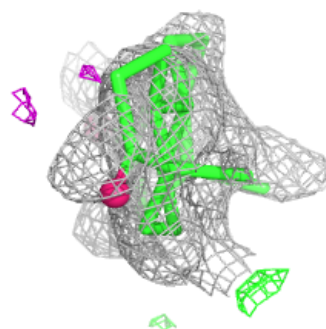
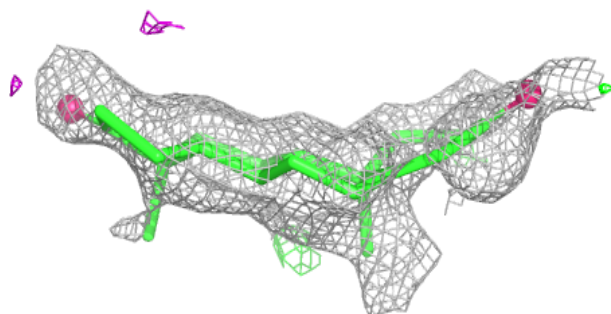
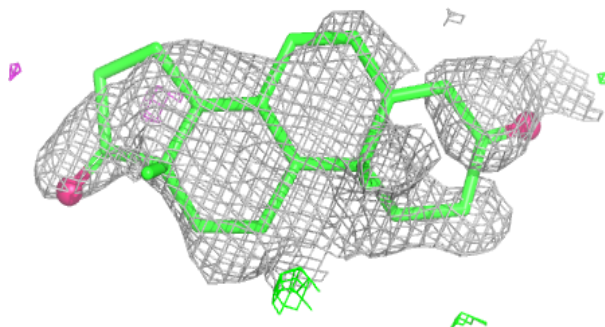
**Electron density around ASD B 1224:**

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

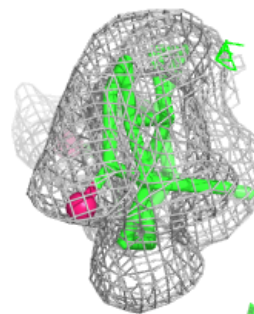
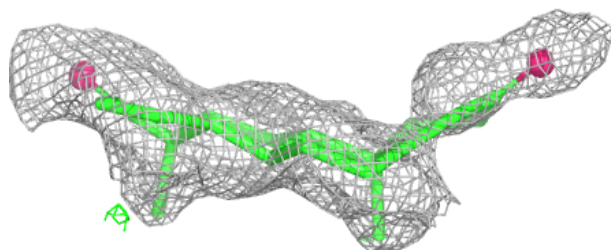
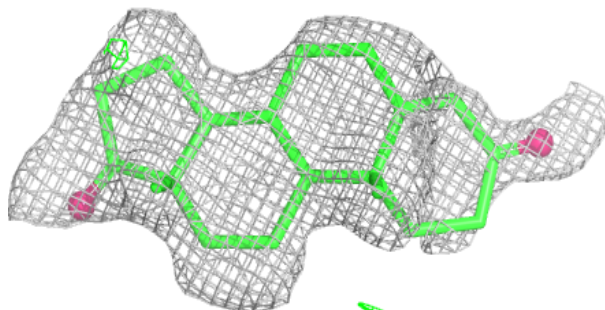


Electron density around ASD D 1224:

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

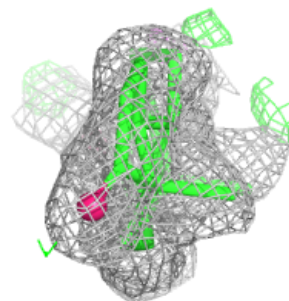
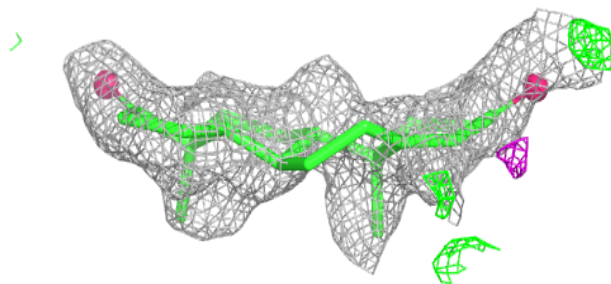
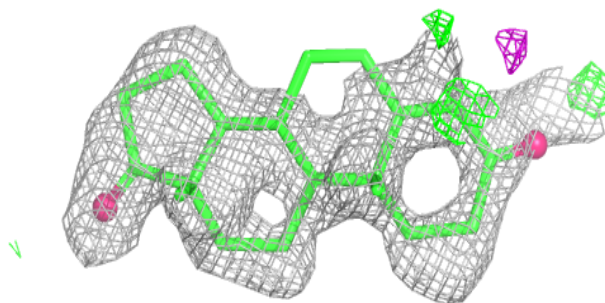
**Electron density around ASD E 1224:**

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

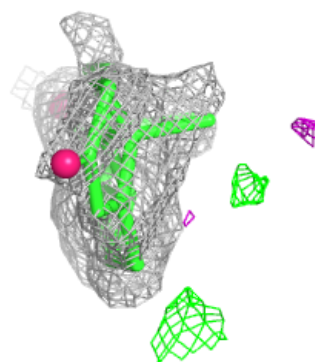
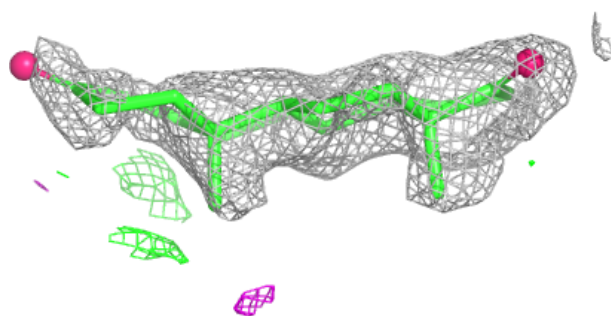
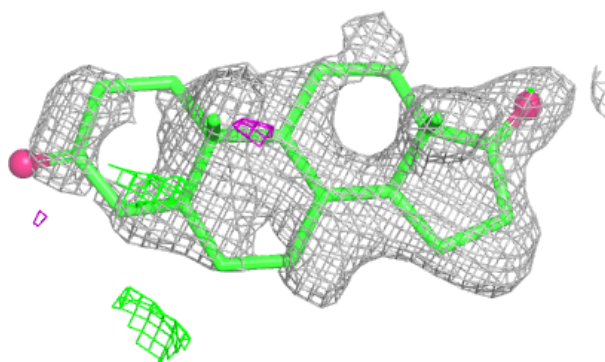


Electron density around ASD F 1224:

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

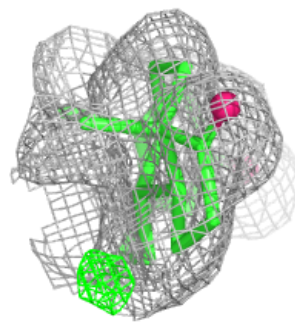
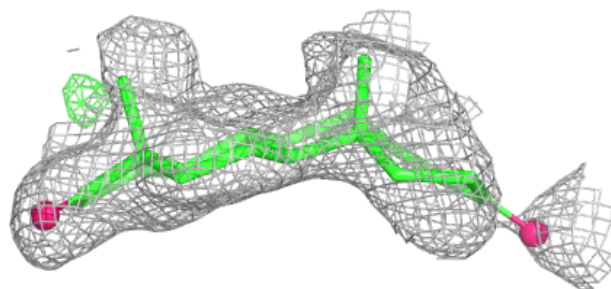
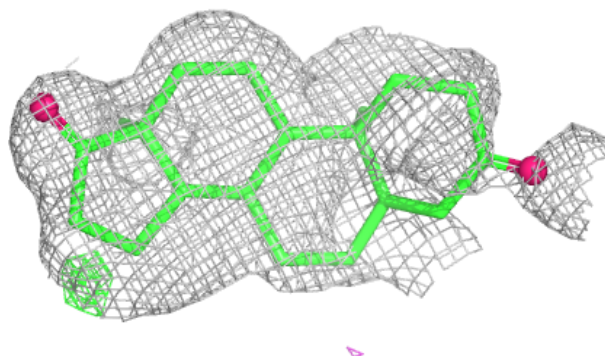
**Electron density around ASD G 1224:**

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

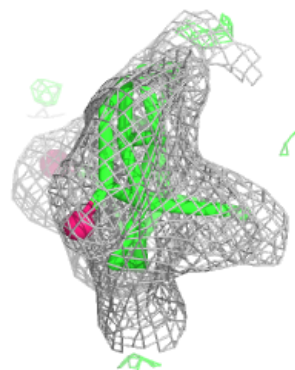
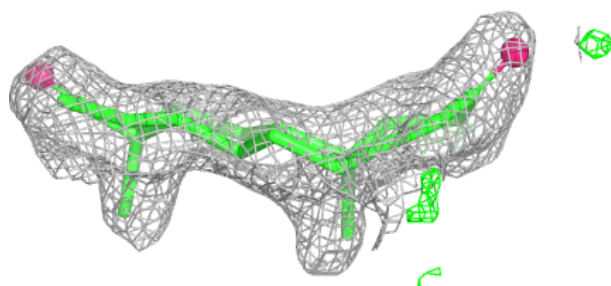
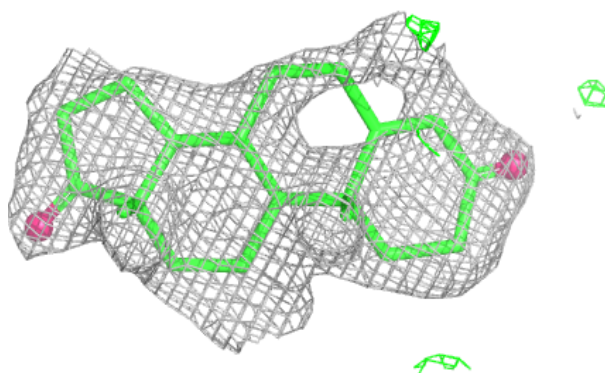


Electron density around ASD H 1224:

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

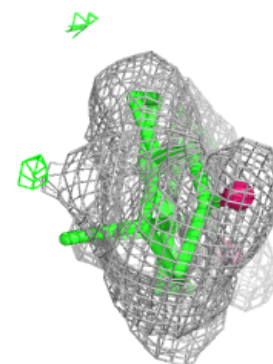
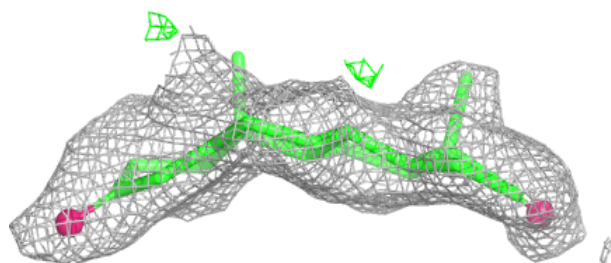
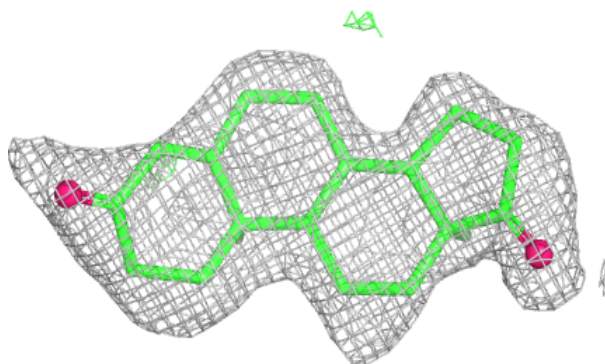
**Electron density around ASD I 1224:**

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

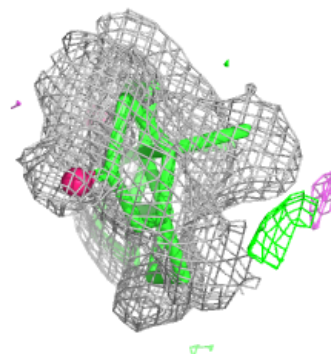
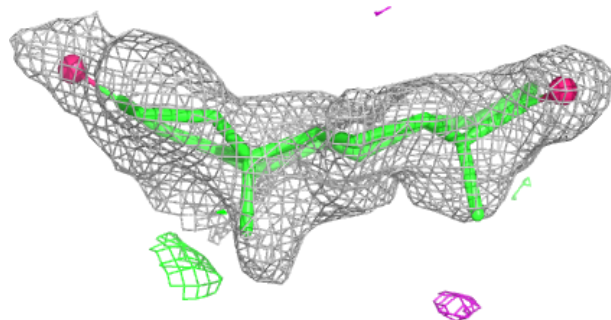
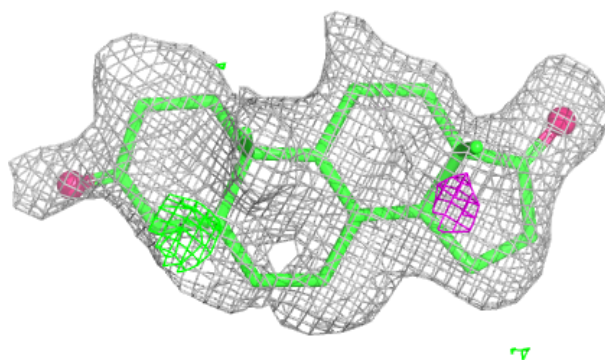


Electron density around ASD L 1224:

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

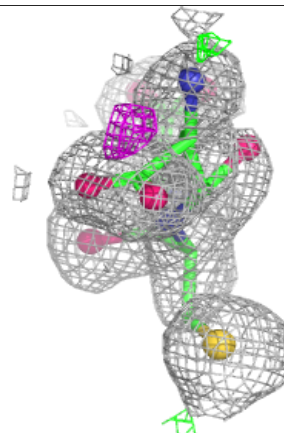
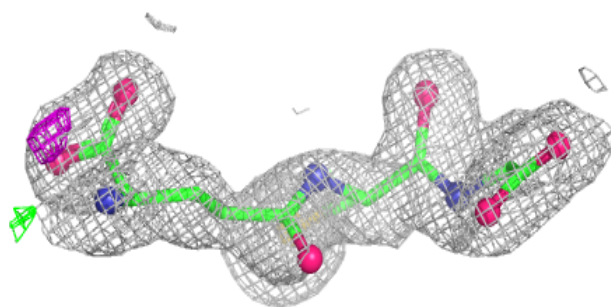
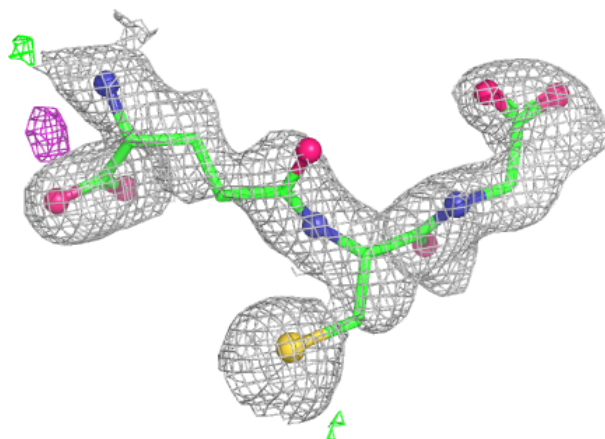
**Electron density around ASD P 1224:**

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

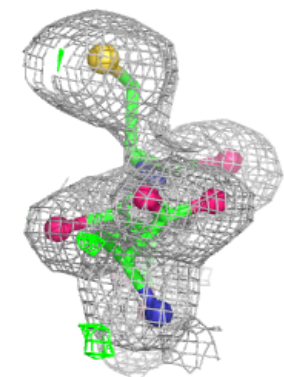
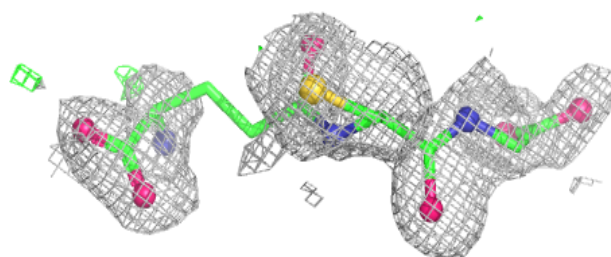
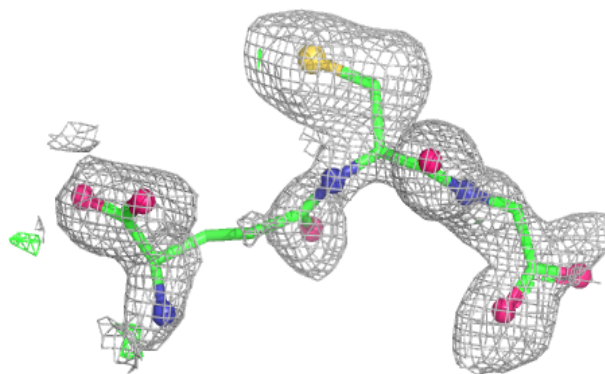


Electron density around GSH A 1223:

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

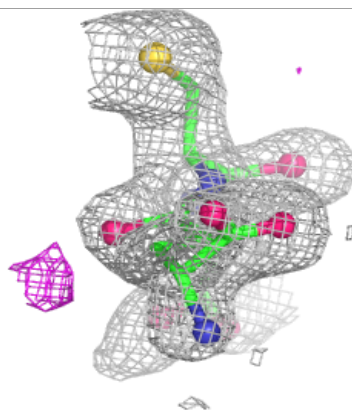
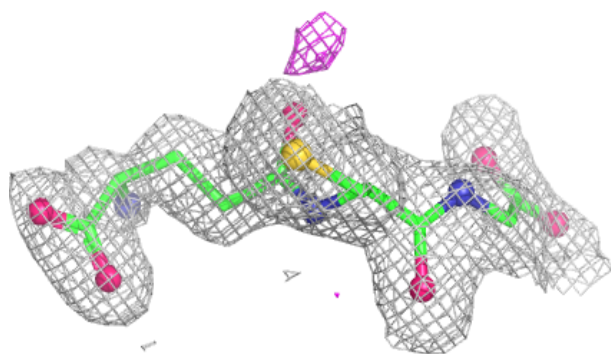
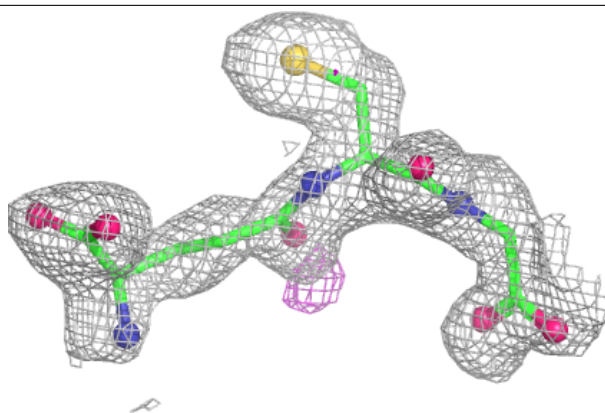
**Electron density around GSH D 1223:**

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

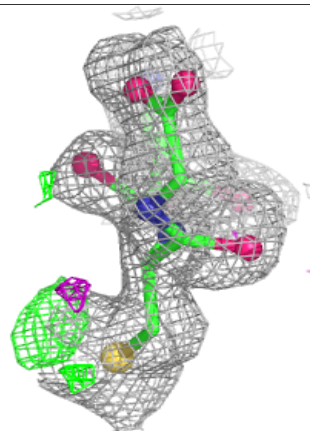
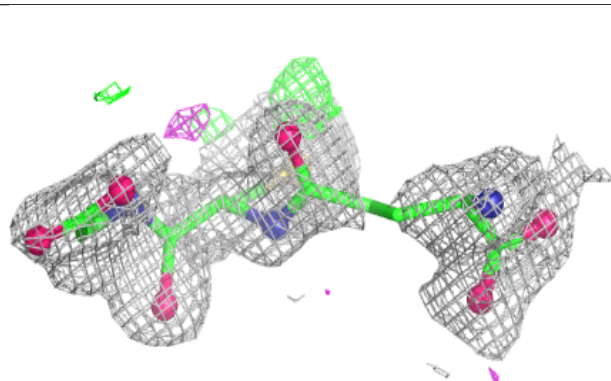
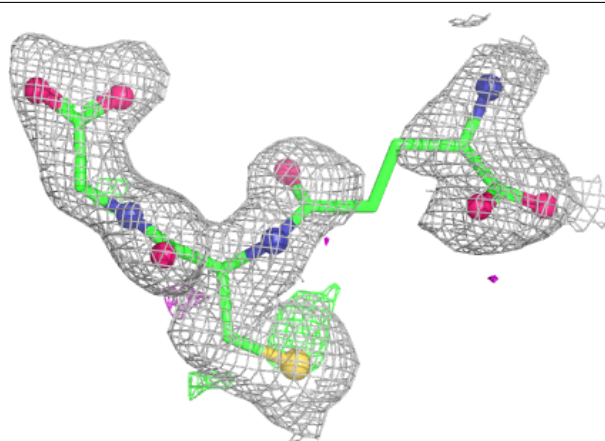


Electron density around GSH E 1223:

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

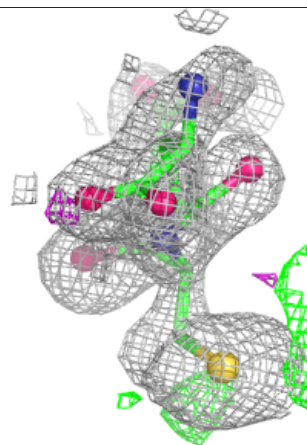
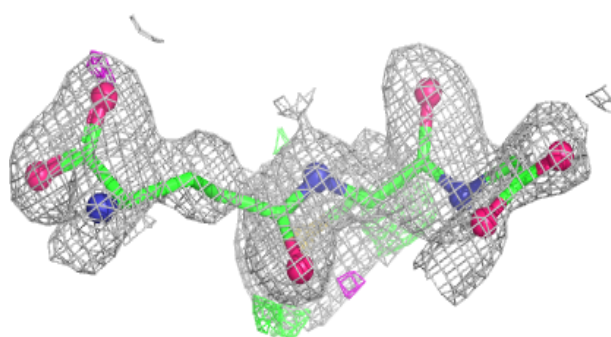
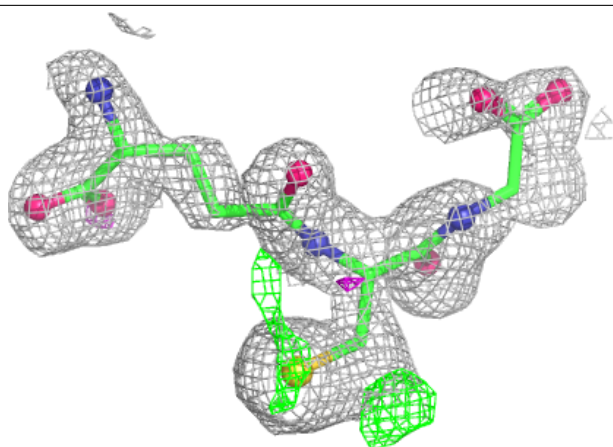
**Electron density around GSH F 1223:**

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



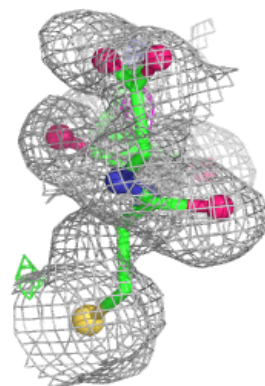
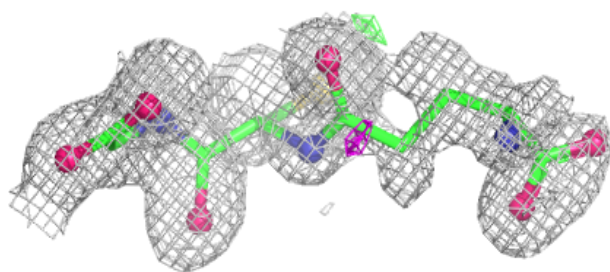
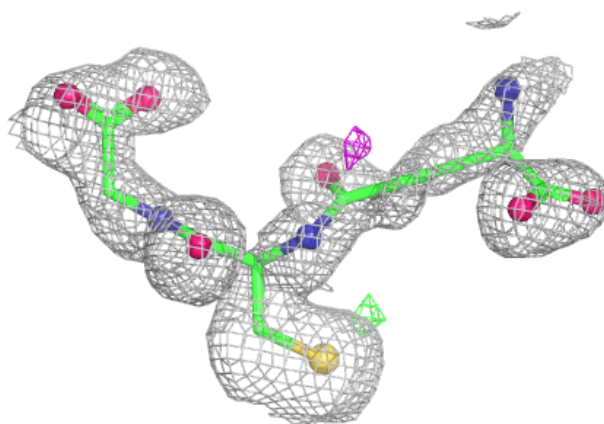
Electron density around GSH G 1223:

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

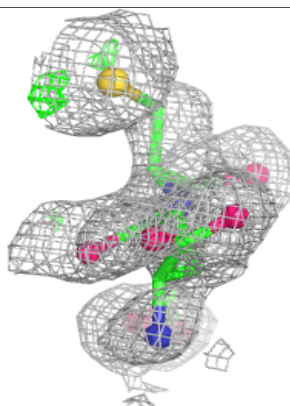
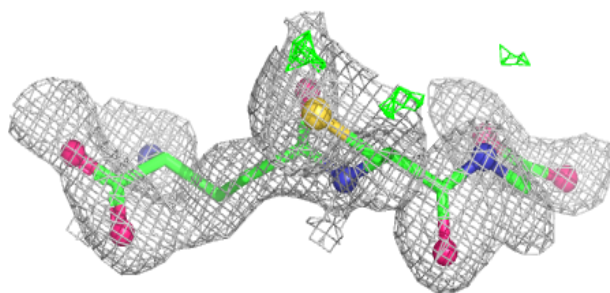
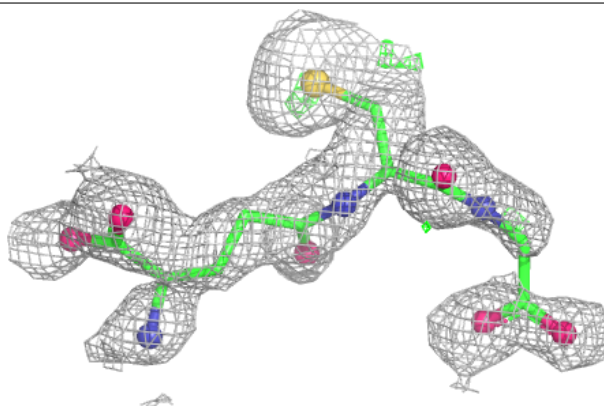


Electron density around GSH H 1223:

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

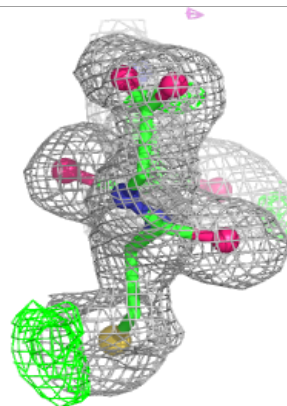
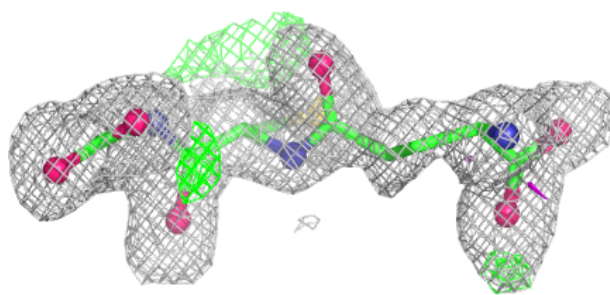
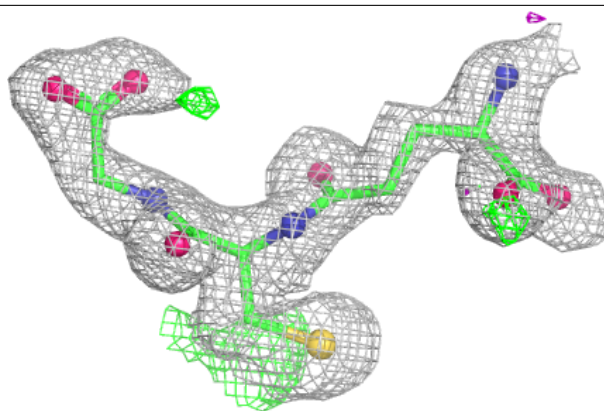
**Electron density around GSH I 1223:**

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

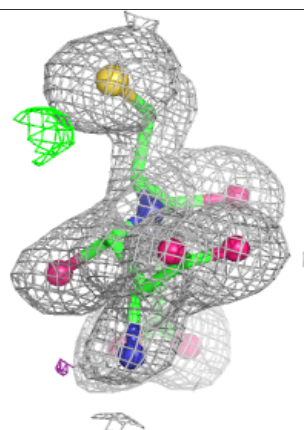
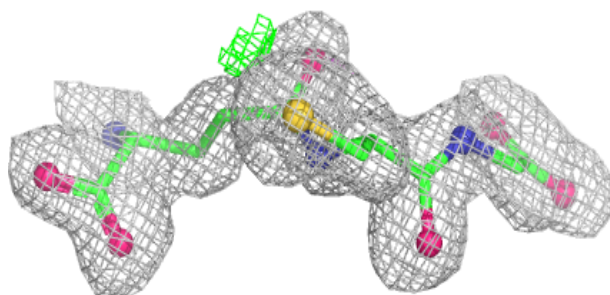
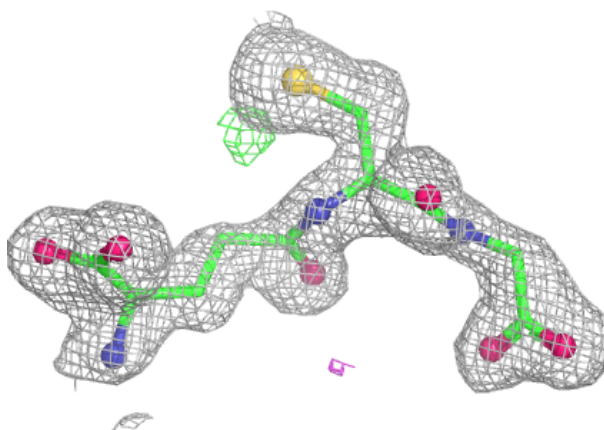


Electron density around GSH J 1223:

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

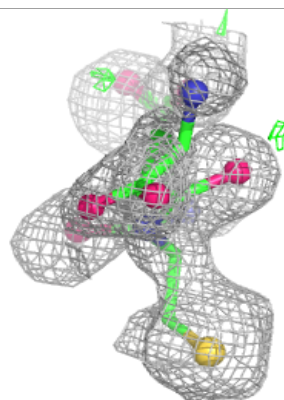
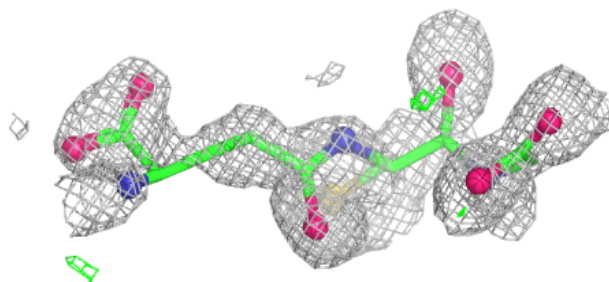
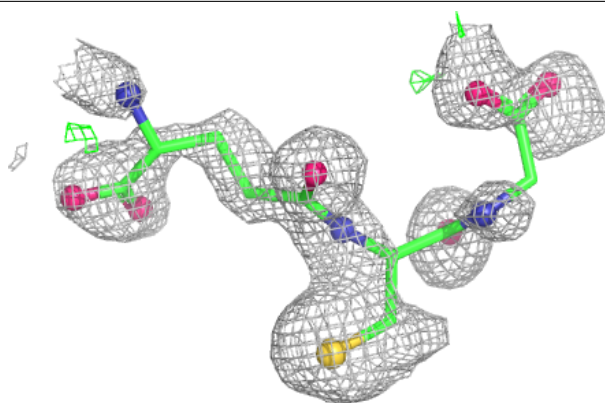
**Electron density around GSH K 1223:**

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

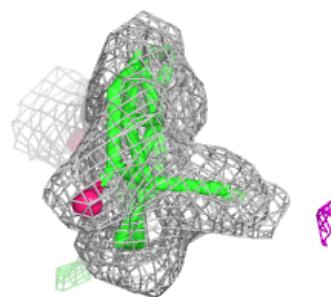
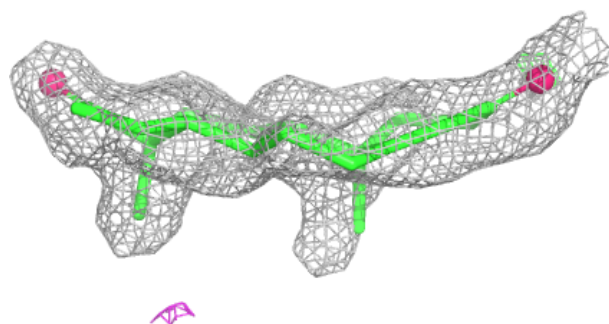
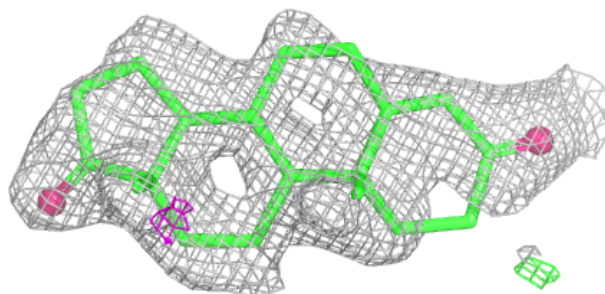


Electron density around GSH B 1223:

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

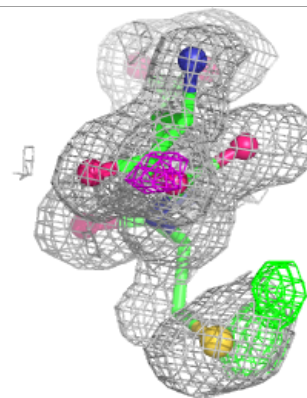
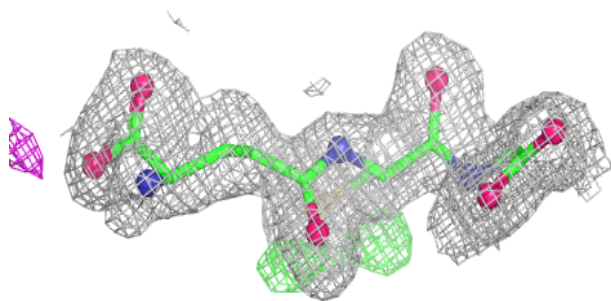
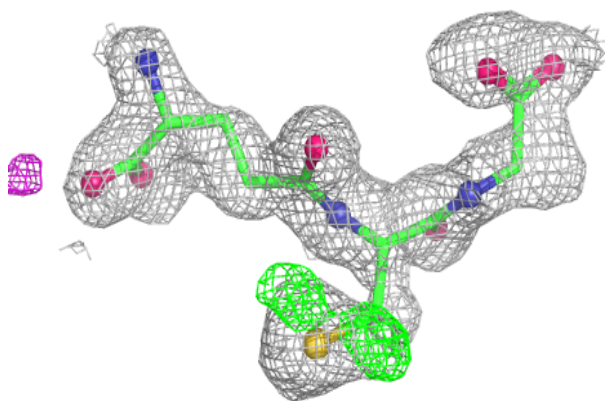
**Electron density around ASD K 1224:**

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

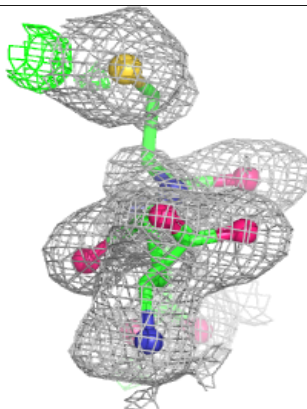
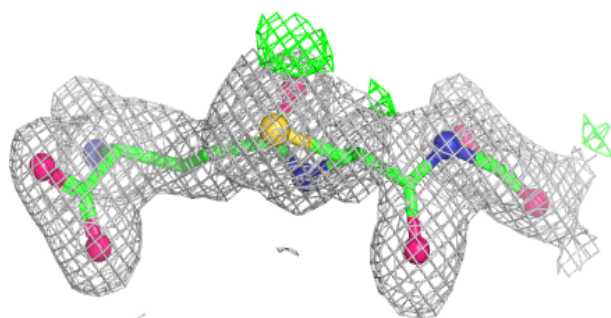
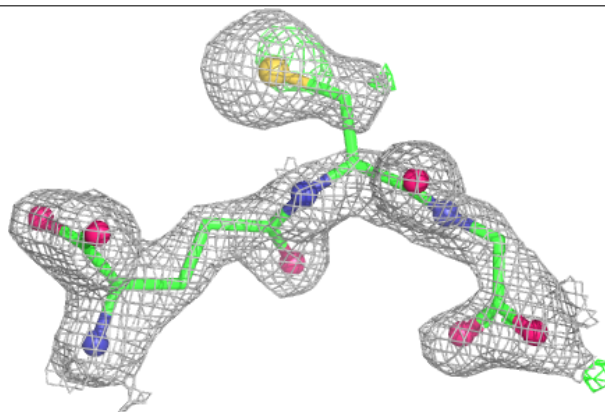


Electron density around GSH M 1223:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.