



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID : 6NB1 / pdb_00006nb1
Title : Crystal structure of Escherichia coli ClpP protease complexed with small molecule activator, ACP1-06
Authors : Mabanglo, M.F.; Houry, W.A.; Eger, B.T.; Bryson, S.; Pai, E.F.
Deposited on : 2018-12-06
Resolution : 1.90 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

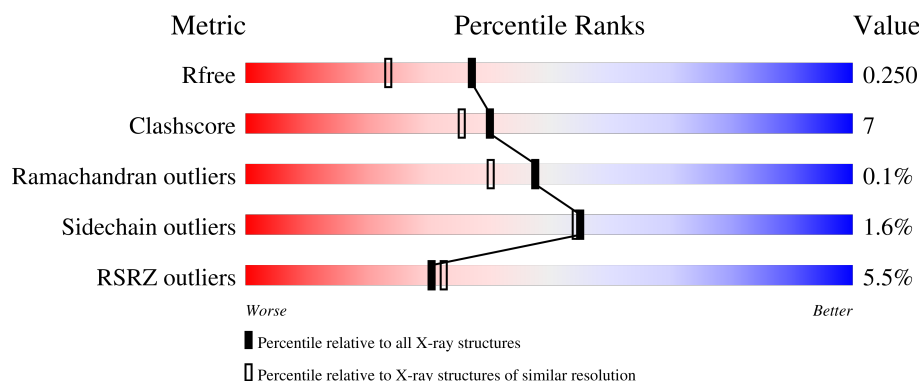
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	207	7% 77% 13% • 9%
1	B	207	5% 79% 14% 7%
1	C	207	7% 76% 12% 11%
1	D	207	7% 76% 12% 11%
1	E	207	2% 79% 10% • 10%

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Mol	Chain	Length	Quality of chain
1	F	207	
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	

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	KHS	N	301[A]	-	-	-	X
2	KHS	N	301[B]	-	-	-	X

2 Entry composition

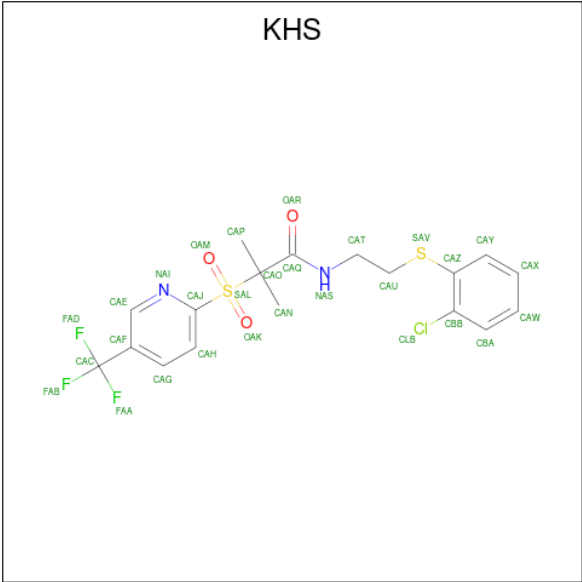
There are 4 unique types of molecules in this entry. The entry contains 21848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit.

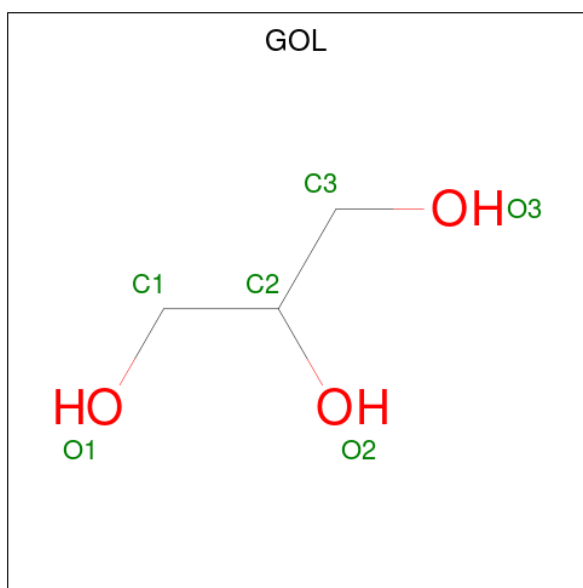
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1472	930	253	277	12			
1	B	193	Total	C	N	O	S	0	0	0
			1509	950	262	285	12			
1	C	184	Total	C	N	O	S	0	0	0
			1441	910	247	272	12			
1	D	184	Total	C	N	O	S	0	0	0
			1442	910	249	271	12			
1	E	186	Total	C	N	O	S	0	0	0
			1458	922	251	273	12			
1	F	183	Total	C	N	O	S	0	0	0
			1429	905	245	267	12			
1	G	183	Total	C	N	O	S	0	0	0
			1428	903	245	268	12			
1	H	181	Total	C	N	O	S	0	0	0
			1416	896	243	265	12			
1	I	176	Total	C	N	O	S	0	0	0
			1376	867	238	260	11			
1	J	180	Total	C	N	O	S	0	0	0
			1403	885	242	264	12			
1	K	181	Total	C	N	O	S	0	0	0
			1413	893	243	265	12			
1	L	182	Total	C	N	O	S	0	0	0
			1424	902	244	266	12			
1	M	180	Total	C	N	O	S	0	0	0
			1409	891	242	264	12			
1	N	180	Total	C	N	O	S	0	0	0
			1409	891	242	264	12			

- Molecule 2 is N-{2-[(2-chlorophenyl)sulfanyl]ethyl}-2-methyl-2-{[5-(trifluoromethyl)pyridin-2-yl]sulfonyl}propanamide (CCD ID: KHS) (formula: C₁₈H₁₈ClF₃N₂O₃S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	B	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	C	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	D	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	E	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	F	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	G	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	H	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	I	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	J	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	K	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	L	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	M	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		
2	N	1	Total	C	Cl	F	N	O	S	0	1
			58	36	2	6	4	6	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total	C	O	0	0
			6	3	3		

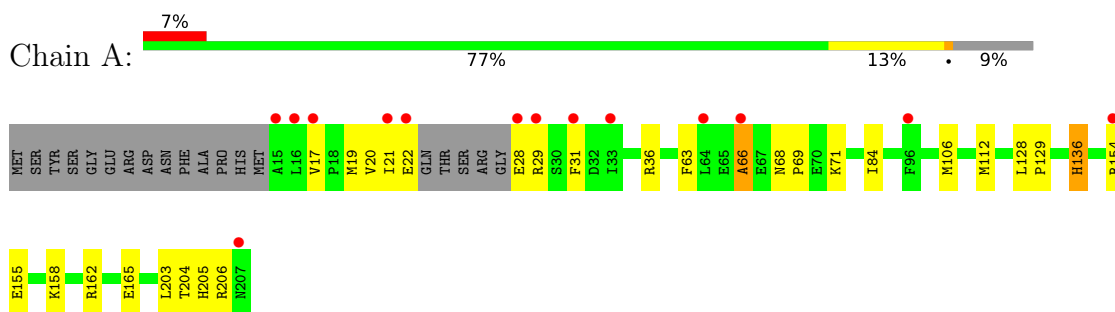
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	65	Total	O	0	0
			65	65		
4	C	44	Total	O	0	0
			44	44		
4	D	43	Total	O	0	0
			43	43		
4	E	64	Total	O	0	0
			64	64		
4	F	89	Total	O	0	0
			89	89		
4	G	90	Total	O	0	0
			90	90		
4	H	66	Total	O	0	0
			66	66		
4	I	61	Total	O	0	0
			61	61		
4	J	43	Total	O	0	0
			43	43		
4	K	55	Total	O	0	0
			55	55		
4	L	70	Total	O	0	0
			70	70		
4	M	89	Total	O	0	0
			89	89		
4	N	72	Total	O	0	0
			72	72		

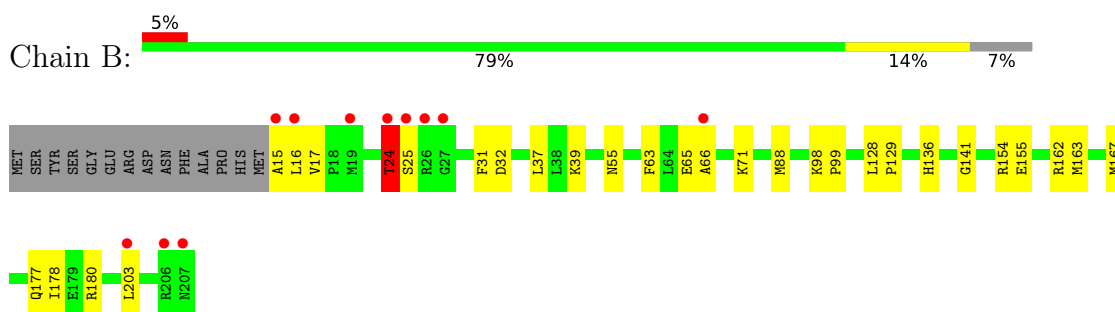
3 Residue-property plots [i](#)

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.

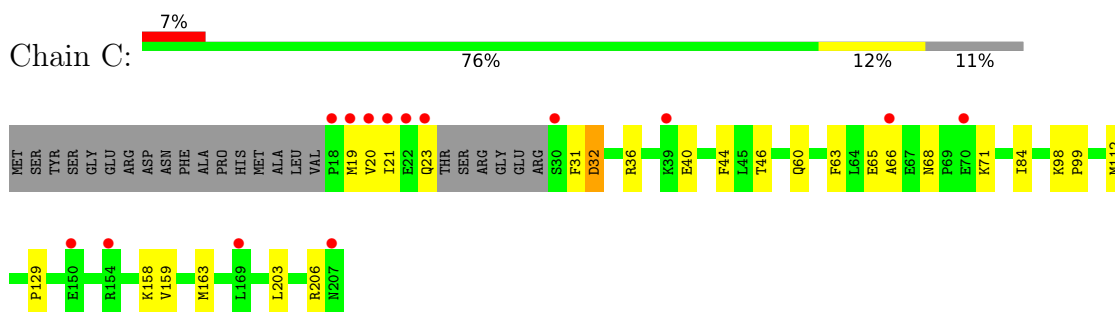
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



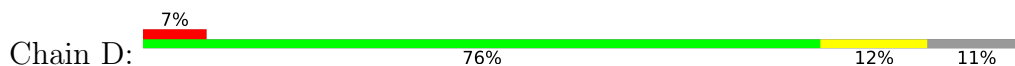
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



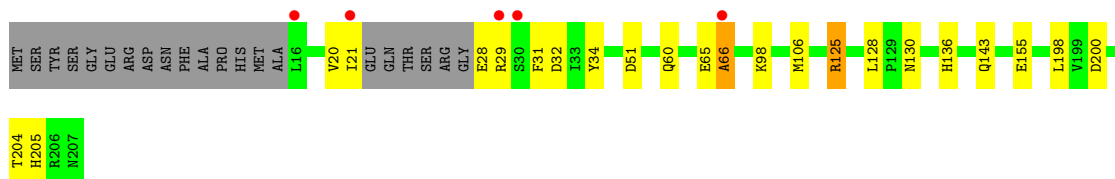
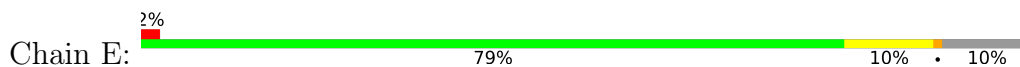
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



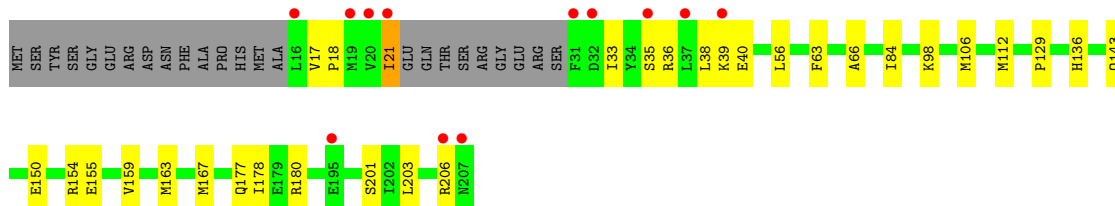
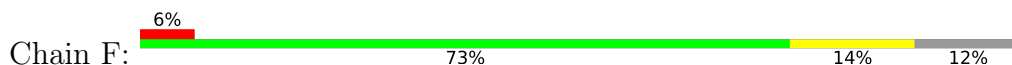
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



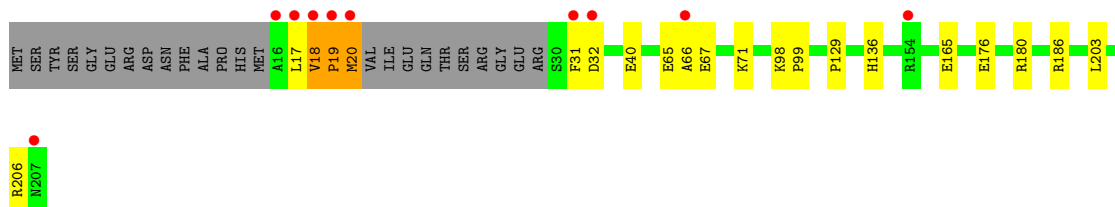
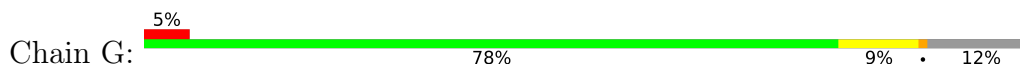
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



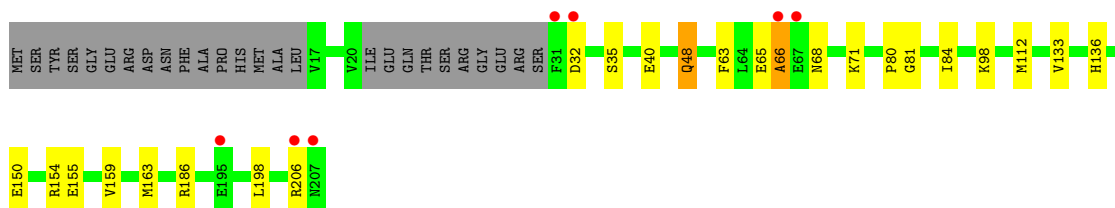
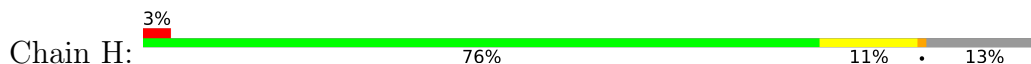
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



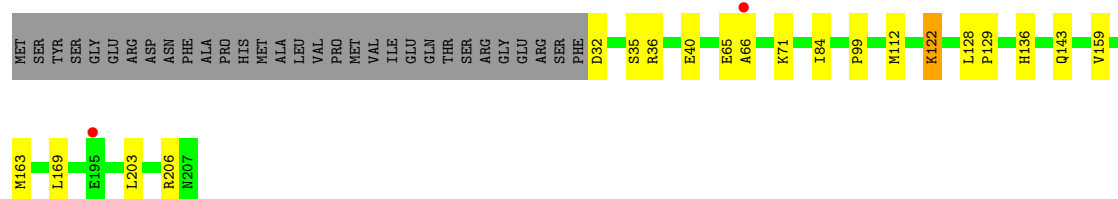
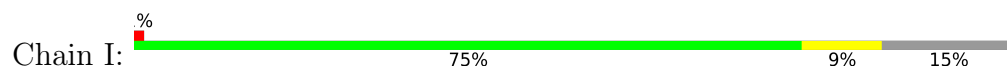
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



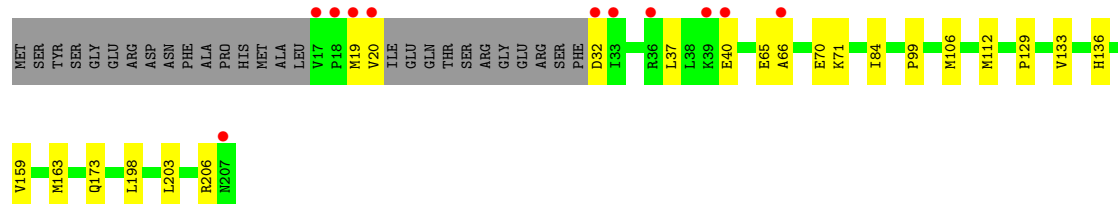
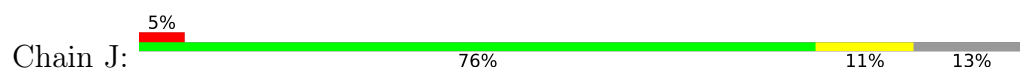
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



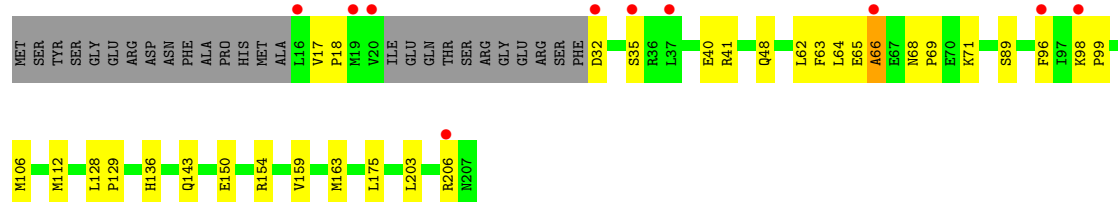
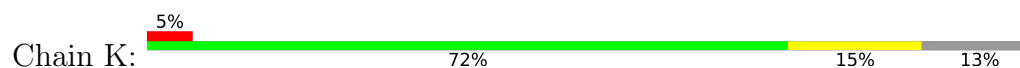
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



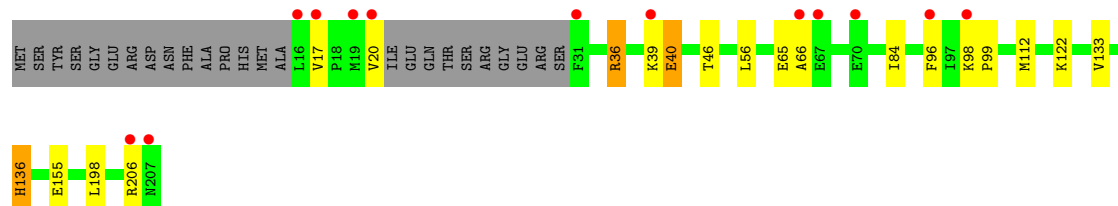
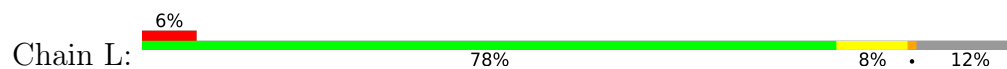
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



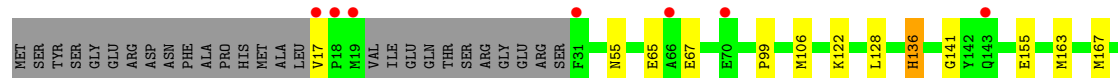
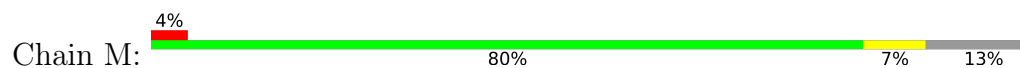
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

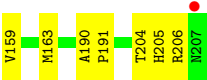
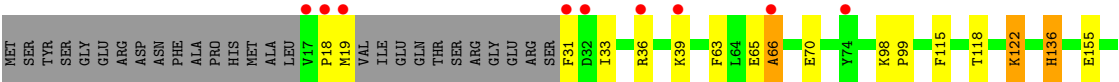
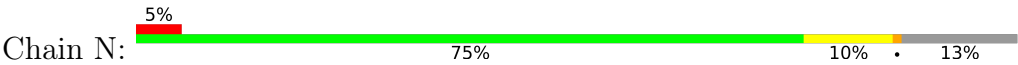


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





● Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.99Å 101.09Å 155.19Å 90.00° 98.29° 90.00°	Depositor
Resolution (Å)	48.00 – 1.90 48.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.00-1.90) 91.9 (48.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.209 , 0.244 0.218 , 0.250	Depositor DCC
R_{free} test set	11300 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21848	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	2/1495 (0.1%)	0.86	1/2013 (0.0%)
1	B	0.57	1/1533 (0.1%)	0.88	1/2065 (0.0%)
1	C	0.61	1/1464 (0.1%)	0.88	2/1970 (0.1%)
1	D	0.55	0/1465	0.87	1/1972 (0.1%)
1	E	0.66	2/1481 (0.1%)	0.88	5/1994 (0.3%)
1	F	0.63	2/1452 (0.1%)	0.89	1/1956 (0.1%)
1	G	0.58	2/1451 (0.1%)	0.83	3/1954 (0.2%)
1	H	0.66	2/1439 (0.1%)	0.87	1/1938 (0.1%)
1	I	0.56	2/1398 (0.1%)	0.82	0/1883
1	J	0.54	1/1425 (0.1%)	0.83	0/1919
1	K	0.65	1/1435 (0.1%)	0.89	4/1933 (0.2%)
1	L	0.68	2/1447 (0.1%)	0.83	2/1949 (0.1%)
1	M	0.57	1/1432 (0.1%)	0.83	2/1928 (0.1%)
1	N	0.64	2/1432 (0.1%)	0.82	1/1928 (0.1%)
All	All	0.61	21/20349 (0.1%)	0.86	24/27402 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66	ALA	CA-CB	-13.07	1.33	1.53
1	H	66	ALA	CA-CB	-12.47	1.34	1.53
1	L	66	ALA	CA-CB	-11.96	1.34	1.53
1	K	66	ALA	CA-CB	-11.86	1.34	1.53
1	C	66	ALA	CA-CB	-10.20	1.37	1.53
1	N	66	ALA	CA-CB	-9.81	1.38	1.53
1	A	66	ALA	CA-CB	-9.65	1.38	1.53
1	B	66	ALA	CA-CB	-9.09	1.39	1.53
1	I	66	ALA	CA-CB	-8.01	1.41	1.53
1	E	136	HIS	C-O	-6.97	1.16	1.23
1	H	136	HIS	C-O	-6.59	1.16	1.23
1	A	136	HIS	C-O	-6.57	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	136	HIS	C-O	-6.54	1.16	1.23
1	M	136	HIS	C-O	-6.39	1.16	1.23
1	G	66	ALA	CA-CB	-6.28	1.43	1.53
1	G	136	HIS	C-O	-6.02	1.17	1.23
1	N	136	HIS	C-O	-5.63	1.18	1.24
1	L	136	HIS	C-O	-5.59	1.17	1.23
1	F	66	ALA	CA-CB	-5.55	1.44	1.53
1	J	66	ALA	CA-CB	-5.33	1.45	1.53
1	I	136	HIS	C-O	-5.18	1.18	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	VAL	CA-C-N	-7.41	110.58	119.84
1	G	18	VAL	C-N-CA	-7.41	110.58	119.84
1	A	66	ALA	N-CA-C	7.22	118.84	110.97
1	H	66	ALA	N-CA-C	7.14	118.71	111.07
1	L	36	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	E	66	ALA	N-CA-C	6.81	118.36	111.07
1	C	32	ASP	N-CA-C	6.40	119.18	110.35
1	N	66	ALA	N-CA-C	6.05	117.54	111.07
1	G	32	ASP	N-CA-C	5.87	118.44	110.35
1	M	17	VAL	CA-C-N	5.77	125.70	119.76
1	M	17	VAL	C-N-CA	5.77	125.70	119.76
1	C	20	VAL	N-CA-C	5.76	116.16	107.75
1	D	48	GLN	CA-CB-CG	5.70	125.49	114.10
1	F	201	SER	N-CA-C	5.56	115.89	108.38
1	E	51	ASP	N-CA-C	5.56	117.78	111.11
1	K	17	VAL	CA-C-N	5.48	125.78	119.92
1	K	17	VAL	C-N-CA	5.48	125.78	119.92
1	K	66	ALA	N-CA-C	5.44	116.89	111.07
1	L	40	GLU	N-CA-C	-5.38	106.59	112.72
1	B	32	ASP	N-CA-C	-5.36	103.46	110.53
1	K	40	GLU	CA-CB-CG	-5.35	103.40	114.10
1	E	32	ASP	N-CA-C	-5.32	103.00	110.50
1	E	98	LYS	CA-C-N	-5.04	114.76	119.85
1	E	98	LYS	C-N-CA	-5.04	114.76	119.85

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	1472	0	1481	22	0
1	B	1509	0	1518	29	1
1	C	1441	0	1446	33	0
1	D	1442	0	1448	29	0
1	E	1458	0	1470	17	0
1	F	1429	0	1437	26	1
1	G	1428	0	1436	18	1
1	H	1416	0	1424	25	0
1	I	1376	0	1382	17	0
1	J	1403	0	1408	15	1
1	K	1413	0	1426	24	0
1	L	1424	0	1435	16	0
1	M	1409	0	1415	15	0
1	N	1409	0	1415	22	0
2	A	58	0	0	3	0
2	B	58	0	0	3	0
2	C	58	0	0	12	0
2	D	58	0	0	5	0
2	E	58	0	0	0	0
2	F	58	0	0	10	0
2	G	58	0	0	7	0
2	H	58	0	0	6	0
2	I	58	0	0	3	0
2	J	58	0	0	3	0
2	K	58	0	0	0	0
2	L	58	0	0	4	0
2	M	58	0	0	3	0
2	N	58	0	0	8	0
3	A	6	0	8	2	0
3	B	6	0	8	2	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
3	E	6	0	8	1	0
3	F	6	0	8	1	0
3	G	6	0	8	0	0
3	H	6	0	8	1	0
3	I	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	6	0	8	0	0
3	K	6	0	8	0	0
3	L	6	0	8	1	0
3	M	6	0	8	1	0
3	N	6	0	8	1	0
4	A	72	0	0	1	0
4	B	65	0	0	0	0
4	C	44	0	0	0	0
4	D	43	0	0	0	0
4	E	64	0	0	1	0
4	F	89	0	0	4	0
4	G	90	0	0	2	0
4	H	66	0	0	1	0
4	I	61	0	0	0	0
4	J	43	0	0	1	0
4	K	55	0	0	1	0
4	L	70	0	0	0	0
4	M	89	0	0	1	0
4	N	72	0	0	1	0
All	All	21848	0	20253	271	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (271) 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:N:206:ARG:NH1	2:N:301[B]:KHS:OAM	2.07	0.87
1:J:106:MET:HG2	1:K:89:SER:HB2	1.59	0.85
1:M:206:ARG:NH1	2:M:301[B]:KHS:OAM	2.11	0.83
1:D:36:ARG:NH1	1:D:40:GLU:OE2	2.11	0.83
1:D:206:ARG:NH1	2:D:301[A]:KHS:OAK	2.13	0.81
1:F:56:LEU:HD11	1:G:17:LEU:HD13	1.62	0.81
1:F:154:ARG:NH1	4:F:401:HOH:O	2.07	0.77
1:F:143:GLN:HG2	1:M:141:GLY:HA3	1.67	0.77
1:M:206:ARG:NH1	2:M:301[A]:KHS:OAK	2.18	0.76
1:D:48:GLN:HA	1:D:48:GLN:HE21	1.50	0.75
1:N:206:ARG:NH1	2:N:301[A]:KHS:OAK	2.18	0.75
1:K:143:GLN:NE2	4:K:401:HOH:O	2.20	0.74
1:B:177:GLN:OE1	1:B:180:ARG:NH2	2.19	0.74
1:F:206:ARG:NH2	2:F:301[A]:KHS:OAK	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:NH1	2:D:301[B]:KHS:OAM	2.21	0.73
1:H:186:ARG:NH1	4:H:401:HOH:O	2.22	0.73
1:H:63:PHE:O	1:H:66:ALA:HB3	1.89	0.72
1:F:155:GLU:OE2	3:F:302:GOL:O1	2.07	0.72
1:I:206:ARG:NH1	2:I:301[A]:KHS:OAK	2.21	0.71
1:C:206:ARG:NH1	2:C:301[B]:KHS:OAM	2.23	0.71
1:I:36:ARG:NH2	1:I:40:GLU:OE2	2.25	0.70
1:A:206:ARG:NH1	2:A:301[A]:KHS:OAK	2.19	0.69
1:B:162:ARG:HH11	1:B:163:MET:HE3	1.57	0.69
1:H:206:ARG:NH1	2:H:301[A]:KHS:OAK	2.24	0.69
1:G:206:ARG:NH1	2:G:301[A]:KHS:OAK	2.25	0.68
1:N:206:ARG:HH22	2:N:301[B]:KHS:CAH	2.07	0.68
1:F:177:GLN:NE2	4:F:402:HOH:O	2.26	0.68
1:D:155:GLU:OE2	3:D:302:GOL:O1	2.12	0.68
1:G:206:ARG:NH1	2:G:301[B]:KHS:OAM	2.23	0.68
1:H:206:ARG:NH1	2:H:301[B]:KHS:OAM	2.26	0.66
1:D:204:THR:HG22	1:D:205:HIS:ND1	2.10	0.66
1:F:40:GLU:HG3	2:F:301[B]:KHS:CAZ	2.25	0.66
1:F:40:GLU:HG3	2:F:301[A]:KHS:CAZ	2.26	0.65
1:E:143:GLN:NE2	4:E:402:HOH:O	2.28	0.64
1:C:158:LYS:HD2	3:C:302:GOL:H11	1.79	0.64
1:A:63:PHE:O	1:A:66:ALA:HB3	1.98	0.63
1:D:48:GLN:NE2	1:D:80:PRO:HG2	2.13	0.63
1:M:155:GLU:OE2	3:M:302:GOL:H11	1.98	0.63
1:H:65:GLU:CD	1:N:206:ARG:HH21	2.07	0.61
1:C:206:ARG:NH1	2:C:301[A]:KHS:OAK	2.34	0.61
1:K:150:GLU:OE2	1:K:154:ARG:NH2	2.35	0.60
1:L:206:ARG:HH22	2:L:301[B]:KHS:CAH	2.14	0.60
1:H:65:GLU:OE1	1:N:206:ARG:NH2	2.24	0.59
1:D:84:ILE:HA	1:D:112:MET:HE3	1.84	0.59
1:D:206:ARG:HG2	1:D:207:ASN:H	1.68	0.58
1:C:206:ARG:HH22	2:C:301[B]:KHS:CAH	2.16	0.58
1:J:206:ARG:NH1	2:J:301[A]:KHS:OAK	2.26	0.58
1:N:65:GLU:HG3	1:N:99:PRO:HD3	1.85	0.58
1:M:206:ARG:HG3	1:M:206:ARG:HH11	1.68	0.58
1:C:63:PHE:HA	2:D:301[B]:KHS:CLB	2.41	0.58
1:I:206:ARG:NH1	2:I:301[B]:KHS:OAM	2.25	0.58
1:B:167:MET:HG2	1:B:178:ILE:HD12	1.86	0.57
1:M:163:MET:HE3	4:M:483:HOH:O	2.04	0.57
1:D:204:THR:C	1:D:205:HIS:HD1	2.12	0.57
1:B:65:GLU:HG3	1:B:99:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:ARG:NH1	2:L:301[A]:KHS:OAK	2.37	0.57
1:D:31:PHE:CE2	1:D:36:ARG:HD3	2.39	0.57
1:A:155:GLU:OE1	3:A:302:GOL:O3	2.18	0.56
1:K:69:PRO:O	1:K:98:LYS:HG3	2.05	0.56
1:F:150:GLU:HG3	4:F:401:HOH:O	2.04	0.56
1:B:55:ASN:ND2	1:C:46:THR:OG1	2.39	0.56
1:N:206:ARG:HG3	1:N:206:ARG:HH11	1.71	0.56
1:B:31:PHE:CZ	1:B:39:LYS:HE2	2.41	0.56
1:F:206:ARG:NH2	2:F:301[A]:KHS:SAL	2.78	0.55
1:I:206:ARG:HG3	1:I:206:ARG:HH11	1.72	0.55
1:A:31:PHE:CE1	1:A:36:ARG:HD3	2.42	0.55
1:C:63:PHE:HA	2:D:301[A]:KHS:CLB	2.42	0.55
1:A:17:VAL:HG21	1:B:15:ALA:HA	1.88	0.55
1:F:180:ARG:NE	4:F:403:HOH:O	2.34	0.55
1:G:206:ARG:HH22	2:G:301[B]:KHS:CAH	2.20	0.55
1:D:204:THR:HG22	1:D:205:HIS:HD1	1.71	0.55
1:D:206:ARG:HH22	2:D:301[B]:KHS:CAH	2.20	0.54
1:C:23:GLN:HE22	1:C:31:PHE:HB2	1.71	0.54
1:E:29:ARG:HD3	1:F:21:ILE:HD12	1.88	0.54
1:K:68:ASN:ND2	1:K:71:LYS:HE2	2.23	0.54
1:A:206:ARG:HD2	1:G:98:LYS:HE3	1.88	0.54
1:C:60:GLN:HA	1:D:33:ILE:HD11	1.89	0.53
1:B:15:ALA:O	1:B:17:VAL:N	2.41	0.53
1:N:19:MET:HE2	1:N:31:PHE:N	2.23	0.53
1:H:32:ASP:OD1	1:H:35:SER:N	2.33	0.53
1:M:206:ARG:NH1	1:M:206:ARG:HG3	2.24	0.53
1:N:155:GLU:OE2	3:N:302:GOL:H11	2.09	0.53
1:B:155:GLU:OE2	3:B:302:GOL:H11	2.08	0.53
1:C:65:GLU:HG3	1:C:99:PRO:HD3	1.90	0.53
1:G:176:GLU:OE2	1:G:180:ARG:NH2	2.42	0.53
1:C:40:GLU:HG3	2:C:301[B]:KHS:CAY	2.38	0.53
1:K:65:GLU:HG3	1:K:99:PRO:HD3	1.92	0.52
1:M:106:MET:HB3	1:M:128:LEU:HD22	1.92	0.52
1:E:155:GLU:OE2	3:E:302:GOL:O3	2.28	0.51
1:L:36:ARG:NH1	1:L:39:LYS:HE2	2.24	0.51
1:H:48:GLN:OE1	1:H:80:PRO:HG2	2.10	0.51
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.75	0.51
1:A:66:ALA:HB2	2:B:301[A]:KHS:CAZ	2.40	0.51
1:B:63:PHE:HD1	2:C:301[B]:KHS:CLB	2.31	0.51
1:J:206:ARG:NH1	2:J:301[B]:KHS:OAM	2.34	0.51
1:J:206:ARG:HE	1:K:65:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:O	1:C:32:ASP:HA	2.11	0.50
1:L:206:ARG:NH1	2:L:301[B]:KHS:OAM	2.41	0.50
1:L:206:ARG:HE	1:M:65:GLU:CD	2.19	0.50
1:L:65:GLU:HG3	1:L:99:PRO:HD3	1.93	0.50
1:A:66:ALA:HB2	2:B:301[B]:KHS:CAZ	2.41	0.50
1:H:155:GLU:OE1	3:H:302:GOL:O1	2.27	0.50
1:B:136:HIS:C	1:B:136:HIS:CD2	2.90	0.50
1:H:159:VAL:O	1:H:163:MET:HG2	2.11	0.50
1:D:100:ASP:OD2	1:D:124:LYS:NZ	2.43	0.49
1:L:84:ILE:HA	1:L:112:MET:HE3	1.94	0.49
1:C:98:LYS:HE3	1:D:206:ARG:HD2	1.95	0.49
1:I:206:ARG:HE	1:J:65:GLU:CD	2.20	0.49
1:A:204:THR:HG22	1:A:205:HIS:CD2	2.48	0.49
1:B:63:PHE:HA	2:C:301[A]:KHS:CLB	2.50	0.49
1:I:129:PRO:HD3	1:I:203:LEU:O	2.13	0.49
1:C:23:GLN:HG2	1:D:30:SER:HB2	1.94	0.49
1:K:206:ARG:HG3	1:L:65:GLU:OE1	2.13	0.49
1:A:22:GLU:HG2	1:A:29:ARG:NH2	2.28	0.48
1:B:24:THR:O	1:B:25:SER:HB3	2.12	0.48
1:C:40:GLU:HG3	2:C:301[A]:KHS:CAZ	2.44	0.48
1:M:167:MET:HG2	1:M:178:ILE:HD12	1.94	0.48
1:E:65:GLU:OE1	1:F:206:ARG:HD2	2.14	0.48
1:K:68:ASN:HD22	1:K:71:LYS:HE2	1.77	0.48
1:A:162:ARG:NH2	1:A:165:GLU:OE1	2.46	0.48
1:N:136:HIS:C	1:N:136:HIS:CD2	2.91	0.48
1:F:84:ILE:HA	1:F:112:MET:HE3	1.95	0.48
1:L:133:VAL:HG11	1:L:198:LEU:HD13	1.94	0.48
1:A:206:ARG:NH1	2:A:301[B]:KHS:OAM	2.28	0.48
1:F:167:MET:HG2	1:F:178:ILE:HD12	1.95	0.47
1:K:159:VAL:O	1:K:163:MET:HG2	2.14	0.47
1:C:40:GLU:HG3	2:C:301[A]:KHS:CAY	2.43	0.47
1:C:206:ARG:HH12	2:C:301[B]:KHS:CAJ	2.27	0.47
1:F:40:GLU:HG3	2:F:301[A]:KHS:CBB	2.44	0.47
1:N:18:PRO:HG2	1:N:33:ILE:HB	1.96	0.47
1:F:206:ARG:NH2	2:F:301[B]:KHS:OAM	2.47	0.47
1:B:31:PHE:CE2	1:B:39:LYS:HE2	2.50	0.47
1:B:63:PHE:HA	2:C:301[B]:KHS:CLB	2.50	0.47
1:B:65:GLU:OE1	1:C:206:ARG:NH2	2.39	0.47
1:H:68:ASN:ND2	1:H:71:LYS:HD3	2.30	0.47
1:M:206:ARG:HH22	2:M:301[B]:KHS:CAH	2.27	0.47
1:A:136:HIS:C	1:A:136:HIS:CD2	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLY:HA3	1:I:143:GLN:HG2	1.98	0.46
1:I:206:ARG:HH22	2:I:301[B]:KHS:CAH	2.28	0.46
1:J:32:ASP:N	4:J:403:HOH:O	2.48	0.46
1:H:40:GLU:HG3	2:H:301[A]:KHS:CBB	2.45	0.46
1:K:206:ARG:HD3	1:L:96:PHE:CE2	2.50	0.46
1:G:65:GLU:HG3	1:G:99:PRO:HD3	1.97	0.46
1:H:206:ARG:HH22	2:H:301[B]:KHS:CAH	2.28	0.46
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.81	0.46
1:H:206:ARG:HE	1:I:65:GLU:CD	2.22	0.46
1:K:63:PHE:O	1:K:66:ALA:HB3	2.15	0.46
1:D:55:ASN:ND2	1:E:34:TYR:CE1	2.84	0.46
1:E:66:ALA:HB1	2:F:301[B]:KHS:CAZ	2.46	0.46
1:N:159:VAL:O	1:N:163:MET:HG2	2.15	0.46
1:B:162:ARG:NH2	3:B:302:GOL:O1	2.48	0.46
1:C:159:VAL:O	1:C:163:MET:HG2	2.16	0.46
1:D:55:ASN:ND2	1:E:34:TYR:HE1	2.14	0.46
1:H:150:GLU:OE2	1:H:154:ARG:HD3	2.15	0.46
1:J:84:ILE:HA	1:J:112:MET:HE3	1.96	0.46
1:G:40:GLU:HG3	2:G:301[B]:KHS:CAY	2.46	0.45
1:G:20:MET:HE3	1:G:20:MET:HB2	1.64	0.45
1:D:112:MET:HE1	1:D:163:MET:HE2	1.97	0.45
1:K:18:PRO:HD2	1:L:56:LEU:HD11	1.97	0.45
1:D:31:PHE:HE2	1:D:36:ARG:HD3	1.79	0.45
1:D:190:ALA:HB3	1:D:191:PRO:HD3	1.99	0.45
1:I:206:ARG:NH1	1:I:206:ARG:HG3	2.31	0.45
1:E:29:ARG:HB2	1:F:21:ILE:HD12	1.97	0.45
1:F:36:ARG:O	1:F:39:LYS:HB2	2.16	0.45
1:H:66:ALA:HB2	2:N:301[B]:KHS:CAZ	2.47	0.45
1:A:84:ILE:HA	1:A:112:MET:HE3	1.98	0.45
1:C:21:ILE:HD13	1:C:36:ARG:NH1	2.32	0.45
1:L:46:THR:OG1	1:M:55:ASN:ND2	2.50	0.45
1:M:136:HIS:CD2	1:M:136:HIS:C	2.95	0.45
1:H:66:ALA:HB2	2:N:301[A]:KHS:CAZ	2.47	0.44
1:E:204:THR:HG22	1:E:205:HIS:CD2	2.52	0.44
1:H:66:ALA:HB1	2:N:301[A]:KHS:CBA	2.47	0.44
1:H:133:VAL:HG11	1:H:198:LEU:HD13	1.99	0.44
1:K:206:ARG:HD2	1:K:206:ARG:HA	1.77	0.44
1:C:40:GLU:HG3	2:C:301[B]:KHS:CAZ	2.47	0.44
1:J:37:LEU:HD23	1:J:37:LEU:HA	1.78	0.44
1:N:122:LYS:HG3	4:N:401:HOH:O	2.16	0.44
1:M:206:ARG:HD2	1:N:98:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASN:HD21	1:C:44:PHE:HB3	1.82	0.44
1:G:40:GLU:HG3	2:G:301[B]:KHS:CAZ	2.48	0.44
1:C:129:PRO:HD3	1:C:203:LEU:O	2.18	0.44
1:J:71:LYS:O	1:J:99:PRO:HB3	2.18	0.44
1:J:203:LEU:HB3	1:K:96:PHE:CE1	2.53	0.44
1:G:129:PRO:HD3	1:G:203:LEU:O	2.18	0.44
1:I:65:GLU:HG3	1:I:99:PRO:HD3	2.00	0.44
1:K:18:PRO:HD3	1:L:56:LEU:HD21	2.00	0.44
1:K:136:HIS:CD2	1:K:136:HIS:C	2.95	0.44
1:E:125:ARG:HD3	1:E:200:ASP:OD2	2.18	0.43
1:I:32:ASP:HB2	1:I:35:SER:HB2	1.99	0.43
1:K:41:ARG:HA	1:K:64:LEU:CD1	2.48	0.43
1:B:98:LYS:HE3	1:C:206:ARG:HG3	1.99	0.43
1:D:206:ARG:NH1	1:D:206:ARG:HG3	2.32	0.43
1:N:206:ARG:NH1	1:N:206:ARG:HG3	2.32	0.43
1:F:129:PRO:HD3	1:F:203:LEU:O	2.19	0.43
1:G:40:GLU:HG3	2:G:301[A]:KHS:CAZ	2.49	0.43
1:I:159:VAL:O	1:I:163:MET:HG2	2.17	0.43
1:I:122:LYS:HE2	1:I:122:LYS:HB2	1.83	0.43
1:C:158:LYS:HE3	1:C:158:LYS:HB2	1.72	0.43
1:F:35:SER:O	1:F:38:LEU:HB3	2.18	0.43
1:J:206:ARG:HH22	2:J:301[B]:KHS:CAH	2.32	0.43
1:B:24:THR:HB	1:B:25:SER:H	1.65	0.43
1:E:66:ALA:HB1	2:F:301[A]:KHS:CAZ	2.48	0.43
1:K:41:ARG:HA	1:K:64:LEU:HD13	2.01	0.43
1:A:158:LYS:HD2	3:A:302:GOL:O3	2.18	0.42
1:F:159:VAL:O	1:F:163:MET:HG2	2.19	0.42
1:A:71:LYS:HG2	4:A:455:HOH:O	2.18	0.42
1:G:71:LYS:O	1:G:99:PRO:HB3	2.19	0.42
1:B:129:PRO:HD3	1:B:203:LEU:O	2.19	0.42
1:C:71:LYS:O	1:C:99:PRO:HB3	2.20	0.42
1:H:66:ALA:HB1	2:N:301[B]:KHS:CBA	2.49	0.42
1:K:129:PRO:HD3	1:K:203:LEU:O	2.19	0.42
1:N:115:PHE:O	1:N:118:THR:HG22	2.20	0.42
1:F:63:PHE:HD1	2:G:301[B]:KHS:CLB	2.39	0.42
1:I:84:ILE:HA	1:I:112:MET:HE3	2.01	0.42
1:D:71:LYS:O	1:D:99:PRO:HB3	2.20	0.42
1:F:17:VAL:HA	1:F:18:PRO:HD3	1.84	0.42
1:J:159:VAL:O	1:J:163:MET:HG2	2.20	0.42
1:B:162:ARG:HE	1:B:163:MET:CE	2.33	0.42
1:J:129:PRO:HD3	1:J:203:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:HIS:CD2	1:L:136:HIS:C	2.98	0.42
1:L:155:GLU:OE1	3:L:302:GOL:H11	2.20	0.42
1:N:204:THR:HG22	1:N:205:HIS:CE1	2.55	0.42
1:B:98:LYS:HE3	1:C:206:ARG:CG	2.49	0.42
1:C:68:ASN:ND2	1:C:71:LYS:HE2	2.35	0.42
1:C:206:ARG:NH1	2:C:301[A]:KHS:SAL	2.90	0.42
1:E:66:ALA:CB	2:F:301[B]:KHS:CAZ	2.98	0.42
1:B:31:PHE:CD2	1:C:21:ILE:HG22	2.55	0.41
1:D:206:ARG:HG2	1:D:207:ASN:N	2.34	0.41
1:F:98:LYS:HE3	1:F:98:LYS:HB2	1.82	0.41
1:E:60:GLN:HA	1:F:33:ILE:HD11	2.02	0.41
1:G:18:VAL:N	4:G:401:HOH:O	2.30	0.41
1:G:18:VAL:N	1:G:19:PRO:HD3	2.35	0.41
1:H:48:GLN:HG3	1:H:81:GLY:O	2.20	0.41
1:H:40:GLU:HG3	2:H:301[B]:KHS:CAZ	2.50	0.41
1:H:84:ILE:HA	1:H:112:MET:HE3	2.02	0.41
1:A:68:ASN:HA	1:A:69:PRO:HD2	1.97	0.41
1:A:106:MET:HB3	1:A:128:LEU:HD12	2.00	0.41
1:K:62:LEU:HA	1:K:62:LEU:HD23	1.78	0.41
1:E:29:ARG:HG3	1:E:31:PHE:CE1	2.55	0.41
1:I:128:LEU:HD23	1:I:128:LEU:HA	1.90	0.41
1:N:63:PHE:O	1:N:66:ALA:HB3	2.20	0.41
1:B:37:LEU:HD23	2:B:301[A]:KHS:CLB	2.58	0.41
1:E:106:MET:HB3	1:E:128:LEU:HD12	2.01	0.41
1:G:206:ARG:HG3	1:G:206:ARG:HH11	1.86	0.41
1:H:40:GLU:HG3	2:H:301[B]:KHS:CBB	2.51	0.41
1:H:66:ALA:HB1	2:N:301[B]:KHS:CAW	2.51	0.41
1:K:112:MET:HE1	1:K:163:MET:HE1	2.03	0.41
1:M:65:GLU:HG3	1:M:99:PRO:HD3	2.03	0.41
1:C:65:GLU:CD	1:D:206:ARG:HE	2.27	0.41
1:J:133:VAL:HG11	1:J:198:LEU:HD13	2.03	0.41
1:B:71:LYS:O	1:B:99:PRO:HB3	2.21	0.41
1:D:133:VAL:HG11	1:D:198:LEU:HD13	2.02	0.41
1:K:32:ASP:OD2	1:K:35:SER:N	2.43	0.41
1:N:190:ALA:HB3	1:N:191:PRO:HD3	2.03	0.41
1:A:129:PRO:HD3	1:A:203:LEU:O	2.20	0.41
1:G:186:ARG:HD3	4:G:428:HOH:O	2.20	0.41
1:I:71:LYS:O	1:I:99:PRO:HB3	2.20	0.41
1:A:19:MET:HE3	1:A:19:MET:HB3	1.97	0.40
1:C:84:ILE:HA	1:C:112:MET:HE3	2.03	0.40
1:J:136:HIS:C	1:J:136:HIS:CD2	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:MET:HB3	1:K:128:LEU:HD12	2.04	0.40
1:N:36:ARG:HD2	1:N:39:LYS:HD3	2.02	0.40
1:N:36:ARG:O	1:N:39:LYS:HB2	2.21	0.40
1:B:88:MET:SD	1:B:163:MET:HE1	2.61	0.40
1:N:31:PHE:HE1	1:N:36:ARG:HB2	1.86	0.40
1:A:21:ILE:HG13	1:G:31:PHE:CD2	2.56	0.40
1:A:206:ARG:HH22	2:A:301[B]:KHS:CAH	2.35	0.40
1:D:162:ARG:NH2	1:E:130:ASN:OD1	2.54	0.40
1:L:40:GLU:HG3	2:L:301[A]:KHS:CBB	2.52	0.40
1:C:23:GLN:OE1	1:C:23:GLN:N	2.55	0.40
1:E:66:ALA:CB	2:F:301[A]:KHS:CAZ	3.00	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ARG:NH1	1:G:165:GLU:OE2[4_645]	2.06	0.14
1:B:154:ARG:NH2	1:J:173:GLN:O[4_656]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	184/207 (89%)	181 (98%)	3 (2%)	0	100	100
1	B	191/207 (92%)	185 (97%)	4 (2%)	2 (1%)	12	5
1	C	180/207 (87%)	175 (97%)	5 (3%)	0	100	100
1	D	180/207 (87%)	177 (98%)	3 (2%)	0	100	100
1	E	182/207 (88%)	180 (99%)	2 (1%)	0	100	100
1	F	179/207 (86%)	177 (99%)	2 (1%)	0	100	100
1	G	179/207 (86%)	174 (97%)	4 (2%)	1 (1%)	21	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	177/207 (86%)	174 (98%)	3 (2%)	0	100	100
1	I	174/207 (84%)	171 (98%)	3 (2%)	0	100	100
1	J	176/207 (85%)	173 (98%)	3 (2%)	0	100	100
1	K	177/207 (86%)	175 (99%)	2 (1%)	0	100	100
1	L	178/207 (86%)	175 (98%)	3 (2%)	0	100	100
1	M	176/207 (85%)	174 (99%)	2 (1%)	0	100	100
1	N	176/207 (85%)	174 (99%)	2 (1%)	0	100	100
All	All	2509/2898 (87%)	2465 (98%)	41 (2%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	LEU
1	B	24	THR
1	G	19	PRO

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	159/175 (91%)	156 (98%)	3 (2%)	50	47
1	B	163/175 (93%)	162 (99%)	1 (1%)	78	81
1	C	156/175 (89%)	156 (100%)	0	100	100
1	D	156/175 (89%)	153 (98%)	3 (2%)	50	47
1	E	158/175 (90%)	153 (97%)	5 (3%)	34	27
1	F	154/175 (88%)	152 (99%)	2 (1%)	61	61
1	G	154/175 (88%)	152 (99%)	2 (1%)	61	61
1	H	153/175 (87%)	151 (99%)	2 (1%)	61	61
1	I	148/175 (85%)	146 (99%)	2 (1%)	59	59
1	J	151/175 (86%)	147 (97%)	4 (3%)	40	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	153/175 (87%)	151 (99%)	2 (1%)	61	61
1	L	154/175 (88%)	150 (97%)	4 (3%)	40	35
1	M	152/175 (87%)	150 (99%)	2 (1%)	61	61
1	N	152/175 (87%)	150 (99%)	2 (1%)	61	61
All	All	2163/2450 (88%)	2129 (98%)	34 (2%)	55	54

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	28	GLU
1	A	154	ARG
1	B	24	THR
1	D	39	LYS
1	D	48	GLN
1	D	207	ASN
1	E	20	VAL
1	E	21	ILE
1	E	28	GLU
1	E	125	ARG
1	E	198	LEU
1	F	21	ILE
1	F	106	MET
1	G	20	MET
1	G	67	GLU
1	H	48	GLN
1	H	98	LYS
1	I	122	LYS
1	I	169	LEU
1	J	19	MET
1	J	20	VAL
1	J	40	GLU
1	J	70	GLU
1	K	48	GLN
1	K	175	LEU
1	L	17	VAL
1	L	20	VAL
1	L	98	LYS
1	L	122	LYS
1	M	67	GLU
1	M	122	LYS

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Mol	Chain	Res	Type
1	N	70	GLU
1	N	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	95	GLN
1	A	177	GLN
1	B	55	ASN
1	B	205	HIS
1	C	108	GLN
1	C	177	GLN
1	D	48	GLN
1	D	177	GLN
1	E	48	GLN
1	E	52	HIS
1	F	177	GLN
1	F	207	ASN
1	G	52	HIS
1	H	205	HIS
1	J	55	ASN
1	J	60	GLN
1	K	108	GLN
1	K	177	GLN
1	K	205	HIS
1	L	55	ASN
1	M	55	ASN
1	M	108	GLN
1	M	205	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

42 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	GOL	J	302	-	5,5,5	0.48	0	5,5,5	0.72	0
2	KHS	J	301[B]	-	29,30,30	2.86	6 (20%)	32,45,45	2.54	5 (15%)
3	GOL	I	302	-	5,5,5	0.55	0	5,5,5	0.37	0
2	KHS	N	301[A]	-	29,30,30	2.89	5 (17%)	32,45,45	2.07	4 (12%)
2	KHS	I	301[A]	-	29,30,30	2.95	6 (20%)	32,45,45	2.20	6 (18%)
3	GOL	B	302	-	5,5,5	0.41	0	5,5,5	0.34	0
3	GOL	K	302	-	5,5,5	0.41	0	5,5,5	0.49	0
2	KHS	G	301[A]	-	29,30,30	3.12	6 (20%)	32,45,45	2.09	6 (18%)
2	KHS	H	301[A]	-	29,30,30	2.87	6 (20%)	32,45,45	2.19	6 (18%)
2	KHS	L	301[A]	-	29,30,30	2.96	7 (24%)	32,45,45	2.20	6 (18%)
2	KHS	F	301[B]	-	29,30,30	2.67	5 (17%)	32,45,45	2.51	7 (21%)
2	KHS	M	301[B]	-	29,30,30	2.80	5 (17%)	32,45,45	2.32	5 (15%)
2	KHS	I	301[B]	-	29,30,30	2.85	5 (17%)	32,45,45	2.41	5 (15%)
2	KHS	C	301[A]	-	29,30,30	3.02	7 (24%)	32,45,45	2.10	6 (18%)
2	KHS	B	301[A]	-	29,30,30	3.02	5 (17%)	32,45,45	2.27	6 (18%)
2	KHS	K	301[A]	-	29,30,30	2.92	5 (17%)	32,45,45	2.21	5 (15%)
2	KHS	N	301[B]	-	29,30,30	2.81	5 (17%)	32,45,45	2.59	5 (15%)
3	GOL	M	302	-	5,5,5	0.55	0	5,5,5	0.22	0
3	GOL	A	302	-	5,5,5	0.41	0	5,5,5	0.60	0
2	KHS	A	301[A]	-	29,30,30	2.96	7 (24%)	32,45,45	2.18	6 (18%)
3	GOL	F	302	-	5,5,5	0.61	0	5,5,5	0.46	0
2	KHS	G	301[B]	-	29,30,30	2.86	5 (17%)	32,45,45	2.61	7 (21%)
2	KHS	H	301[B]	-	29,30,30	2.79	5 (17%)	32,45,45	2.42	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KHS	L	301[B]	-	29,30,30	2.87	5 (17%)	32,45,45	2.53	6 (18%)
2	KHS	D	301[A]	-	29,30,30	2.96	6 (20%)	32,45,45	2.15	6 (18%)
2	KHS	E	301[A]	-	29,30,30	3.01	5 (17%)	32,45,45	2.19	5 (15%)
2	KHS	B	301[B]	-	29,30,30	2.88	6 (20%)	32,45,45	2.52	5 (15%)
2	KHS	C	301[B]	-	29,30,30	2.79	5 (17%)	32,45,45	2.52	6 (18%)
2	KHS	K	301[B]	-	29,30,30	2.87	5 (17%)	32,45,45	2.56	5 (15%)
3	GOL	H	302	-	5,5,5	0.40	0	5,5,5	0.26	0
3	GOL	L	302	-	5,5,5	0.42	0	5,5,5	0.10	0
2	KHS	J	301[A]	-	29,30,30	2.90	6 (20%)	32,45,45	2.09	5 (15%)
3	GOL	E	302	-	5,5,5	0.57	0	5,5,5	0.90	0
3	GOL	C	302	-	5,5,5	0.37	0	5,5,5	0.66	0
2	KHS	A	301[B]	-	29,30,30	2.84	5 (17%)	32,45,45	2.51	5 (15%)
3	GOL	D	302	-	5,5,5	0.47	0	5,5,5	0.19	0
2	KHS	D	301[B]	-	29,30,30	2.85	5 (17%)	32,45,45	2.43	5 (15%)
2	KHS	E	301[B]	-	29,30,30	2.95	7 (24%)	32,45,45	2.40	5 (15%)
3	GOL	N	302	-	5,5,5	0.43	0	5,5,5	0.44	0
3	GOL	G	302	-	5,5,5	0.41	0	5,5,5	0.37	0
2	KHS	F	301[A]	-	29,30,30	3.12	5 (17%)	32,45,45	2.63	12 (37%)
2	KHS	M	301[A]	-	29,30,30	2.93	6 (20%)	32,45,45	2.22	7 (21%)

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	GOL	J	302	-	-	2/4/4/4	-
2	KHS	J	301[B]	-	-	8/31/34/34	0/2/2/2
3	GOL	I	302	-	-	1/4/4/4	-
2	KHS	N	301[A]	-	-	5/31/34/34	0/2/2/2
2	KHS	I	301[A]	-	-	2/31/34/34	0/2/2/2
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	K	302	-	-	4/4/4/4	-
2	KHS	G	301[A]	-	-	4/31/34/34	0/2/2/2
2	KHS	H	301[A]	-	-	6/31/34/34	0/2/2/2
2	KHS	L	301[A]	-	-	2/31/34/34	0/2/2/2
2	KHS	F	301[B]	-	-	7/31/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KHS	M	301[B]	-	-	3/31/34/34	0/2/2/2
2	KHS	I	301[B]	-	-	2/31/34/34	0/2/2/2
2	KHS	C	301[A]	-	-	5/31/34/34	0/2/2/2
2	KHS	B	301[A]	-	-	4/31/34/34	0/2/2/2
2	KHS	K	301[A]	-	-	2/31/34/34	0/2/2/2
2	KHS	N	301[B]	-	-	4/31/34/34	0/2/2/2
3	GOL	M	302	-	-	2/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
2	KHS	A	301[A]	-	-	2/31/34/34	0/2/2/2
3	GOL	F	302	-	-	1/4/4/4	-
2	KHS	G	301[B]	-	-	5/31/34/34	0/2/2/2
2	KHS	H	301[B]	-	-	7/31/34/34	0/2/2/2
2	KHS	L	301[B]	-	-	7/31/34/34	0/2/2/2
2	KHS	D	301[A]	-	-	4/31/34/34	0/2/2/2
2	KHS	E	301[A]	-	-	4/31/34/34	0/2/2/2
2	KHS	B	301[B]	-	-	3/31/34/34	0/2/2/2
2	KHS	C	301[B]	-	-	5/31/34/34	0/2/2/2
2	KHS	K	301[B]	-	-	1/31/34/34	0/2/2/2
3	GOL	H	302	-	-	0/4/4/4	-
3	GOL	L	302	-	-	2/4/4/4	-
2	KHS	J	301[A]	-	-	3/31/34/34	0/2/2/2
3	GOL	E	302	-	-	4/4/4/4	-
3	GOL	C	302	-	-	2/4/4/4	-
2	KHS	A	301[B]	-	-	2/31/34/34	0/2/2/2
3	GOL	D	302	-	-	2/4/4/4	-
2	KHS	D	301[B]	-	-	6/31/34/34	0/2/2/2
2	KHS	E	301[B]	-	-	5/31/34/34	0/2/2/2
3	GOL	N	302	-	-	2/4/4/4	-
3	GOL	G	302	-	-	4/4/4/4	-
2	KHS	F	301[A]	-	-	6/31/34/34	0/2/2/2
2	KHS	M	301[A]	-	-	4/31/34/34	0/2/2/2

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301[A]	KHS	OAM-SAL	9.84	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[A]	KHS	OAM-SAL	9.83	1.54	1.44
2	B	301[A]	KHS	OAK-SAL	9.66	1.53	1.44
2	G	301[A]	KHS	OAM-SAL	9.61	1.53	1.44
2	K	301[A]	KHS	OAM-SAL	9.57	1.53	1.44
2	F	301[A]	KHS	OAM-SAL	9.49	1.53	1.44
2	I	301[A]	KHS	OAM-SAL	9.47	1.53	1.44
2	G	301[A]	KHS	OAK-SAL	9.46	1.53	1.44
2	A	301[A]	KHS	OAM-SAL	9.46	1.53	1.44
2	L	301[A]	KHS	OAM-SAL	9.45	1.53	1.44
2	H	301[A]	KHS	OAM-SAL	9.44	1.53	1.44
2	M	301[A]	KHS	OAM-SAL	9.44	1.53	1.44
2	B	301[B]	KHS	OAM-SAL	9.44	1.53	1.44
2	D	301[A]	KHS	OAM-SAL	9.43	1.53	1.44
2	E	301[A]	KHS	OAK-SAL	9.42	1.53	1.44
2	N	301[A]	KHS	OAM-SAL	9.42	1.53	1.44
2	J	301[A]	KHS	OAM-SAL	9.39	1.53	1.44
2	C	301[A]	KHS	OAM-SAL	9.34	1.53	1.44
2	E	301[B]	KHS	OAM-SAL	9.34	1.53	1.44
2	F	301[A]	KHS	OAK-SAL	9.30	1.53	1.44
2	L	301[A]	KHS	OAK-SAL	9.27	1.53	1.44
2	E	301[B]	KHS	OAK-SAL	9.26	1.53	1.44
2	N	301[A]	KHS	OAK-SAL	9.26	1.53	1.44
2	G	301[B]	KHS	OAM-SAL	9.23	1.53	1.44
2	I	301[B]	KHS	OAK-SAL	9.21	1.53	1.44
2	H	301[B]	KHS	OAK-SAL	9.19	1.53	1.44
2	C	301[A]	KHS	OAK-SAL	9.19	1.53	1.44
2	K	301[A]	KHS	OAK-SAL	9.18	1.53	1.44
2	M	301[B]	KHS	OAK-SAL	9.17	1.53	1.44
2	M	301[A]	KHS	OAK-SAL	9.15	1.53	1.44
2	D	301[B]	KHS	OAK-SAL	9.15	1.53	1.44
2	A	301[B]	KHS	OAK-SAL	9.15	1.53	1.44
2	K	301[B]	KHS	OAM-SAL	9.14	1.53	1.44
2	L	301[B]	KHS	OAM-SAL	9.13	1.53	1.44
2	D	301[A]	KHS	OAK-SAL	9.13	1.53	1.44
2	A	301[B]	KHS	OAM-SAL	9.12	1.53	1.44
2	A	301[A]	KHS	OAK-SAL	9.10	1.53	1.44
2	K	301[B]	KHS	OAK-SAL	9.09	1.53	1.44
2	J	301[B]	KHS	OAK-SAL	9.09	1.53	1.44
2	I	301[B]	KHS	OAM-SAL	9.06	1.53	1.44
2	L	301[B]	KHS	OAK-SAL	9.04	1.53	1.44
2	N	301[B]	KHS	OAK-SAL	9.03	1.53	1.44
2	I	301[A]	KHS	OAK-SAL	9.02	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301[B]	KHS	OAM-SAL	9.01	1.53	1.44
2	J	301[A]	KHS	OAK-SAL	9.00	1.53	1.44
2	G	301[B]	KHS	OAK-SAL	9.00	1.53	1.44
2	J	301[B]	KHS	OAM-SAL	8.98	1.53	1.44
2	B	301[B]	KHS	OAK-SAL	8.98	1.53	1.44
2	H	301[A]	KHS	OAK-SAL	8.97	1.53	1.44
2	C	301[B]	KHS	OAK-SAL	8.96	1.53	1.44
2	M	301[B]	KHS	OAM-SAL	8.82	1.53	1.44
2	C	301[B]	KHS	OAM-SAL	8.80	1.52	1.44
2	N	301[B]	KHS	OAM-SAL	8.68	1.52	1.44
2	H	301[B]	KHS	OAM-SAL	8.63	1.52	1.44
2	F	301[B]	KHS	OAK-SAL	8.61	1.52	1.44
2	F	301[B]	KHS	OAM-SAL	8.24	1.52	1.44
2	F	301[A]	KHS	CAC-CAF	-6.60	1.36	1.49
2	G	301[A]	KHS	CAC-CAF	-6.28	1.37	1.49
2	C	301[A]	KHS	CAC-CAF	-5.98	1.37	1.49
2	I	301[A]	KHS	CAC-CAF	-5.91	1.37	1.49
2	L	301[A]	KHS	CAC-CAF	-5.85	1.38	1.49
2	A	301[A]	KHS	CAC-CAF	-5.79	1.38	1.49
2	B	301[A]	KHS	CAC-CAF	-5.78	1.38	1.49
2	M	301[A]	KHS	CAC-CAF	-5.77	1.38	1.49
2	D	301[A]	KHS	CAC-CAF	-5.73	1.38	1.49
2	J	301[A]	KHS	CAC-CAF	-5.71	1.38	1.49
2	H	301[A]	KHS	CAC-CAF	-5.67	1.38	1.49
2	E	301[A]	KHS	CAC-CAF	-5.48	1.38	1.49
2	K	301[A]	KHS	CAC-CAF	-5.45	1.38	1.49
2	G	301[A]	KHS	CAJ-SAL	-5.44	1.70	1.78
2	F	301[A]	KHS	CAJ-SAL	-5.34	1.70	1.78
2	L	301[B]	KHS	CAC-CAF	-5.17	1.39	1.49
2	N	301[A]	KHS	CAC-CAF	-5.14	1.39	1.49
2	J	301[B]	KHS	CAC-CAF	-5.11	1.39	1.49
2	D	301[B]	KHS	CAC-CAF	-5.10	1.39	1.49
2	M	301[B]	KHS	CAC-CAF	-5.08	1.39	1.49
2	E	301[B]	KHS	CAO-SAL	5.03	1.96	1.82
2	A	301[B]	KHS	CAC-CAF	-5.02	1.39	1.49
2	H	301[B]	KHS	CAC-CAF	-5.01	1.39	1.49
2	E	301[A]	KHS	CAO-SAL	4.95	1.96	1.82
2	I	301[B]	KHS	CAC-CAF	-4.94	1.39	1.49
2	G	301[B]	KHS	CAC-CAF	-4.90	1.39	1.49
2	E	301[B]	KHS	CAC-CAF	-4.89	1.39	1.49
2	D	301[B]	KHS	CAO-SAL	4.88	1.96	1.82
2	A	301[B]	KHS	CAO-SAL	4.82	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[B]	KHS	CAC-CAF	-4.82	1.40	1.49
2	I	301[B]	KHS	CAO-SAL	4.80	1.95	1.82
2	C	301[B]	KHS	CAC-CAF	-4.80	1.40	1.49
2	N	301[B]	KHS	CAC-CAF	-4.76	1.40	1.49
2	K	301[B]	KHS	CAO-SAL	4.75	1.95	1.82
2	D	301[A]	KHS	CAO-SAL	4.75	1.95	1.82
2	I	301[A]	KHS	CAO-SAL	4.71	1.95	1.82
2	B	301[B]	KHS	CAO-SAL	4.70	1.95	1.82
2	M	301[B]	KHS	CAO-SAL	4.69	1.95	1.82
2	K	301[A]	KHS	CAO-SAL	4.69	1.95	1.82
2	L	301[B]	KHS	CAO-SAL	4.68	1.95	1.82
2	H	301[B]	KHS	CAO-SAL	4.67	1.95	1.82
2	K	301[B]	KHS	CAC-CAF	-4.64	1.40	1.49
2	G	301[B]	KHS	CAO-SAL	4.63	1.95	1.82
2	C	301[B]	KHS	CAO-SAL	4.63	1.95	1.82
2	J	301[B]	KHS	CAO-SAL	4.63	1.95	1.82
2	F	301[B]	KHS	CAO-SAL	4.62	1.95	1.82
2	M	301[A]	KHS	CAO-SAL	4.61	1.95	1.82
2	F	301[B]	KHS	CAC-CAF	-4.59	1.40	1.49
2	A	301[A]	KHS	CAO-SAL	4.54	1.95	1.82
2	L	301[A]	KHS	CAO-SAL	4.49	1.95	1.82
2	H	301[A]	KHS	CAO-SAL	4.48	1.95	1.82
2	B	301[A]	KHS	CAO-SAL	4.47	1.95	1.82
2	C	301[A]	KHS	CAO-SAL	4.46	1.94	1.82
2	C	301[A]	KHS	CAJ-SAL	-4.45	1.72	1.78
2	N	301[B]	KHS	CAO-SAL	4.43	1.94	1.82
2	F	301[A]	KHS	CAO-SAL	4.39	1.94	1.82
2	N	301[A]	KHS	CAO-SAL	4.30	1.94	1.82
2	J	301[A]	KHS	CAO-SAL	4.27	1.94	1.82
2	G	301[A]	KHS	CAO-SAL	4.25	1.94	1.82
2	N	301[B]	KHS	CAE-NAI	3.93	1.42	1.34
2	G	301[B]	KHS	CAE-NAI	3.92	1.42	1.34
2	K	301[B]	KHS	CAE-NAI	3.80	1.42	1.34
2	C	301[B]	KHS	CAE-NAI	3.78	1.42	1.34
2	F	301[B]	KHS	CAE-NAI	3.69	1.41	1.34
2	J	301[B]	KHS	CAE-NAI	3.67	1.41	1.34
2	B	301[B]	KHS	CAE-NAI	3.64	1.41	1.34
2	L	301[B]	KHS	CAE-NAI	3.63	1.41	1.34
2	H	301[B]	KHS	CAE-NAI	3.54	1.41	1.34
2	A	301[B]	KHS	CAE-NAI	3.52	1.41	1.34
2	I	301[B]	KHS	CAE-NAI	3.49	1.41	1.34
2	M	301[B]	KHS	CAE-NAI	3.44	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301[B]	KHS	CAE-NAI	3.34	1.41	1.34
2	A	301[A]	KHS	CAJ-SAL	-3.28	1.73	1.78
2	E	301[B]	KHS	CAE-NAI	3.28	1.41	1.34
2	D	301[A]	KHS	CAJ-SAL	-3.03	1.74	1.78
2	K	301[A]	KHS	CAE-NAI	2.96	1.40	1.34
2	N	301[A]	KHS	CAE-NAI	2.85	1.40	1.34
2	E	301[A]	KHS	CAE-NAI	2.83	1.40	1.34
2	B	301[A]	KHS	CAE-NAI	2.82	1.40	1.34
2	I	301[A]	KHS	CAE-NAI	2.80	1.40	1.34
2	E	301[B]	KHS	CAZ-SAV	2.74	1.81	1.77
2	A	301[A]	KHS	CAE-NAI	2.73	1.40	1.34
2	D	301[A]	KHS	CAE-NAI	2.73	1.40	1.34
2	J	301[A]	KHS	CAE-NAI	2.72	1.39	1.34
2	M	301[A]	KHS	CAE-NAI	2.71	1.39	1.34
2	L	301[A]	KHS	CAE-NAI	2.71	1.39	1.34
2	H	301[A]	KHS	CAE-NAI	2.66	1.39	1.34
2	C	301[A]	KHS	CAE-NAI	2.58	1.39	1.34
2	L	301[A]	KHS	CAJ-SAL	-2.58	1.74	1.78
2	I	301[A]	KHS	CAJ-SAL	-2.55	1.74	1.78
2	B	301[B]	KHS	CAZ-SAV	-2.55	1.73	1.77
2	M	301[A]	KHS	CAJ-SAL	-2.50	1.74	1.78
2	J	301[A]	KHS	CAJ-SAL	-2.47	1.74	1.78
2	G	301[A]	KHS	CAE-NAI	2.41	1.39	1.34
2	C	301[A]	KHS	FAB-CAC	-2.35	1.24	1.33
2	J	301[B]	KHS	CAZ-SAV	-2.30	1.73	1.77
2	L	301[A]	KHS	FAB-CAC	-2.30	1.24	1.33
2	E	301[B]	KHS	CAJ-SAL	2.22	1.81	1.78
2	A	301[A]	KHS	FAB-CAC	-2.09	1.25	1.33
2	H	301[A]	KHS	FAB-CAC	-2.08	1.25	1.33

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301[B]	KHS	SAL-CAJ-NAI	8.04	121.91	114.40
2	K	301[B]	KHS	OAK-SAL-OAM	-8.00	109.01	119.06
2	N	301[B]	KHS	SAL-CAJ-NAI	7.98	121.86	114.40
2	F	301[A]	KHS	OAK-SAL-OAM	-7.97	109.05	119.06
2	B	301[A]	KHS	OAK-SAL-OAM	-7.86	109.20	119.06
2	N	301[B]	KHS	OAK-SAL-OAM	-7.82	109.24	119.06
2	E	301[B]	KHS	OAK-SAL-OAM	-7.81	109.26	119.06
2	B	301[B]	KHS	SAL-CAJ-NAI	7.76	121.65	114.40
2	L	301[B]	KHS	SAL-CAJ-NAI	7.73	121.62	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[B]	KHS	OAK-SAL-OAM	-7.69	109.40	119.06
2	K	301[A]	KHS	OAK-SAL-OAM	-7.69	109.41	119.06
2	C	301[B]	KHS	OAK-SAL-OAM	-7.68	109.42	119.06
2	J	301[B]	KHS	SAL-CAJ-NAI	7.64	121.53	114.40
2	B	301[B]	KHS	OAK-SAL-OAM	-7.61	109.51	119.06
2	F	301[B]	KHS	OAK-SAL-OAM	-7.60	109.52	119.06
2	A	301[B]	KHS	SAL-CAJ-NAI	7.60	121.49	114.40
2	J	301[B]	KHS	OAK-SAL-OAM	-7.58	109.55	119.06
2	E	301[A]	KHS	OAK-SAL-OAM	-7.57	109.56	119.06
2	A	301[B]	KHS	OAK-SAL-OAM	-7.56	109.57	119.06
2	K	301[B]	KHS	SAL-CAJ-NAI	7.56	121.46	114.40
2	I	301[B]	KHS	OAK-SAL-OAM	-7.56	109.57	119.06
2	H	301[B]	KHS	OAK-SAL-OAM	-7.56	109.58	119.06
2	H	301[A]	KHS	OAK-SAL-OAM	-7.48	109.67	119.06
2	M	301[B]	KHS	OAK-SAL-OAM	-7.46	109.69	119.06
2	C	301[B]	KHS	SAL-CAJ-NAI	7.46	121.37	114.40
2	L	301[B]	KHS	OAK-SAL-OAM	-7.41	109.76	119.06
2	M	301[A]	KHS	OAK-SAL-OAM	-7.38	109.80	119.06
2	A	301[A]	KHS	OAK-SAL-OAM	-7.33	109.86	119.06
2	L	301[A]	KHS	OAK-SAL-OAM	-7.23	109.98	119.06
2	G	301[B]	KHS	OAK-SAL-OAM	-7.18	110.05	119.06
2	I	301[A]	KHS	OAK-SAL-OAM	-7.17	110.06	119.06
2	D	301[A]	KHS	OAK-SAL-OAM	-7.02	110.25	119.06
2	I	301[B]	KHS	SAL-CAJ-NAI	7.01	120.94	114.40
2	J	301[A]	KHS	OAK-SAL-OAM	-6.94	110.35	119.06
2	N	301[A]	KHS	OAK-SAL-OAM	-6.94	110.35	119.06
2	D	301[B]	KHS	SAL-CAJ-NAI	6.85	120.80	114.40
2	C	301[A]	KHS	OAK-SAL-OAM	-6.85	110.47	119.06
2	H	301[B]	KHS	SAL-CAJ-NAI	6.74	120.69	114.40
2	E	301[B]	KHS	SAL-CAJ-NAI	6.65	120.61	114.40
2	G	301[A]	KHS	OAK-SAL-OAM	-6.58	110.80	119.06
2	M	301[B]	KHS	SAL-CAJ-NAI	6.45	120.42	114.40
2	F	301[B]	KHS	SAL-CAJ-NAI	6.34	120.33	114.40
2	N	301[B]	KHS	CAH-CAJ-NAI	-5.86	119.15	125.39
2	F	301[A]	KHS	CAH-CAJ-SAL	5.84	125.07	119.70
2	H	301[B]	KHS	CAH-CAJ-NAI	-5.67	119.35	125.39
2	G	301[B]	KHS	CAH-CAJ-NAI	-5.63	119.40	125.39
2	B	301[B]	KHS	CAH-CAJ-NAI	-5.55	119.48	125.39
2	F	301[B]	KHS	CAH-CAJ-NAI	-5.53	119.50	125.39
2	C	301[B]	KHS	CAH-CAJ-NAI	-5.46	119.58	125.39
2	E	301[B]	KHS	CAH-CAJ-NAI	-5.45	119.59	125.39
2	L	301[B]	KHS	CAH-CAJ-NAI	-5.43	119.61	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301[B]	KHS	CAH-CAJ-NAI	-5.42	119.62	125.39
2	M	301[B]	KHS	CAH-CAJ-NAI	-5.33	119.71	125.39
2	K	301[B]	KHS	CAH-CAJ-NAI	-5.33	119.72	125.39
2	I	301[B]	KHS	CAH-CAJ-NAI	-5.32	119.73	125.39
2	A	301[B]	KHS	CAH-CAJ-NAI	-5.29	119.76	125.39
2	B	301[A]	KHS	SAL-CAJ-NAI	5.24	119.30	114.40
2	D	301[B]	KHS	CAH-CAJ-NAI	-5.17	119.89	125.39
2	F	301[A]	KHS	CAF-CAE-NAI	-5.12	118.58	123.38
2	G	301[A]	KHS	CAF-CAE-NAI	-5.06	118.63	123.38
2	I	301[A]	KHS	SAL-CAJ-NAI	5.02	119.09	114.40
2	L	301[A]	KHS	SAL-CAJ-NAI	4.99	119.06	114.40
2	M	301[A]	KHS	CAF-CAE-NAI	-4.97	118.72	123.38
2	K	301[B]	KHS	CAF-CAE-NAI	-4.96	118.72	123.38
2	G	301[B]	KHS	CAF-CAE-NAI	-4.92	118.77	123.38
2	K	301[A]	KHS	SAL-CAJ-NAI	4.91	118.99	114.40
2	C	301[A]	KHS	CAF-CAE-NAI	-4.83	118.85	123.38
2	L	301[A]	KHS	CAF-CAE-NAI	-4.81	118.87	123.38
2	I	301[A]	KHS	CAF-CAE-NAI	-4.81	118.87	123.38
2	A	301[A]	KHS	CAF-CAE-NAI	-4.76	118.92	123.38
2	F	301[B]	KHS	CAF-CAE-NAI	-4.73	118.94	123.38
2	C	301[B]	KHS	CAF-CAE-NAI	-4.72	118.95	123.38
2	N	301[A]	KHS	CAH-CAJ-NAI	-4.71	120.38	125.39
2	J	301[B]	KHS	CAF-CAE-NAI	-4.69	118.98	123.38
2	D	301[A]	KHS	CAF-CAE-NAI	-4.67	119.00	123.38
2	M	301[A]	KHS	SAL-CAJ-NAI	4.64	118.73	114.40
2	E	301[A]	KHS	CAH-CAJ-NAI	-4.63	120.46	125.39
2	H	301[A]	KHS	CAF-CAE-NAI	-4.61	119.05	123.38
2	K	301[A]	KHS	CAH-CAJ-NAI	-4.61	120.49	125.39
2	E	301[A]	KHS	SAL-CAJ-NAI	4.57	118.67	114.40
2	N	301[B]	KHS	CAF-CAE-NAI	-4.56	119.10	123.38
2	B	301[A]	KHS	CAH-CAJ-NAI	-4.54	120.56	125.39
2	J	301[A]	KHS	SAL-CAJ-NAI	4.51	118.61	114.40
2	D	301[A]	KHS	SAL-CAJ-NAI	4.49	118.59	114.40
2	B	301[A]	KHS	CAF-CAE-NAI	-4.47	119.19	123.38
2	L	301[B]	KHS	CAF-CAE-NAI	-4.46	119.19	123.38
2	A	301[A]	KHS	SAL-CAJ-NAI	4.41	118.52	114.40
2	H	301[A]	KHS	CAH-CAJ-NAI	-4.39	120.72	125.39
2	E	301[A]	KHS	CAF-CAE-NAI	-4.37	119.28	123.38
2	B	301[B]	KHS	CAF-CAE-NAI	-4.35	119.30	123.38
2	F	301[A]	KHS	CAE-CAF-CAC	-4.31	115.90	120.69
2	N	301[A]	KHS	SAL-CAJ-NAI	4.31	118.42	114.40
2	J	301[A]	KHS	CAF-CAE-NAI	-4.30	119.34	123.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301[B]	KHS	CAF-CAE-NAI	-4.30	119.35	123.38
2	A	301[B]	KHS	CAF-CAE-NAI	-4.23	119.41	123.38
2	L	301[A]	KHS	CAH-CAJ-NAI	-4.23	120.89	125.39
2	J	301[A]	KHS	CAH-CAJ-NAI	-4.21	120.91	125.39
2	D	301[A]	KHS	CAH-CAJ-NAI	-4.21	120.91	125.39
2	D	301[B]	KHS	CAF-CAE-NAI	-4.19	119.45	123.38
2	H	301[B]	KHS	CAF-CAE-NAI	-4.18	119.46	123.38
2	M	301[A]	KHS	CAH-CAJ-NAI	-4.17	120.95	125.39
2	H	301[A]	KHS	SAL-CAJ-NAI	4.15	118.27	114.40
2	K	301[A]	KHS	CAF-CAE-NAI	-4.14	119.49	123.38
2	I	301[A]	KHS	CAH-CAJ-NAI	-4.13	120.99	125.39
2	E	301[B]	KHS	CAF-CAE-NAI	-4.10	119.53	123.38
2	M	301[B]	KHS	CAF-CAE-NAI	-4.10	119.53	123.38
2	N	301[A]	KHS	CAF-CAE-NAI	-4.06	119.57	123.38
2	C	301[A]	KHS	SAL-CAJ-NAI	4.05	118.19	114.40
2	A	301[A]	KHS	CAH-CAJ-NAI	-4.05	121.08	125.39
2	C	301[A]	KHS	CAH-CAJ-NAI	-3.78	121.37	125.39
2	F	301[B]	KHS	CAO-SAL-CAJ	3.76	112.99	106.32
2	F	301[A]	KHS	CAG-CAF-CAE	3.72	121.77	117.73
2	G	301[A]	KHS	SAL-CAJ-NAI	3.47	117.64	114.40
2	G	301[A]	KHS	CAH-CAJ-NAI	-3.43	121.74	125.39
2	D	301[B]	KHS	CAO-SAL-CAJ	3.41	112.36	106.32
2	G	301[A]	KHS	CAG-CAF-CAE	3.31	121.33	117.73
2	F	301[A]	KHS	CAH-CAJ-NAI	-3.31	121.87	125.39
2	L	301[B]	KHS	CAO-SAL-CAJ	3.25	112.09	106.32
2	A	301[B]	KHS	CAO-SAL-CAJ	3.17	111.94	106.32
2	G	301[B]	KHS	CAO-SAL-CAJ	3.15	111.90	106.32
2	J	301[B]	KHS	CAO-SAL-CAJ	3.15	111.90	106.32
2	H	301[B]	KHS	CAO-SAL-CAJ	3.07	111.77	106.32
2	C	301[A]	KHS	CAG-CAF-CAE	2.90	120.89	117.73
2	E	301[B]	KHS	CAO-SAL-CAJ	2.86	111.39	106.32
2	B	301[B]	KHS	CAO-SAL-CAJ	2.80	111.28	106.32
2	L	301[A]	KHS	CAG-CAF-CAE	2.77	120.74	117.73
2	I	301[A]	KHS	CAG-CAF-CAE	2.76	120.73	117.73
2	I	301[B]	KHS	CAO-SAL-CAJ	2.75	111.19	106.32
2	F	301[B]	KHS	CAU-CAT-NAS	2.73	118.10	112.41
2	A	301[A]	KHS	CAG-CAF-CAE	2.72	120.69	117.73
2	C	301[B]	KHS	CAO-SAL-CAJ	2.65	111.03	106.32
2	G	301[B]	KHS	CAE-CAF-CAC	2.64	123.62	120.69
2	M	301[A]	KHS	CAG-CAF-CAE	2.64	120.60	117.73
2	H	301[A]	KHS	CAG-CAF-CAE	2.57	120.52	117.73
2	F	301[A]	KHS	CAO-SAL-CAJ	2.56	110.86	106.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[A]	KHS	FAB-CAC-CAF	-2.52	107.50	112.90
2	D	301[A]	KHS	CAG-CAF-CAE	2.52	120.47	117.73
2	B	301[A]	KHS	CAG-CAF-CAE	2.50	120.45	117.73
2	K	301[B]	KHS	CAO-SAL-CAJ	2.49	110.74	106.32
2	F	301[B]	KHS	CAT-NAS-CAQ	2.46	127.58	121.97
2	J	301[A]	KHS	CAG-CAF-CAE	2.42	120.36	117.73
2	N	301[B]	KHS	CAO-SAL-CAJ	2.38	110.55	106.32
2	F	301[A]	KHS	CAT-NAS-CAQ	2.37	127.38	121.97
2	I	301[A]	KHS	FAB-CAC-CAF	-2.32	107.94	112.90
2	M	301[B]	KHS	CAO-SAL-CAJ	2.30	110.41	106.32
2	M	301[A]	KHS	FAB-CAC-CAF	-2.26	108.06	112.90
2	G	301[A]	KHS	FAB-CAC-CAF	-2.23	108.11	112.90
2	B	301[A]	KHS	FAB-CAC-CAF	-2.20	108.18	112.90
2	H	301[A]	KHS	FAB-CAC-CAF	-2.19	108.21	112.90
2	F	301[A]	KHS	FAA-CAC-CAF	-2.18	108.24	112.90
2	G	301[B]	KHS	CAT-NAS-CAQ	2.17	126.92	121.97
2	F	301[A]	KHS	CAU-CAT-NAS	2.16	116.93	112.41
2	M	301[A]	KHS	CAO-SAL-CAJ	2.16	110.14	106.32
2	K	301[A]	KHS	CAG-CAF-CAE	2.15	120.07	117.73
2	D	301[A]	KHS	FAB-CAC-CAF	-2.15	108.30	112.90
2	C	301[A]	KHS	FAB-CAC-CAF	-2.12	108.36	112.90
2	E	301[A]	KHS	CAG-CAF-CAE	2.10	120.01	117.73
2	A	301[A]	KHS	FAB-CAC-CAF	-2.10	108.40	112.90
2	L	301[A]	KHS	FAB-CAC-CAF	-2.10	108.41	112.90
2	C	301[B]	KHS	CAE-CAF-CAC	2.08	123.00	120.69
2	F	301[A]	KHS	CAH-CAG-CAF	-2.04	118.35	121.17
2	L	301[B]	KHS	CAY-CAZ-CBB	2.03	120.20	117.55

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	KHS	NAI-CAJ-SAL-OAM
2	A	301[A]	KHS	CAH-CAJ-SAL-OAM
2	A	301[B]	KHS	NAI-CAJ-SAL-OAM
2	A	301[B]	KHS	CAH-CAJ-SAL-OAM
2	B	301[A]	KHS	NAI-CAJ-SAL-OAM
2	B	301[A]	KHS	CAH-CAJ-SAL-OAM
2	B	301[B]	KHS	NAI-CAJ-SAL-OAM
2	B	301[B]	KHS	CAH-CAJ-SAL-OAM
2	C	301[A]	KHS	NAI-CAJ-SAL-CAO
2	C	301[A]	KHS	NAI-CAJ-SAL-OAM

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Mol	Chain	Res	Type	Atoms
2	C	301[A]	KHS	CAH-CAJ-SAL-OAM
2	C	301[B]	KHS	NAI-CAJ-SAL-CAO
2	C	301[B]	KHS	NAI-CAJ-SAL-OAM
2	C	301[B]	KHS	CAH-CAJ-SAL-OAM
2	D	301[A]	KHS	NAI-CAJ-SAL-OAM
2	D	301[A]	KHS	CAH-CAJ-SAL-OAM
2	D	301[B]	KHS	NAI-CAJ-SAL-CAO
2	D	301[B]	KHS	NAI-CAJ-SAL-OAM
2	D	301[B]	KHS	CAH-CAJ-SAL-OAM
2	E	301[A]	KHS	NAI-CAJ-SAL-OAM
2	E	301[A]	KHS	CAH-CAJ-SAL-OAM
2	E	301[B]	KHS	NAI-CAJ-SAL-OAM
2	E	301[B]	KHS	CAH-CAJ-SAL-OAM
2	F	301[A]	KHS	CAU-CAT-NAS-CAQ
2	F	301[A]	KHS	NAI-CAJ-SAL-OAM
2	F	301[A]	KHS	CAH-CAJ-SAL-OAM
2	F	301[B]	KHS	CAU-CAT-NAS-CAQ
2	F	301[B]	KHS	NAI-CAJ-SAL-CAO
2	F	301[B]	KHS	NAI-CAJ-SAL-OAM
2	F	301[B]	KHS	CAH-CAJ-SAL-OAM
2	F	301[B]	KHS	NAI-CAJ-SAL-OAK
2	F	301[B]	KHS	CAH-CAJ-SAL-OAK
2	G	301[A]	KHS	NAI-CAJ-SAL-OAM
2	G	301[A]	KHS	CAH-CAJ-SAL-OAM
2	G	301[B]	KHS	CAU-CAT-NAS-CAQ
2	G	301[B]	KHS	NAI-CAJ-SAL-OAM
2	G	301[B]	KHS	CAH-CAJ-SAL-OAM
2	H	301[A]	KHS	NAI-CAJ-SAL-CAO
2	H	301[A]	KHS	NAI-CAJ-SAL-OAM
2	H	301[A]	KHS	CAH-CAJ-SAL-OAM
2	H	301[A]	KHS	CAH-CAJ-SAL-OAK
2	H	301[B]	KHS	NAI-CAJ-SAL-OAM
2	H	301[B]	KHS	CAH-CAJ-SAL-OAM
2	I	301[A]	KHS	NAI-CAJ-SAL-OAM
2	I	301[A]	KHS	CAH-CAJ-SAL-OAM
2	I	301[B]	KHS	NAI-CAJ-SAL-OAM
2	I	301[B]	KHS	CAH-CAJ-SAL-OAM
2	J	301[A]	KHS	NAI-CAJ-SAL-OAM
2	J	301[A]	KHS	CAH-CAJ-SAL-OAM
2	J	301[B]	KHS	NAI-CAJ-SAL-OAM
2	J	301[B]	KHS	CAH-CAJ-SAL-OAM
2	K	301[A]	KHS	NAI-CAJ-SAL-OAM

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Mol	Chain	Res	Type	Atoms
2	K	301[A]	KHS	CAH-CAJ-SAL-OAM
2	L	301[A]	KHS	NAI-CAJ-SAL-OAM
2	L	301[A]	KHS	CAH-CAJ-SAL-OAM
2	L	301[B]	KHS	NAI-CAJ-SAL-CAO
2	L	301[B]	KHS	NAI-CAJ-SAL-OAM
2	L	301[B]	KHS	CAH-CAJ-SAL-OAM
2	M	301[A]	KHS	NAI-CAJ-SAL-OAM
2	M	301[A]	KHS	CAH-CAJ-SAL-OAM
2	M	301[B]	KHS	NAI-CAJ-SAL-OAM
2	M	301[B]	KHS	CAH-CAJ-SAL-OAM
2	N	301[A]	KHS	NAI-CAJ-SAL-OAM
2	N	301[A]	KHS	CAH-CAJ-SAL-OAM
2	N	301[B]	KHS	NAI-CAJ-SAL-OAM
2	N	301[B]	KHS	CAH-CAJ-SAL-OAM
3	B	302	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-C3
3	C	302	GOL	O1-C1-C2-C3
3	D	302	GOL	O1-C1-C2-O2
3	D	302	GOL	O1-C1-C2-C3
3	E	302	GOL	O1-C1-C2-O2
3	E	302	GOL	O1-C1-C2-C3
3	E	302	GOL	C1-C2-C3-O3
3	E	302	GOL	O2-C2-C3-O3
3	J	302	GOL	O1-C1-C2-C3
3	K	302	GOL	O1-C1-C2-C3
3	L	302	GOL	O1-C1-C2-C3
3	M	302	GOL	O1-C1-C2-O2
3	M	302	GOL	O1-C1-C2-C3
3	N	302	GOL	O1-C1-C2-C3
3	L	302	GOL	O1-C1-C2-O2
3	A	302	GOL	C1-C2-C3-O3
3	G	302	GOL	O1-C1-C2-C3
3	G	302	GOL	C1-C2-C3-O3
3	K	302	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	G	302	GOL	O2-C2-C3-O3
3	J	302	GOL	O1-C1-C2-O2
3	K	302	GOL	O1-C1-C2-O2
3	N	302	GOL	O1-C1-C2-O2
3	G	302	GOL	O1-C1-C2-O2
3	F	302	GOL	O1-C1-C2-C3
2	G	301[A]	KHS	CAU-CAT-NAS-CAQ

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Mol	Chain	Res	Type	Atoms
2	B	301[A]	KHS	CAT-CAU-SAV-CAZ
2	B	301[B]	KHS	CAT-CAU-SAV-CAZ
2	C	301[A]	KHS	CAH-CAJ-SAL-OAK
2	C	301[B]	KHS	CAH-CAJ-SAL-OAK
2	H	301[A]	KHS	NAI-CAJ-SAL-OAK
2	F	301[B]	KHS	CAH-CAJ-SAL-CAO
3	I	302	GOL	C1-C2-C3-O3
2	C	301[A]	KHS	NAI-CAJ-SAL-OAK
2	C	301[B]	KHS	NAI-CAJ-SAL-OAK
2	D	301[A]	KHS	CAH-CAJ-SAL-OAK
2	D	301[B]	KHS	NAI-CAJ-SAL-OAK
2	D	301[B]	KHS	CAH-CAJ-SAL-OAK
2	E	301[A]	KHS	CAH-CAJ-SAL-OAK
2	E	301[B]	KHS	NAI-CAJ-SAL-OAK
2	E	301[B]	KHS	CAH-CAJ-SAL-OAK
2	F	301[A]	KHS	NAI-CAJ-SAL-OAK
2	F	301[A]	KHS	CAH-CAJ-SAL-OAK
2	G	301[A]	KHS	CAH-CAJ-SAL-OAK
2	G	301[B]	KHS	CAH-CAJ-SAL-OAK
2	H	301[B]	KHS	CAH-CAJ-SAL-OAK
2	J	301[B]	KHS	NAI-CAJ-SAL-OAK
2	J	301[B]	KHS	CAH-CAJ-SAL-OAK
2	K	301[B]	KHS	CAH-CAJ-SAL-OAM
2	L	301[B]	KHS	NAI-CAJ-SAL-OAK
2	L	301[B]	KHS	CAH-CAJ-SAL-OAK
2	M	301[A]	KHS	CAH-CAJ-SAL-OAK
2	N	301[A]	KHS	NAI-CAJ-SAL-OAK
2	N	301[A]	KHS	CAH-CAJ-SAL-OAK
2	N	301[B]	KHS	CAH-CAJ-SAL-OAK
3	A	302	GOL	O2-C2-C3-O3
3	K	302	GOL	O2-C2-C3-O3
2	E	301[A]	KHS	NAI-CAJ-SAL-CAO
2	E	301[B]	KHS	NAI-CAJ-SAL-CAO
2	F	301[A]	KHS	NAI-CAJ-SAL-CAO
2	G	301[B]	KHS	NAI-CAJ-SAL-CAO
2	H	301[B]	KHS	NAI-CAJ-SAL-CAO
2	J	301[B]	KHS	NAI-CAJ-SAL-CAO
2	M	301[A]	KHS	NAI-CAJ-SAL-CAO
2	N	301[A]	KHS	NAI-CAJ-SAL-CAO
2	N	301[B]	KHS	NAI-CAJ-SAL-CAO
2	B	301[A]	KHS	CAP-CAO-CAQ-NAS
2	H	301[B]	KHS	CAP-CAO-CAQ-NAS

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Mol	Chain	Res	Type	Atoms
2	H	301[B]	KHS	CAN-CAO-CAQ-NAS
2	J	301[B]	KHS	CAP-CAO-CAQ-NAS
2	J	301[B]	KHS	CAN-CAO-CAQ-NAS
2	L	301[B]	KHS	CAP-CAO-CAQ-NAS
2	L	301[B]	KHS	CAN-CAO-CAQ-NAS
2	M	301[B]	KHS	CAP-CAO-CAQ-NAS
2	D	301[A]	KHS	CAU-CAT-NAS-CAQ
2	D	301[B]	KHS	CAU-CAT-NAS-CAQ
2	H	301[A]	KHS	CAU-CAT-NAS-CAQ
2	H	301[B]	KHS	CAU-CAT-NAS-CAQ
2	J	301[A]	KHS	CAU-CAT-NAS-CAQ
2	J	301[B]	KHS	CAU-CAT-NAS-CAQ

There are no ring outliers.

34 monomers are involved in 79 short contacts:

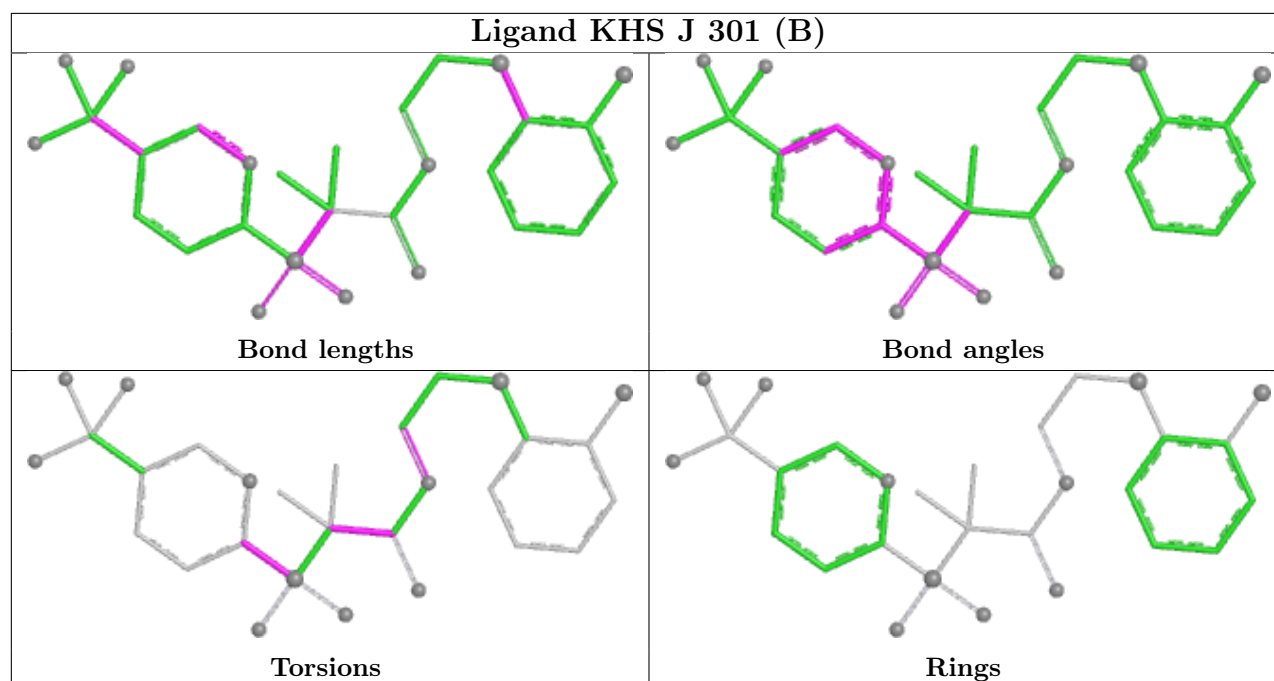
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301[B]	KHS	2	0
2	N	301[A]	KHS	3	0
2	I	301[A]	KHS	1	0
3	B	302	GOL	2	0
2	G	301[A]	KHS	2	0
2	H	301[A]	KHS	2	0
2	L	301[A]	KHS	2	0
2	F	301[B]	KHS	4	0
2	M	301[B]	KHS	2	0
2	I	301[B]	KHS	2	0
2	C	301[A]	KHS	5	0
2	B	301[A]	KHS	2	0
2	N	301[B]	KHS	5	0
3	M	302	GOL	1	0
3	A	302	GOL	2	0
2	A	301[A]	KHS	1	0
3	F	302	GOL	1	0
2	G	301[B]	KHS	5	0
2	H	301[B]	KHS	4	0
2	L	301[B]	KHS	2	0
2	D	301[A]	KHS	2	0
2	B	301[B]	KHS	1	0
2	C	301[B]	KHS	7	0
3	H	302	GOL	1	0
3	L	302	GOL	1	0

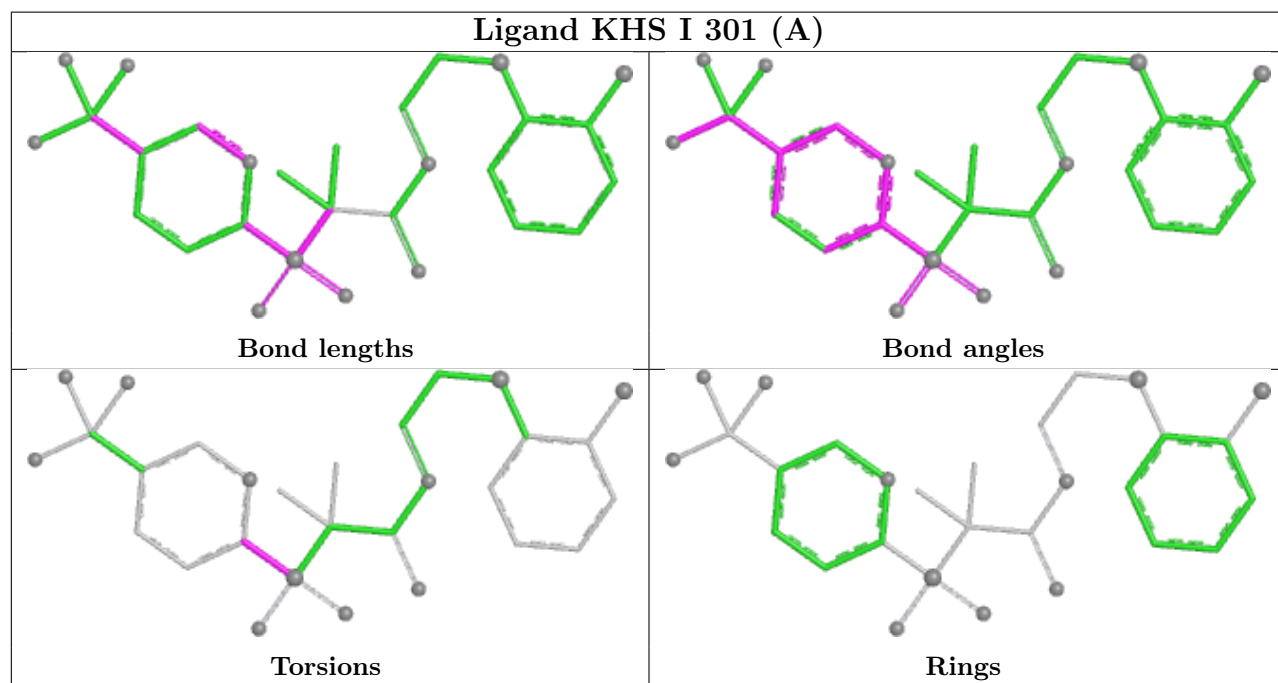
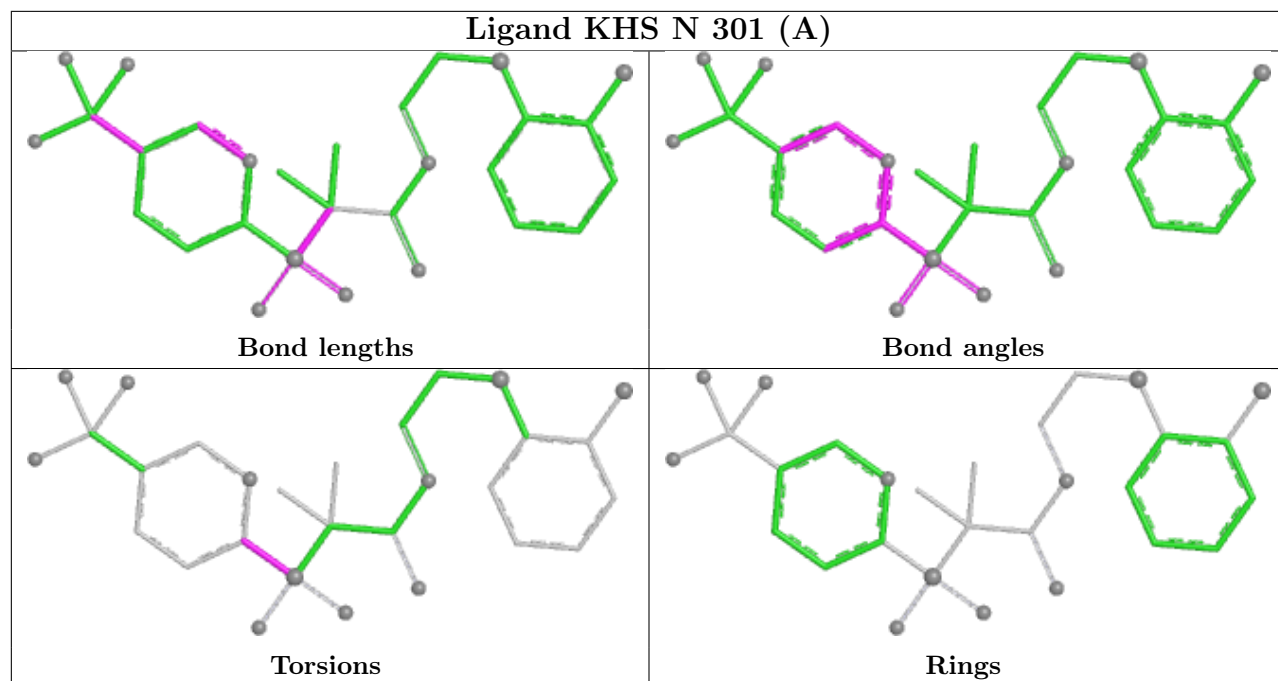
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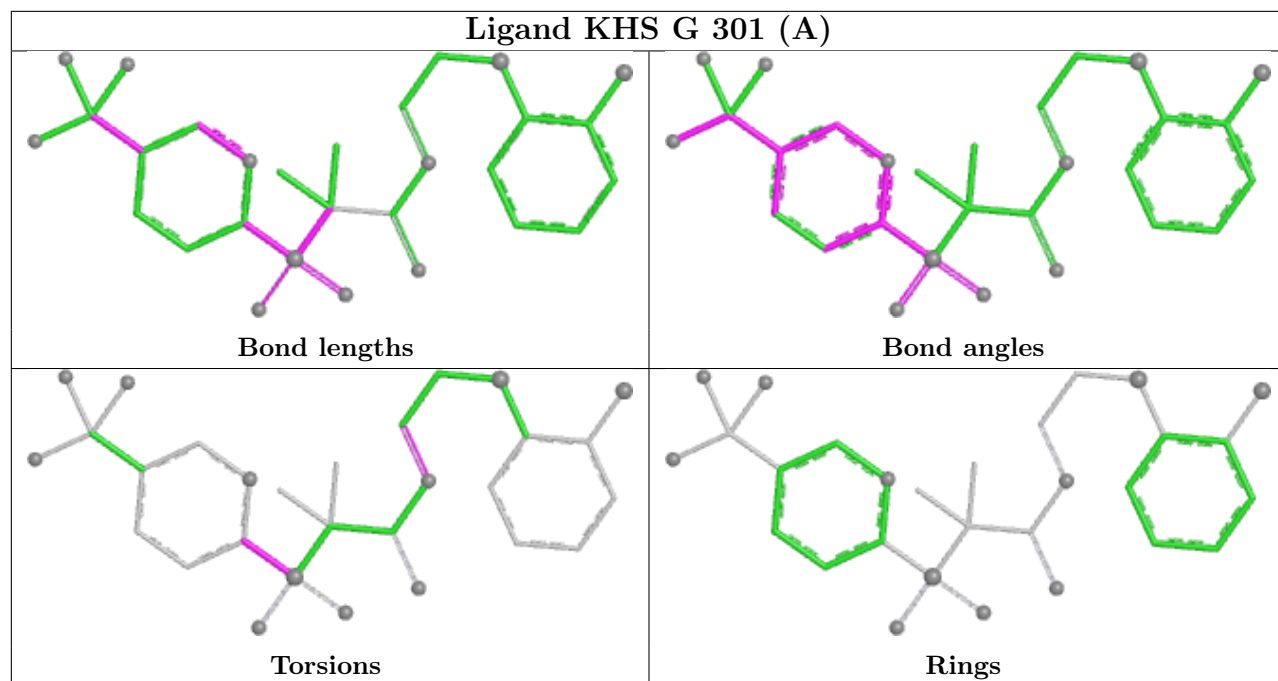
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301[A]	KHS	1	0
3	E	302	GOL	1	0
3	C	302	GOL	1	0
2	A	301[B]	KHS	2	0
3	D	302	GOL	1	0
2	D	301[B]	KHS	3	0
3	N	302	GOL	1	0
2	F	301[A]	KHS	6	0
2	M	301[A]	KHS	1	0

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

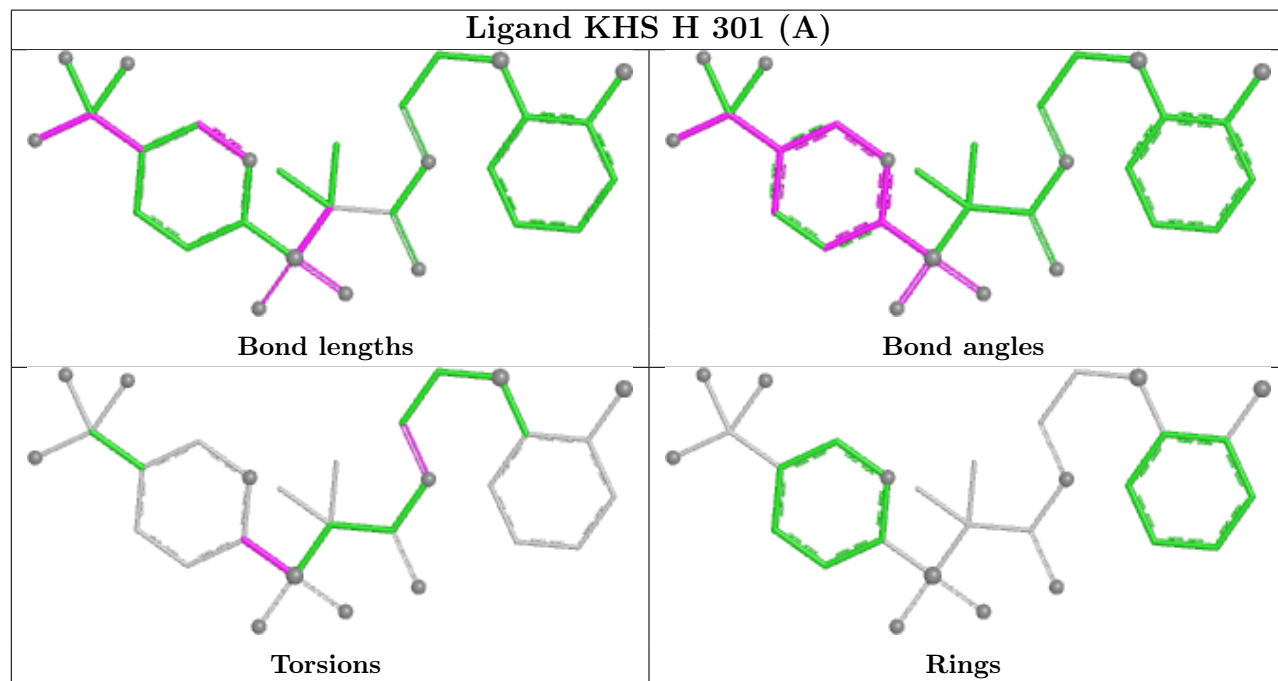


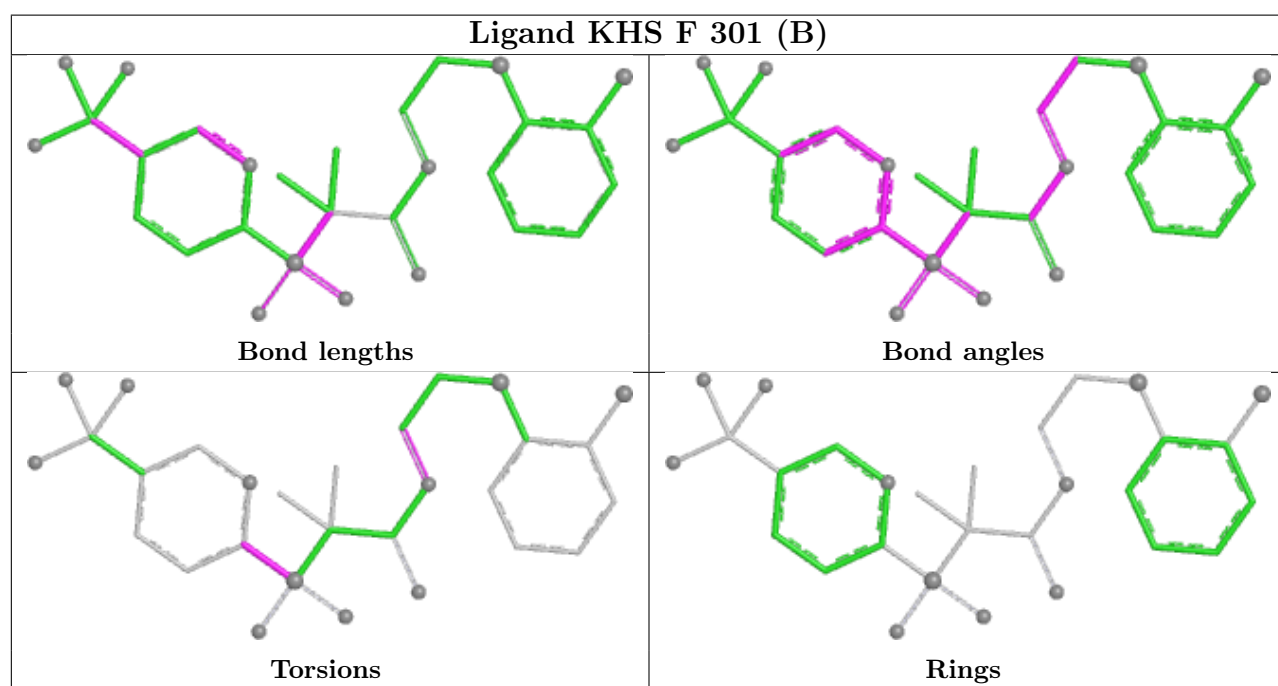
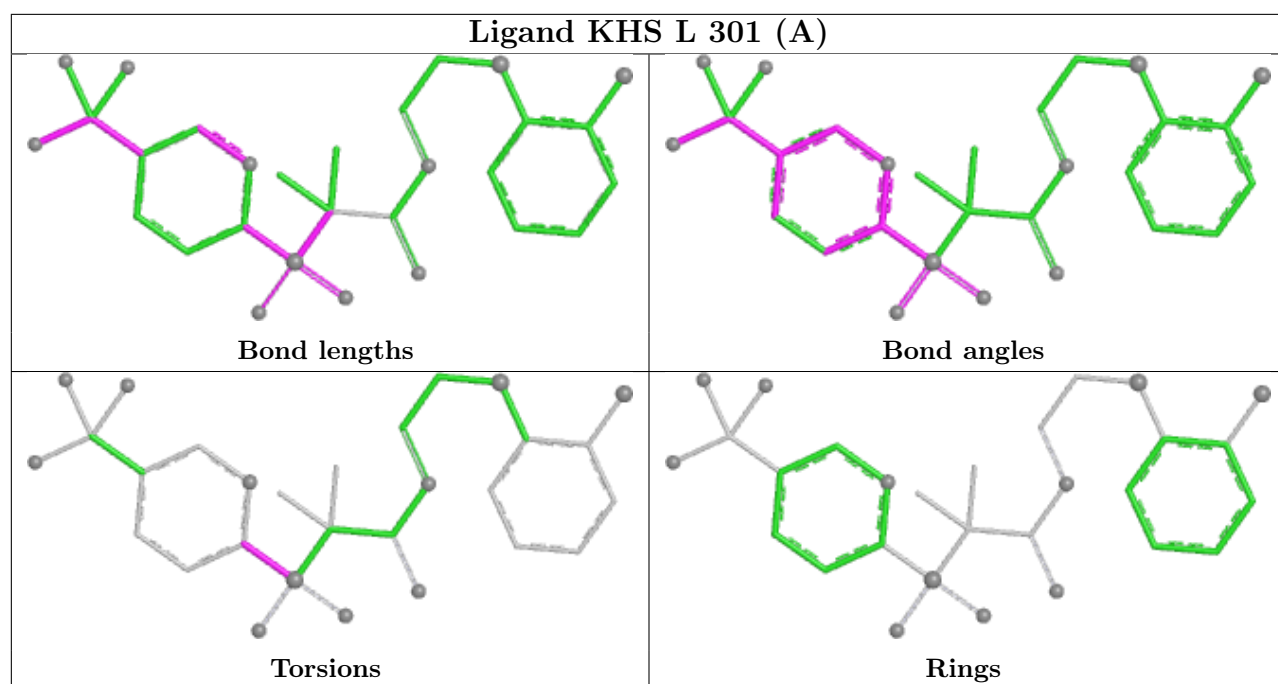


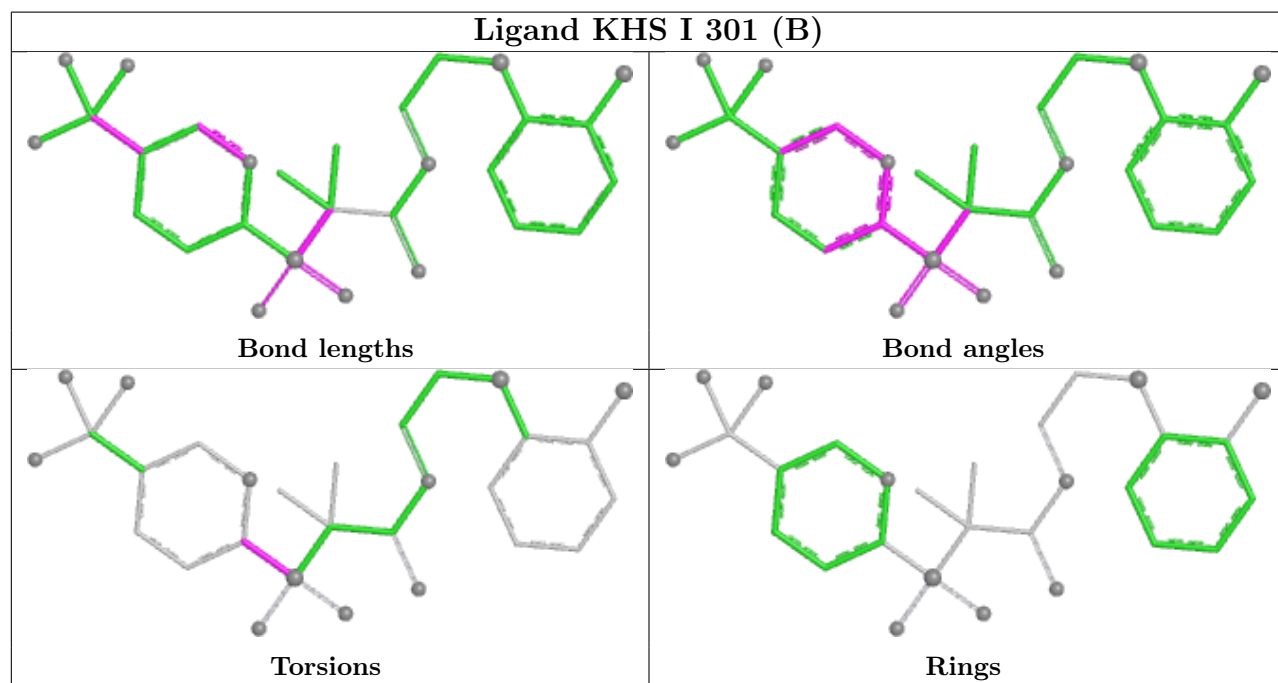
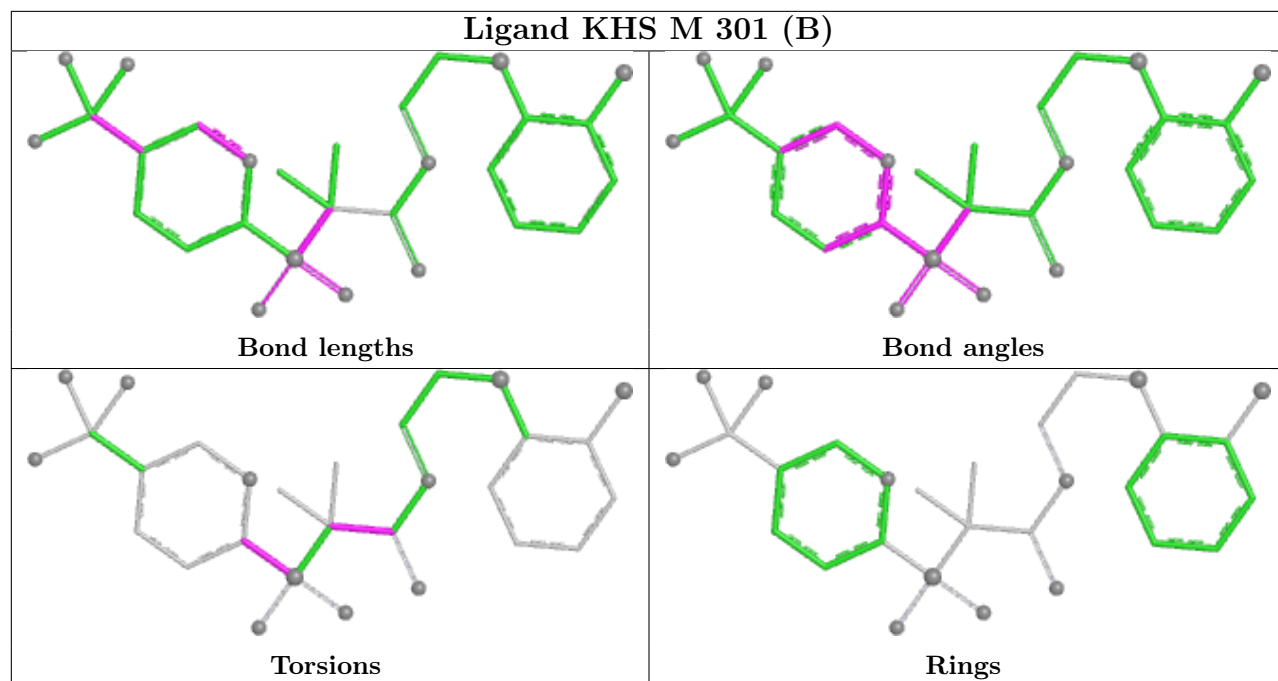
Ligand KHS G 301 (A)

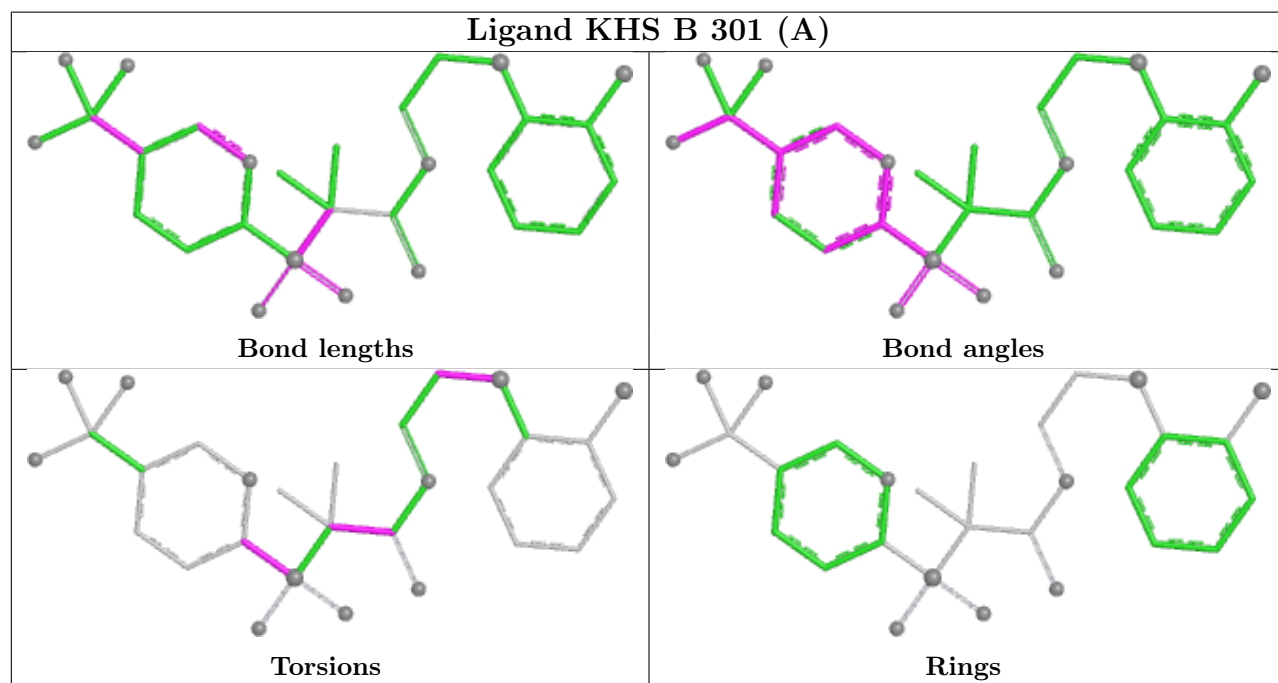
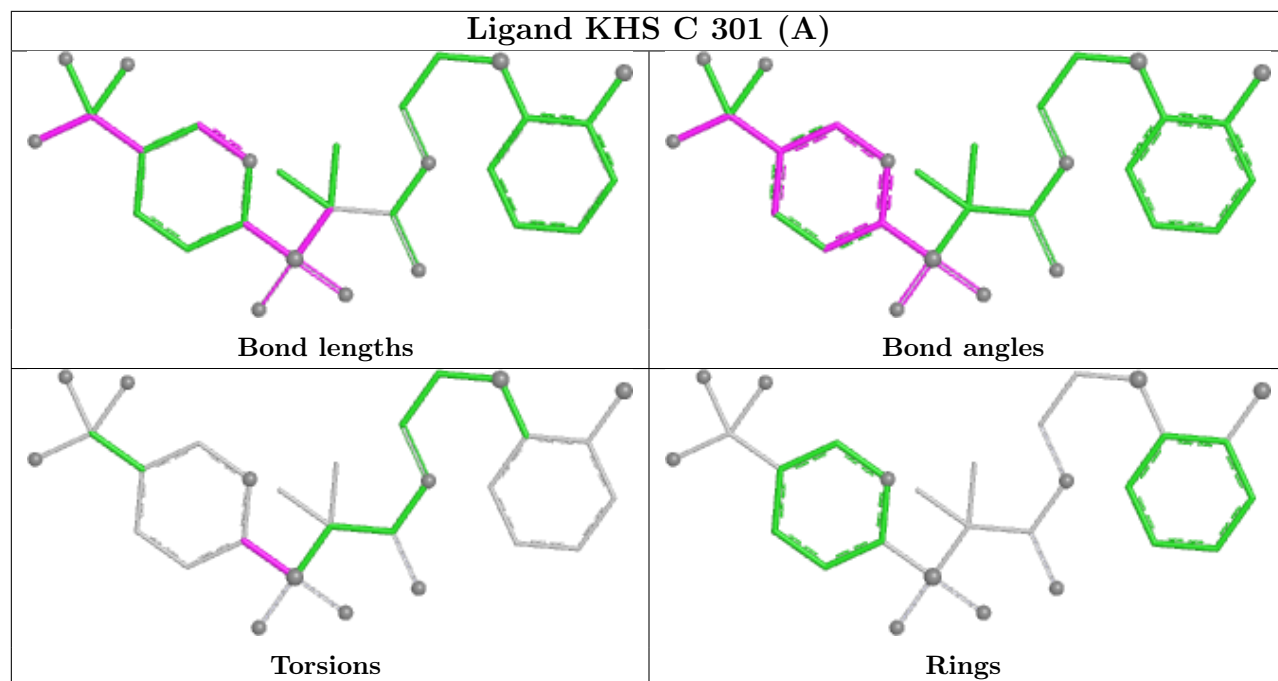


Ligand KHS H 301 (A)

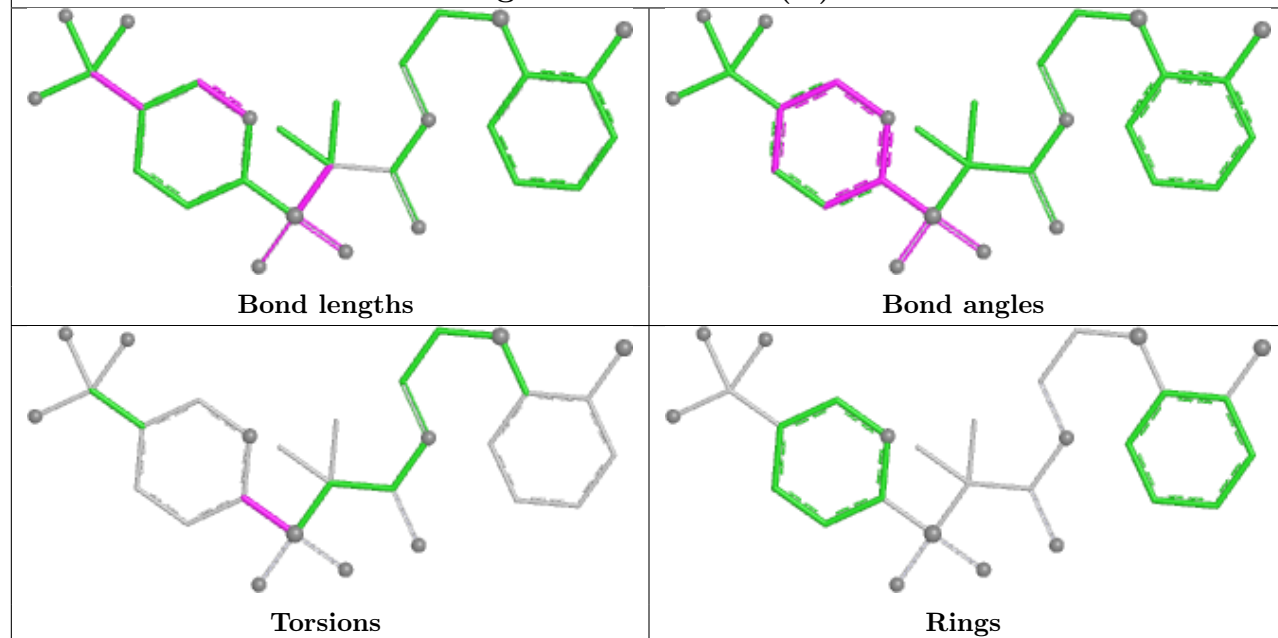




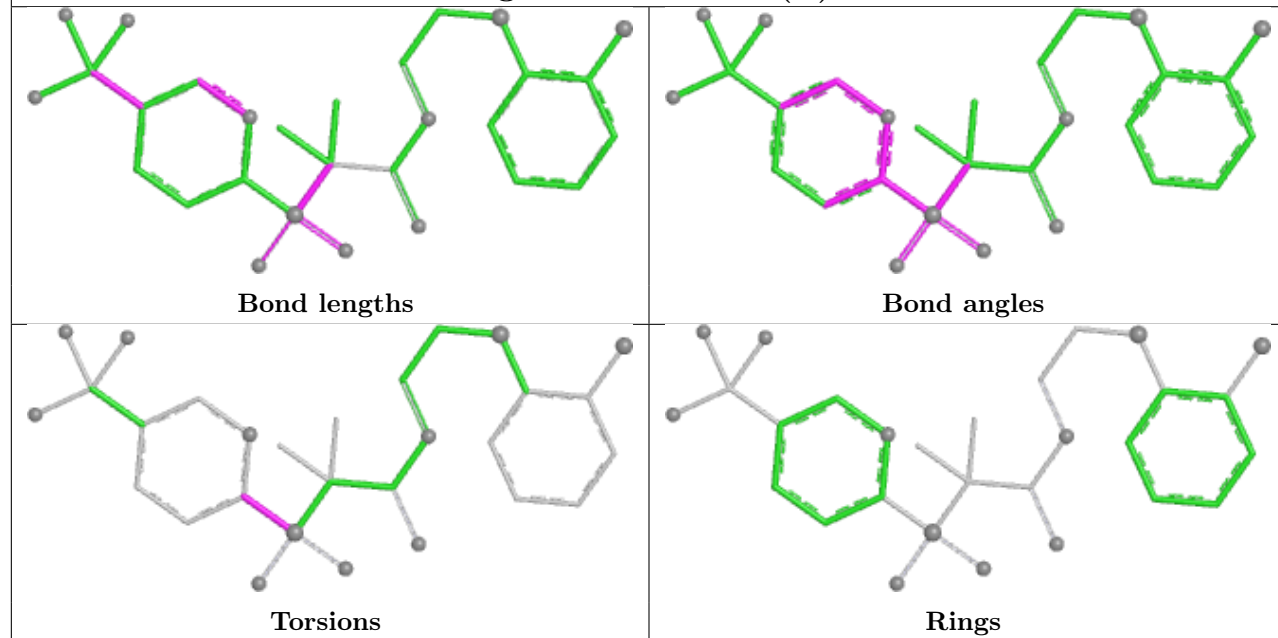


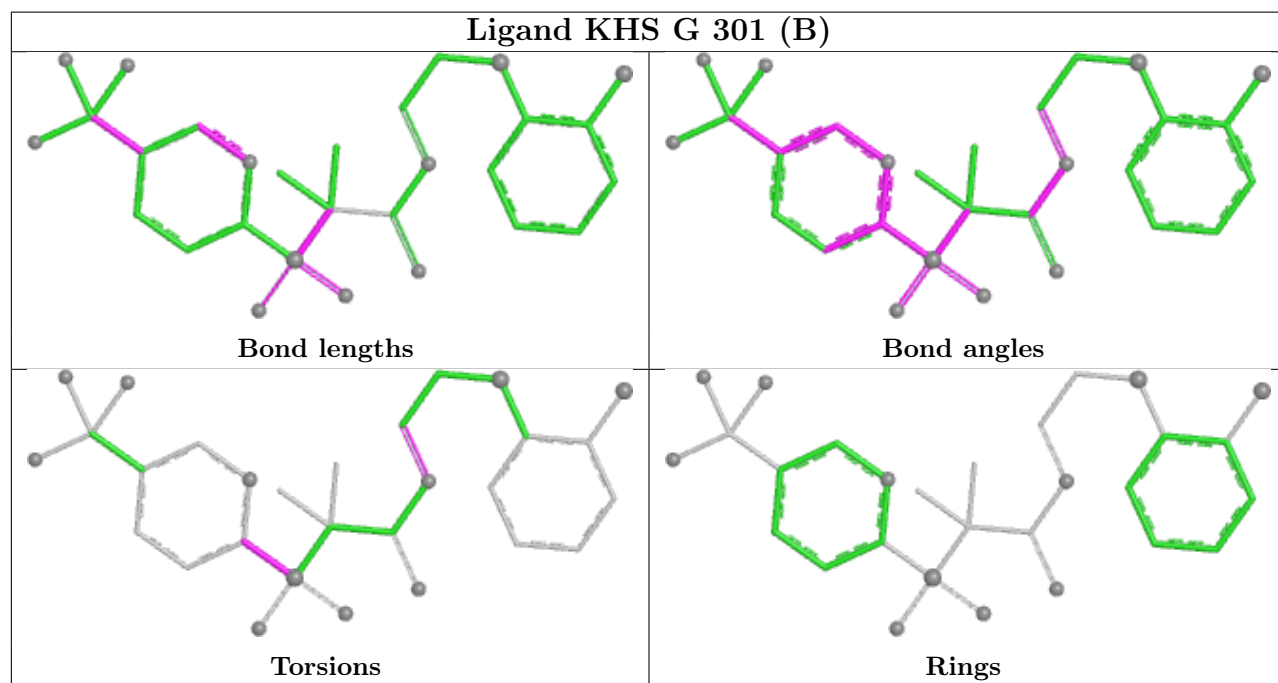
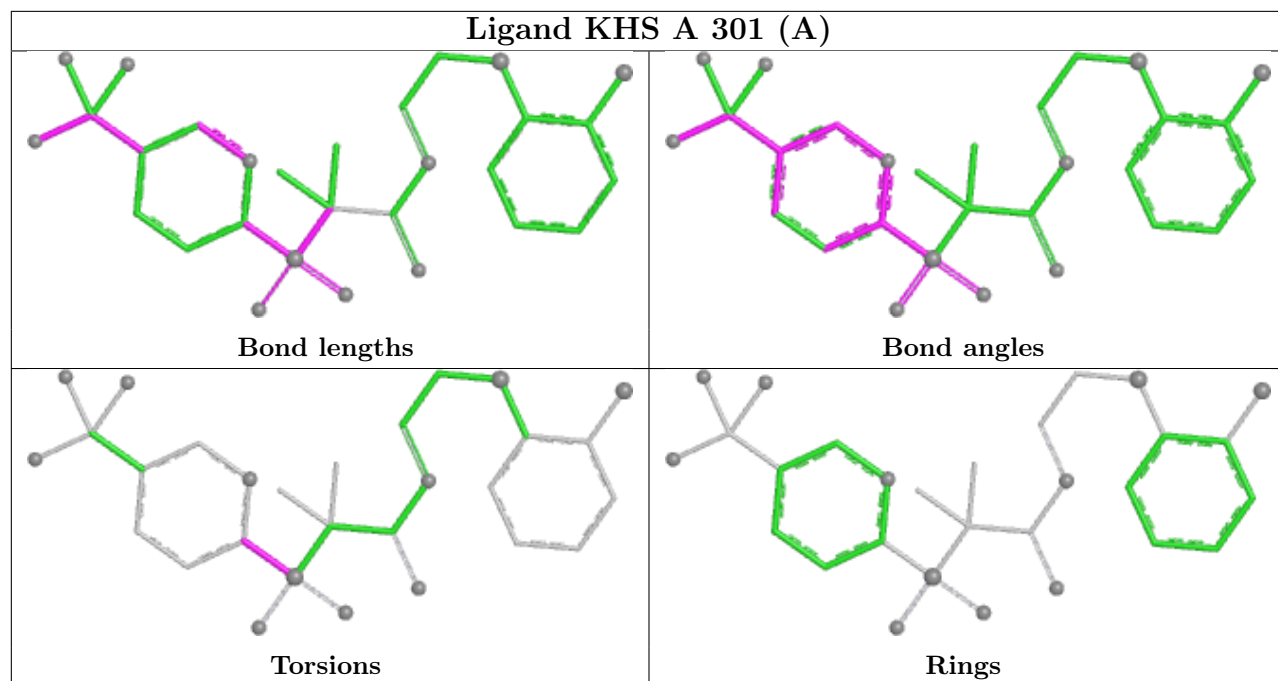


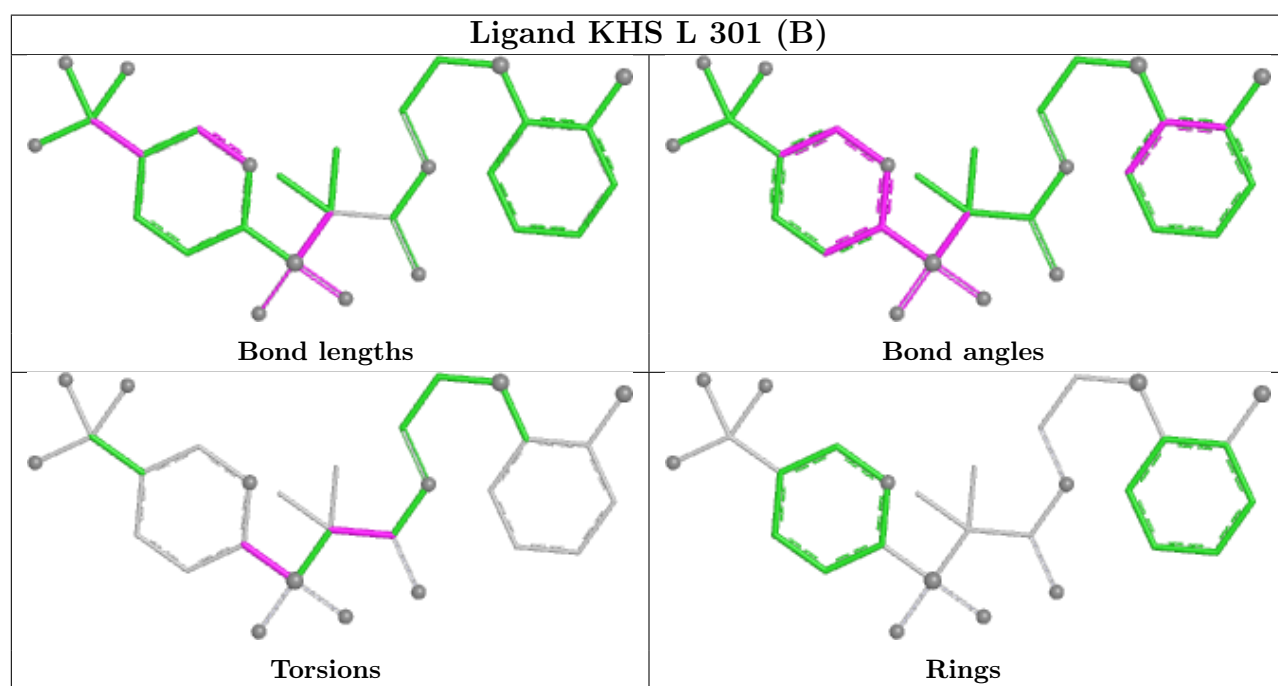
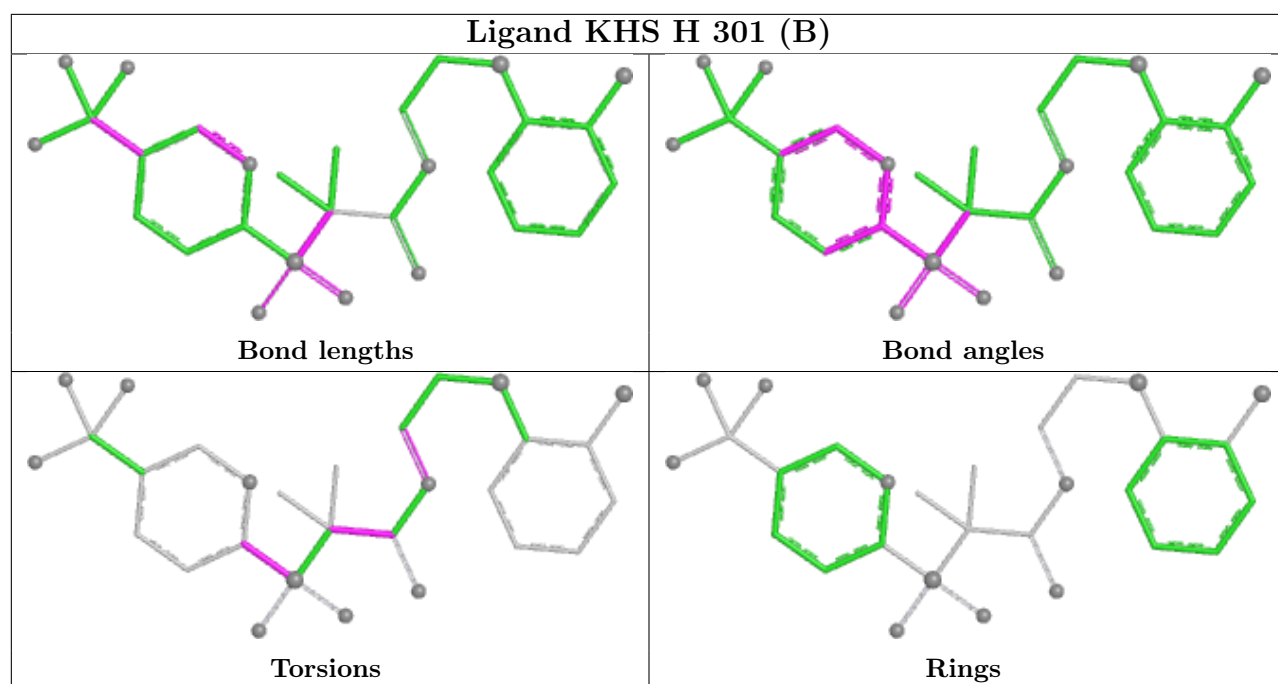
Ligand KHS K 301 (A)



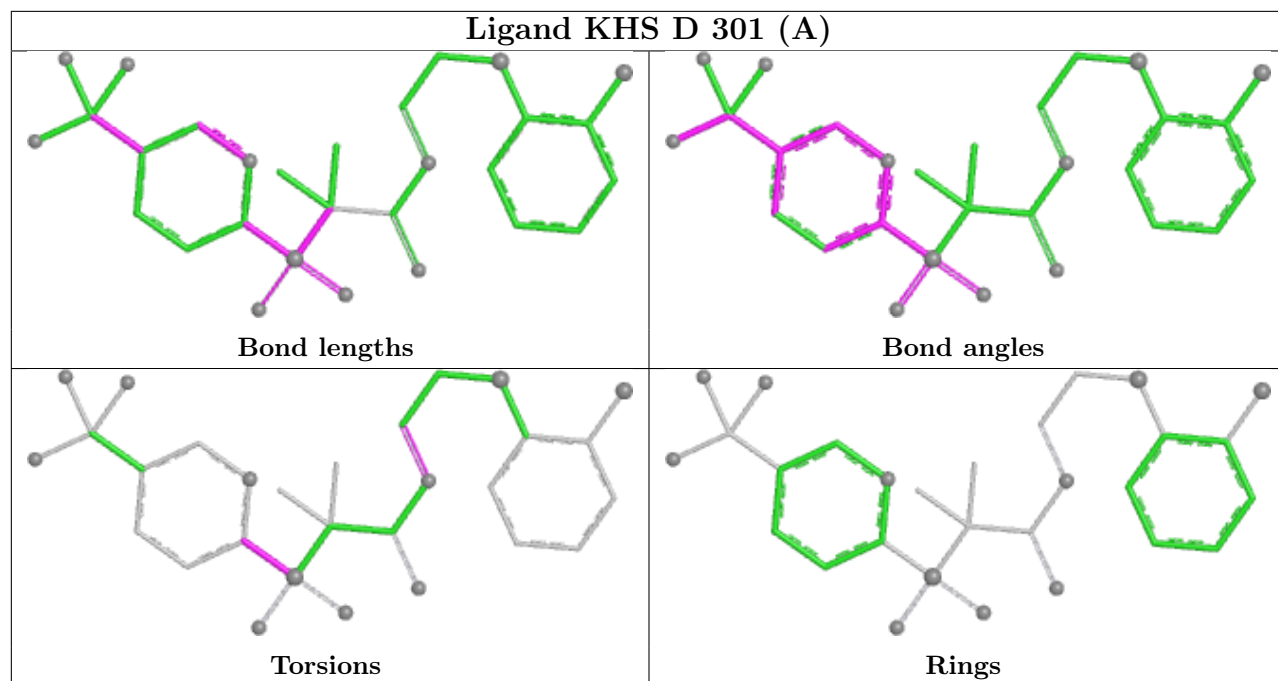
Ligand KHS N 301 (B)



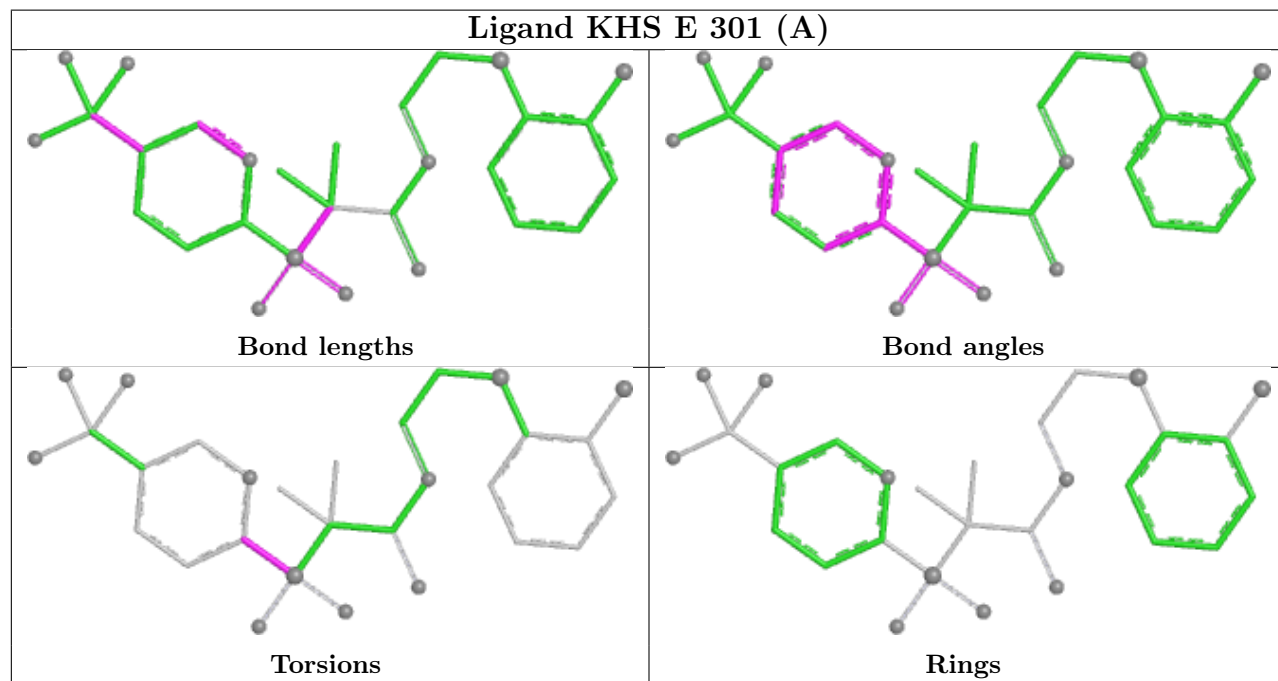




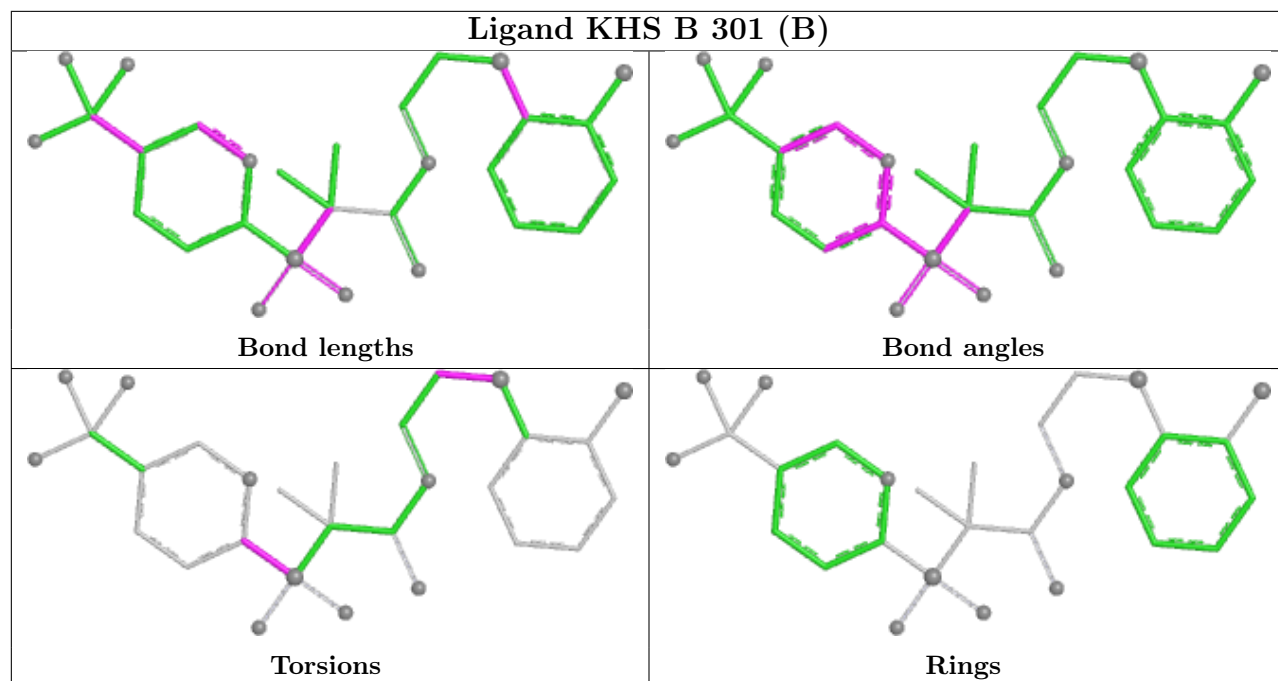
Ligand KHS D 301 (A)



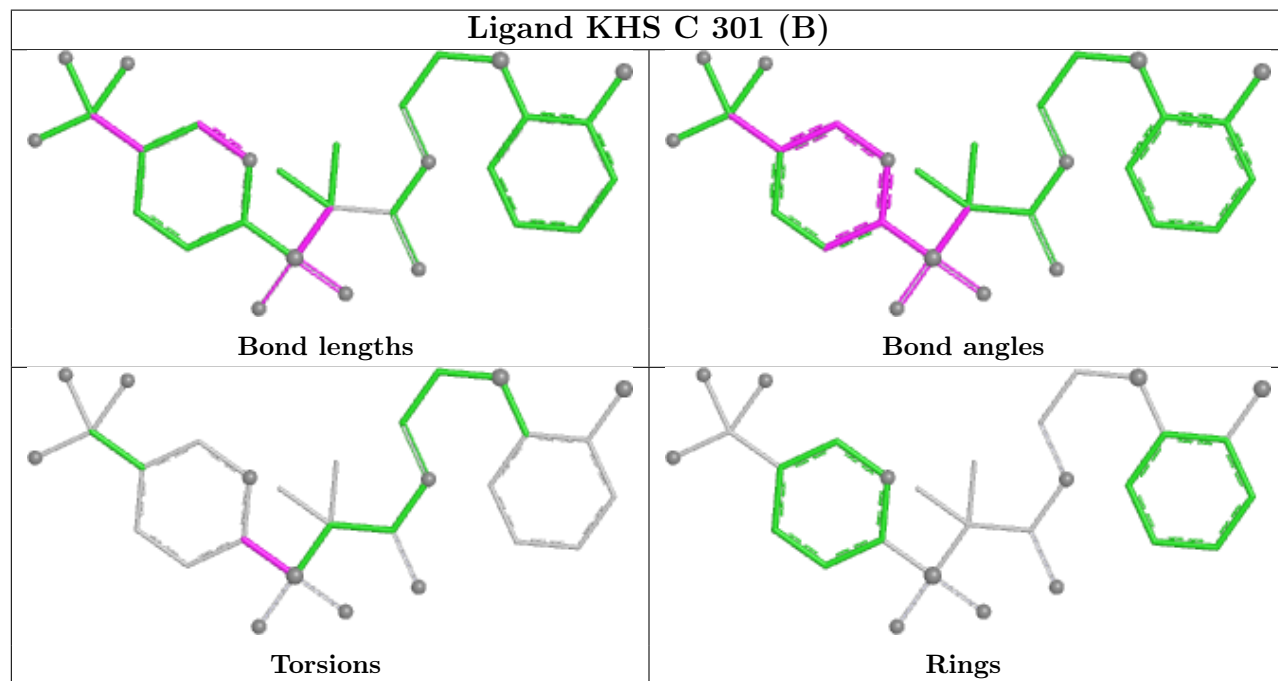
Ligand KHS E 301 (A)



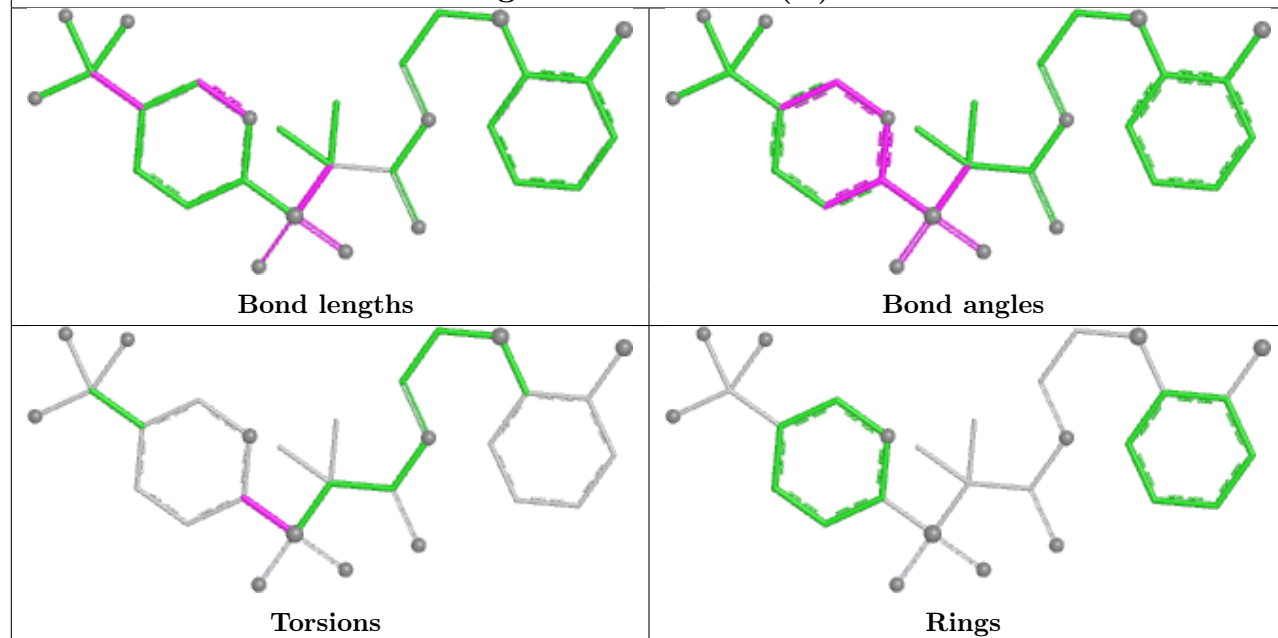
Ligand KHS B 301 (B)



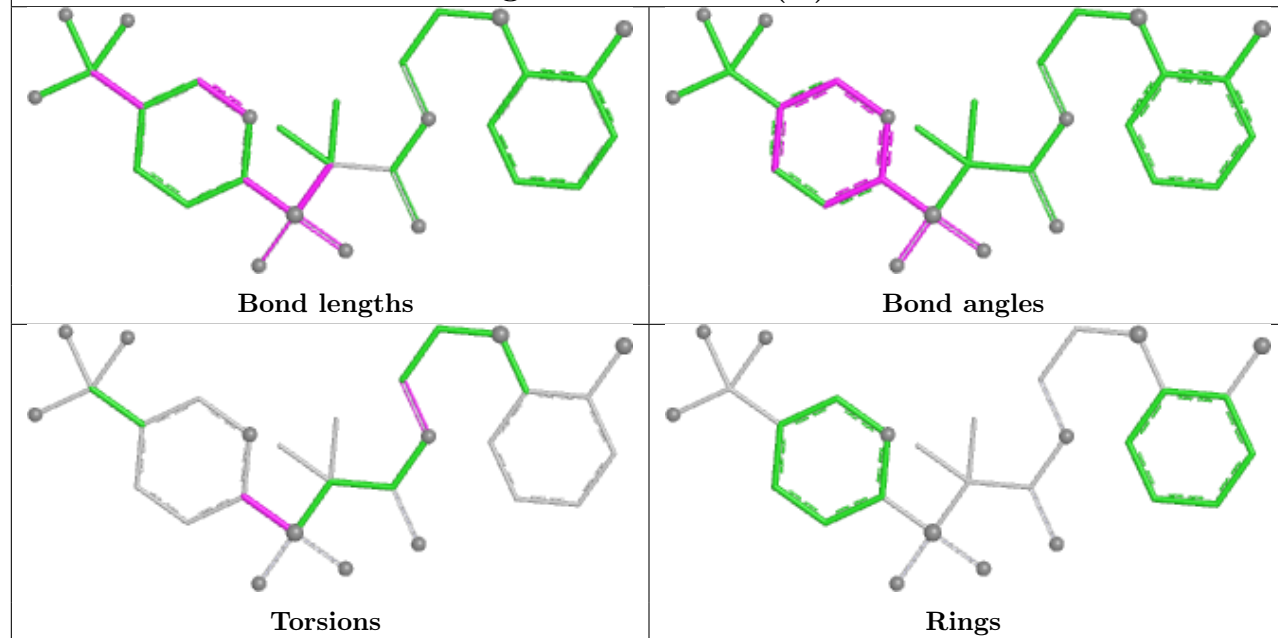
Ligand KHS C 301 (B)



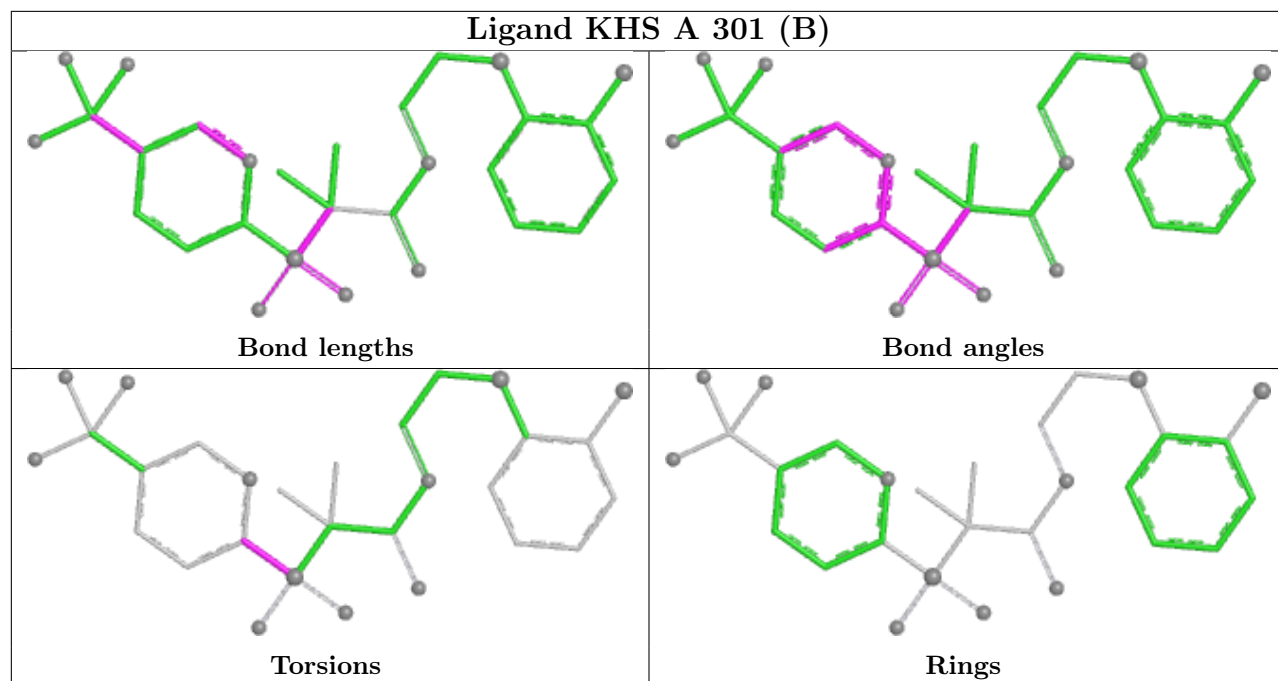
Ligand KHS K 301 (B)



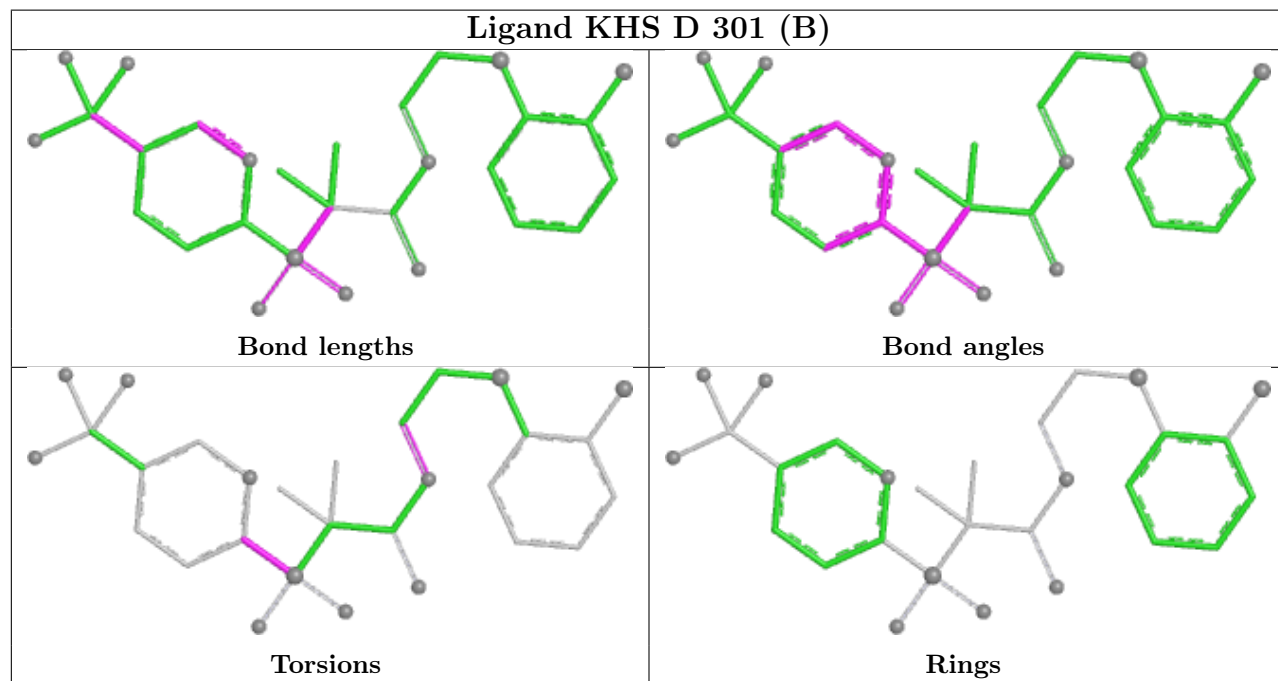
Ligand KHS J 301 (A)



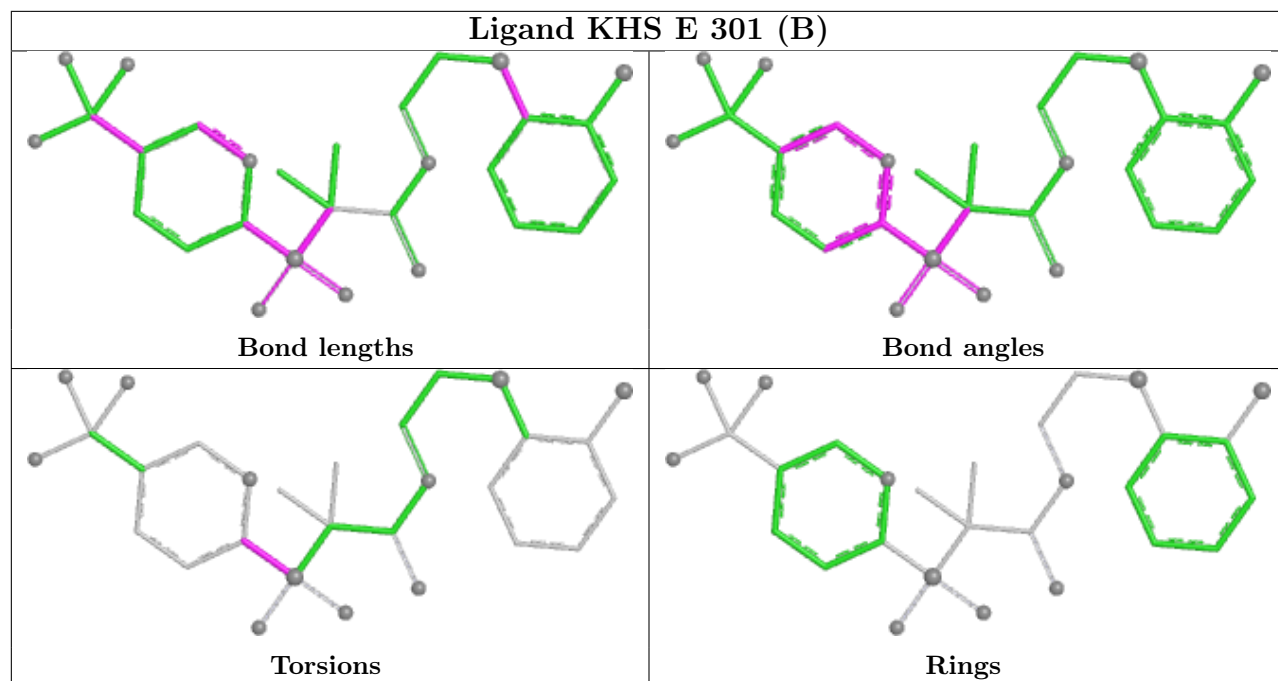
Ligand KHS A 301 (B)



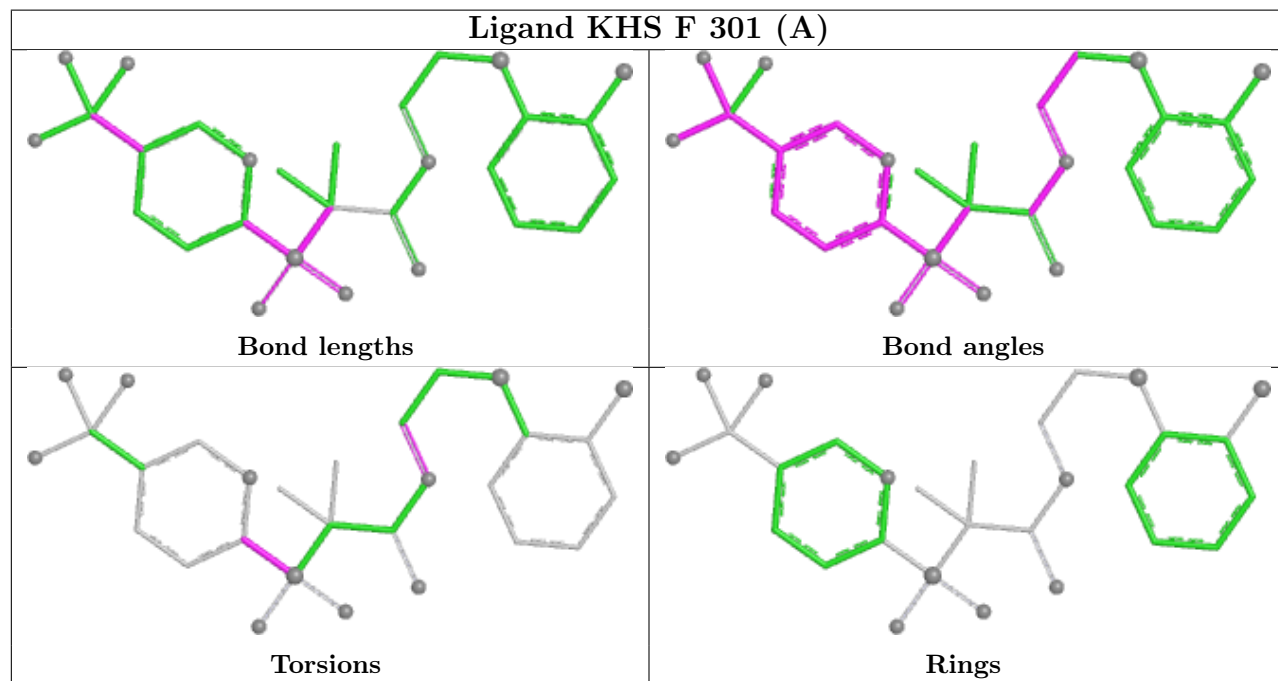
Ligand KHS D 301 (B)

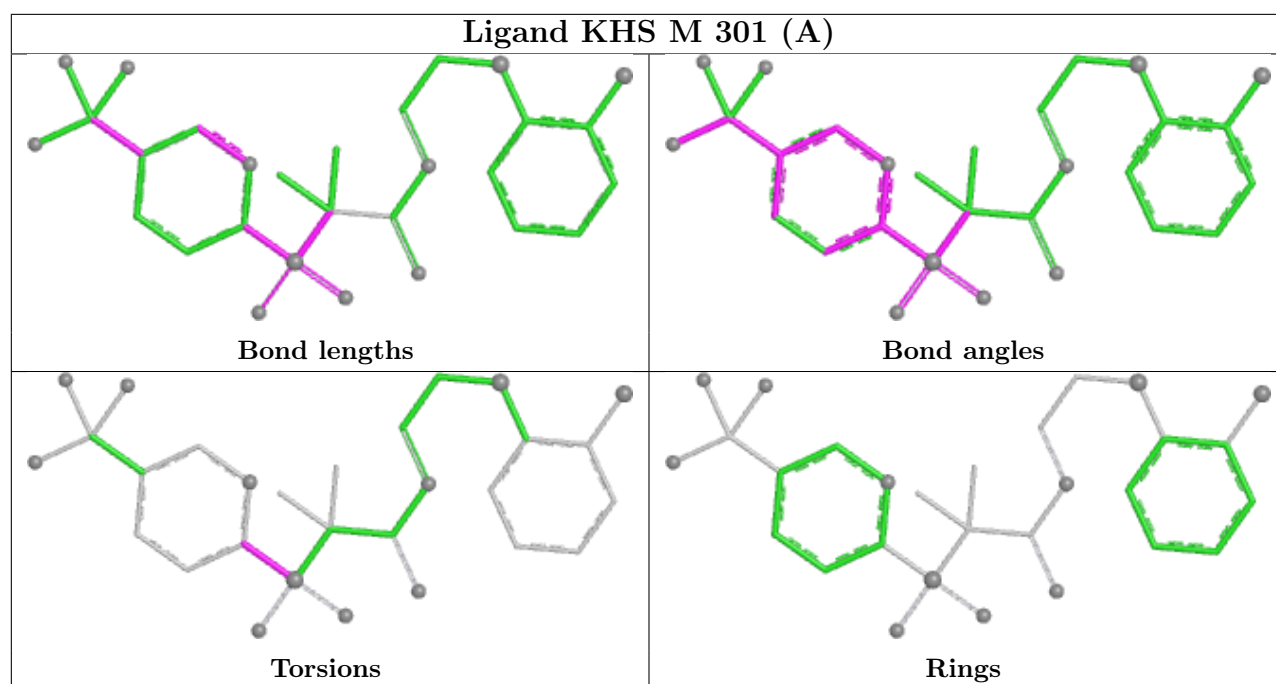


Ligand KHS E 301 (B)



Ligand KHS F 301 (A)





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	188/207 (90%)	0.42	14 (7%)	20 22	18, 25, 50, 77	0
1	B	193/207 (93%)	0.60	11 (5%)	29 31	20, 27, 54, 89	4 (2%)
1	C	184/207 (88%)	0.67	14 (7%)	20 21	19, 27, 48, 72	3 (1%)
1	D	184/207 (88%)	0.62	14 (7%)	20 21	21, 27, 50, 83	0
1	E	186/207 (89%)	0.44	5 (2%)	56 60	17, 26, 46, 89	0
1	F	183/207 (88%)	0.27	12 (6%)	24 26	16, 22, 47, 67	1 (0%)
1	G	183/207 (88%)	0.20	10 (5%)	30 32	16, 22, 46, 72	0
1	H	181/207 (87%)	0.38	7 (3%)	43 46	19, 26, 49, 65	0
1	I	176/207 (85%)	0.27	2 (1%)	78 80	19, 25, 45, 68	0
1	J	180/207 (86%)	0.42	11 (6%)	27 29	20, 26, 48, 71	1 (0%)
1	K	181/207 (87%)	0.45	10 (5%)	30 32	20, 26, 46, 73	0
1	L	182/207 (87%)	0.33	13 (7%)	22 23	17, 24, 48, 70	2 (1%)
1	M	180/207 (86%)	0.22	8 (4%)	39 41	16, 24, 49, 68	2 (1%)
1	N	180/207 (86%)	0.28	10 (5%)	30 32	19, 25, 48, 75	0
All	All	2561/2898 (88%)	0.40	141 (5%)	30 32	16, 25, 49, 89	13 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	17	VAL	6.3
1	B	15	ALA	6.0
1	M	31	PHE	5.8
1	N	19	MET	5.6
1	F	19	MET	5.6
1	N	17	VAL	5.4
1	M	17	VAL	5.3
1	E	21	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	4.9
1	N	31	PHE	4.8
1	B	16	LEU	4.8
1	K	16	LEU	4.7
1	A	15	ALA	4.6
1	J	17	VAL	4.5
1	J	19	MET	4.5
1	L	16	LEU	4.4
1	A	31	PHE	4.3
1	F	31	PHE	4.2
1	D	17	VAL	4.2
1	M	19	MET	4.1
1	B	66	ALA	4.0
1	G	16	ALA	4.0
1	L	31	PHE	4.0
1	C	21	ILE	4.0
1	G	31	PHE	4.0
1	B	24	THR	3.9
1	C	20	VAL	3.9
1	F	21	ILE	3.9
1	H	31	PHE	3.9
1	E	29	ARG	3.7
1	G	17	LEU	3.7
1	J	18	PRO	3.7
1	I	66	ALA	3.6
1	D	31	PHE	3.6
1	A	22	GLU	3.5
1	G	19	PRO	3.4
1	D	20	VAL	3.4
1	C	66	ALA	3.4
1	A	16	LEU	3.4
1	F	16	LEU	3.4
1	L	96	PHE	3.4
1	E	66	ALA	3.3
1	L	66	ALA	3.3
1	A	28	GLU	3.3
1	F	207	ASN	3.3
1	D	207	ASN	3.3
1	K	96	PHE	3.2
1	H	207	ASN	3.2
1	D	29	ARG	3.1
1	C	23	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	N	66	ALA	3.1
1	A	207	ASN	3.1
1	F	39	LYS	3.0
1	L	67	GLU	3.0
1	L	39	LYS	3.0
1	C	19	MET	3.0
1	M	66	ALA	3.0
1	D	28	GLU	2.9
1	D	66	ALA	2.9
1	E	30	SER	2.9
1	A	96	PHE	2.8
1	A	21	ILE	2.8
1	F	20	VAL	2.8
1	J	20	VAL	2.8
1	H	195	GLU	2.8
1	A	29	ARG	2.8
1	B	25	SER	2.7
1	H	66	ALA	2.7
1	B	203	LEU	2.7
1	L	19	MET	2.7
1	B	206	ARG	2.7
1	K	66	ALA	2.7
1	B	207	ASN	2.7
1	J	33	ILE	2.7
1	D	122	LYS	2.6
1	B	26	ARG	2.6
1	G	207	ASN	2.6
1	J	32	ASP	2.6
1	C	39	LYS	2.6
1	F	35	SER	2.5
1	A	17	VAL	2.5
1	G	18	VAL	2.5
1	L	70	GLU	2.5
1	N	39	LYS	2.5
1	C	169	LEU	2.5
1	F	195	GLU	2.5
1	K	19	MET	2.4
1	J	66	ALA	2.4
1	K	98	LYS	2.4
1	C	154	ARG	2.4
1	H	206	ARG	2.4
1	J	39	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	2.4
1	N	36	ARG	2.4
1	J	40	GLU	2.4
1	G	32	ASP	2.3
1	F	206	ARG	2.3
1	K	32	ASP	2.3
1	D	96	PHE	2.3
1	D	205	HIS	2.3
1	B	19	MET	2.3
1	G	20	MET	2.3
1	K	20	VAL	2.3
1	C	150	GLU	2.3
1	J	207	ASN	2.3
1	A	154	ARG	2.3
1	I	195	GLU	2.3
1	E	16	LEU	2.3
1	C	22	GLU	2.2
1	C	30	SER	2.2
1	K	35	SER	2.2
1	F	32	ASP	2.2
1	L	20	VAL	2.2
1	M	207	ASN	2.2
1	N	207	ASN	2.2
1	K	206	ARG	2.2
1	D	197	GLY	2.2
1	N	18	PRO	2.2
1	D	33	ILE	2.2
1	C	70	GLU	2.2
1	G	66	ALA	2.2
1	C	207	ASN	2.1
1	H	32	ASP	2.1
1	M	18	PRO	2.1
1	M	143	GLN	2.1
1	J	36	ARG	2.1
1	H	67	GLU	2.1
1	N	32	ASP	2.1
1	G	154	ARG	2.1
1	L	98	LYS	2.1
1	M	70	GLU	2.1
1	F	37	LEU	2.1
1	K	37	LEU	2.1
1	D	48	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	207	ASN	2.0
1	A	64	LEU	2.0
1	D	206	ARG	2.0
1	A	33	ILE	2.0
1	N	74	TYR	2.0
1	C	18	PRO	2.0
1	L	206	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KHS	G	301[A]	29/29	0.46	0.38	47,59,69,76	29
2	KHS	G	301[B]	29/29	0.46	0.38	32,58,69,76	29
2	KHS	M	301[A]	29/29	0.50	0.33	46,60,69,73	29
2	KHS	M	301[B]	29/29	0.50	0.33	33,59,67,73	29
2	KHS	H	301[A]	29/29	0.51	0.38	52,62,75,82	29
2	KHS	H	301[B]	29/29	0.51	0.38	38,60,75,82	29
2	KHS	C	301[A]	29/29	0.51	0.34	55,68,83,94	29
2	KHS	C	301[B]	29/29	0.51	0.34	42,68,83,94	29
2	KHS	N	301[A]	29/29	0.51	0.41	56,70,83,106	29
2	KHS	N	301[B]	29/29	0.51	0.41	37,68,83,106	29
2	KHS	J	301[A]	29/29	0.53	0.38	50,67,77,97	29
2	KHS	J	301[B]	29/29	0.53	0.38	40,67,77,97	29
2	KHS	D	301[A]	29/29	0.54	0.33	55,68,78,86	29
2	KHS	D	301[B]	29/29	0.54	0.33	42,67,78,87	29
2	KHS	L	301[A]	29/29	0.55	0.29	46,62,69,70	29
2	KHS	L	301[B]	29/29	0.55	0.29	33,62,68,69	29

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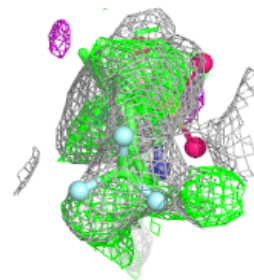
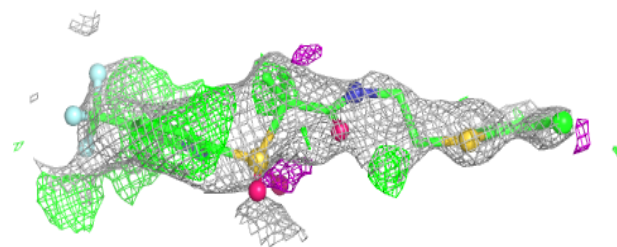
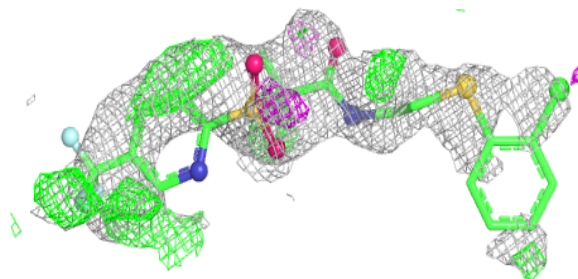
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KHS	I	301[A]	29/29	0.56	0.29	51,59,75,83	29
2	KHS	I	301[B]	29/29	0.56	0.29	36,58,74,84	29
2	KHS	A	301[A]	29/29	0.58	0.32	52,63,67,77	29
2	KHS	A	301[B]	29/29	0.58	0.32	32,61,67,77	29
2	KHS	F	301[A]	29/29	0.58	0.38	47,64,82,101	29
2	KHS	F	301[B]	29/29	0.58	0.38	41,64,82,101	29
2	KHS	K	301[A]	29/29	0.58	0.31	50,62,73,83	29
2	KHS	K	301[B]	29/29	0.58	0.31	37,60,73,83	29
2	KHS	E	301[A]	29/29	0.65	0.29	45,51,56,63	29
2	KHS	E	301[B]	29/29	0.65	0.29	32,48,54,63	29
2	KHS	B	301[A]	29/29	0.67	0.35	57,68,80,93	29
2	KHS	B	301[B]	29/29	0.67	0.35	38,65,80,94	29
3	GOL	D	302	6/6	0.81	0.16	33,44,52,62	0
3	GOL	C	302	6/6	0.82	0.13	33,39,43,54	0
3	GOL	B	302	6/6	0.83	0.14	34,45,50,50	0
3	GOL	H	302	6/6	0.83	0.14	26,35,43,52	0
3	GOL	I	302	6/6	0.83	0.15	28,40,45,54	0
3	GOL	K	302	6/6	0.84	0.12	33,36,45,50	0
3	GOL	G	302	6/6	0.85	0.12	33,34,45,51	0
3	GOL	F	302	6/6	0.85	0.16	15,34,37,54	0
3	GOL	E	302	6/6	0.86	0.15	30,33,35,48	0
3	GOL	L	302	6/6	0.88	0.12	35,36,39,49	0
3	GOL	M	302	6/6	0.88	0.11	25,28,34,44	0
3	GOL	A	302	6/6	0.90	0.10	29,35,36,41	0
3	GOL	N	302	6/6	0.90	0.12	32,34,36,55	0
3	GOL	J	302	6/6	0.93	0.10	29,43,47,49	0

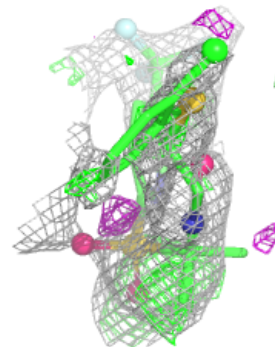
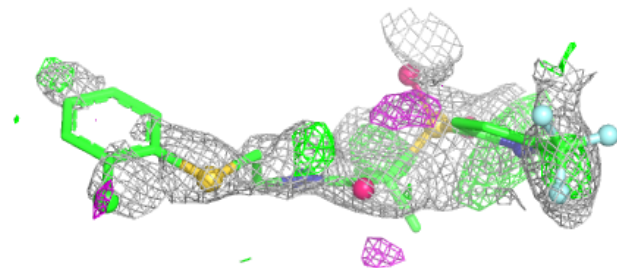
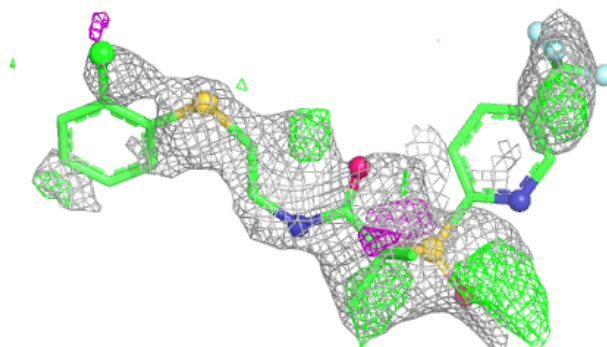
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KHS G 301 (A):

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

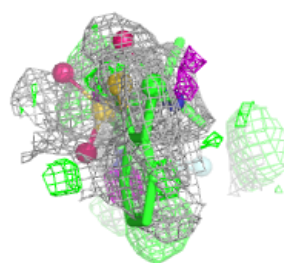
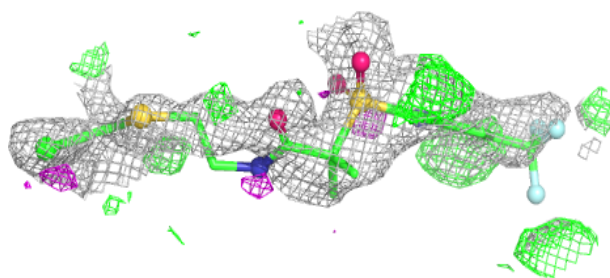
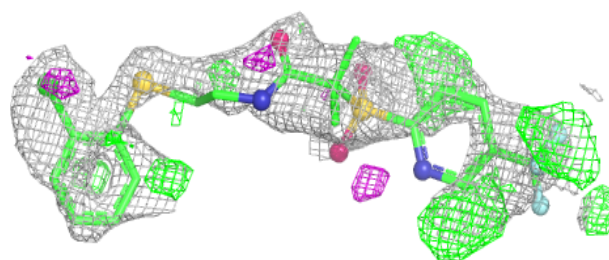
**Electron density around KHS G 301 (B):**

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

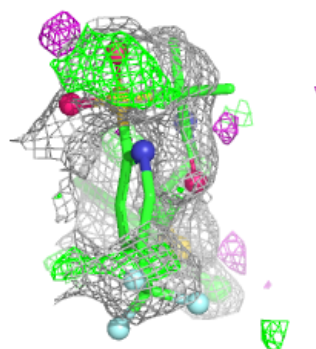
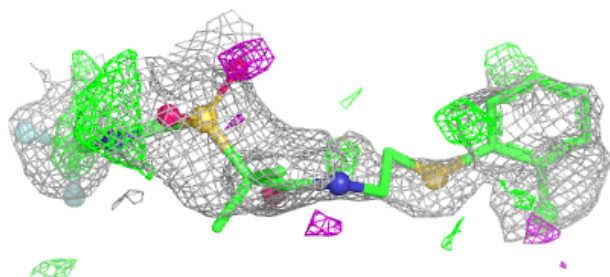
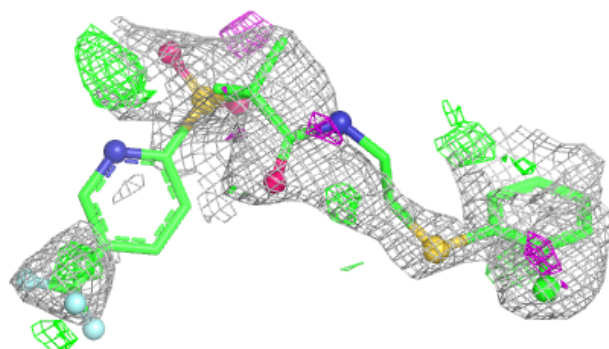


Electron density around KHS M 301 (A):

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

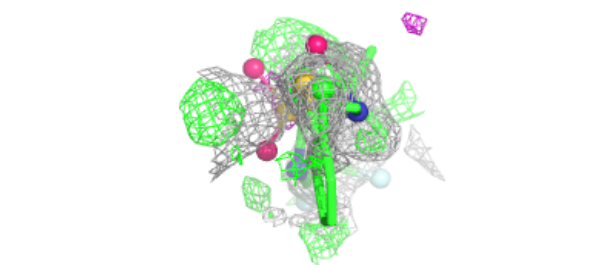
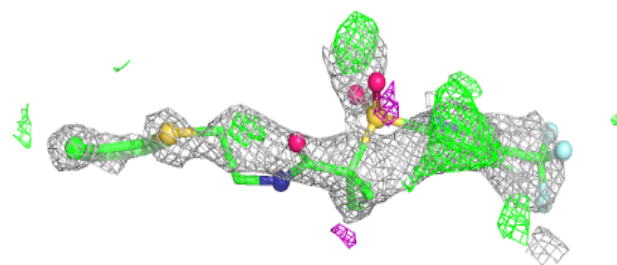
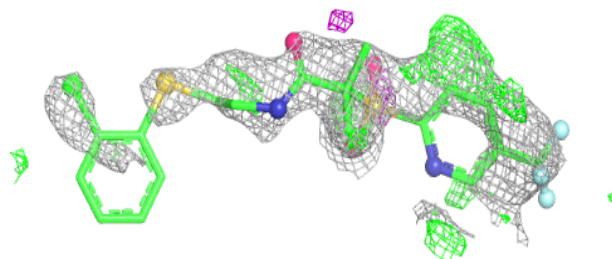
**Electron density around KHS M 301 (B):**

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

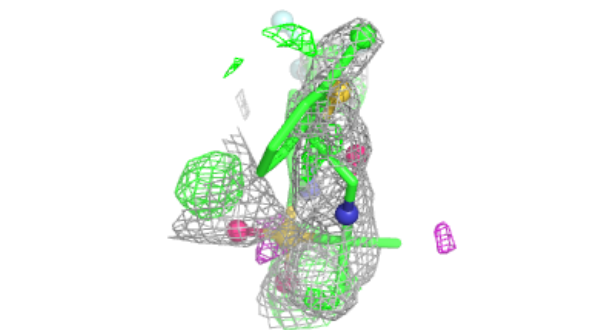
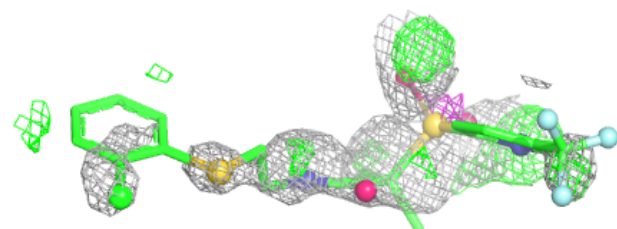
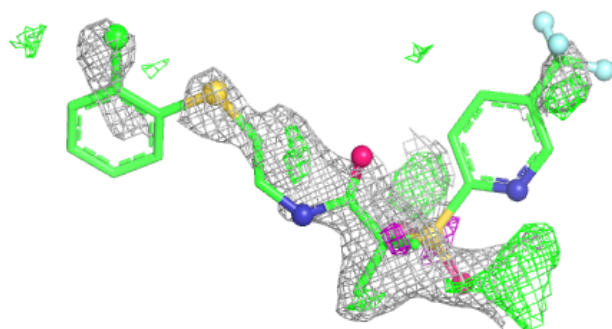


Electron density around KHS H 301 (A):

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

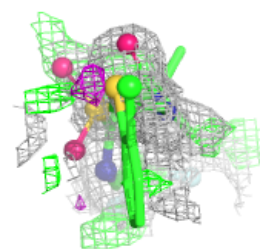
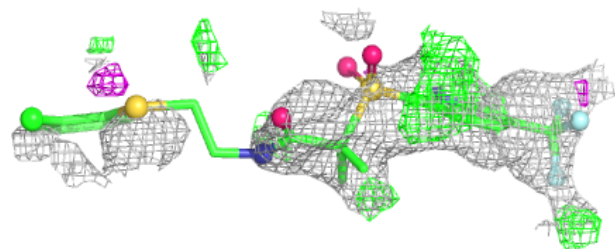
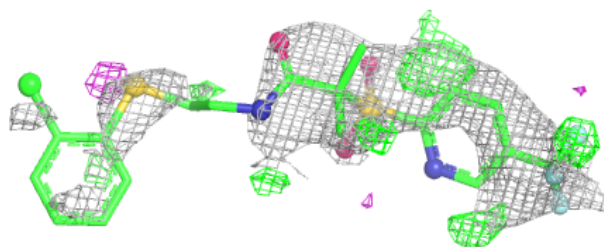
**Electron density around KHS H 301 (B):**

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

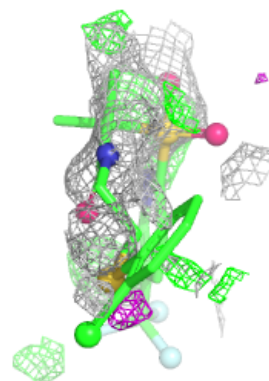
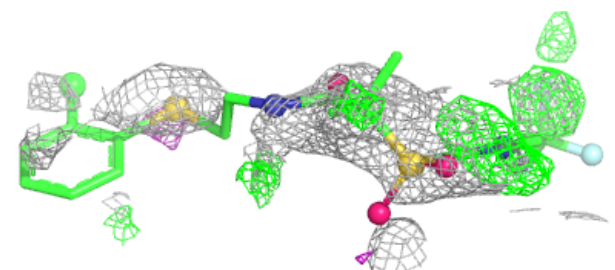
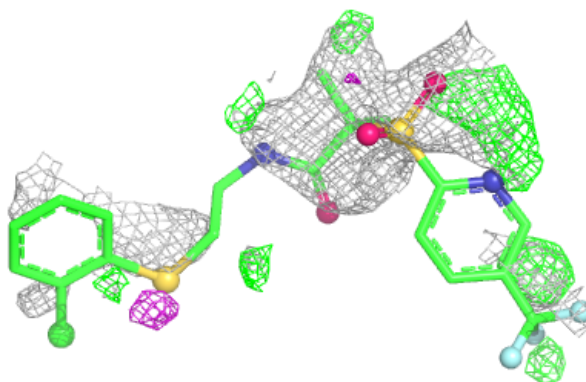


Electron density around KHS C 301 (A):

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

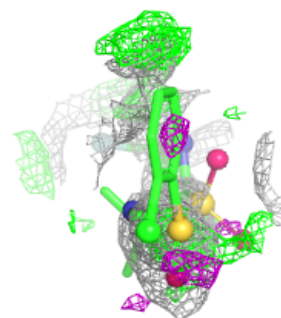
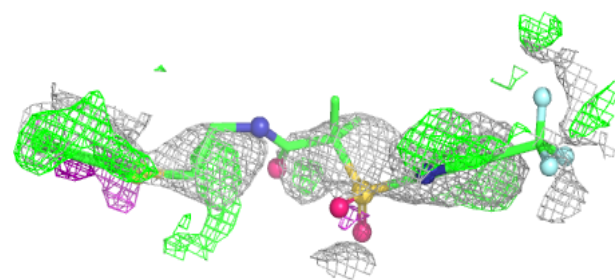
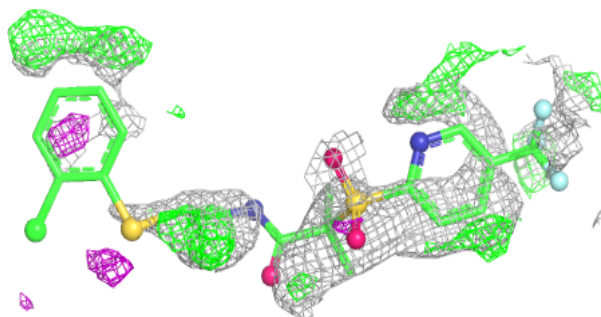
**Electron density around KHS C 301 (B):**

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

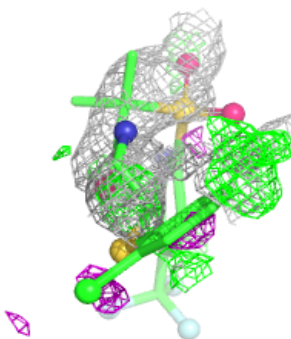
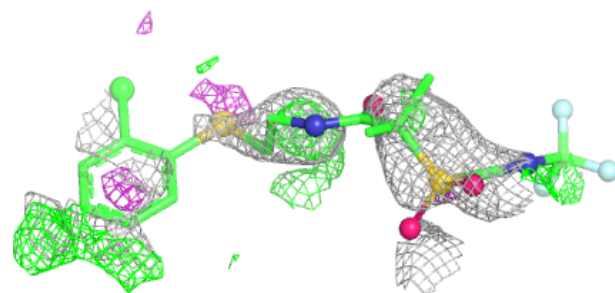
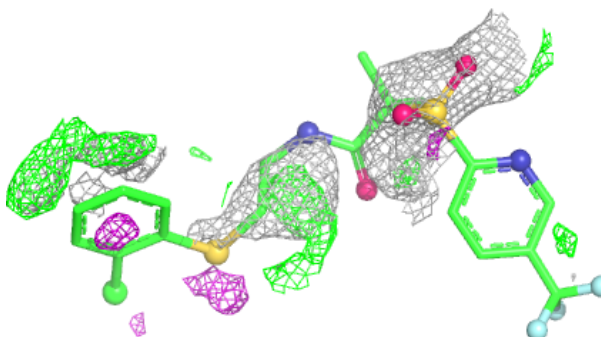


Electron density around KHS N 301 (A):

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

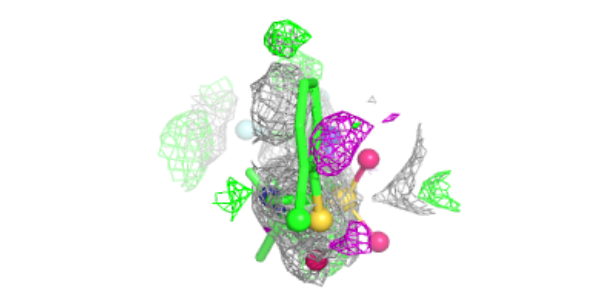
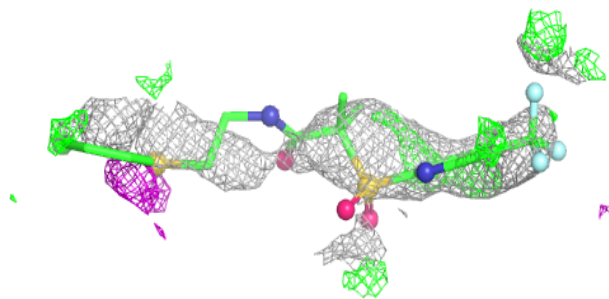
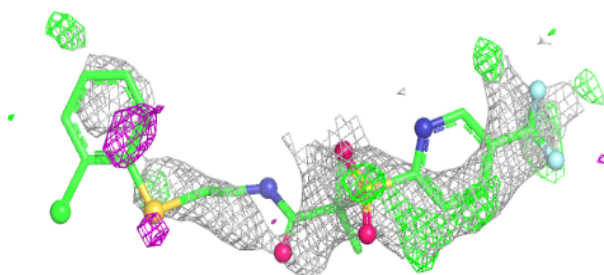
**Electron density around KHS N 301 (B):**

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

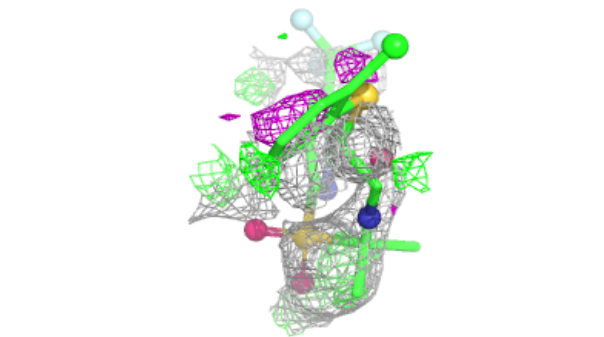
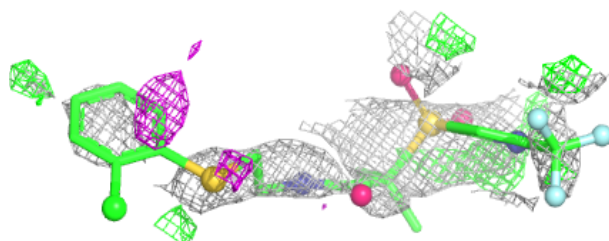
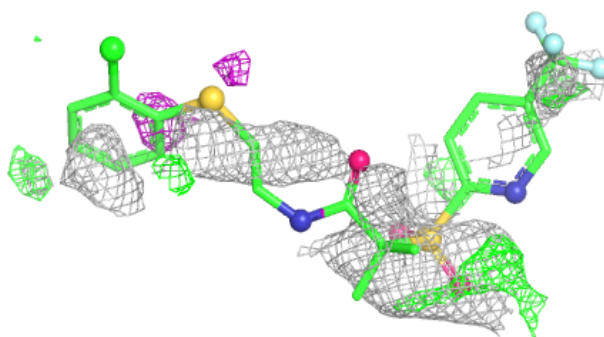


Electron density around KHS J 301 (A):

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

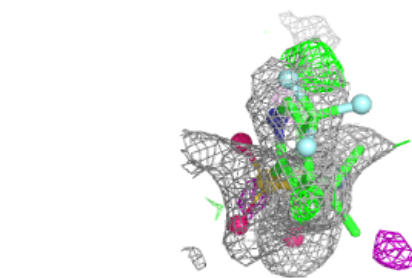
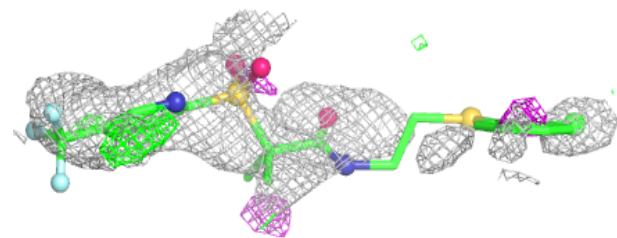
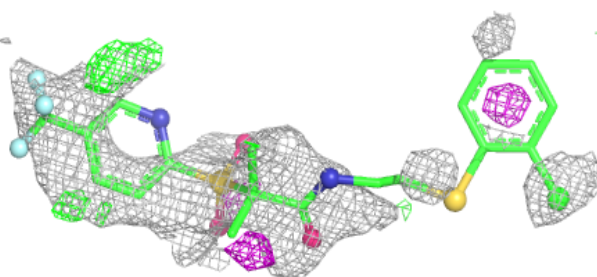
**Electron density around KHS J 301 (B):**

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

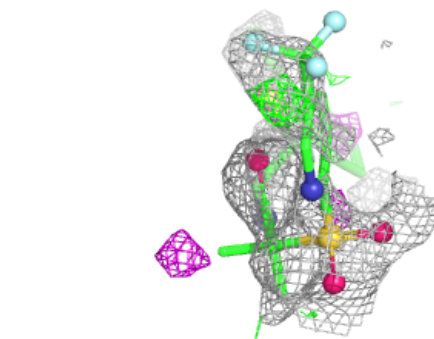
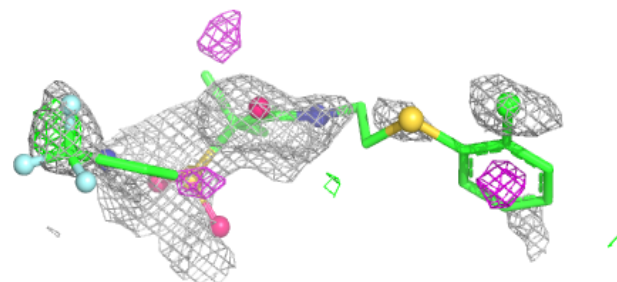
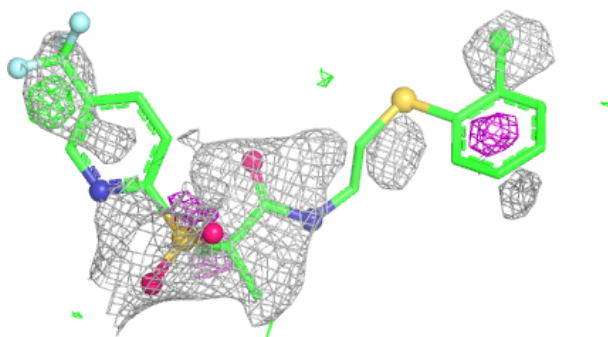


Electron density around KHS D 301 (A):

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

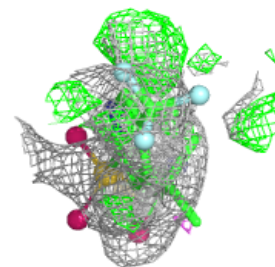
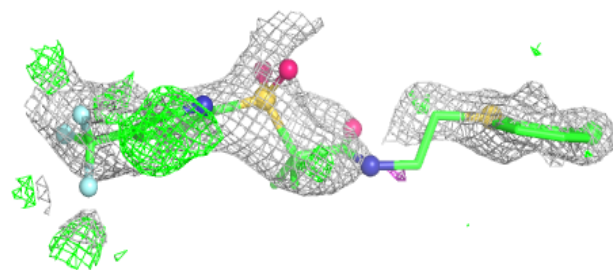
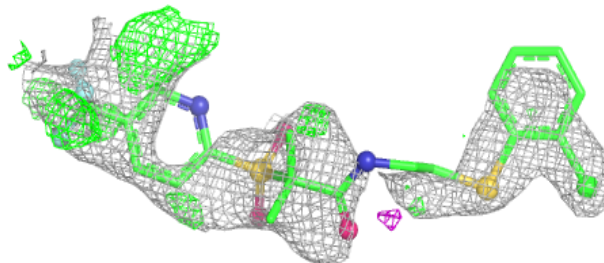
**Electron density around KHS D 301 (B):**

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

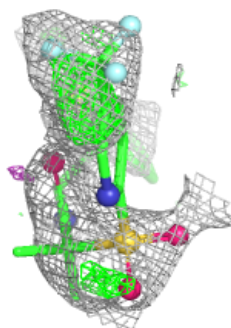
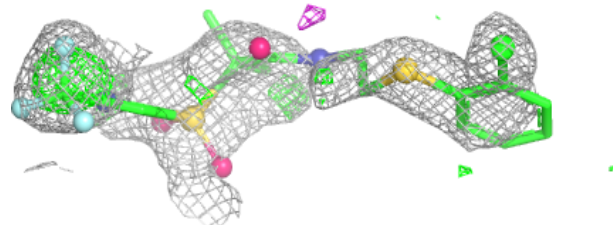
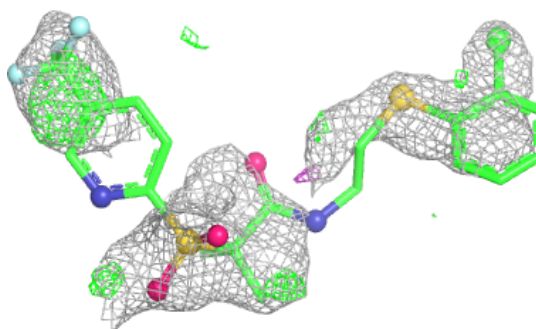


Electron density around KHS L 301 (A):

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

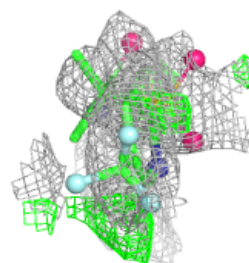
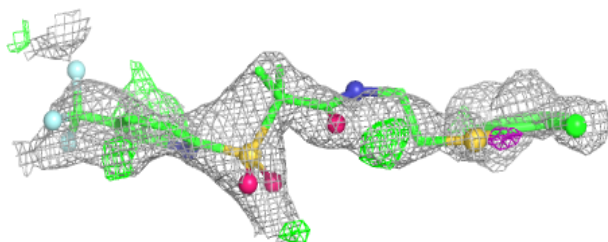
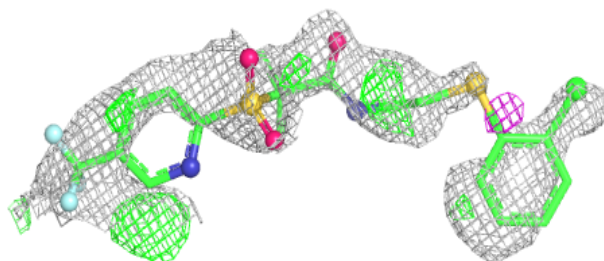
**Electron density around KHS L 301 (B):**

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

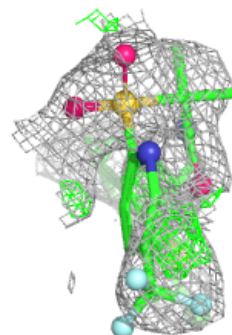
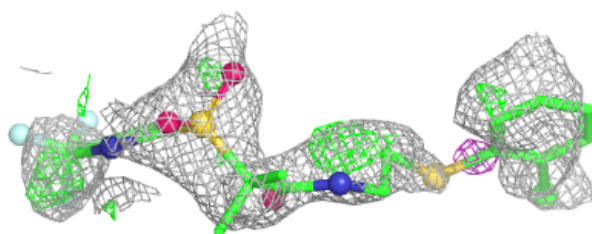
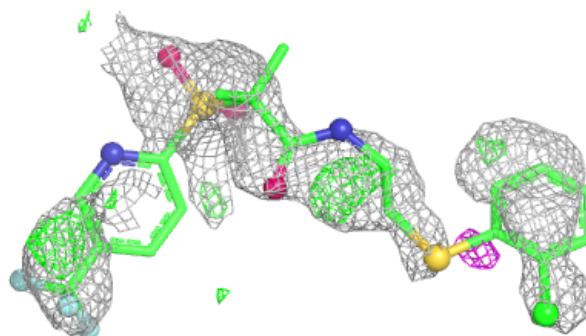


Electron density around KHS I 301 (A):

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

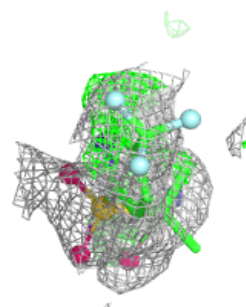
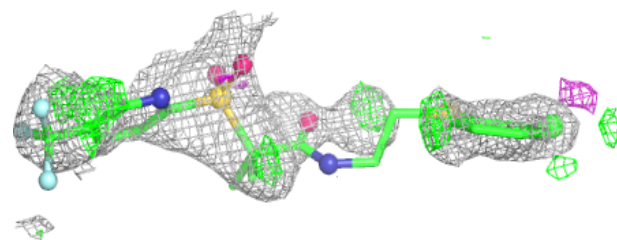
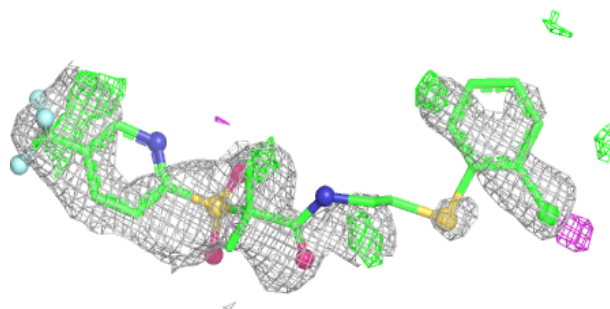
**Electron density around KHS I 301 (B):**

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

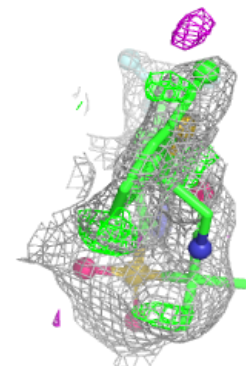
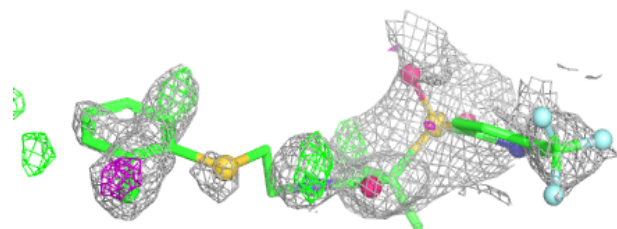
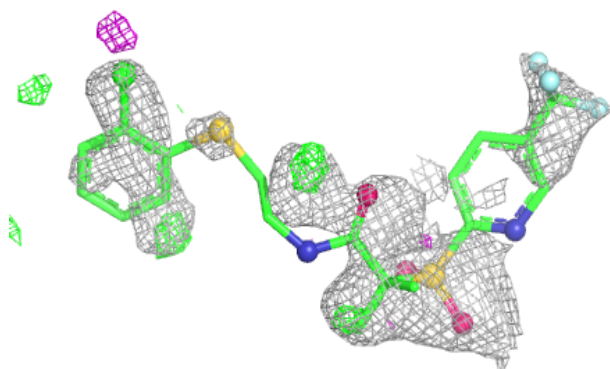


Electron density around KHS A 301 (A):

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

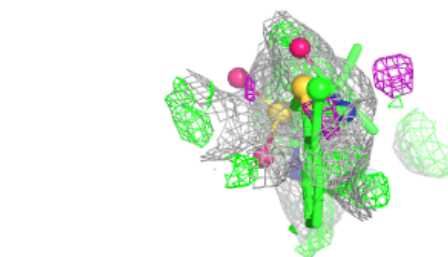
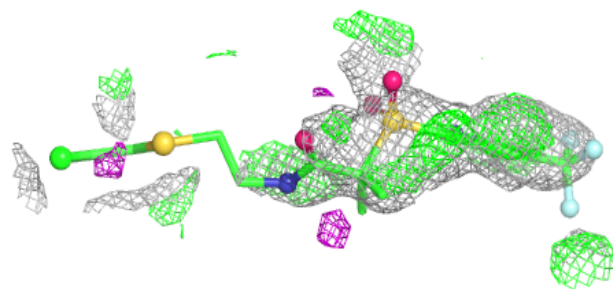
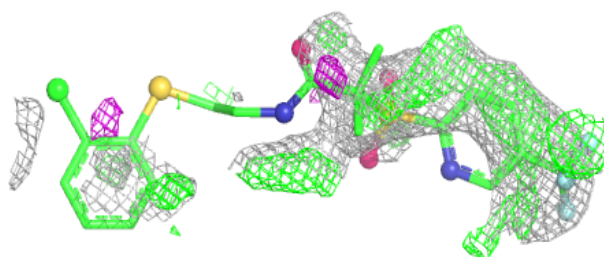
**Electron density around KHS A 301 (B):**

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

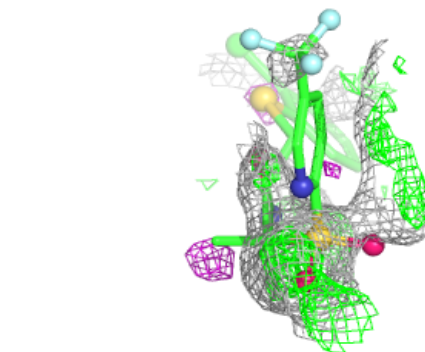
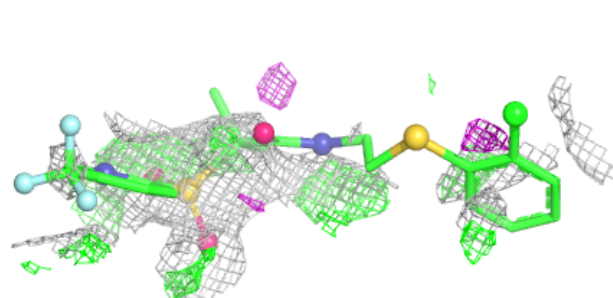
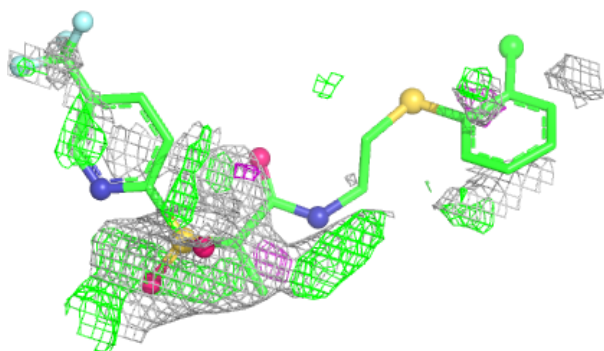


Electron density around KHS F 301 (A):

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

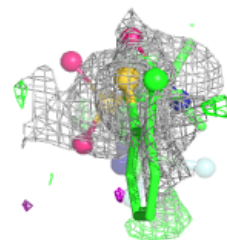
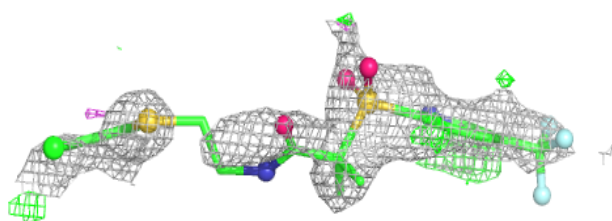
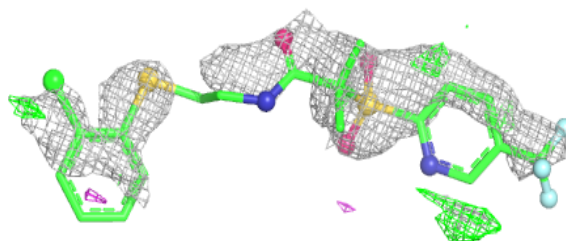
**Electron density around KHS F 301 (B):**

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

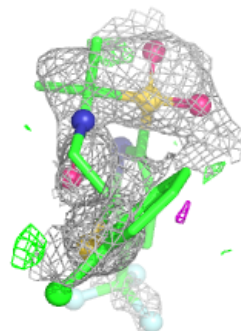
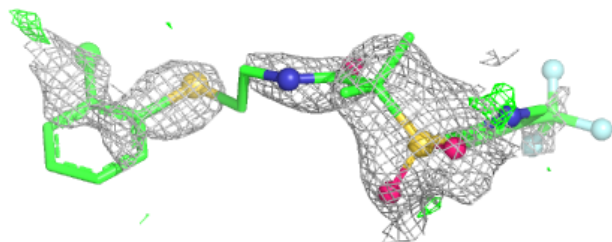
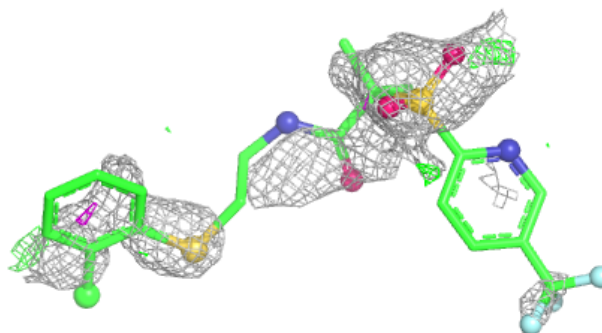


Electron density around KHS K 301 (A):

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

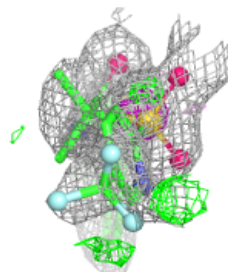
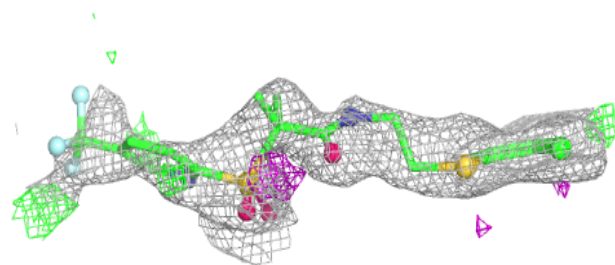
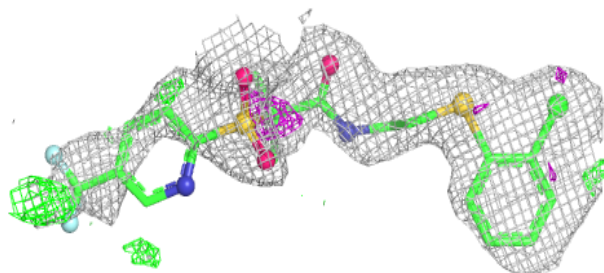
**Electron density around KHS K 301 (B):**

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

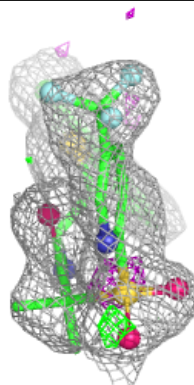
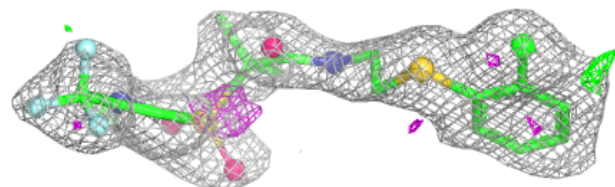
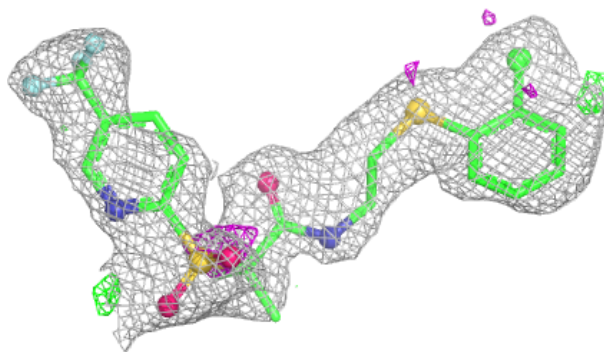


Electron density around KHS E 301 (A):

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

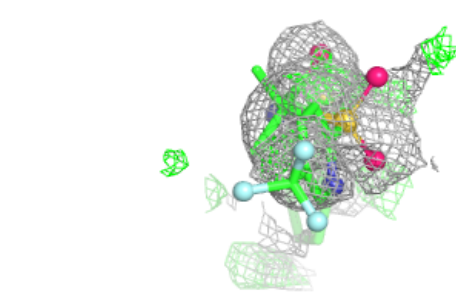
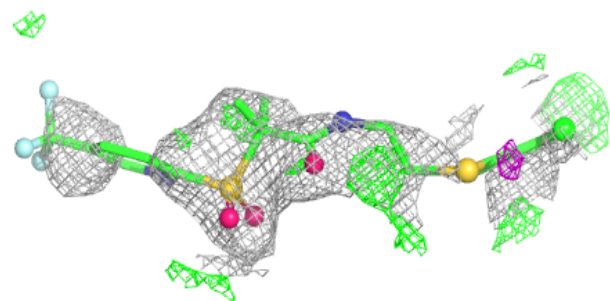
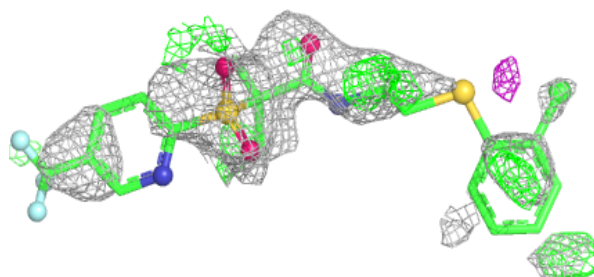
**Electron density around KHS E 301 (B):**

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

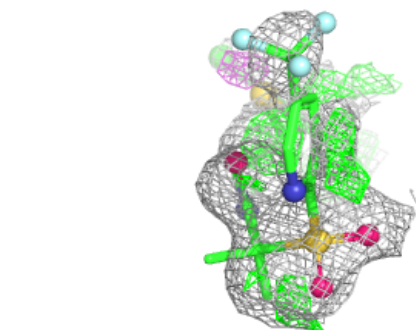
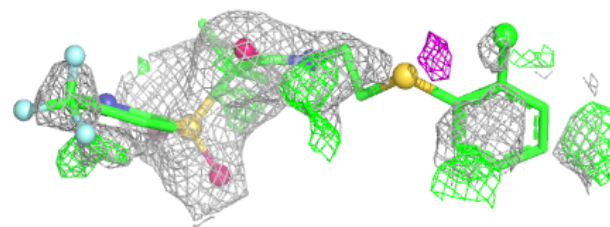
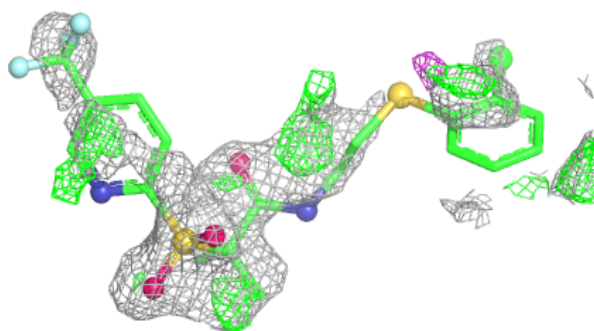


Electron density around KHS B 301 (A):

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

**Electron density around KHS B 301 (B):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.