



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2021 – 10:09 AM EDT

PDB ID : 6UVG  
Title : Crystal structure of BCL-XL bound to compound 13: (R)-2-(3-([1,1'-Biphenyl]-4-carbonyl)-3-(4-methylbenzyl)ureido)-3-(((3R,5R,7R)-adamantan-1-ylmethyl)sulfonyl)propanoic acid  
Authors : Roy, M.J.; Lessene, G.; Czabotar, P.E.  
Deposited on : 2019-11-02  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

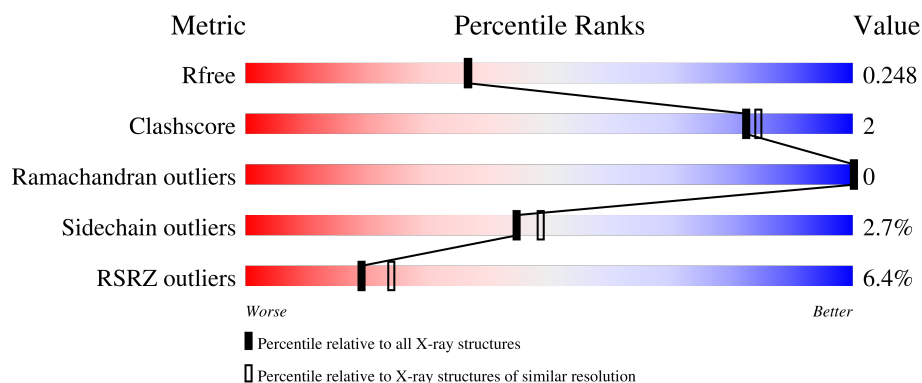
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	<div> <div>18%</div> <div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	158	<div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	C	158	<div> <div>82%</div> <div>13%</div> </div>
1	D	158	<div> <div>18%</div> <div>78%</div> <div>9%</div> <div>11%</div> </div>
1	E	158	<div> <div>2%</div> <div>84%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	158	<div><div></div><div>4%</div><div>82%</div><div>6%</div><div>•</div><div>11%</div></div>
1	G	158	<div><div></div><div>2%</div><div>85%</div><div>•</div><div>11%</div></div>
1	H	158	<div><div></div><div>%</div><div>82%</div><div>8%</div><div>10%</div></div>
1	I	158	<div><div></div><div>14%</div><div>83%</div><div>•</div><div>13%</div></div>
1	J	158	<div><div></div><div>13%</div><div>78%</div><div>6%</div><div>16%</div></div>
1	K	158	<div><div></div><div>7%</div><div>79%</div><div>10%</div><div>•</div><div>10%</div></div>
1	L	158	<div><div></div><div>4%</div><div>81%</div><div>6%</div><div>•</div><div>11%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14083 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	1	0
			1174	749	198	222	5			
1	B	144	Total	C	N	O	S	0	0	0
			1154	739	192	218	5			
1	C	138	Total	C	N	O	S	0	0	0
			1116	714	188	210	4			
1	D	140	Total	C	N	O	S	0	0	0
			1082	691	181	206	4			
1	E	140	Total	C	N	O	S	0	0	0
			1132	724	191	213	4			
1	F	141	Total	C	N	O	S	0	0	0
			1114	710	189	211	4			
1	G	141	Total	C	N	O	S	0	0	0
			1131	724	189	213	5			
1	H	142	Total	C	N	O	S	0	0	0
			1142	730	193	215	4			
1	I	138	Total	C	N	O	S	0	0	0
			1043	673	178	188	4			
1	J	133	Total	C	N	O	S	0	0	0
			1028	662	171	191	4			
1	K	142	Total	C	N	O	S	0	0	0
			1133	723	191	215	4			
1	L	140	Total	C	N	O	S	0	0	0
			1074	691	180	198	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q07817
A	-4	PRO	-	expression tag	UNP Q07817
A	-3	LEU	-	expression tag	UNP Q07817
A	-2	GLY	-	expression tag	UNP Q07817
A	-1	SER	-	expression tag	UNP Q07817

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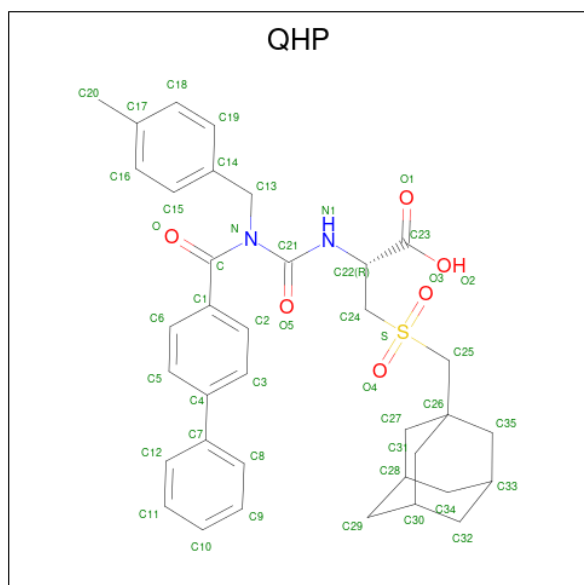
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q07817
B	-4	PRO	-	expression tag	UNP Q07817
B	-3	LEU	-	expression tag	UNP Q07817
B	-2	GLY	-	expression tag	UNP Q07817
B	-1	SER	-	expression tag	UNP Q07817
C	-4	GLY	-	expression tag	UNP Q07817
C	-3	PRO	-	expression tag	UNP Q07817
C	-2	LEU	-	expression tag	UNP Q07817
C	-1	GLY	-	expression tag	UNP Q07817
C	0	SER	-	expression tag	UNP Q07817
D	-5	GLY	-	expression tag	UNP Q07817
D	-4	PRO	-	expression tag	UNP Q07817
D	-3	LEU	-	expression tag	UNP Q07817
D	-2	GLY	-	expression tag	UNP Q07817
D	-1	SER	-	expression tag	UNP Q07817
E	-4	GLY	-	expression tag	UNP Q07817
E	-3	PRO	-	expression tag	UNP Q07817
E	-2	LEU	-	expression tag	UNP Q07817
E	-1	GLY	-	expression tag	UNP Q07817
E	0	SER	-	expression tag	UNP Q07817
F	-4	GLY	-	expression tag	UNP Q07817
F	-3	PRO	-	expression tag	UNP Q07817
F	-2	LEU	-	expression tag	UNP Q07817
F	-1	GLY	-	expression tag	UNP Q07817
F	0	SER	-	expression tag	UNP Q07817
G	-5	GLY	-	expression tag	UNP Q07817
G	-4	PRO	-	expression tag	UNP Q07817
G	-3	LEU	-	expression tag	UNP Q07817
G	-2	GLY	-	expression tag	UNP Q07817
G	-1	SER	-	expression tag	UNP Q07817
H	-4	GLY	-	expression tag	UNP Q07817
H	-3	PRO	-	expression tag	UNP Q07817
H	-2	LEU	-	expression tag	UNP Q07817
H	-1	GLY	-	expression tag	UNP Q07817
H	0	SER	-	expression tag	UNP Q07817
I	-4	GLY	-	expression tag	UNP Q07817
I	-3	PRO	-	expression tag	UNP Q07817
I	-2	LEU	-	expression tag	UNP Q07817
I	-1	GLY	-	expression tag	UNP Q07817
I	0	SER	-	expression tag	UNP Q07817
J	-4	GLY	-	expression tag	UNP Q07817
J	-3	PRO	-	expression tag	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	LEU	-	expression tag	UNP Q07817
J	-1	GLY	-	expression tag	UNP Q07817
J	0	SER	-	expression tag	UNP Q07817
K	-5	GLY	-	expression tag	UNP Q07817
K	-4	PRO	-	expression tag	UNP Q07817
K	-3	LEU	-	expression tag	UNP Q07817
K	-2	GLY	-	expression tag	UNP Q07817
K	-1	SER	-	expression tag	UNP Q07817
L	-5	GLY	-	expression tag	UNP Q07817
L	-4	PRO	-	expression tag	UNP Q07817
L	-3	LEU	-	expression tag	UNP Q07817
L	-2	GLY	-	expression tag	UNP Q07817
L	-1	SER	-	expression tag	UNP Q07817

- Molecule 2 is (R)-2-(3-([1,1'-Biphenyl]-4-carbonyl)-3-(4-methylbenzyl)ureido)-3-(((3R,5R,7R)-adamantan-1-ylmethyl)sulfonyl)propanoic acid (three-letter code: QHP) (formula: C<sub>36</sub>H<sub>40</sub>N<sub>2</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	B	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	C	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	D	1	Total	C	N	O	S	0	0
			45	36	2	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	F	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	G	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	H	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	I	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	J	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	K	1	Total	C	N	O	S	0	0
			45	36	2	6	1		
2	L	1	Total	C	N	O	S	0	0
			45	36	2	6	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



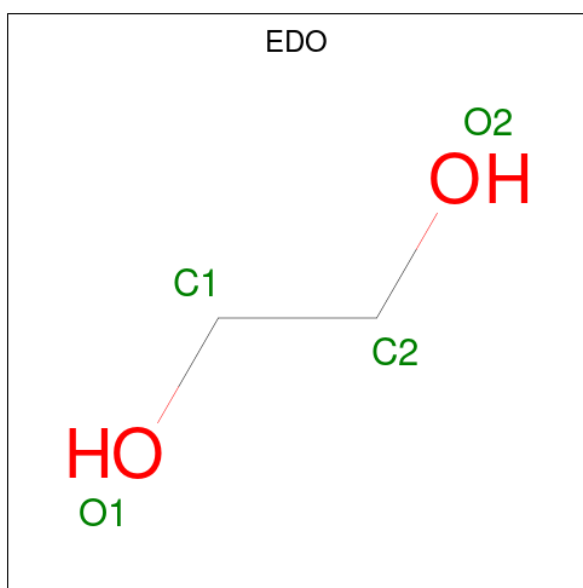
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

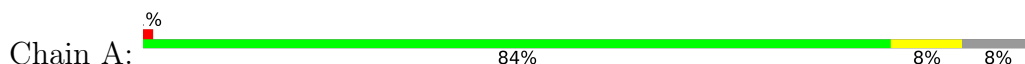


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total 44	O 44	0	0
5	B	25	Total 25	O 25	0	0
5	C	24	Total 24	O 24	0	0
5	D	1	Total 1	O 1	0	0
5	E	14	Total 14	O 14	0	0
5	F	4	Total 4	O 4	0	0
5	G	13	Total 13	O 13	0	0
5	H	23	Total 23	O 23	0	0
5	I	1	Total 1	O 1	0	0
5	J	4	Total 4	O 4	0	0
5	K	3	Total 3	O 3	0	0
5	L	4	Total 4	O 4	0	0

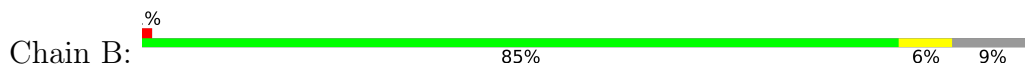
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

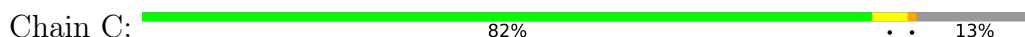
- Molecule 1: Bcl-2-like protein 1



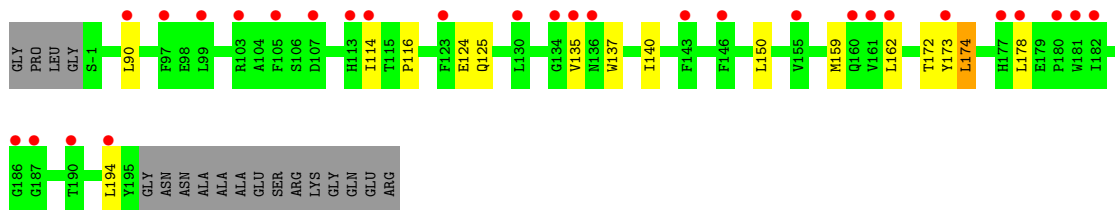
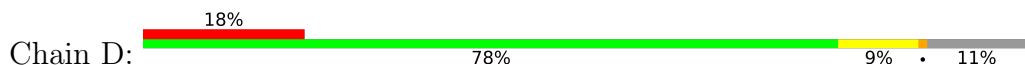
- Molecule 1: Bcl-2-like protein 1



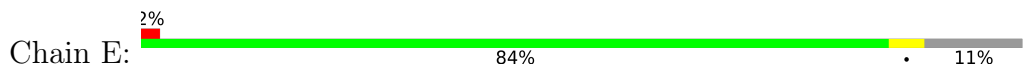
- Molecule 1: Bcl-2-like protein 1



- Molecule 1: Bcl-2-like protein 1

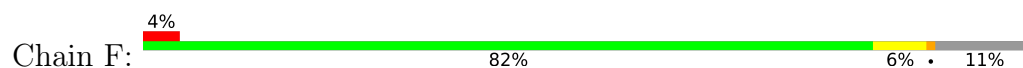


- Molecule 1: Bcl-2-like protein 1

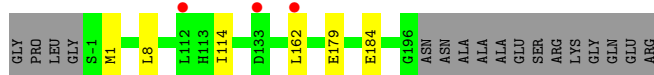
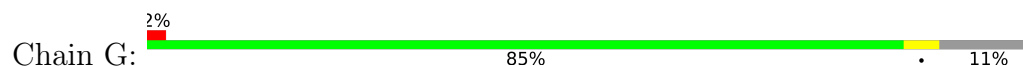




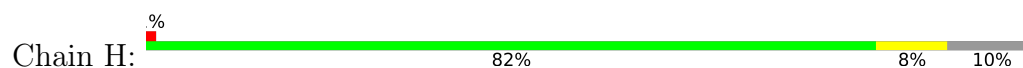
- Molecule 1: Bcl-2-like protein 1



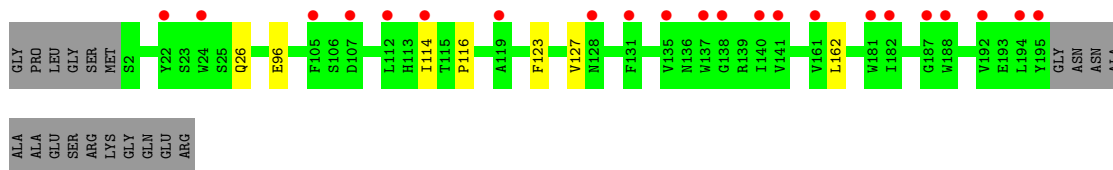
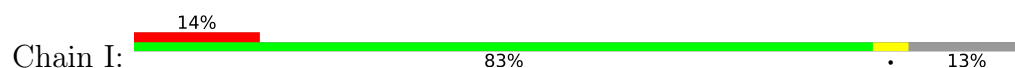
- Molecule 1: Bcl-2-like protein 1



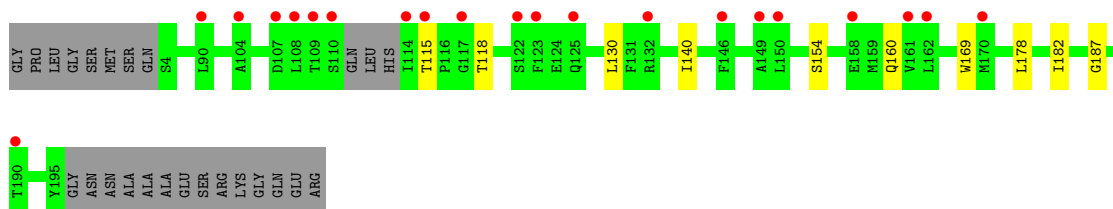
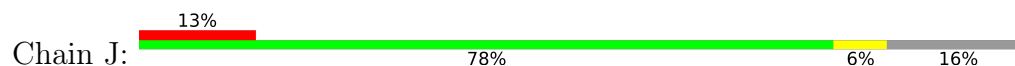
- Molecule 1: Bcl-2-like protein 1



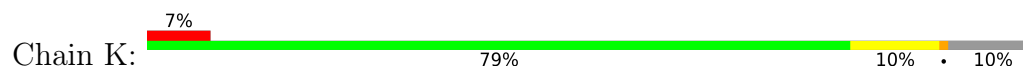
- Molecule 1: Bcl-2-like protein 1

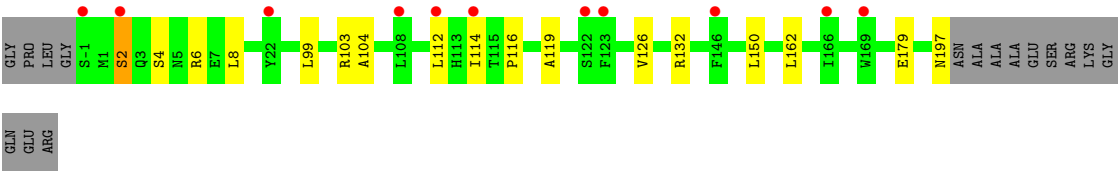


- Molecule 1: Bcl-2-like protein 1

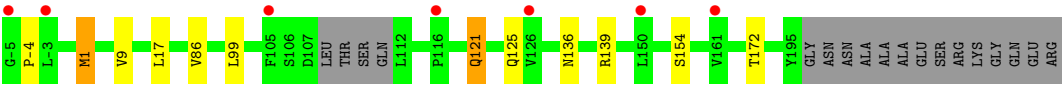
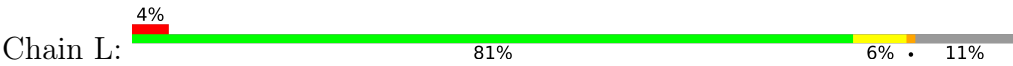


- Molecule 1: Bcl-2-like protein 1





● Molecule 1: Bcl-2-like protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.59Å 103.70Å 111.12Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	30.22 – 2.10 86.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.22-2.10) 98.7 (86.33-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.10Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.205 , 0.228 0.220 , 0.248	Depositor DCC
$R_{free}$ test set	5651 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, QHP

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	0.63	0/1203	0.63	0/1628
1	B	0.53	0/1183	0.61	0/1602
1	C	0.58	0/1144	0.63	0/1551
1	D	0.52	0/1109	0.63	0/1508
1	E	0.57	0/1160	0.63	0/1571
1	F	0.52	0/1141	0.63	0/1547
1	G	0.51	0/1158	0.61	0/1568
1	H	0.55	0/1170	0.62	0/1585
1	I	0.51	0/1070	0.60	0/1458
1	J	0.52	0/1053	0.61	0/1432
1	K	0.50	0/1160	0.61	0/1573
1	L	0.51	0/1101	0.64	0/1494
All	All	0.54	0/13652	0.62	0/18517

There are no bond length outliers.

There are no bond angle outliers.

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	1174	0	1119	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1154	0	1098	7	0
1	C	1116	0	1053	6	0
1	D	1082	0	982	8	0
1	E	1132	0	1076	4	0
1	F	1114	0	1037	7	0
1	G	1131	0	1074	3	0
1	H	1142	0	1080	8	0
1	I	1043	0	948	3	0
1	J	1028	0	938	5	0
1	K	1133	0	1067	12	0
1	L	1074	0	980	6	0
2	A	45	0	0	0	0
2	B	45	0	0	0	0
2	C	45	0	0	2	0
2	D	45	0	0	1	0
2	E	45	0	0	0	0
2	F	45	0	0	0	0
2	G	45	0	0	0	0
2	H	45	0	0	0	0
2	I	45	0	0	0	0
2	J	45	0	0	0	0
2	K	45	0	0	0	0
2	L	45	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	H	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	4	0	6	0	0
4	E	4	0	6	0	0
4	G	8	0	12	0	0
4	H	4	0	6	2	0
5	A	44	0	0	1	0
5	B	25	0	0	1	0
5	C	24	0	0	0	0
5	D	1	0	0	0	0
5	E	14	0	0	0	0
5	F	4	0	0	0	0
5	G	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	23	0	0	0	0
5	I	1	0	0	0	0
5	J	4	0	0	0	0
5	K	3	0	0	0	0
5	L	4	0	0	0	0
All	All	14083	0	12482	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (66) 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:D:114:ILE:HG13	1:D:150:LEU:HD22	1.52	0.90
1:A:1:MET:SD	1:B:179:GLU:HG2	2.20	0.82
1:G:8:LEU:HD21	1:H:86:VAL:HG23	1.62	0.80
1:B:164:SER:HB2	1:K:2:SER:HB2	1.67	0.74
1:C:114:ILE:HD12	1:C:169:TRP:HZ3	1.55	0.72
1:G:1:MET:SD	1:H:179:GLU:HG3	2.34	0.68
1:E:114:ILE:HG13	1:E:162:LEU:HD13	1.76	0.68
1:K:103:ARG:HG3	1:K:104:ALA:H	1.59	0.66
1:J:118:THR:HG23	1:J:169:TRP:HH2	1.60	0.66
1:C:8:LEU:HD23	1:D:90:LEU:HD22	1.80	0.64
1:K:179:GLU:HG2	1:L:1:MET:HG2	1.81	0.63
1:K:114:ILE:HG22	1:K:162:LEU:HD13	1.79	0.62
1:F:189:ASP:O	1:F:192:VAL:HG22	1.99	0.62
1:I:116:PRO:HA	1:I:162:LEU:HD21	1.83	0.60
1:D:116:PRO:HA	1:D:162:LEU:HD21	1.85	0.59
1:B:116:PRO:HA	1:B:162:LEU:HD21	1.85	0.59
1:L:136:ASN:OD1	1:L:139:ARG:HG3	2.03	0.59
1:H:83:MET:O	1:H:86:VAL:HG22	2.05	0.56
1:I:114:ILE:HG13	1:I:162:LEU:HD13	1.88	0.56
1:D:114:ILE:CG1	1:D:150:LEU:HD22	2.31	0.56
1:K:114:ILE:CD1	1:K:150:LEU:HD13	2.37	0.55
1:A:127:VAL:O	1:A:130:LEU:HB2	2.08	0.54
1:H:127:VAL:O	1:H:130:LEU:HB2	2.10	0.52
1:I:123:PHE:O	1:I:127:VAL:HG23	2.09	0.52
1:K:116:PRO:HA	1:K:162:LEU:HD21	1.90	0.52
1:F:133:ASP:HB2	1:F:139:ARG:HH22	1.75	0.52
1:C:114:ILE:HD12	1:C:169:TRP:CZ3	2.41	0.52
1:D:174:LEU:HA	1:D:178:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:ILE:HG13	1:G:162:LEU:HD13	1.92	0.50
1:K:8:LEU:HD21	1:L:86:VAL:HG12	1.93	0.50
1:H:139:ARG:HE	4:H:303:EDO:H11	1.76	0.50
1:A:5:ASN:HD22	1:B:175:ASN:ND2	2.10	0.49
1:A:114:ILE:HD12	1:A:169:TRP:HZ3	1.77	0.49
1:A:116:PRO:HA	1:A:162:LEU:HD21	1.94	0.49
1:K:112:LEU:HB2	1:K:126:VAL:HG21	1.95	0.48
1:K:114:ILE:HD12	1:K:150:LEU:HD13	1.93	0.48
1:K:103:ARG:CG	1:K:104:ALA:H	2.26	0.48
1:H:139:ARG:HE	4:H:303:EDO:C1	2.27	0.48
1:F:133:ASP:HB2	1:F:139:ARG:HH12	1.79	0.48
1:D:124:GLU:HA	1:D:173:TYR:HE2	1.79	0.48
1:H:114:ILE:HD12	1:H:169:TRP:HZ3	1.78	0.48
1:C:116:PRO:HA	1:C:162:LEU:HD21	1.96	0.46
1:C:172:THR:O	1:C:176:ASP:HB2	2.15	0.46
1:A:8:LEU:HD21	1:B:86:VAL:HG12	1.99	0.45
1:A:180:PRO:HD3	5:A:401:HOH:O	2.15	0.45
1:J:118:THR:HG23	1:J:169:TRP:CH2	2.46	0.45
1:J:140:ILE:HG12	1:J:178:LEU:HD13	1.99	0.45
2:C:301:QHP:C23	1:K:119:ALA:HA	2.47	0.45
2:D:301:QHP:C13	2:D:301:QHP:C6	2.95	0.44
1:L:121:GLN:O	1:L:125:GLN:HG2	2.17	0.44
1:F:130:LEU:HD13	1:F:139:ARG:HG3	1.99	0.44
1:E:116:PRO:HA	1:E:162:LEU:HD21	2.00	0.43
2:C:301:QHP:O1	1:K:119:ALA:HA	2.18	0.43
1:J:115:THR:O	1:J:118:THR:HG22	2.18	0.43
1:B:172:THR:HG21	1:L:172:THR:OG1	2.19	0.43
1:C:5:ASN:HD22	1:D:174:LEU:HD22	1.84	0.43
1:B:177:HIS:HE1	5:B:401:HOH:O	2.00	0.42
1:A:168:ALA:HB1	1:L:-4:PRO:HB2	2.01	0.42
1:H:26:GLN:O	1:H:86:VAL:HG13	2.20	0.42
1:J:182:ILE:HG22	1:J:187:GLY:HA2	2.02	0.41
1:F:136:ASN:OD1	1:F:139:ARG:HD3	2.20	0.41
1:E:180:PRO:O	1:E:184:GLU:HG3	2.20	0.41
1:F:83:MET:HG3	1:F:87:LYS:HE3	2.03	0.41
1:D:137:TRP:CE3	1:D:140:ILE:HD11	2.57	0.40
1:F:130:LEU:HD11	1:F:139:ARG:O	2.21	0.40
1:E:114:ILE:HG12	1:E:166:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

## 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	144/158 (91%)	143 (99%)	1 (1%)	0	100	100
1	B	142/158 (90%)	142 (100%)	0	0	100	100
1	C	136/158 (86%)	135 (99%)	1 (1%)	0	100	100
1	D	138/158 (87%)	133 (96%)	5 (4%)	0	100	100
1	E	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
1	F	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
1	G	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
1	H	140/158 (89%)	139 (99%)	1 (1%)	0	100	100
1	I	136/158 (86%)	136 (100%)	0	0	100	100
1	J	129/158 (82%)	126 (98%)	3 (2%)	0	100	100
1	K	140/158 (89%)	137 (98%)	3 (2%)	0	100	100
1	L	136/158 (86%)	135 (99%)	1 (1%)	0	100	100
All	All	1657/1896 (87%)	1636 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	124/131 (95%)	123 (99%)	1 (1%)	81	86
1	B	121/131 (92%)	120 (99%)	1 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	116/131 (88%)	114 (98%)	2 (2%)	60	67
1	D	106/131 (81%)	100 (94%)	6 (6%)	20	18
1	E	118/131 (90%)	117 (99%)	1 (1%)	81	86
1	F	112/131 (86%)	108 (96%)	4 (4%)	35	36
1	G	117/131 (89%)	115 (98%)	2 (2%)	60	67
1	H	118/131 (90%)	115 (98%)	3 (2%)	47	52
1	I	98/131 (75%)	96 (98%)	2 (2%)	55	60
1	J	99/131 (76%)	96 (97%)	3 (3%)	41	44
1	K	117/131 (89%)	111 (95%)	6 (5%)	24	22
1	L	103/131 (79%)	97 (94%)	6 (6%)	20	17
All	All	1349/1572 (86%)	1312 (97%)	37 (3%)	44	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	B	114	ILE
1	C	8	LEU
1	C	176	ASP
1	D	125	GLN
1	D	135	VAL
1	D	159	MET
1	D	172	THR
1	D	174	LEU
1	D	194	LEU
1	E	113	HIS
1	F	99	LEU
1	F	113	HIS
1	F	139	ARG
1	F	162	LEU
1	G	179	GLU
1	G	184	GLU
1	H	6	ARG
1	H	8	LEU
1	H	99	LEU
1	I	26	GLN
1	I	96	GLU
1	J	130	LEU

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Mol	Chain	Res	Type
1	J	154	SER
1	J	160	GLN
1	K	2	SER
1	K	4	SER
1	K	6	ARG
1	K	99	LEU
1	K	132	ARG
1	K	197	ASN
1	L	1	MET
1	L	9	VAL
1	L	17	LEU
1	L	99	LEU
1	L	121	GLN
1	L	154	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	175	ASN
1	C	5	ASN
1	F	111	GLN
1	G	175	ASN
1	I	136	ASN
1	K	3	GLN
1	K	160	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

25 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	SO4	L	302	-	4,4,4	0.22	0	6,6,6	0.15	0
4	EDO	G	303	-	3,3,3	0.66	0	2,2,2	0.30	0
4	EDO	A	303	-	3,3,3	0.50	0	2,2,2	0.56	0
2	QHP	H	301	-	45,50,50	1.20	2 (4%)	62,74,74	0.41	1 (1%)
2	QHP	C	301	-	45,50,50	0.47	0	62,74,74	0.41	0
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.16	0
2	QHP	A	301	-	45,50,50	1.04	1 (2%)	62,74,74	0.50	0
3	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.16	0
2	QHP	I	301	-	45,50,50	0.72	1 (2%)	62,74,74	0.30	0
2	QHP	L	301	-	45,50,50	0.78	1 (2%)	62,74,74	0.28	0
2	QHP	K	301	-	45,50,50	0.42	0	62,74,74	0.34	0
3	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.17	0
4	EDO	H	303	-	3,3,3	0.61	0	2,2,2	0.46	0
2	QHP	B	301	-	45,50,50	0.69	1 (2%)	62,74,74	0.43	0
2	QHP	E	301	-	45,50,50	0.95	1 (2%)	62,74,74	0.33	0
3	SO4	D	302	-	4,4,4	0.28	0	6,6,6	0.24	0
3	SO4	A	302	-	4,4,4	0.16	0	6,6,6	0.22	0
2	QHP	G	301	-	45,50,50	0.61	1 (2%)	62,74,74	0.48	1 (1%)
4	EDO	E	302	-	3,3,3	0.70	0	2,2,2	0.21	0
2	QHP	F	301	-	45,50,50	0.98	1 (2%)	62,74,74	0.44	0
4	EDO	G	302	-	3,3,3	0.70	0	2,2,2	0.09	0
2	QHP	D	301	-	45,50,50	0.73	1 (2%)	62,74,74	0.39	0
3	SO4	H	302	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	K	302	-	4,4,4	0.24	0	6,6,6	0.20	0
2	QHP	J	301	-	45,50,50	1.01	1 (2%)	62,74,74	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	302	-	-	0/1/1/1	-
2	QHP	F	301	-	-	6/35/66/66	0/7/6/6
4	EDO	H	303	-	-	0/1/1/1	-
2	QHP	B	301	-	-	5/35/66/66	0/7/6/6
4	EDO	G	303	-	-	1/1/1/1	-
2	QHP	J	301	-	-	8/35/66/66	0/7/6/6
4	EDO	G	302	-	-	0/1/1/1	-
2	QHP	D	301	-	-	13/35/66/66	0/7/6/6
4	EDO	A	303	-	-	0/1/1/1	-
2	QHP	L	301	-	-	7/35/66/66	0/7/6/6
2	QHP	H	301	-	-	4/35/66/66	0/7/6/6
2	QHP	C	301	-	-	4/35/66/66	0/7/6/6
2	QHP	K	301	-	-	14/35/66/66	0/7/6/6
2	QHP	E	301	-	-	8/35/66/66	0/7/6/6
2	QHP	A	301	-	-	4/35/66/66	0/7/6/6
2	QHP	G	301	-	-	4/35/66/66	0/7/6/6
2	QHP	I	301	-	-	11/35/66/66	0/7/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	QHP	C24-C22	7.27	1.58	1.53
2	A	301	QHP	C24-C22	6.22	1.58	1.53
2	J	301	QHP	C24-C22	6.18	1.58	1.53
2	F	301	QHP	C24-C22	5.71	1.57	1.53
2	E	301	QHP	C24-C22	5.57	1.57	1.53
2	L	301	QHP	C24-C22	4.39	1.56	1.53
2	I	301	QHP	C24-C22	4.29	1.56	1.53
2	D	301	QHP	C24-C22	3.98	1.56	1.53
2	B	301	QHP	C24-C22	3.62	1.56	1.53
2	G	301	QHP	C24-C22	2.80	1.55	1.53
2	H	301	QHP	C-N	2.16	1.44	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	QHP	C22-C24-S	2.18	119.61	114.56
2	H	301	QHP	C22-C24-S	2.04	119.31	114.56

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	QHP	N1-C22-C24-S
2	D	301	QHP	S-C25-C26-C35
2	D	301	QHP	S-C25-C26-C31
2	D	301	QHP	S-C25-C26-C27
2	E	301	QHP	N-C21-N1-C22
2	I	301	QHP	C23-C22-C24-S
2	I	301	QHP	N1-C22-C24-S
2	I	301	QHP	C14-C13-N-C
2	I	301	QHP	O-C-N-C21
2	I	301	QHP	C1-C-N-C21
2	I	301	QHP	O-C-N-C13
2	I	301	QHP	C1-C-N-C13
2	K	301	QHP	O5-C21-N1-C22
2	K	301	QHP	N-C21-N1-C22
2	K	301	QHP	C22-C24-S-C25
2	L	301	QHP	O-C-N-C21
2	J	301	QHP	C5-C4-C7-C12
2	J	301	QHP	C3-C4-C7-C12
2	J	301	QHP	C3-C4-C7-C8
2	J	301	QHP	C5-C4-C7-C8
2	F	301	QHP	N-C21-N1-C22
2	E	301	QHP	O5-C21-N1-C22
2	K	301	QHP	C3-C4-C7-C8
2	L	301	QHP	S-C25-C26-C27
2	A	301	QHP	O-C-N-C21
2	B	301	QHP	O-C-N-C21
2	C	301	QHP	O-C-N-C21
2	D	301	QHP	O-C-N-C21
2	E	301	QHP	O-C-N-C21
2	F	301	QHP	O-C-N-C21
2	G	301	QHP	O-C-N-C21
2	H	301	QHP	O-C-N-C21
2	J	301	QHP	O-C-N-C21
2	K	301	QHP	O-C-N-C21
2	K	301	QHP	C26-C25-S-O3
2	K	301	QHP	C26-C25-S-O4
2	C	301	QHP	C1-C-N-C21
2	D	301	QHP	C1-C-N-C21
2	G	301	QHP	C1-C-N-C21
2	J	301	QHP	C1-C-N-C21
2	K	301	QHP	C1-C-N-C21
2	L	301	QHP	C1-C-N-C21

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Mol	Chain	Res	Type	Atoms
2	E	301	QHP	N1-C22-C24-S
2	F	301	QHP	N1-C22-C24-S
2	H	301	QHP	N1-C22-C24-S
2	I	301	QHP	C14-C13-N-C21
2	D	301	QHP	O-C-C1-C6
2	I	301	QHP	C23-C22-N1-C21
2	D	301	QHP	C23-C22-C24-S
2	D	301	QHP	C3-C4-C7-C12
4	G	303	EDO	O1-C1-C2-O2
2	K	301	QHP	C5-C4-C7-C8
2	I	301	QHP	C26-C25-S-O3
2	A	301	QHP	O-C-N-C13
2	B	301	QHP	O-C-N-C13
2	C	301	QHP	O-C-N-C13
2	E	301	QHP	O-C-N-C13
2	F	301	QHP	O-C-N-C13
2	L	301	QHP	O-C-N-C13
2	L	301	QHP	S-C25-C26-C31
2	K	301	QHP	C3-C4-C7-C12
2	D	301	QHP	N-C-C1-C6
2	K	301	QHP	N1-C22-C24-S
2	K	301	QHP	C26-C25-S-C24
2	I	301	QHP	C26-C25-S-O4
2	B	301	QHP	C3-C4-C7-C8
2	F	301	QHP	C14-C13-N-C21
2	B	301	QHP	C22-C24-S-C25
2	A	301	QHP	C1-C-N-C13
2	B	301	QHP	C1-C-N-C13
2	C	301	QHP	C1-C-N-C13
2	D	301	QHP	O-C-N-C13
2	D	301	QHP	C1-C-N-C13
2	E	301	QHP	C1-C-N-C13
2	F	301	QHP	C1-C-N-C13
2	G	301	QHP	O-C-N-C13
2	G	301	QHP	C1-C-N-C13
2	H	301	QHP	O-C-N-C13
2	H	301	QHP	C1-C-N-C13
2	J	301	QHP	O-C-N-C13
2	J	301	QHP	C1-C-N-C13
2	K	301	QHP	O-C-N-C13
2	K	301	QHP	C1-C-N-C13
2	L	301	QHP	C1-C-N-C13

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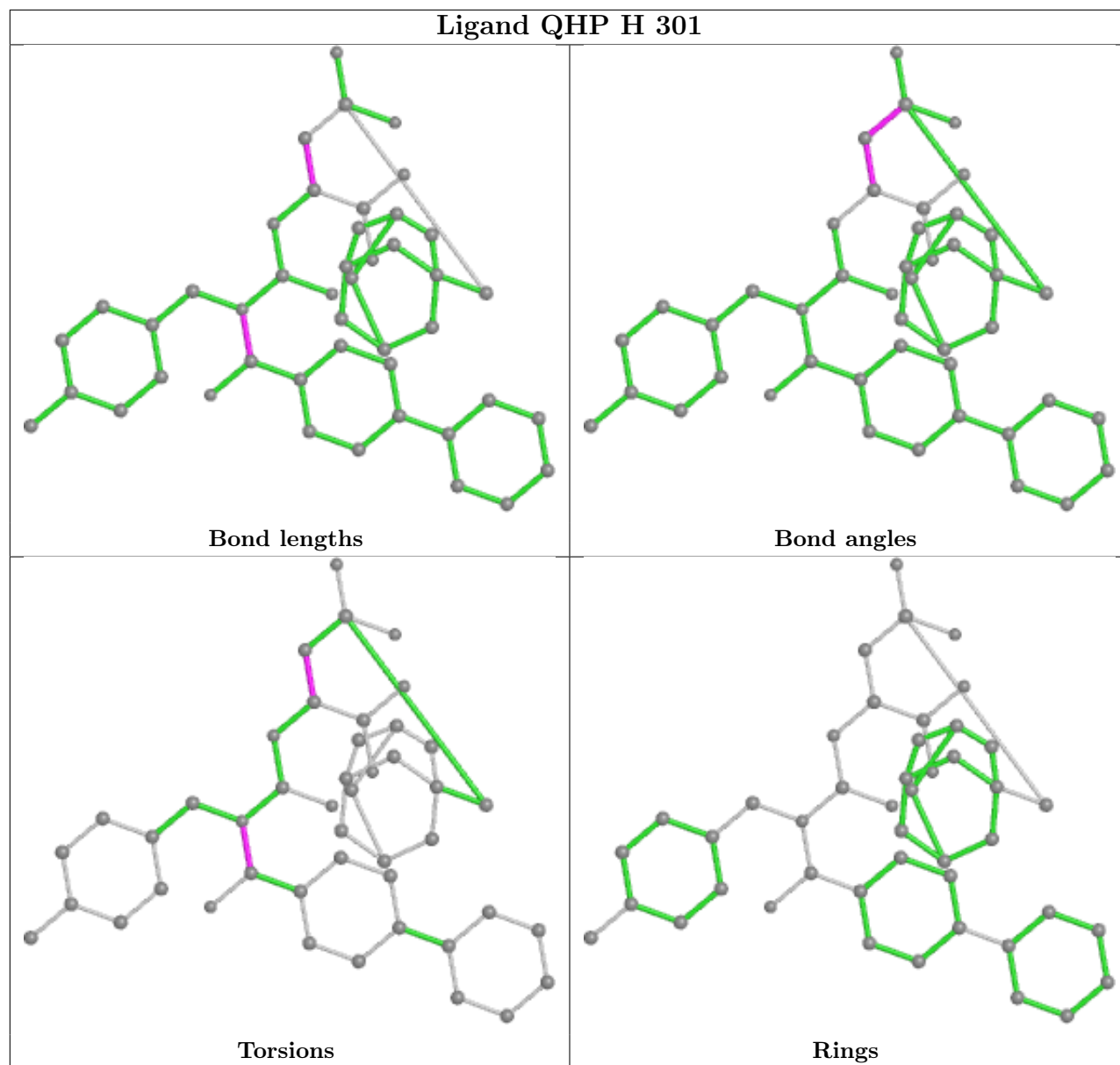
Mol	Chain	Res	Type	Atoms
2	L	301	QHP	S-C25-C26-C35
2	A	301	QHP	C1-C-N-C21
2	E	301	QHP	C1-C-N-C21
2	E	301	QHP	C23-C22-C24-S
2	D	301	QHP	O-C-C1-C2

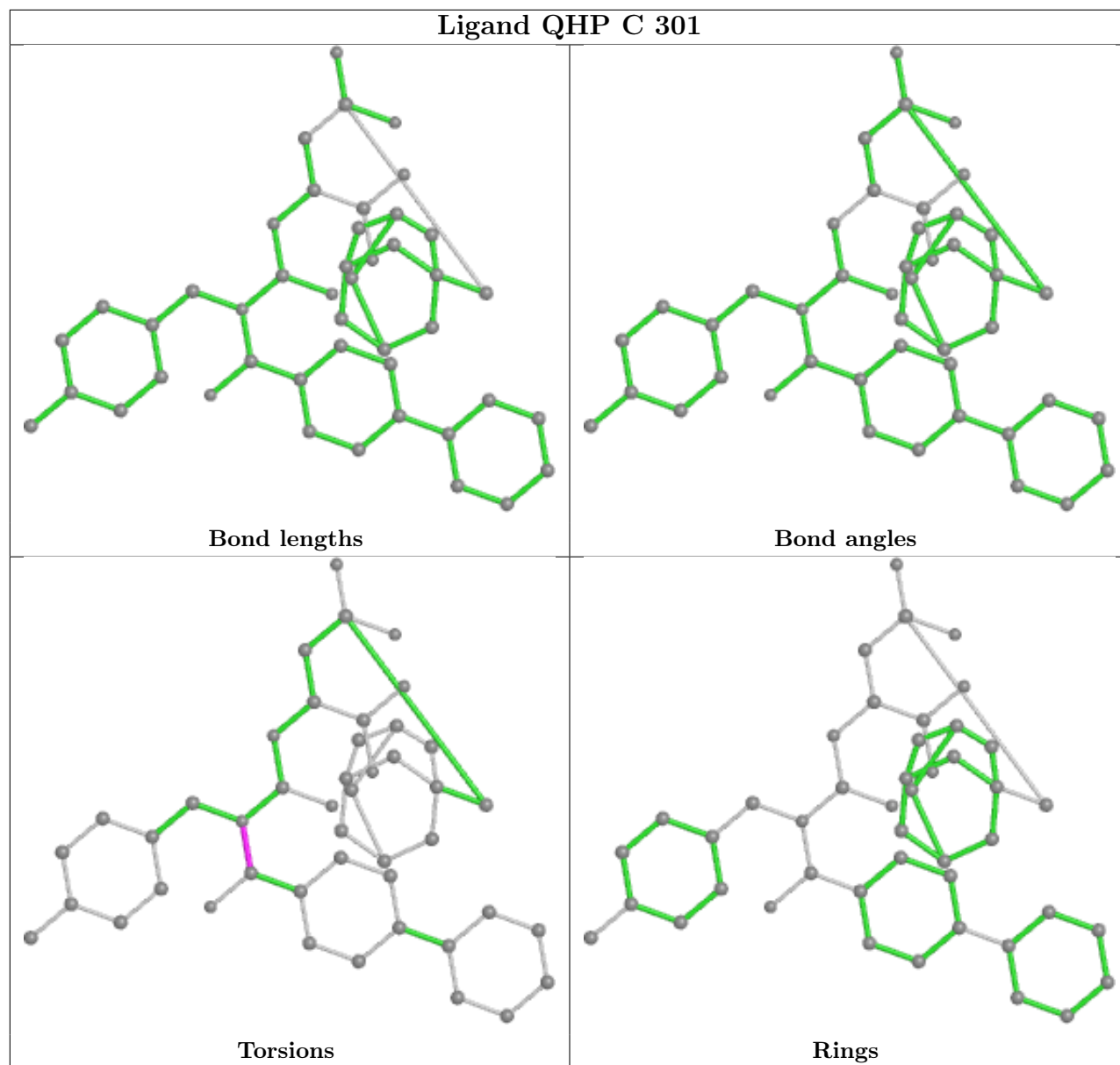
There are no ring outliers.

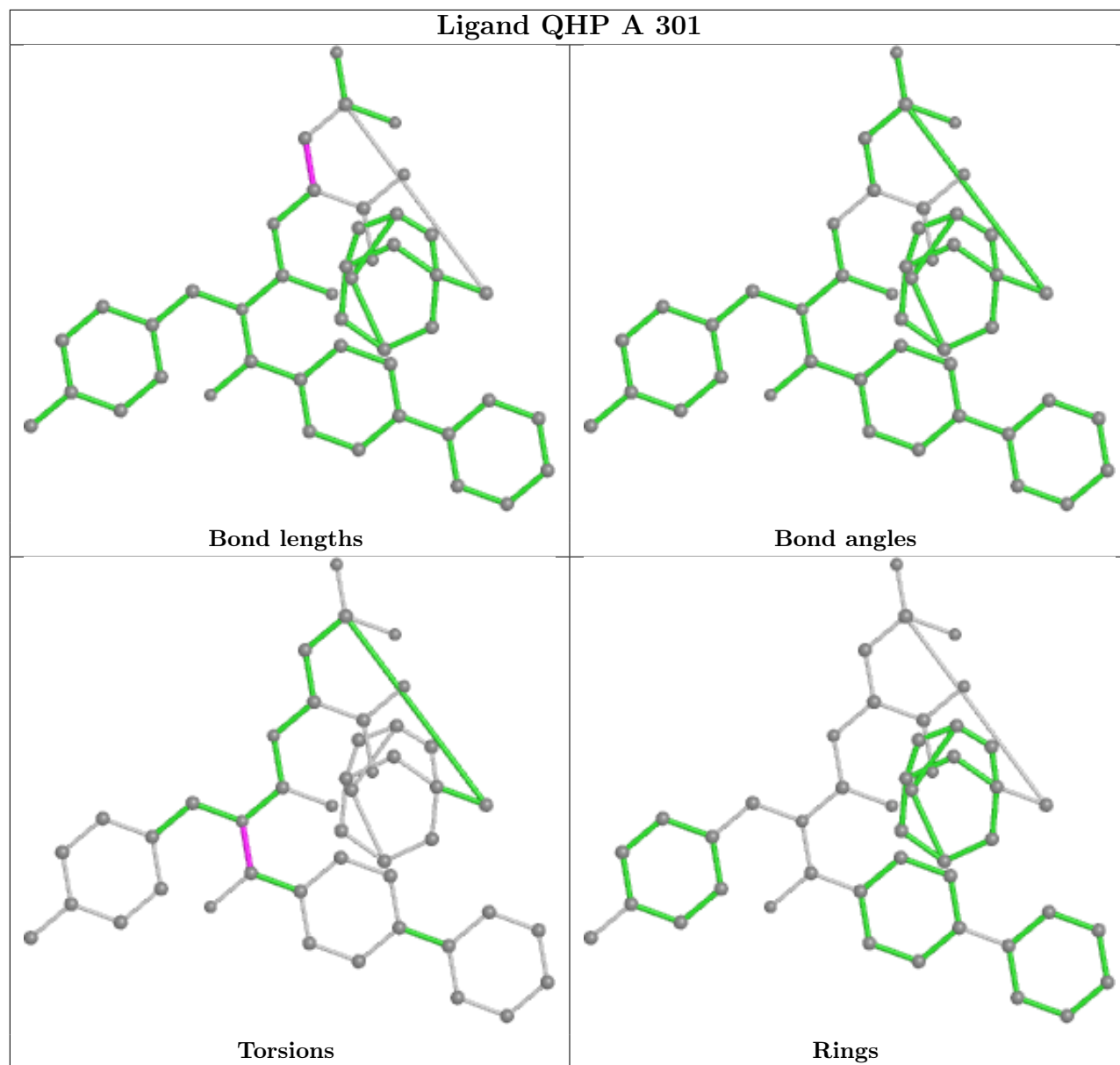
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	QHP	2	0
4	H	303	EDO	2	0
2	D	301	QHP	1	0

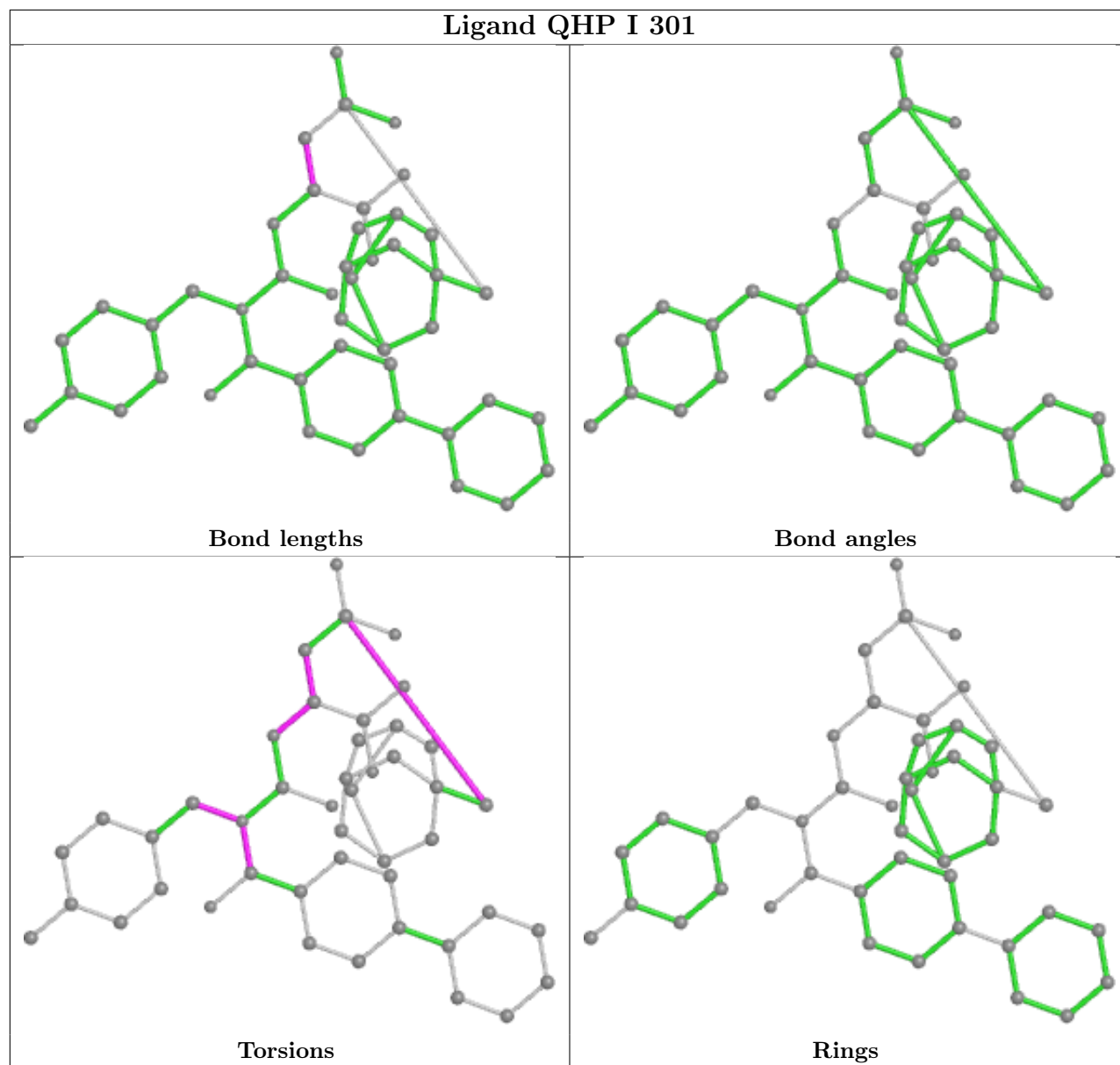
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

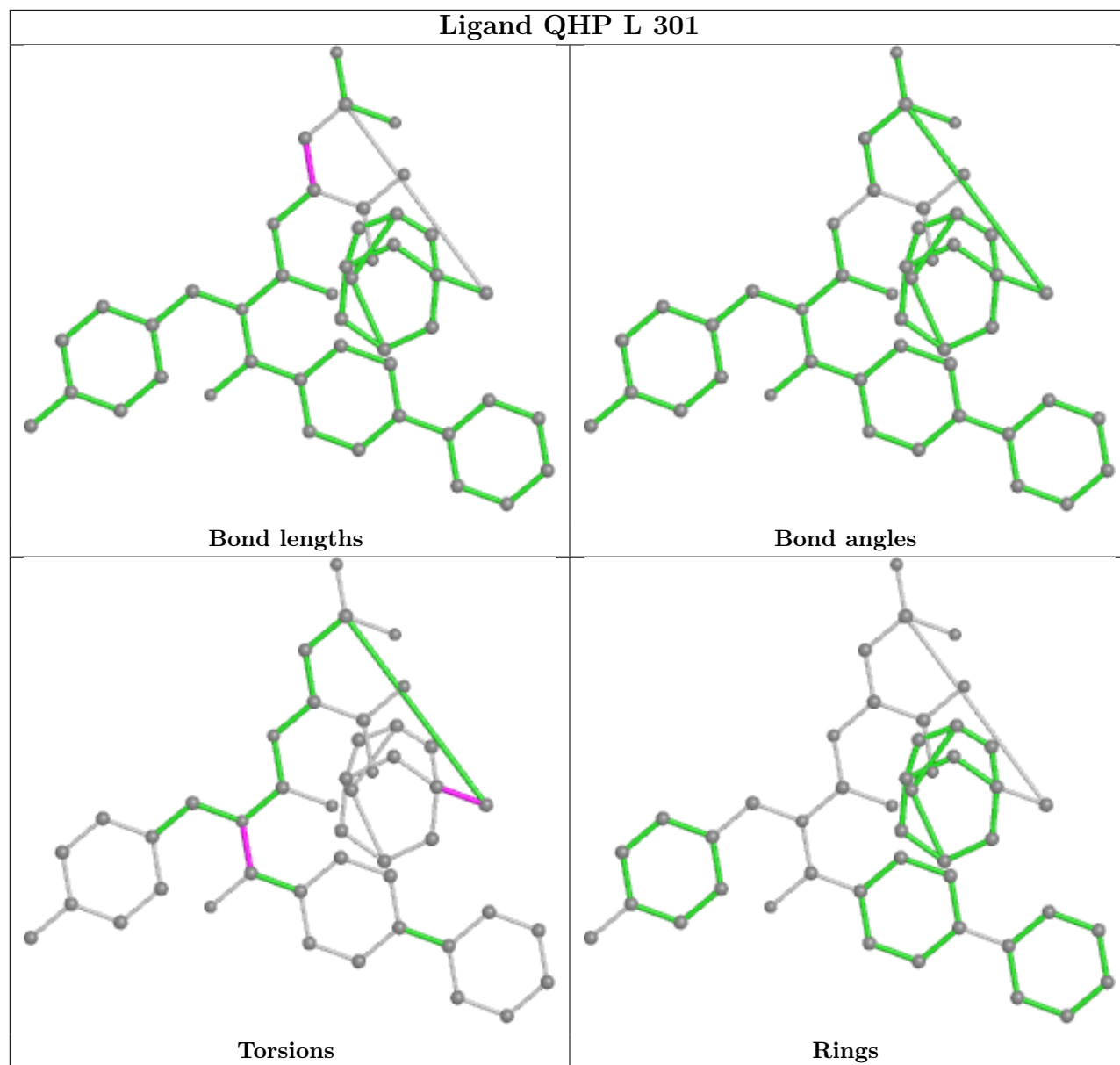


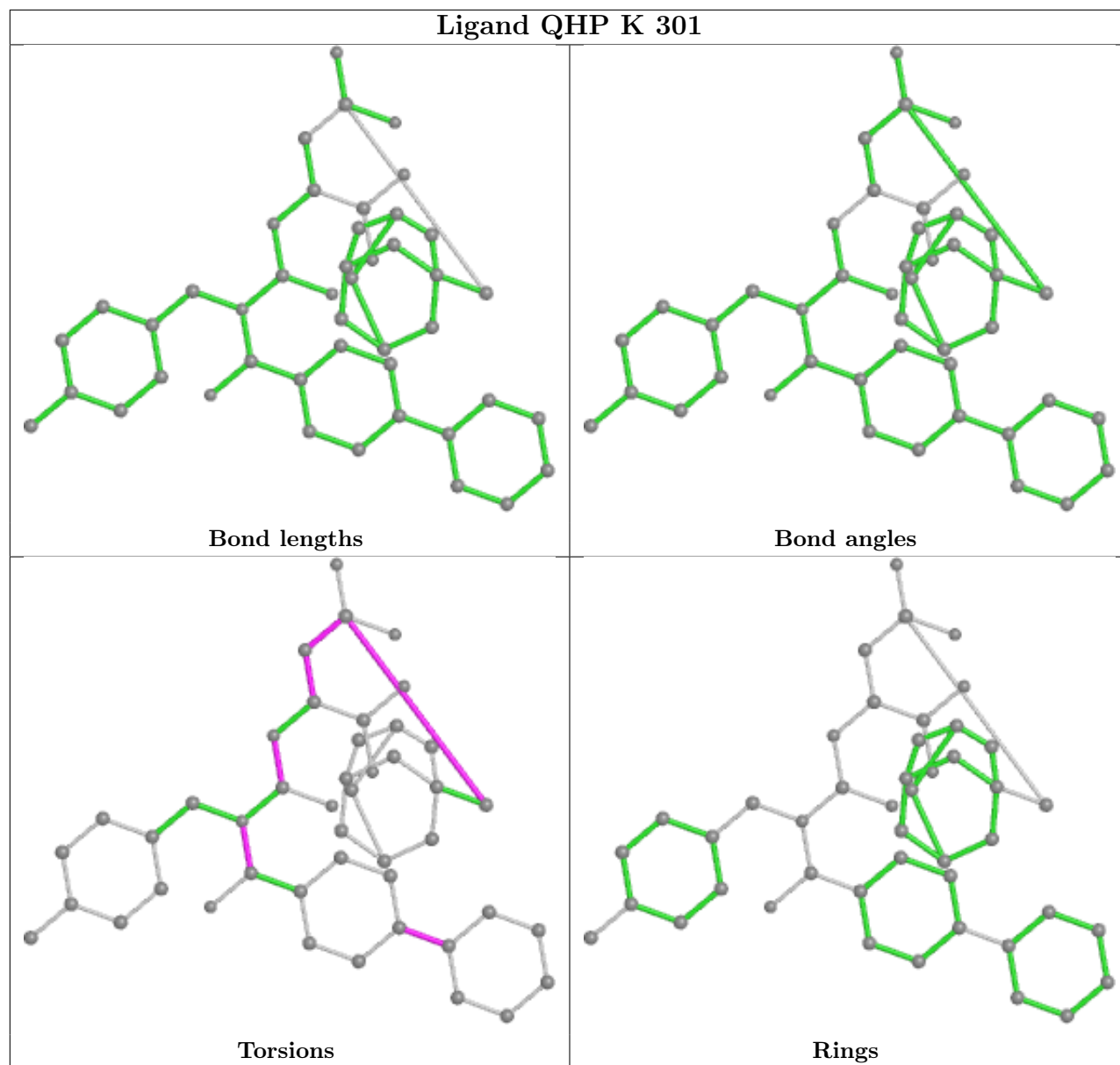


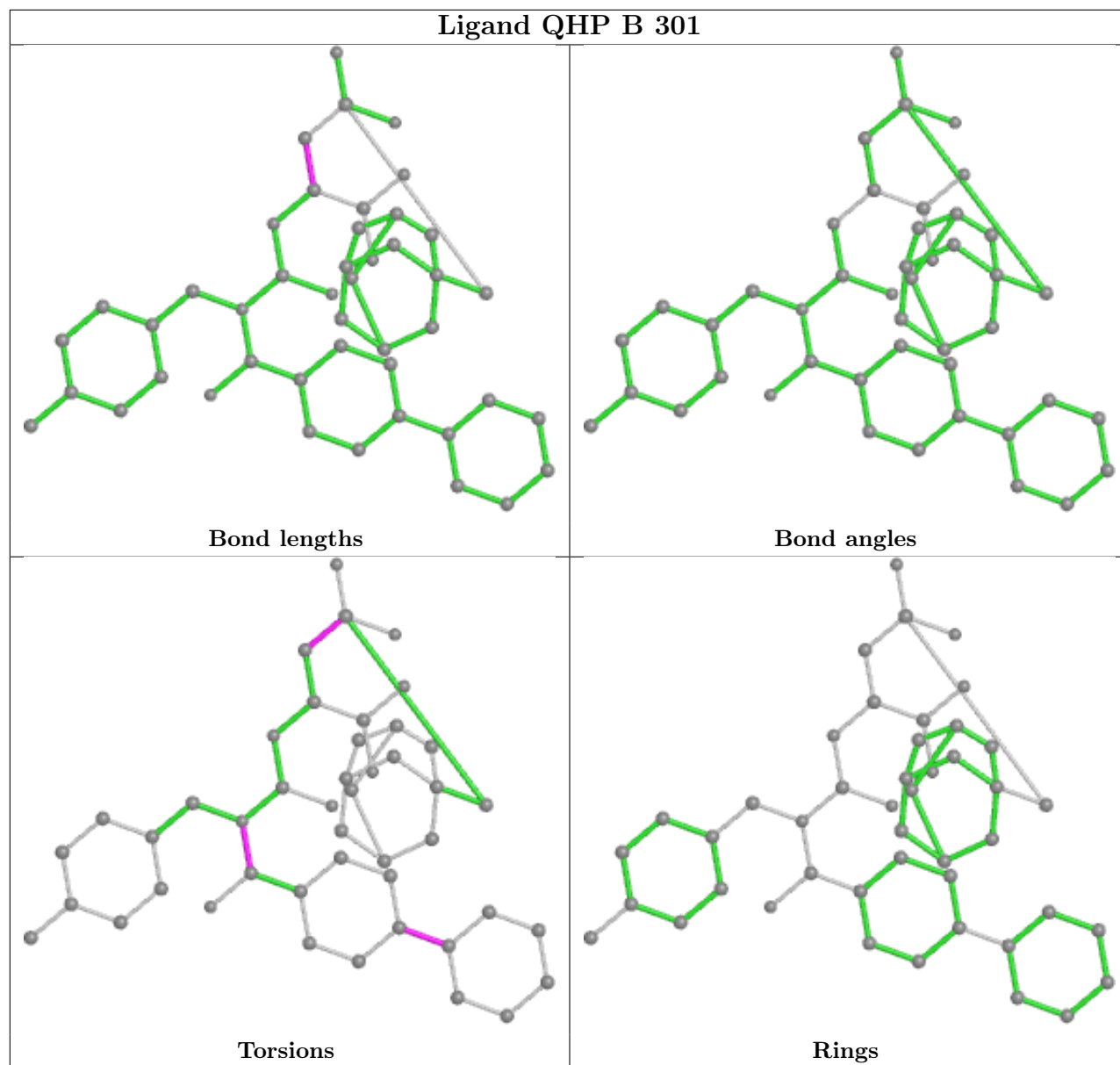


## Ligand QHP I 301



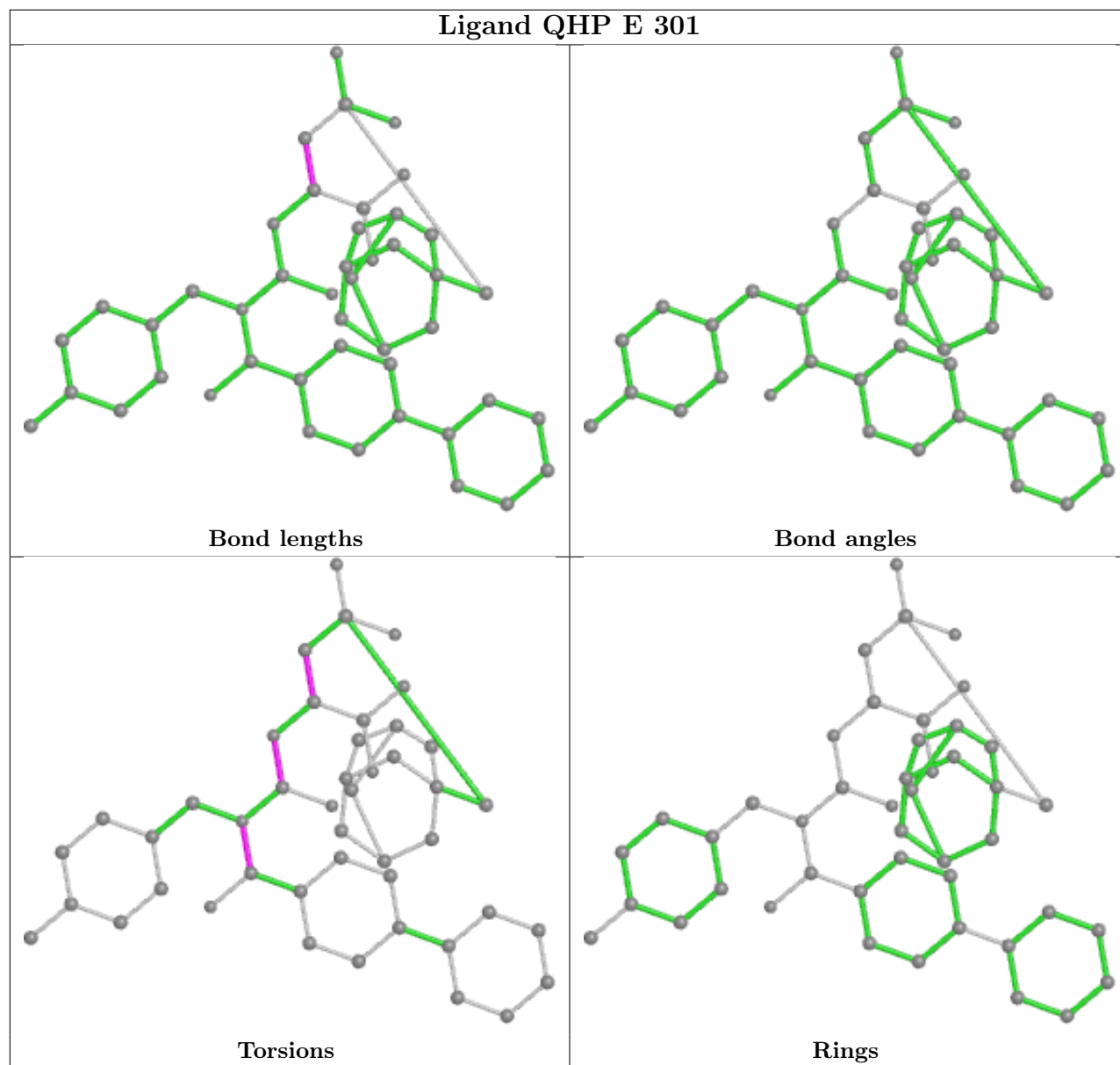


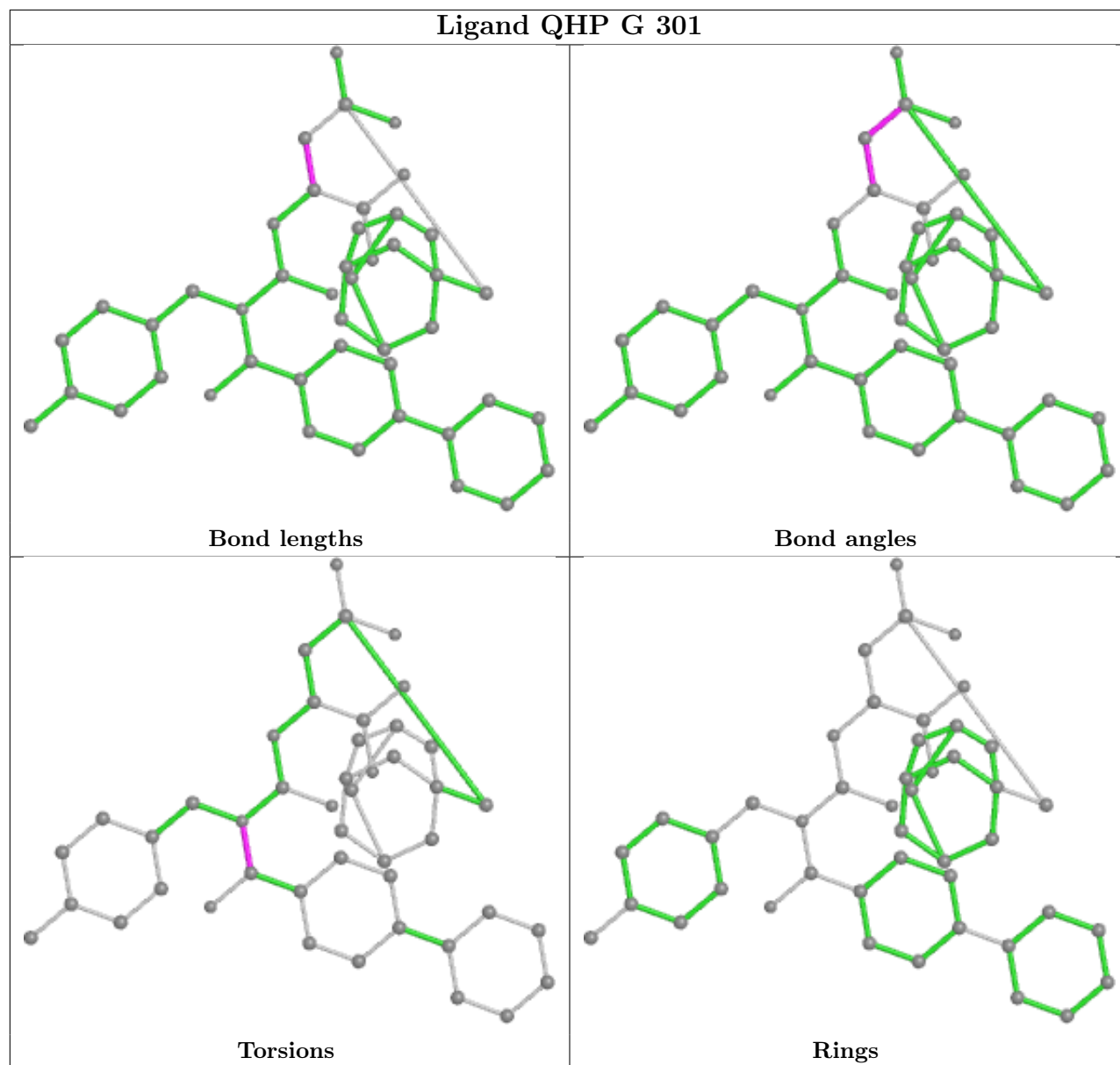




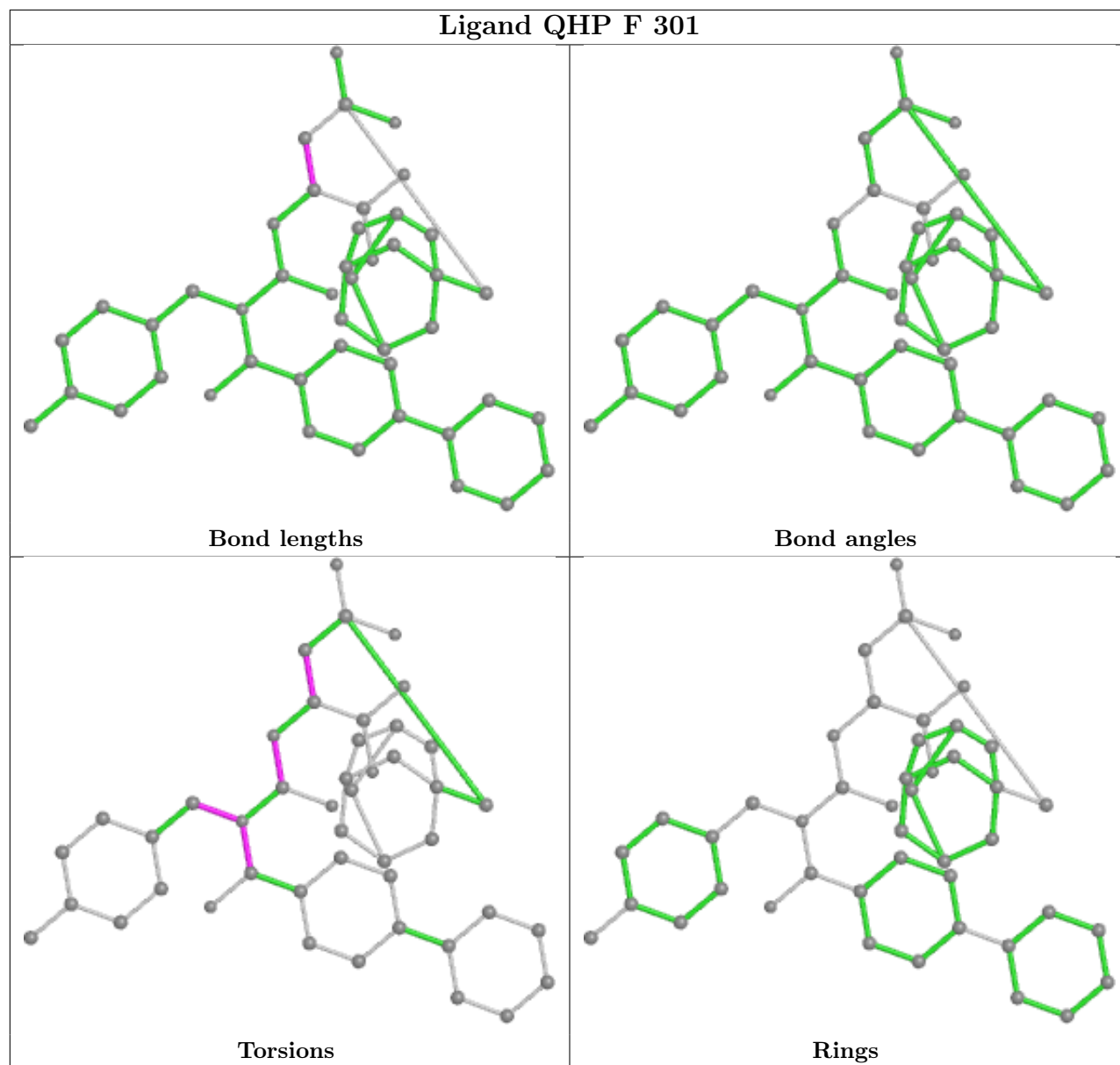


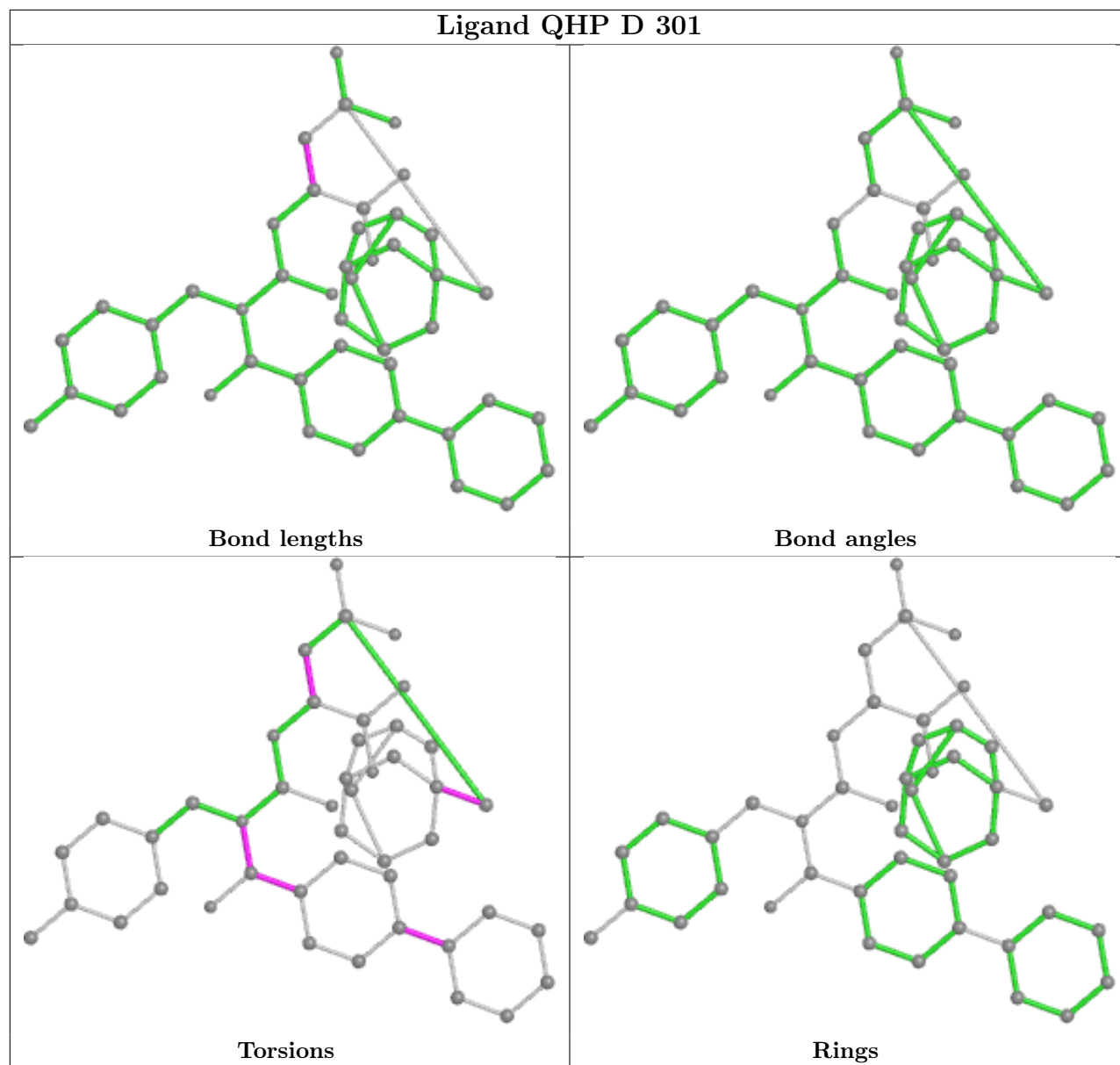
## Ligand QHP E 301

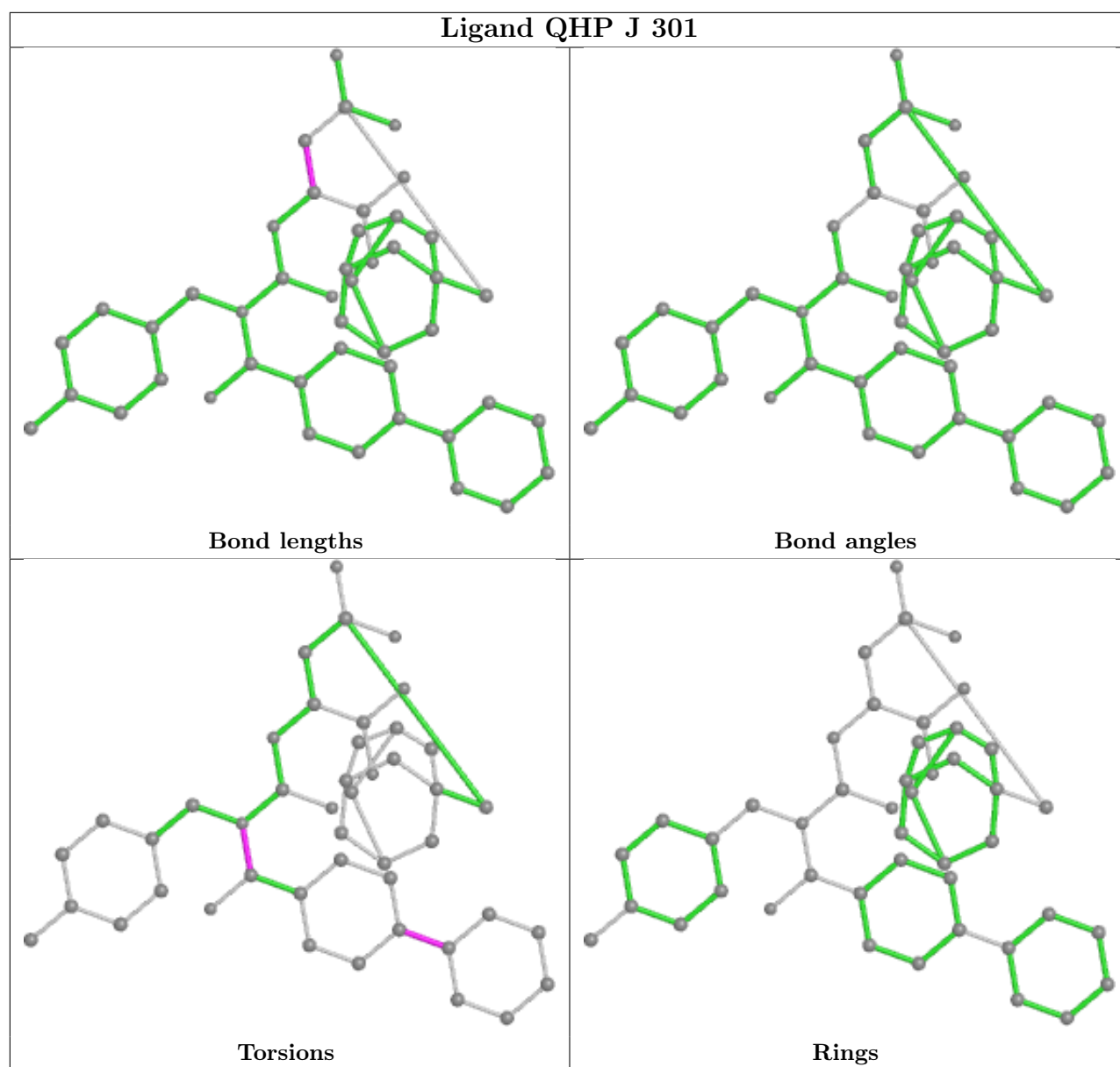




## Ligand QHP F 301







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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	145/158 (91%)	0.19	2 (1%) 75 78	35, 45, 77, 95	0
1	B	144/158 (91%)	0.19	2 (1%) 75 78	36, 58, 84, 90	0
1	C	138/158 (87%)	0.20	0 100 100	36, 52, 81, 101	0
1	D	140/158 (88%)	1.01	29 (20%) 1 1	39, 90, 125, 139	0
1	E	140/158 (88%)	0.36	3 (2%) 63 68	39, 61, 91, 105	0
1	F	141/158 (89%)	0.58	7 (4%) 28 34	41, 84, 116, 130	0
1	G	141/158 (89%)	0.42	3 (2%) 63 68	40, 67, 108, 114	0
1	H	142/158 (89%)	0.19	1 (0%) 87 89	37, 52, 84, 96	0
1	I	138/158 (87%)	1.01	22 (15%) 1 2	58, 92, 124, 132	0
1	J	133/158 (84%)	1.00	21 (15%) 2 2	47, 86, 116, 131	0
1	K	142/158 (89%)	0.73	11 (7%) 13 17	52, 77, 115, 127	0
1	L	140/158 (88%)	0.51	7 (5%) 28 34	58, 82, 112, 139	0
All	All	1684/1896 (88%)	0.53	108 (6%) 19 24	35, 69, 113, 139	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	112	LEU	7.2
1	I	188	TRP	5.7
1	D	105	PHE	5.6
1	I	22	TYR	5.4
1	D	186	GLY	5.3
1	J	108	LEU	5.2
1	J	104	ALA	4.8
1	J	162	LEU	4.6
1	J	161	VAL	4.6
1	K	114	ILE	4.5
1	K	22	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	143	PHE	4.3
1	K	108	LEU	4.3
1	D	160	GLN	4.2
1	I	137	TRP	4.2
1	F	108	LEU	4.1
1	I	181	TRP	4.1
1	I	161	VAL	4.1
1	I	135	VAL	3.9
1	J	125	GLN	3.9
1	J	110	SER	3.8
1	D	113	HIS	3.8
1	L	161	VAL	3.7
1	I	194	LEU	3.7
1	D	177	HIS	3.7
1	I	128	ASN	3.7
1	D	107	ASP	3.6
1	D	99	LEU	3.5
1	A	-3	LEU	3.5
1	I	131	PHE	3.4
1	I	192	VAL	3.4
1	D	182	ILE	3.3
1	J	114	ILE	3.3
1	D	173	TYR	3.3
1	I	138	GLY	3.3
1	J	122	SER	3.2
1	K	-1	SER	3.2
1	D	178	LEU	3.2
1	I	105	PHE	3.1
1	K	169	TRP	3.1
1	J	109	THR	3.1
1	D	135	VAL	3.1
1	J	115	THR	3.0
1	F	129	GLU	3.0
1	J	132	ARG	3.0
1	I	140	ILE	3.0
1	E	114	ILE	2.9
1	J	150	LEU	2.9
1	D	155	VAL	2.9
1	K	166	ILE	2.9
1	I	195	TYR	2.9
1	I	187	GLY	2.8
1	J	149	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	119	ALA	2.8
1	K	122	SER	2.8
1	K	123	PHE	2.8
1	D	90	LEU	2.8
1	D	146	PHE	2.6
1	J	146	PHE	2.6
1	L	150	LEU	2.6
1	D	134	GLY	2.6
1	D	130	LEU	2.6
1	D	187	GLY	2.6
1	I	112	LEU	2.6
1	J	123	PHE	2.6
1	J	90	LEU	2.6
1	D	123	PHE	2.5
1	G	162	LEU	2.5
1	F	99	LEU	2.4
1	L	-3	LEU	2.4
1	E	121	GLN	2.4
1	J	158	GLU	2.4
1	D	97	PHE	2.4
1	I	141	VAL	2.4
1	L	-5	GLY	2.4
1	F	112	LEU	2.4
1	I	114	ILE	2.4
1	D	136	ASN	2.3
1	I	24	TRP	2.3
1	E	108	LEU	2.3
1	I	182	ILE	2.3
1	G	133	ASP	2.2
1	D	181	TRP	2.2
1	L	105	PHE	2.2
1	F	181	TRP	2.2
1	J	117	GLY	2.2
1	D	103	ARG	2.2
1	D	180	PRO	2.2
1	A	3	GLN	2.1
1	K	2	SER	2.1
1	B	-3	LEU	2.1
1	K	146	PHE	2.1
1	D	190	THR	2.1
1	J	190	THR	2.1
1	J	107	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	162	LEU	2.1
1	D	161	VAL	2.1
1	I	119	ALA	2.1
1	D	194	LEU	2.1
1	H	86	VAL	2.1
1	L	116	PRO	2.1
1	L	126	VAL	2.1
1	I	107	ASP	2.0
1	J	170	MET	2.0
1	F	104	ALA	2.0
1	D	114	ILE	2.0
1	G	112	LEU	2.0
1	B	161	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	H	302	5/5	0.67	0.18	149,149,150,150	0
2	QHP	I	301	45/45	0.72	0.38	127,134,146,147	0
4	EDO	E	302	4/4	0.78	0.12	65,70,73,75	0
2	QHP	D	301	45/45	0.80	0.26	105,115,118,119	0
3	SO4	C	302	5/5	0.80	0.31	138,139,140,140	0
3	SO4	L	302	5/5	0.83	0.12	134,134,135,136	0
4	EDO	G	302	4/4	0.84	0.18	69,71,71,72	0
3	SO4	B	302	5/5	0.85	0.18	132,133,134,134	0
2	QHP	J	301	45/45	0.88	0.22	94,109,123,128	0
3	SO4	A	302	5/5	0.88	0.14	127,128,129,129	0

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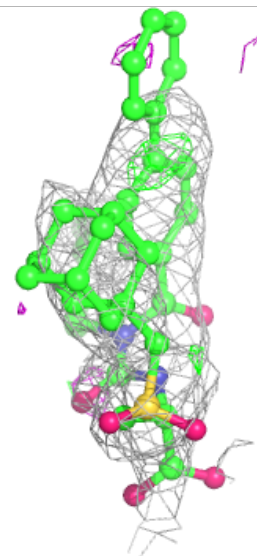
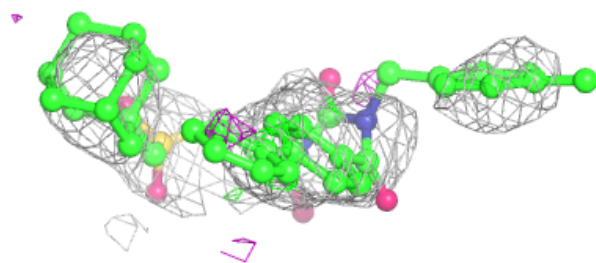
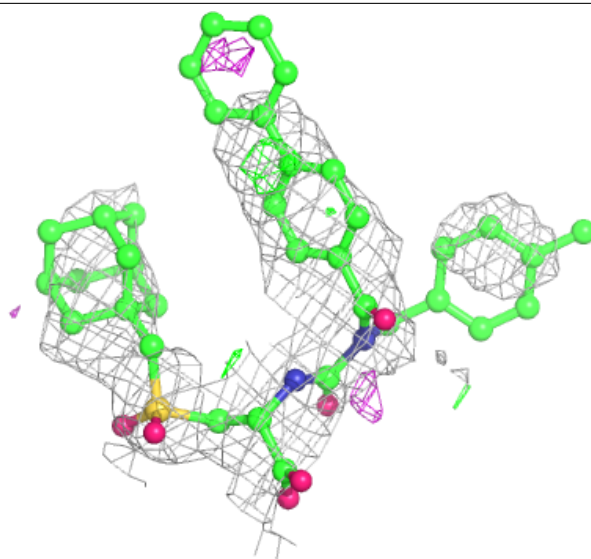
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	302	5/5	0.89	0.26	122,123,123,124	0
2	QHP	F	301	45/45	0.90	0.24	80,91,107,110	0
2	QHP	L	301	45/45	0.91	0.21	80,90,105,110	0
4	EDO	A	303	4/4	0.92	0.17	68,68,68,69	0
2	QHP	K	301	45/45	0.93	0.17	57,82,98,106	0
3	SO4	K	302	5/5	0.93	0.17	114,115,116,117	0
4	EDO	H	303	4/4	0.93	0.11	65,67,69,73	0
4	EDO	G	303	4/4	0.94	0.33	59,65,67,72	0
2	QHP	B	301	45/45	0.94	0.16	48,64,80,90	0
3	SO4	J	302	5/5	0.95	0.10	133,134,134,135	0
2	QHP	H	301	45/45	0.95	0.13	39,55,76,81	0
2	QHP	E	301	45/45	0.96	0.12	40,50,68,68	0
2	QHP	C	301	45/45	0.96	0.13	34,49,58,66	0
2	QHP	G	301	45/45	0.96	0.14	46,62,82,87	0
2	QHP	A	301	45/45	0.97	0.13	33,47,59,73	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.

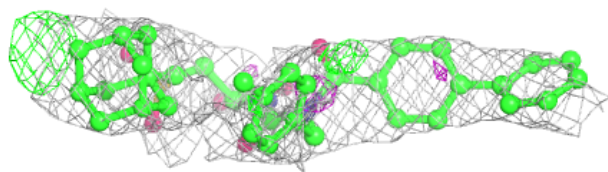
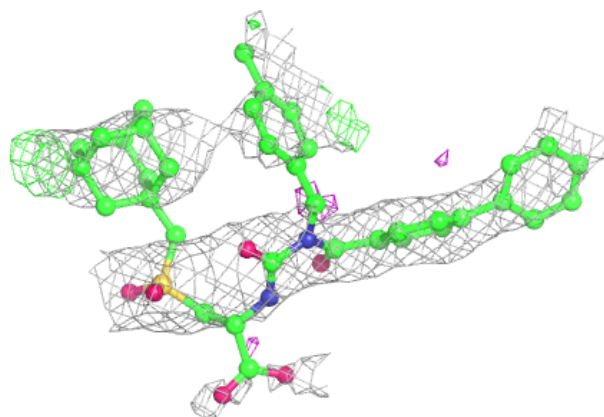
**Electron density around QHP I 301:**

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

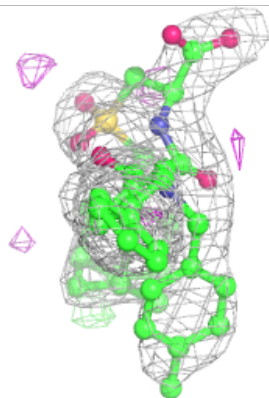
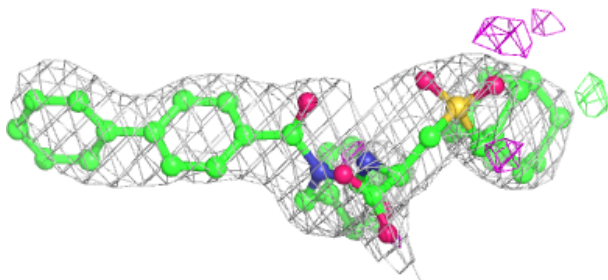
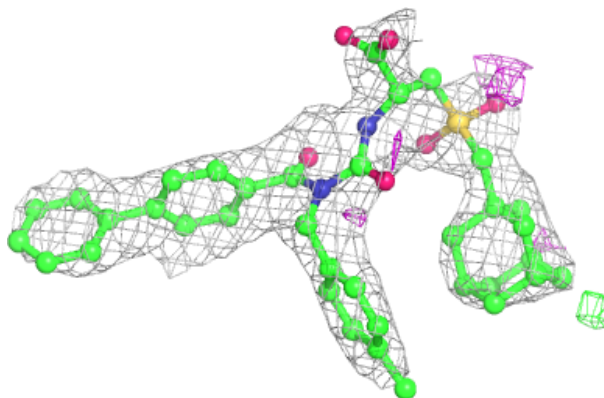


**Electron density around QHP D 301:**

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and green (positive)

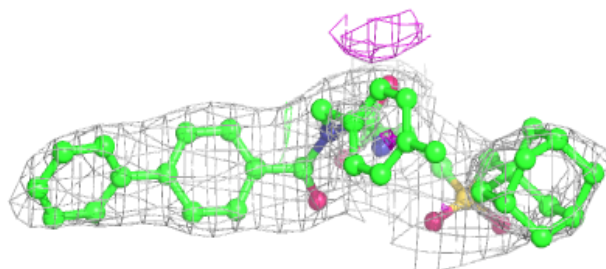
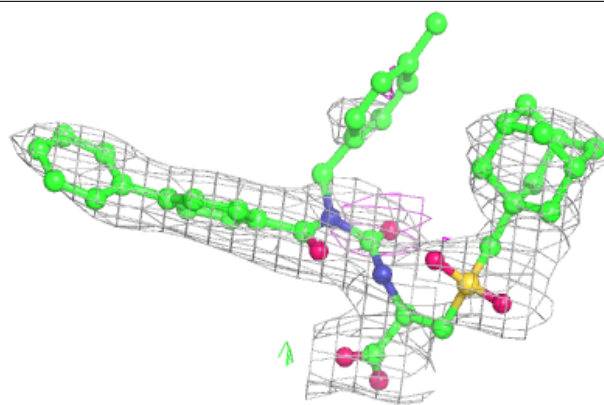
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and green (positive)

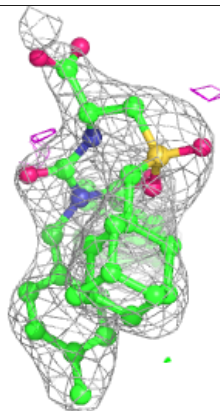
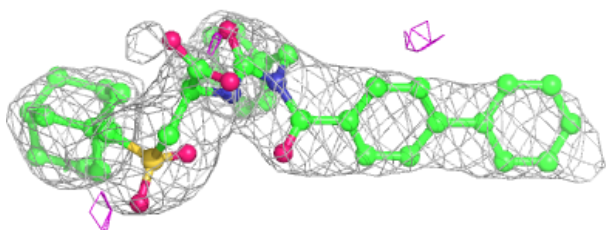
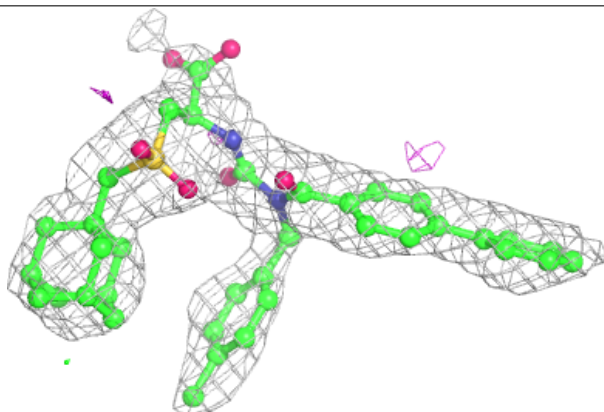


**Electron density around QHP F 301:**

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and green (positive)

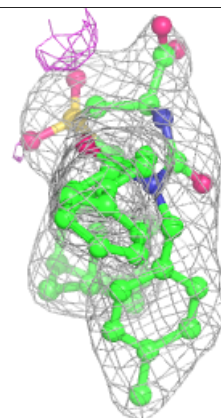
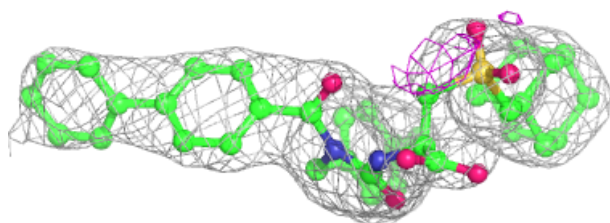
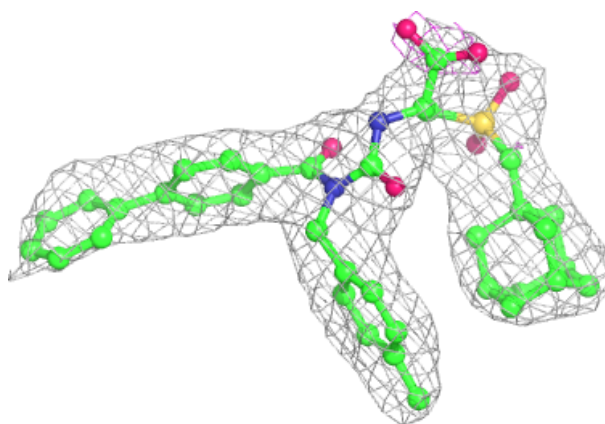
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and green (positive)

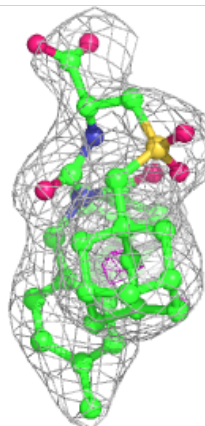
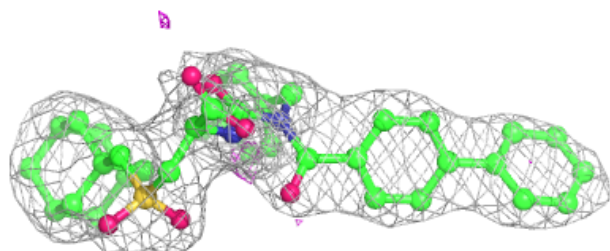
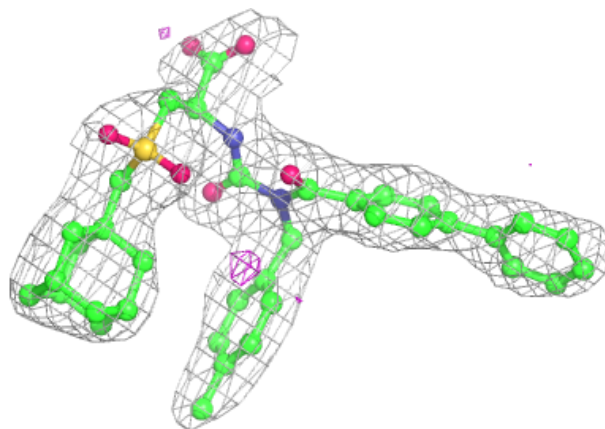


**Electron density around QHP K 301:**

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and green (positive)

**Electron density around QHP B 301:**

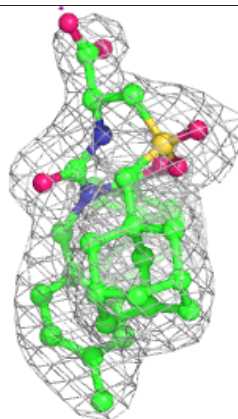
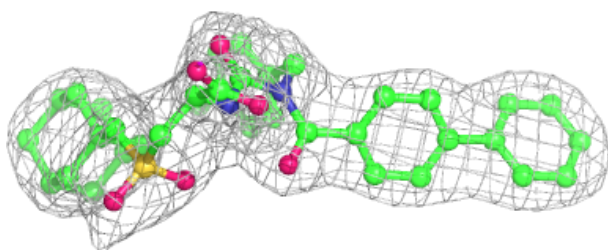
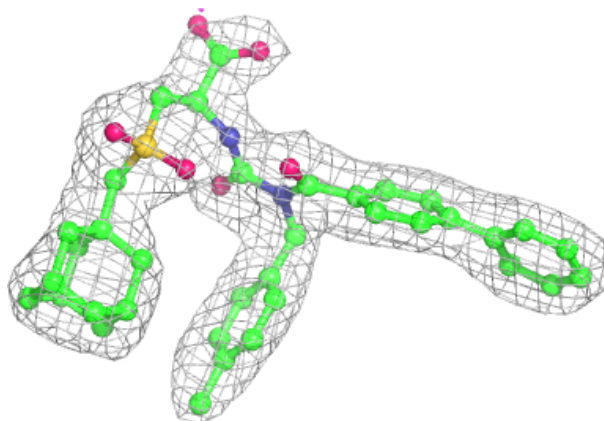
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



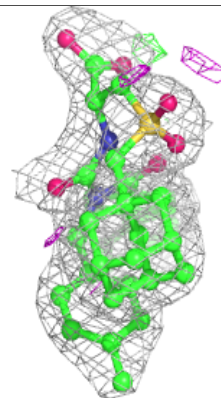
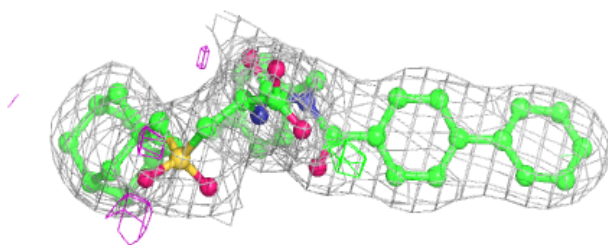
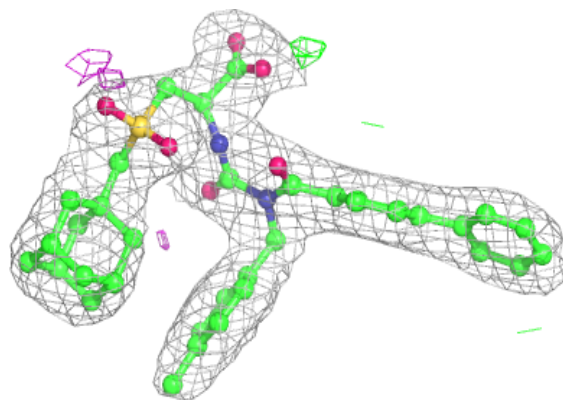


**Electron density around QHP H 301:**

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

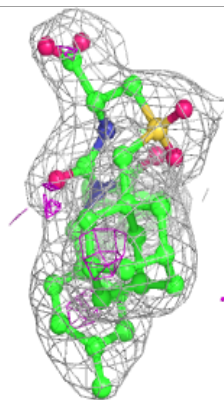
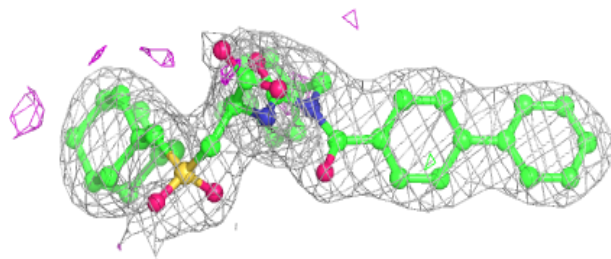
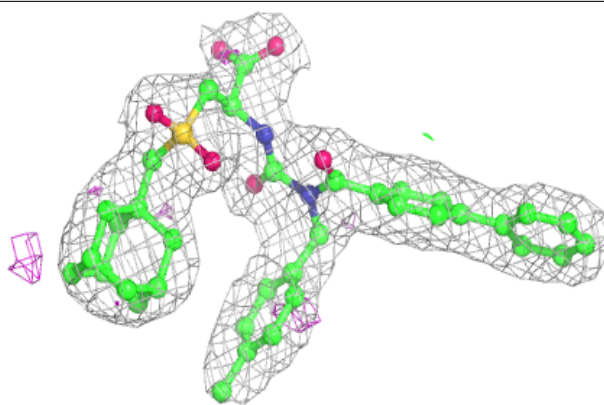
**Electron density around QHP E 301:**

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and green (positive)

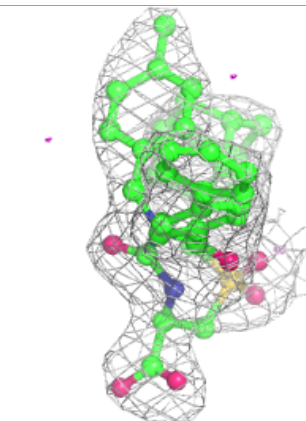
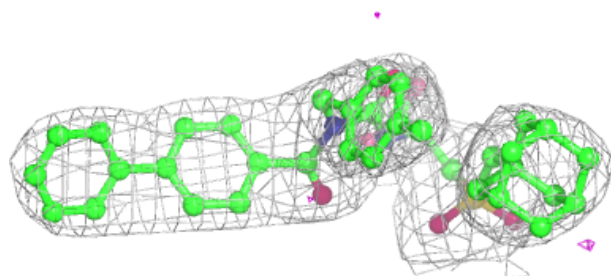
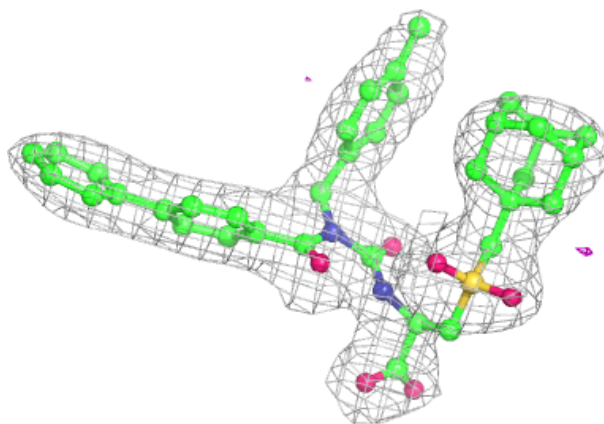


**Electron density around QHP C 301:**

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

**Electron density around QHP G 301:**

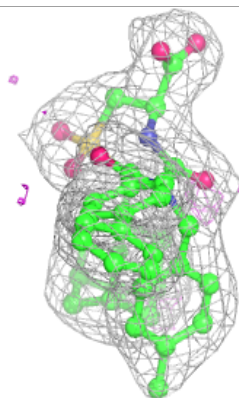
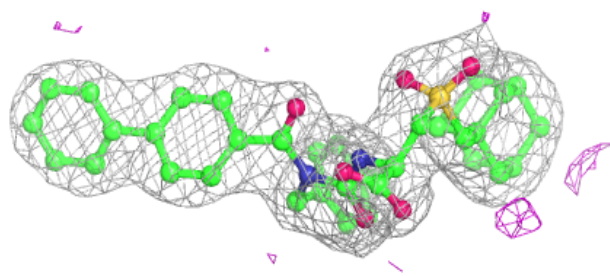
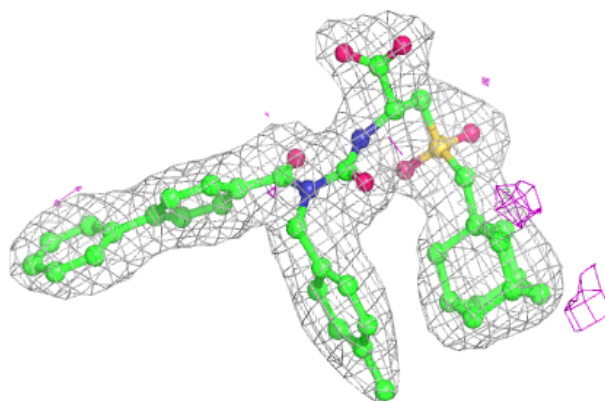
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QHP A 301:**

$2mF_o-DF_c$  (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.