



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 10:27 AM UTC

PDB ID : 6NFN / pdb_00006nfn
Title : Fab fragment of anti-cocaine antibody h2E2 bound to benzoylecgonine
Authors : Pokkuluri, P.R.; Tan, K.
Deposited on : 2018-12-20
Resolution : 2.63 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

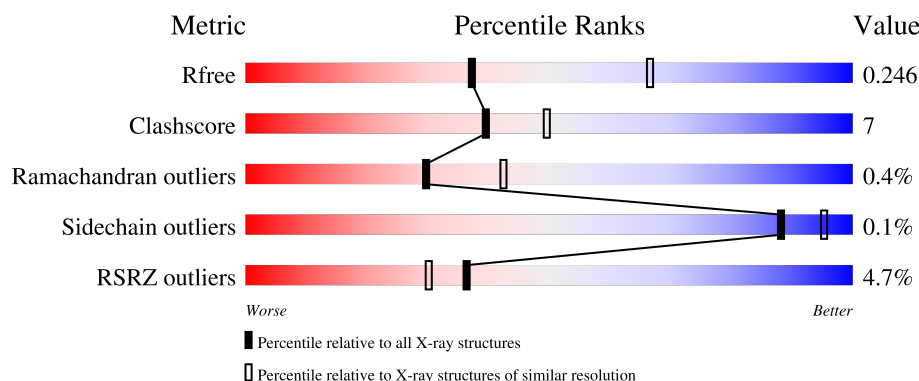
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	215	4% 84% 15% .
1	C	215	% 87% 12% .
1	E	215	% 85% 14% .
1	I	215	86% 13% .
1	L	215	86% 13% .

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Mol	Chain	Length	Quality of chain
1	M	215	
1	O	215	
1	Q	215	
2	B	222	
2	D	222	
2	F	222	
2	H	222	
2	J	222	
2	N	222	
2	P	222	
2	R	222	

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
6	ACT	M	302	-	-	X	-
6	ACT	O	302	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25262 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 Fab h2E2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1559	990	261	303	5			
1	A	213	Total	C	N	O	S	0	0	0
			1554	987	258	304	5			
1	C	212	Total	C	N	O	S	0	0	0
			1570	996	259	310	5			
1	E	213	Total	C	N	O	S	0	0	0
			1582	1003	264	309	6			
1	I	213	Total	C	N	O	S	0	0	0
			1586	1005	264	311	6			
1	O	212	Total	C	N	O	S	0	0	0
			1574	999	261	309	5			
1	Q	210	Total	C	N	O	S	0	0	0
			1447	907	246	289	5			
1	M	213	Total	C	N	O	S	0	0	0
			1546	983	255	302	6			

- Molecule 2 is a protein called Fab h2E2 heavy chain.

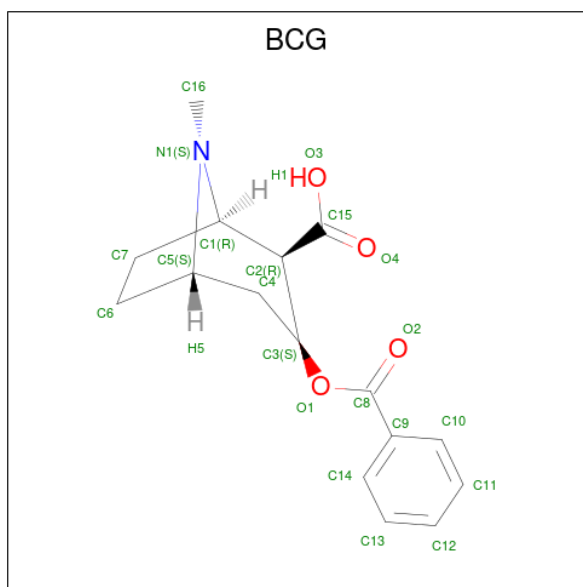
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	204	Total	C	N	O	S	0	0	0
			1507	953	252	296	6			
2	B	206	Total	C	N	O	S	0	0	0
			1533	968	258	301	6			
2	D	209	Total	C	N	O	S	0	0	0
			1556	982	261	307	6			
2	F	212	Total	C	N	O	S	0	0	0
			1585	999	267	312	7			
2	J	219	Total	C	N	O	S	0	0	0
			1624	1021	276	320	7			
2	P	209	Total	C	N	O	S	0	0	0
			1557	983	262	306	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	201	Total	C	N	O	S	0	0	0
			1492	939	252	295	6			
2	N	214	Total	C	N	O	S	0	0	0
			1597	1007	277	306	7			

- Molecule 3 is 3-(BENZOYLOXY)-8-METHYL-8-AZABICYCLO[3.2.1]OCTANE-2-CARBOXYLIC ACID (CCD ID: BCG) (formula: $C_{16}H_{19}NO_4$) (labeled as "Ligand of Interest" by depositor).



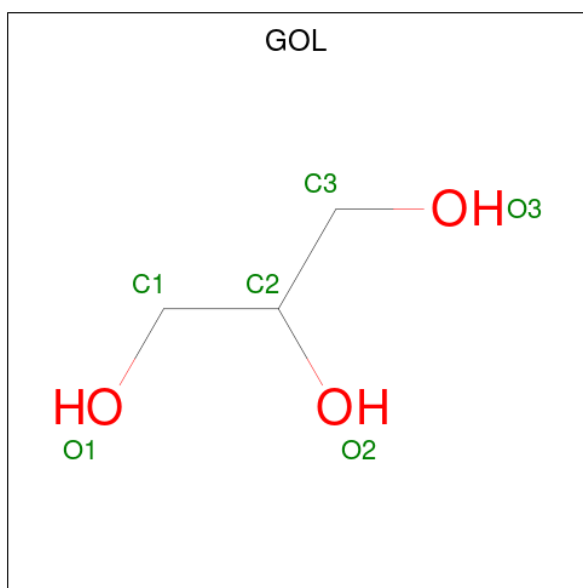
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			21	16	1	4		
3	B	1	Total	C	N	O	0	0
			21	16	1	4		
3	C	1	Total	C	N	O	0	0
			21	16	1	4		
3	E	1	Total	C	N	O	0	0
			21	16	1	4		
3	J	1	Total	C	N	O	0	0
			21	16	1	4		
3	O	1	Total	C	N	O	0	0
			21	16	1	4		
3	Q	1	Total	C	N	O	0	0
			21	16	1	4		
3	M	1	Total	C	N	O	0	0
			21	16	1	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



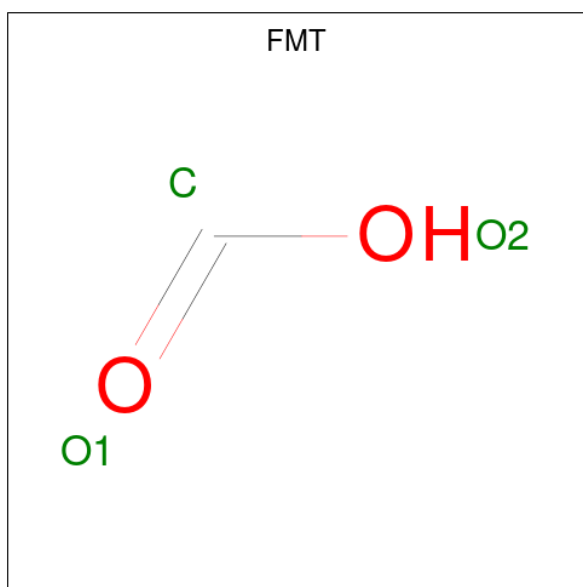
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	O	1	Total	C	O	0	0
			4	2	2		
6	P	1	Total	C	O	0	0
			4	2	2		
6	Q	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	O	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	20	Total	O	0	0
			20	20		
8	H	15	Total	O	0	0
			15	15		
8	A	6	Total	O	0	0
			6	6		
8	B	9	Total	O	0	0
			9	9		
8	C	7	Total	O	0	0
			7	7		
8	D	11	Total	O	0	0
			11	11		
8	E	8	Total	O	0	0
			8	8		
8	F	13	Total	O	0	0
			13	13		
8	I	8	Total	O	0	0
			8	8		
8	J	25	Total	O	0	0
			25	25		
8	O	12	Total	O	0	0
			12	12		

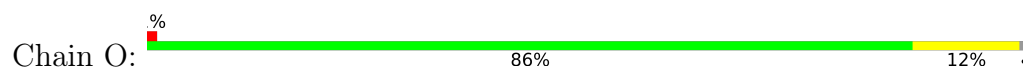
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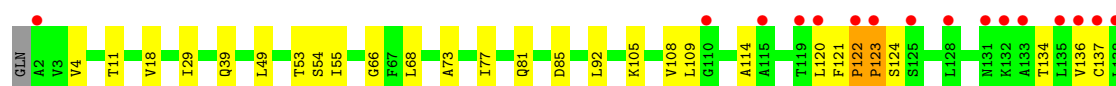
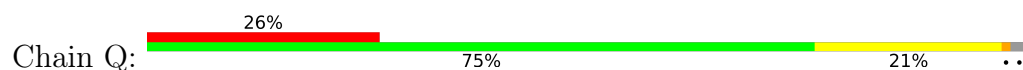
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	17	Total 17	O 17	0	0
8	Q	4	Total 4	O 4	0	0
8	R	6	Total 6	O 6	0	0
8	M	6	Total 6	O 6	0	0
8	N	6	Total 6	O 6	0	0



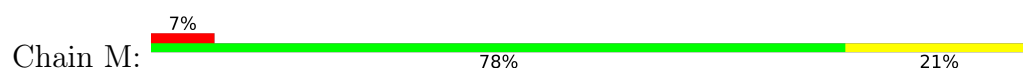
- Molecule 1: Fab h2E2 light chain



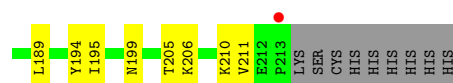
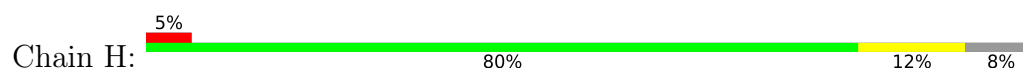
- Molecule 1: Fab h2E2 light chain



- Molecule 1: Fab h2E2 light chain

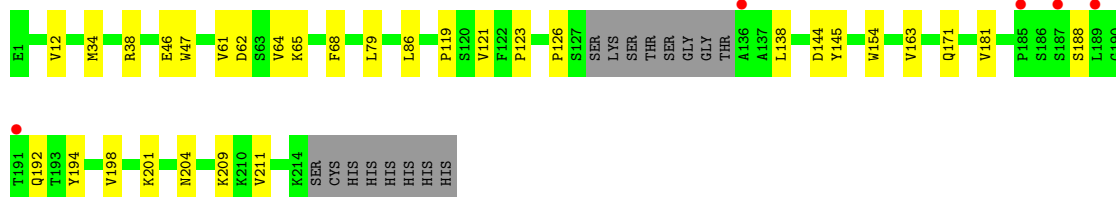


- Molecule 2: Fab h2E2 heavy chain



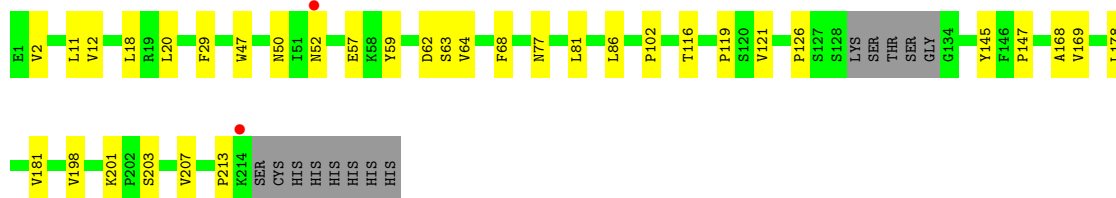
- Molecule 2: Fab h2E2 heavy chain

Chain B:  79% 14% 7% 2%



- Molecule 2: Fab h2E2 heavy chain

Chain D:  79% 15% 6% 0%



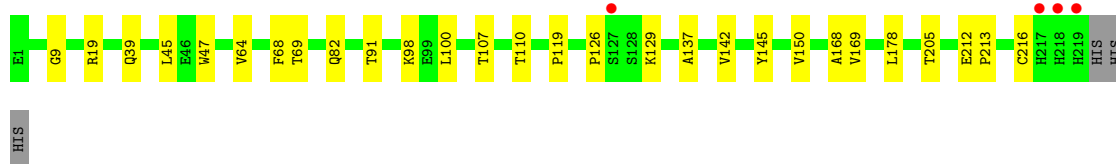
- Molecule 2: Fab h2E2 heavy chain

Chain F:  86% 9% 5% 0%



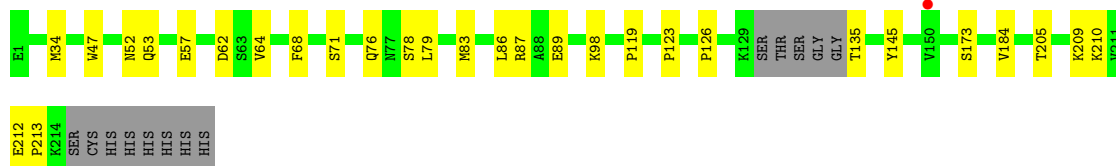
- Molecule 2: Fab h2E2 heavy chain

Chain J:  86% 13% 0% 2%

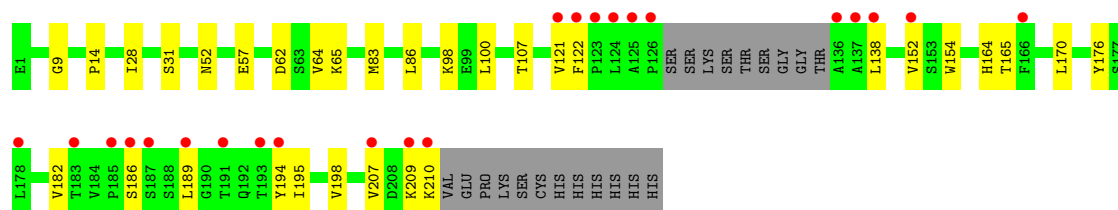
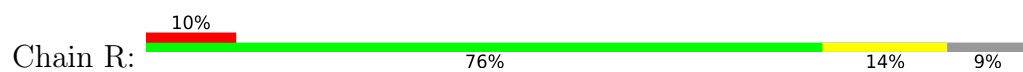


- Molecule 2: Fab h2E2 heavy chain

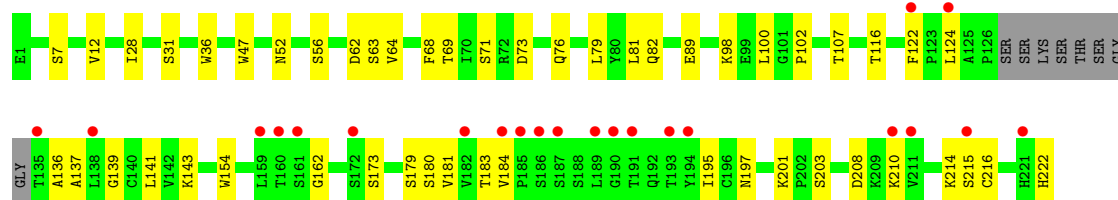
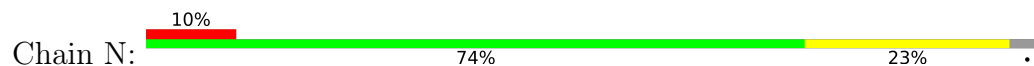
Chain P:  81% 13% 6% 0%



- Molecule 2: Fab h2E2 heavy chain



• Molecule 2: Fab h2E2 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.05Å 85.84Å 164.40Å 82.93° 81.77° 71.28°	Depositor
Resolution (Å)	38.67 – 2.63 38.67 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.67-2.63) 92.4 (38.67-2.63)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.185 , 0.244 0.187 , 0.246	Depositor DCC
R_{free} test set	5131 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25262	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4700e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, FMT, ACT, BCG, GOL

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	0.21	0/1593	0.45	0/2185
1	C	0.15	0/1609	0.35	0/2204
1	E	0.16	0/1621	0.38	0/2218
1	I	0.15	0/1625	0.39	0/2223
1	L	0.24	0/1598	0.40	0/2189
1	M	0.28	0/1584	0.53	2/2172 (0.1%)
1	O	0.27	0/1613	0.48	2/2208 (0.1%)
1	Q	0.32	1/1480 (0.1%)	0.52	0/2037
2	B	0.15	0/1569	0.40	0/2140
2	D	0.16	0/1592	0.36	0/2170
2	F	0.14	0/1621	0.35	0/2206
2	H	0.29	0/1543	0.51	0/2108
2	J	0.16	0/1662	0.39	0/2264
2	N	0.24	0/1639	0.49	1/2237 (0.0%)
2	P	0.15	0/1593	0.37	0/2172
2	R	0.16	0/1527	0.38	0/2083
All	All	0.21	1/25469 (0.0%)	0.43	5/34816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	55	ILE	C-O	-6.58	1.16	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	212	THR	CA-C-N	8.88	136.47	122.62
1	M	212	THR	C-N-CA	8.88	136.47	122.62
2	N	173	SER	N-CA-C	-8.52	102.44	113.17
1	O	93	TRP	CA-C-N	6.69	132.44	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	93	TRP	C-N-CA	6.69	132.44	123.20

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	1554	0	1508	20	0
1	C	1570	0	1537	18	0
1	E	1582	0	1559	21	0
1	I	1586	0	1563	18	0
1	L	1559	0	1531	17	0
1	M	1546	0	1495	33	0
1	O	1574	0	1553	17	0
1	Q	1447	0	1317	28	0
2	B	1533	0	1483	21	0
2	D	1556	0	1514	24	0
2	F	1585	0	1553	16	0
2	H	1507	0	1438	24	0
2	J	1624	0	1581	20	0
2	N	1597	0	1523	41	0
2	P	1557	0	1515	20	0
2	R	1492	0	1427	24	0
3	B	21	0	18	0	0
3	C	21	0	18	0	0
3	E	21	0	18	0	0
3	J	21	0	18	0	0
3	L	21	0	18	0	0
3	M	21	0	18	0	0
3	O	21	0	18	0	0
3	Q	21	0	18	0	0
4	L	7	0	10	0	0
5	L	6	0	8	0	0
6	B	4	0	3	0	0
6	C	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	4	0	3	0	0
6	H	4	0	3	0	0
6	J	4	0	3	0	0
6	M	4	0	3	2	0
6	O	4	0	3	2	0
6	P	4	0	3	0	0
6	Q	4	0	3	0	0
7	O	3	0	1	0	0
8	A	6	0	0	0	0
8	B	9	0	0	0	0
8	C	7	0	0	0	0
8	D	11	0	0	0	0
8	E	8	0	0	0	0
8	F	13	0	0	0	0
8	H	15	0	0	0	0
8	I	8	0	0	0	0
8	J	25	0	0	0	0
8	L	20	0	0	0	0
8	M	6	0	0	0	0
8	N	6	0	0	0	0
8	O	12	0	0	0	0
8	P	17	0	0	1	0
8	Q	4	0	0	0	0
8	R	6	0	0	0	0
All	All	25262	0	24287	329	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 7.

The worst 5 of 329 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:E:163:GLU:HG2	2:F:169:VAL:HG11	1.41	1.02
1:A:111:GLN:HE22	1:A:174:LYS:HE3	1.36	0.91
1:A:125:SER:HA	1:A:128:LEU:HD12	1.53	0.89
2:B:121:VAL:HG21	2:B:198:VAL:HG11	1.53	0.88
2:P:52:ASN:OD1	2:P:53:GLN:NE2	2.07	0.86

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	211/215 (98%)	195 (92%)	14 (7%)	2 (1%)	14	21
1	C	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
1	E	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
1	I	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
1	L	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
1	M	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	14	21
1	O	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
1	Q	208/215 (97%)	179 (86%)	23 (11%)	6 (3%)	3	4
2	B	202/222 (91%)	194 (96%)	7 (4%)	1 (0%)	24	36
2	D	205/222 (92%)	199 (97%)	5 (2%)	1 (0%)	24	36
2	F	208/222 (94%)	198 (95%)	10 (5%)	0	100	100
2	H	200/222 (90%)	193 (96%)	7 (4%)	0	100	100
2	J	217/222 (98%)	207 (95%)	9 (4%)	1 (0%)	24	36
2	N	210/222 (95%)	201 (96%)	9 (4%)	0	100	100
2	P	205/222 (92%)	200 (98%)	5 (2%)	0	100	100
2	R	197/222 (89%)	192 (98%)	5 (2%)	0	100	100
All	All	3325/3496 (95%)	3161 (95%)	151 (4%)	13 (0%)	30	42

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	122	PRO
1	Q	144	PRO
1	Q	173	ASN
1	A	141	ASP
2	B	144	ASP

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	166/177 (94%)	166 (100%)	0	100	100
1	C	172/177 (97%)	172 (100%)	0	100	100
1	E	174/177 (98%)	174 (100%)	0	100	100
1	I	175/177 (99%)	174 (99%)	1 (1%)	78	87
1	L	170/177 (96%)	170 (100%)	0	100	100
1	M	165/177 (93%)	165 (100%)	0	100	100
1	O	173/177 (98%)	173 (100%)	0	100	100
1	Q	141/177 (80%)	141 (100%)	0	100	100
2	B	169/187 (90%)	168 (99%)	1 (1%)	78	87
2	D	173/187 (92%)	173 (100%)	0	100	100
2	F	178/187 (95%)	178 (100%)	0	100	100
2	H	164/187 (88%)	164 (100%)	0	100	100
2	J	181/187 (97%)	181 (100%)	0	100	100
2	N	174/187 (93%)	174 (100%)	0	100	100
2	P	173/187 (92%)	173 (100%)	0	100	100
2	R	163/187 (87%)	163 (100%)	0	100	100
All	All	2711/2912 (93%)	2709 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	201	LYS
1	I	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	173	ASN

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Continued from previous page...

Mol	Chain	Res	Type
2	N	39	GLN
2	N	199	ASN
1	E	187	GLN
1	E	43	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	BCG	L	301	-	23,23,23	0.78	1 (4%)	31,33,33	0.94	2 (6%)
6	ACT	P	301	-	3,3,3	1.46	1 (33%)	3,3,3	1.35	0
6	ACT	J	302	-	3,3,3	1.46	1 (33%)	3,3,3	1.32	0
6	ACT	O	302	-	3,3,3	1.25	0	3,3,3	1.39	0
3	BCG	E	301	-	23,23,23	0.76	1 (4%)	31,33,33	0.98	2 (6%)
6	ACT	C	302	-	3,3,3	1.35	0	3,3,3	1.37	0
3	BCG	B	301	-	23,23,23	0.78	1 (4%)	31,33,33	0.91	2 (6%)
6	ACT	E	302	-	3,3,3	1.34	0	3,3,3	1.35	0
6	ACT	M	302	-	3,3,3	1.23	0	3,3,3	1.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	Q	302	-	3,3,3	1.28	0	3,3,3	1.41	0
6	ACT	H	301	-	3,3,3	1.17	0	3,3,3	1.43	0
3	BCG	J	301	-	23,23,23	0.75	1 (4%)	31,33,33	1.00	2 (6%)
3	BCG	O	301	-	23,23,23	0.74	1 (4%)	31,33,33	1.02	2 (6%)
6	ACT	B	302	-	3,3,3	1.27	0	3,3,3	1.40	0
5	GOL	L	303	-	5,5,5	0.99	0	5,5,5	1.05	0
3	BCG	M	301	-	23,23,23	0.78	1 (4%)	31,33,33	0.94	2 (6%)
4	PEG	L	302	-	6,6,6	0.14	0	5,5,5	0.06	0
3	BCG	Q	301	-	23,23,23	0.77	1 (4%)	31,33,33	0.94	2 (6%)
7	FMT	O	303	-	2,2,2	0.73	0	1,1,1	0.21	0
3	BCG	C	301	-	23,23,23	0.76	1 (4%)	31,33,33	0.94	2 (6%)

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	BCG	Q	301	-	-	2/12/37/37	0/4/3/3
4	PEG	L	302	-	-	0/4/4/4	-
3	BCG	L	301	-	-	2/12/37/37	0/4/3/3
3	BCG	J	301	-	-	0/12/37/37	0/4/3/3
3	BCG	O	301	-	-	2/12/37/37	0/4/3/3
3	BCG	B	301	-	-	0/12/37/37	0/4/3/3
5	GOL	L	303	-	-	2/4/4/4	-
3	BCG	E	301	-	-	1/12/37/37	0/4/3/3
3	BCG	M	301	-	-	0/12/37/37	0/4/3/3
3	BCG	C	301	-	-	2/12/37/37	0/4/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	301	BCG	O3-C15	-3.01	1.21	1.30
3	B	301	BCG	O3-C15	-2.98	1.21	1.30
3	M	301	BCG	O3-C15	-2.97	1.21	1.30
3	J	301	BCG	O3-C15	-2.96	1.21	1.30
3	C	301	BCG	O3-C15	-2.94	1.21	1.30

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	BCG	C7-C1-C2	3.28	117.11	112.28
3	O	301	BCG	C7-C1-N1	-3.25	101.84	105.18
3	J	301	BCG	C7-C1-N1	-3.23	101.86	105.18
3	O	301	BCG	C7-C1-C2	3.12	116.88	112.28
3	L	301	BCG	C7-C1-C2	3.08	116.82	112.28

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	BCG	O3-C15-C2-C3
5	L	303	GOL	C1-C2-C3-O3
5	L	303	GOL	O2-C2-C3-O3
3	O	301	BCG	O3-C15-C2-C3
3	Q	301	BCG	O4-C15-C2-C3

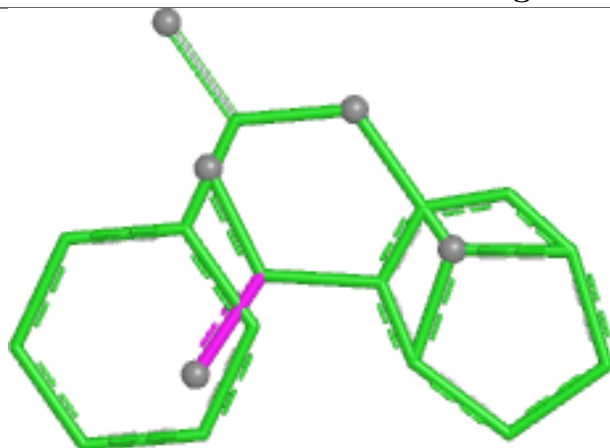
There are no ring outliers.

3 monomers are involved in 5 short contacts:

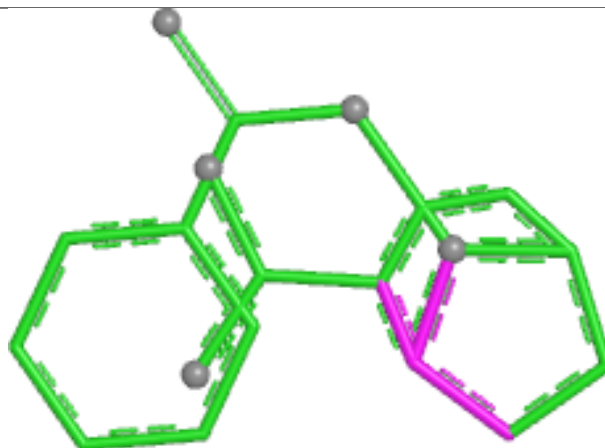
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	302	ACT	2	0
6	C	302	ACT	1	0
6	M	302	ACT	2	0

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.

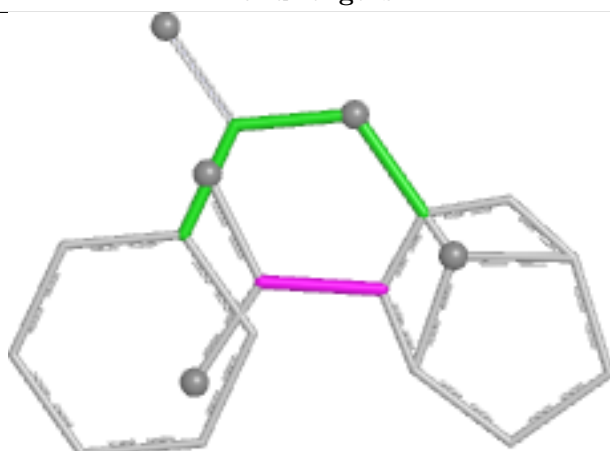
Ligand BCG L 301



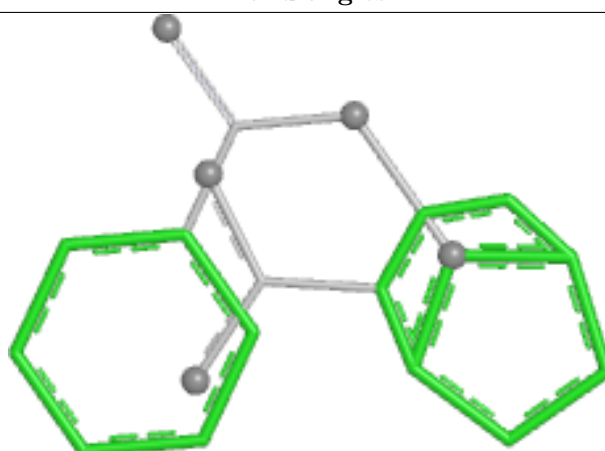
Bond lengths



Bond angles

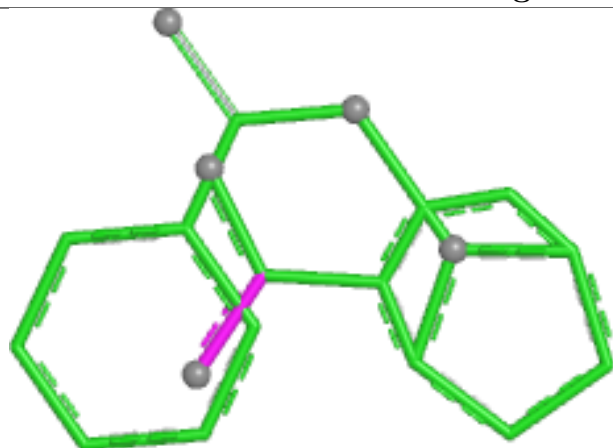


Torsions

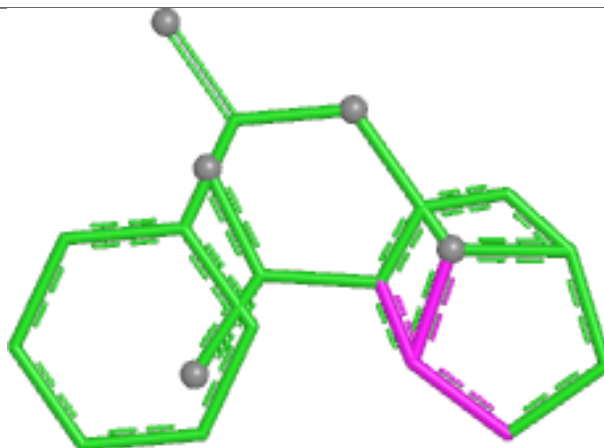


Rings

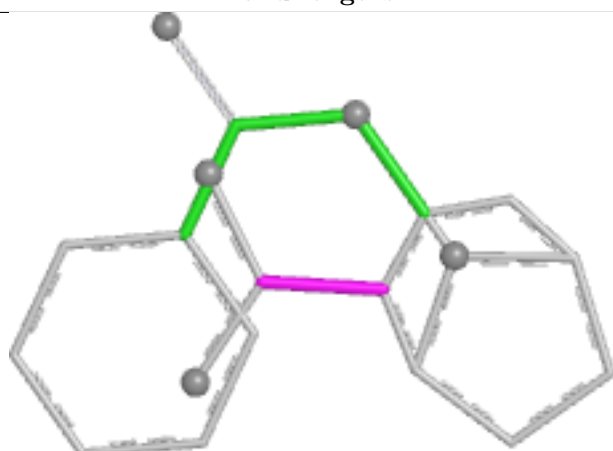
Ligand BCG E 301



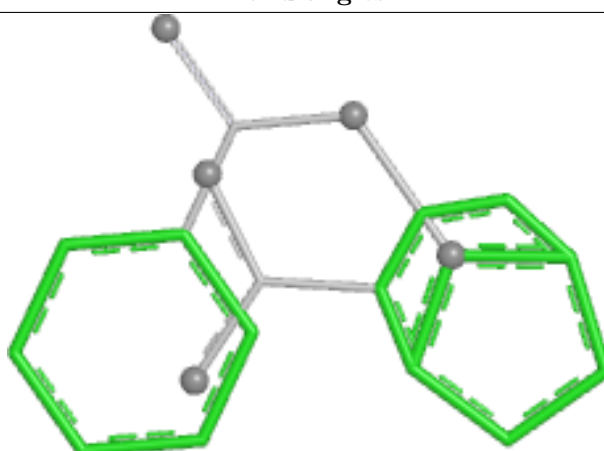
Bond lengths



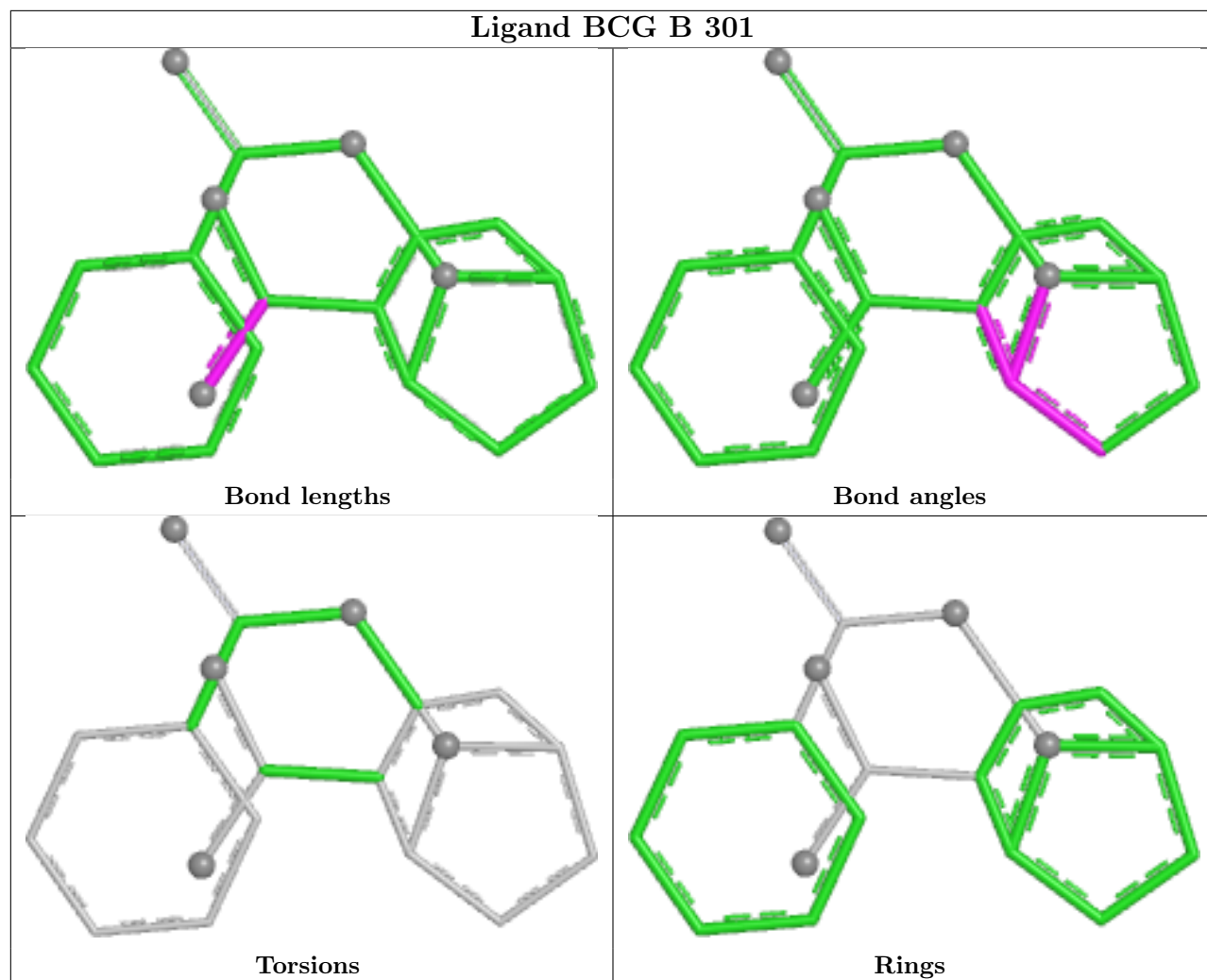
Bond angles



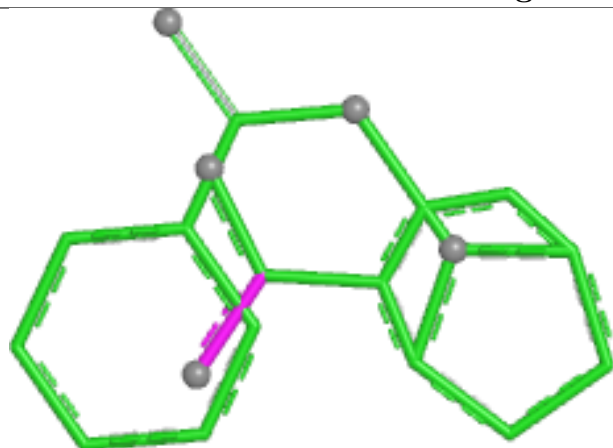
Torsions



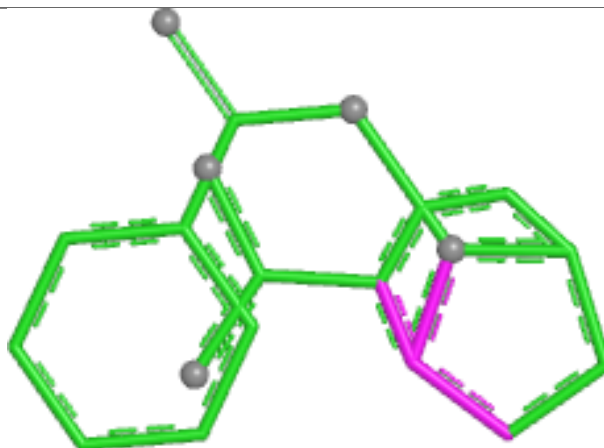
Rings



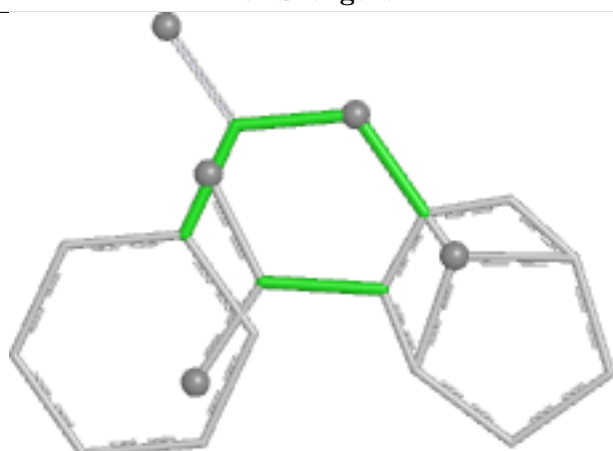
Ligand BCG J 301



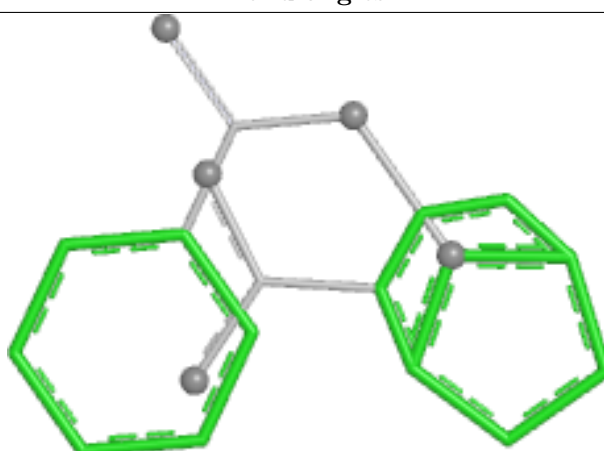
Bond lengths



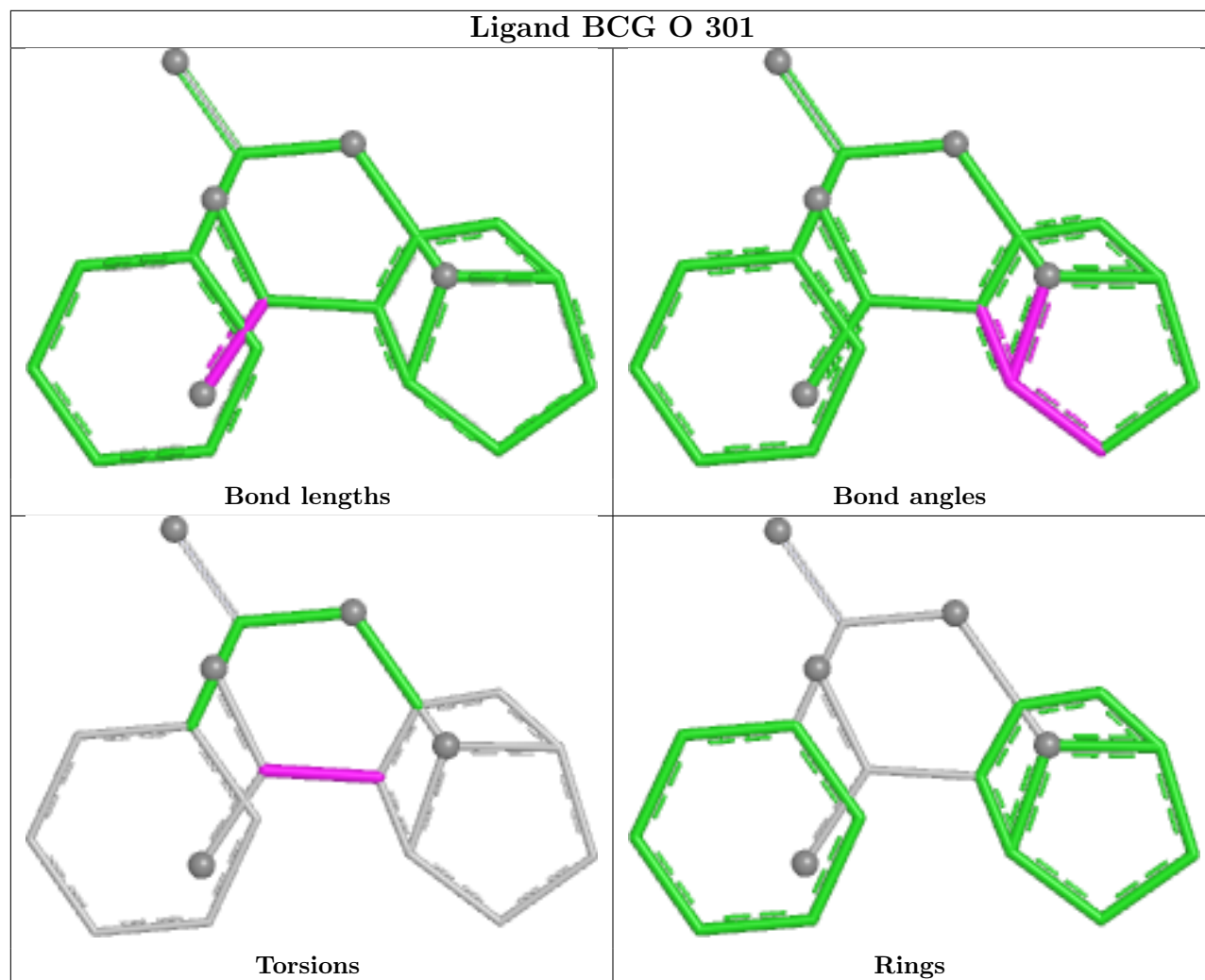
Bond angles

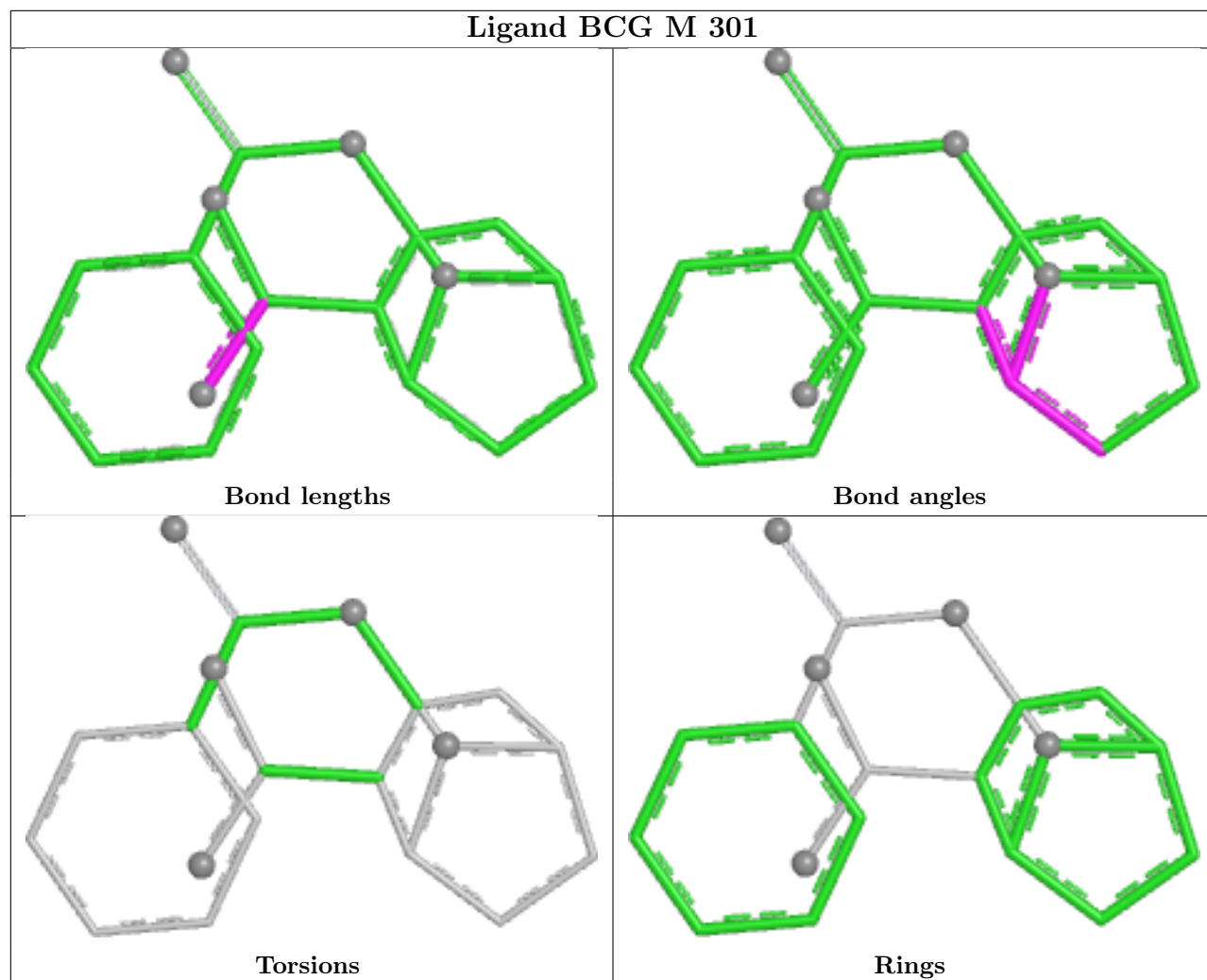


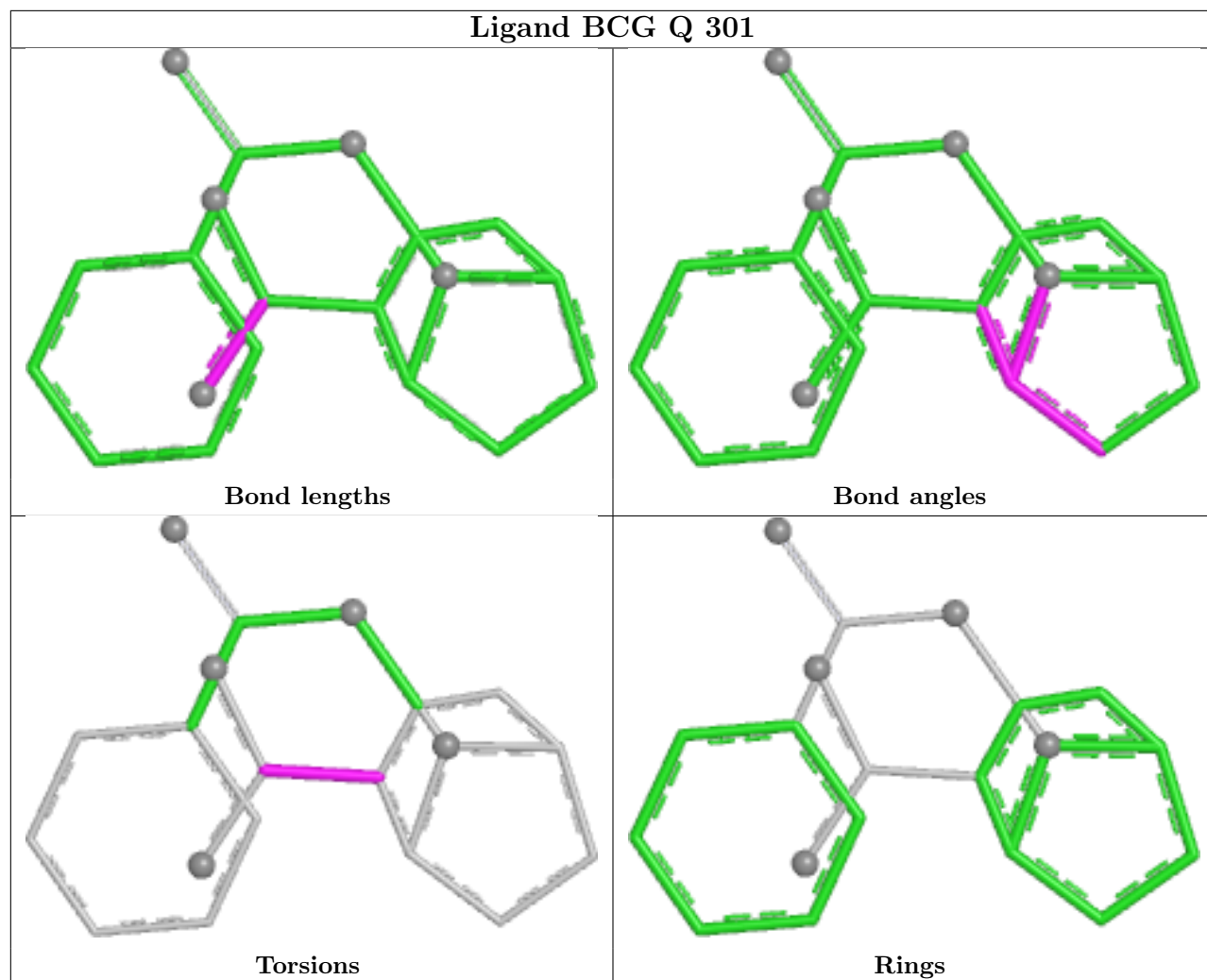
Torsions

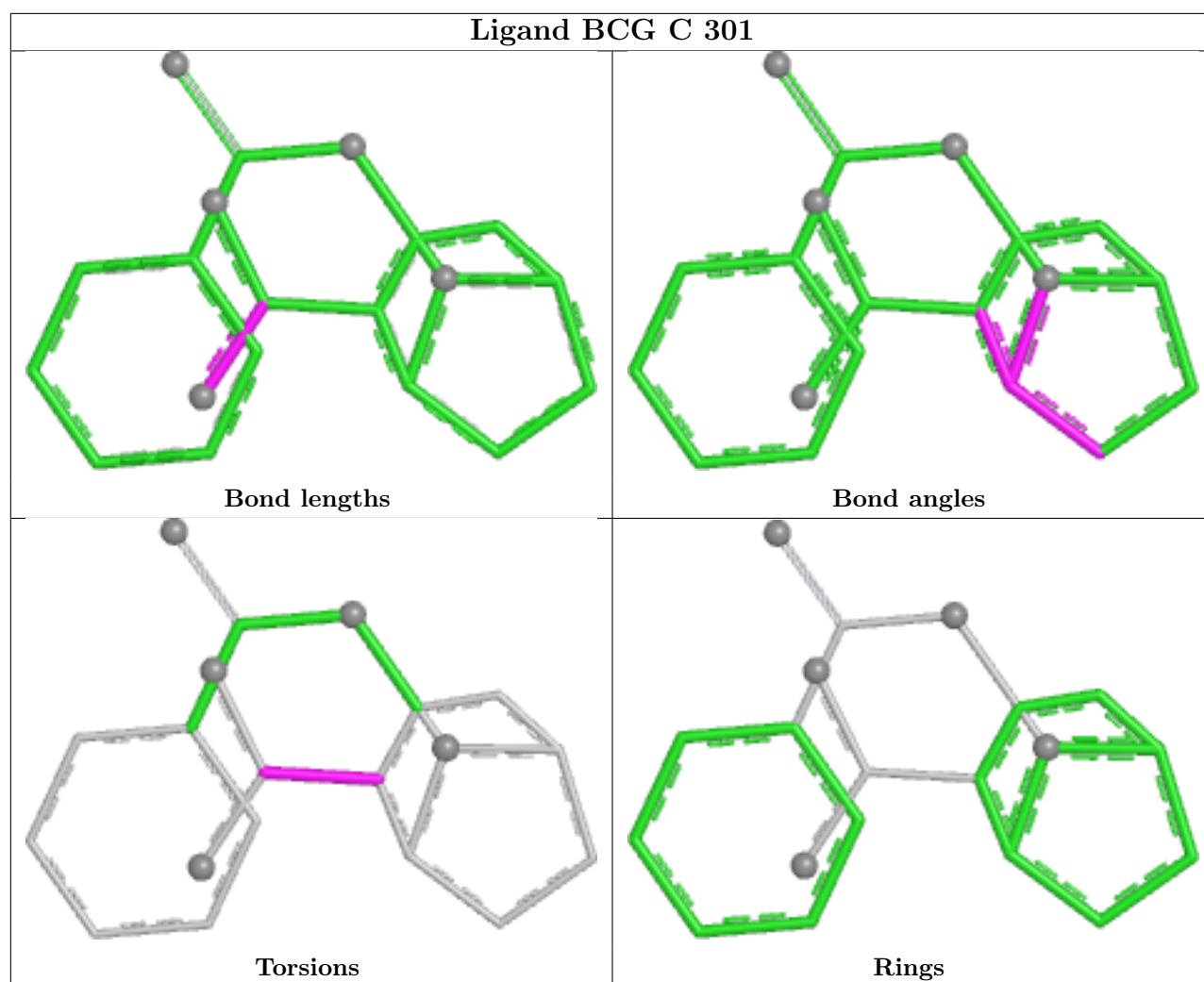


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	213/215 (99%)	0.12	8 (3%) 44 38	30, 62, 121, 147	0
1	C	212/215 (98%)	0.03	2 (0%) 81 78	34, 62, 101, 117	0
1	E	213/215 (99%)	-0.18	2 (0%) 81 78	30, 52, 76, 130	0
1	I	213/215 (99%)	-0.17	1 (0%) 87 85	26, 51, 97, 137	0
1	L	211/215 (98%)	-0.29	1 (0%) 87 85	26, 46, 71, 94	0
1	M	213/215 (99%)	0.37	14 (6%) 24 20	36, 66, 135, 155	0
1	O	212/215 (98%)	-0.11	3 (1%) 73 70	31, 53, 79, 99	0
1	Q	210/215 (97%)	0.89	55 (26%) 1 1	36, 77, 174, 186	0
2	B	206/222 (92%)	0.20	5 (2%) 59 55	35, 63, 116, 148	0
2	D	209/222 (94%)	-0.12	2 (0%) 79 76	34, 52, 89, 118	0
2	F	212/222 (95%)	-0.23	4 (1%) 66 62	31, 47, 99, 133	0
2	H	204/222 (91%)	0.14	10 (4%) 35 29	30, 52, 112, 143	0
2	J	219/222 (98%)	-0.25	4 (1%) 67 64	22, 43, 98, 138	0
2	N	214/222 (96%)	0.44	22 (10%) 12 9	32, 66, 134, 184	0
2	P	209/222 (94%)	-0.19	1 (0%) 87 85	24, 46, 75, 99	0
2	R	201/222 (90%)	0.47	23 (11%) 10 8	37, 62, 140, 161	0
All	All	3371/3496 (96%)	0.07	157 (4%) 36 30	22, 53, 125, 186	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	74	ASN	4.8
1	O	2	ALA	4.8
2	J	219	HIS	4.7
1	Q	149	VAL	4.5
1	Q	192	ARG	4.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

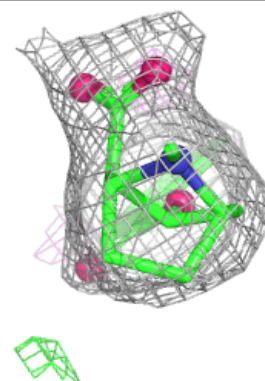
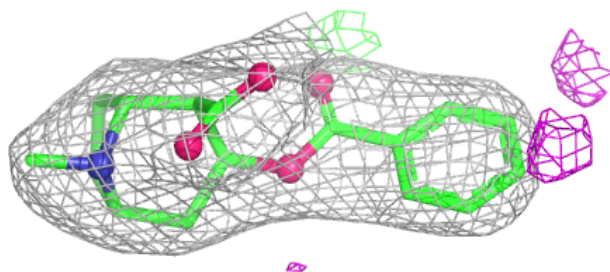
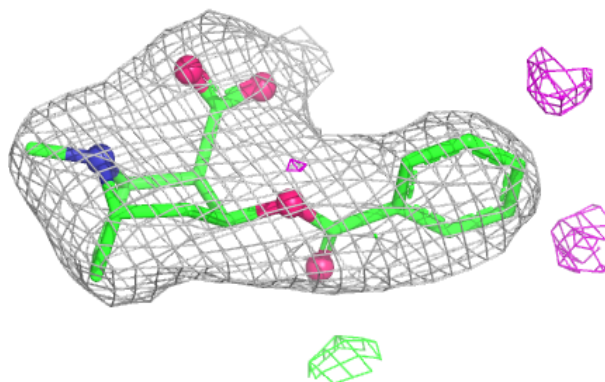
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	Q	302	4/4	0.78	0.28	67,79,80,89	0
7	FMT	O	303	3/3	0.79	0.19	56,56,61,66	0
4	PEG	L	302	7/7	0.82	0.15	50,59,71,72	0
6	ACT	M	302	4/4	0.86	0.21	73,75,79,81	0
6	ACT	P	301	4/4	0.87	0.14	56,58,61,62	0
5	GOL	L	303	6/6	0.89	0.13	51,67,77,77	0
6	ACT	E	302	4/4	0.89	0.18	53,60,65,75	0
6	ACT	C	302	4/4	0.90	0.16	49,60,60,60	0
6	ACT	J	302	4/4	0.90	0.18	41,66,72,75	0
6	ACT	H	301	4/4	0.91	0.20	50,69,73,73	0
6	ACT	O	302	4/4	0.93	0.16	55,62,63,70	0
3	BCG	Q	301	21/21	0.94	0.10	36,54,69,73	0
3	BCG	L	301	21/21	0.95	0.08	27,36,51,61	0
6	ACT	B	302	4/4	0.95	0.18	55,66,68,77	0
3	BCG	M	301	21/21	0.95	0.09	42,50,57,60	0
3	BCG	C	301	21/21	0.95	0.09	42,54,60,65	0
3	BCG	O	301	21/21	0.95	0.08	37,47,60,66	0
3	BCG	E	301	21/21	0.96	0.08	28,44,61,65	0
3	BCG	B	301	21/21	0.96	0.08	28,43,52,55	0
3	BCG	J	301	21/21	0.97	0.06	29,38,49,55	0

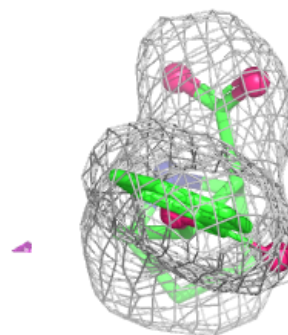
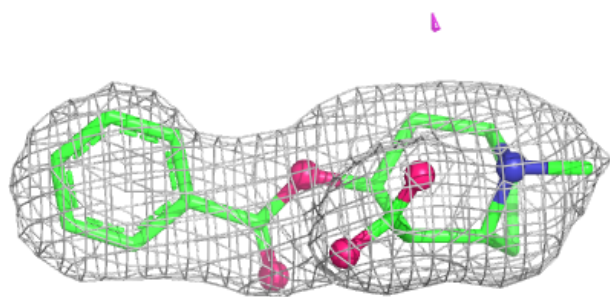
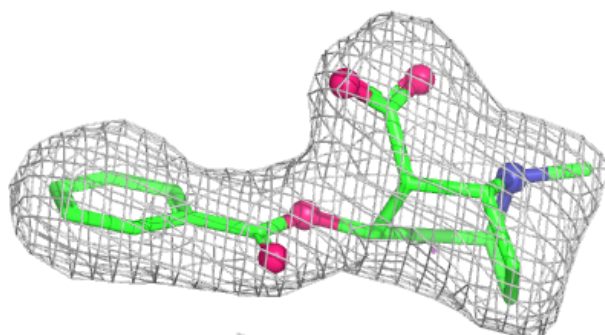
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCG Q 301:

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

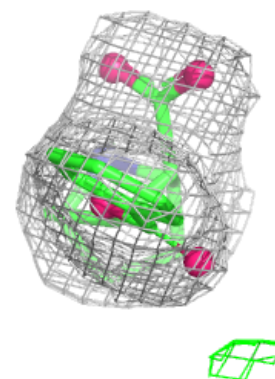
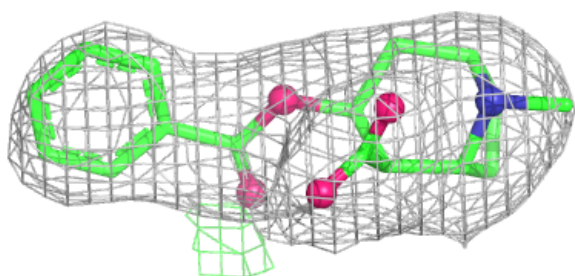
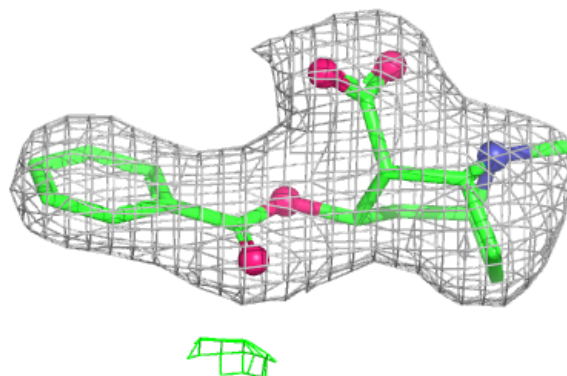
**Electron density around BCG L 301:**

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

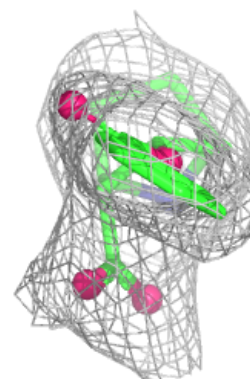
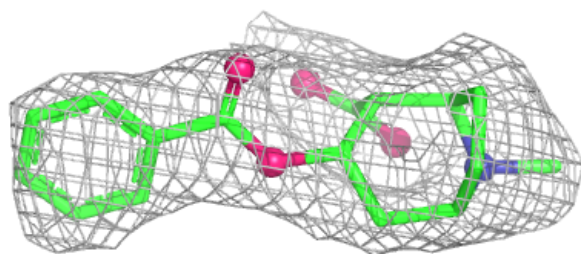
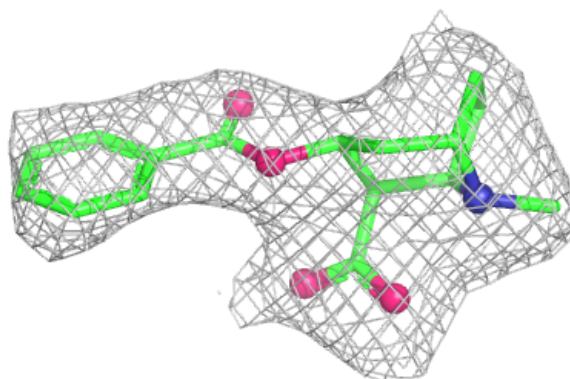


Electron density around BCG M 301:

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and green (positive)

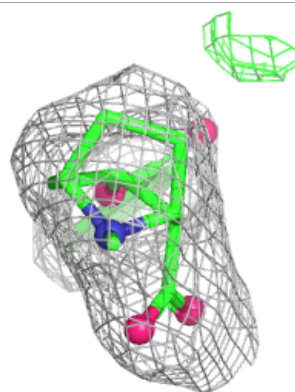
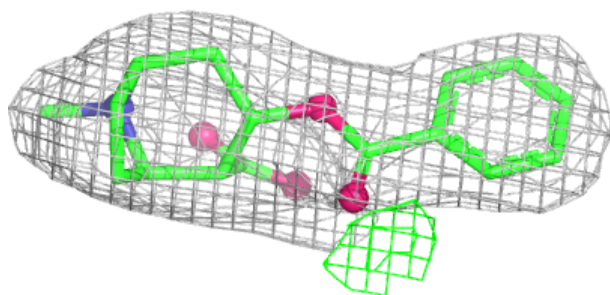
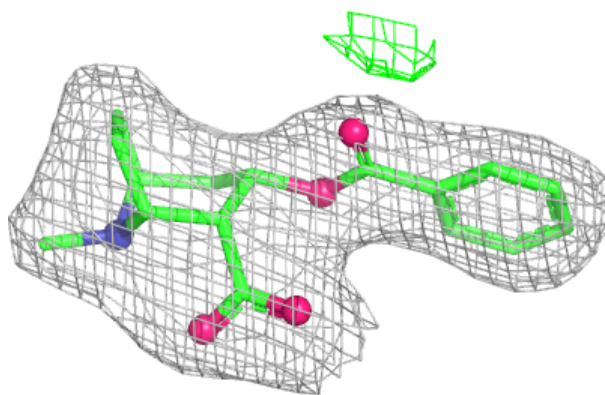
**Electron density around BCG C 301:**

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

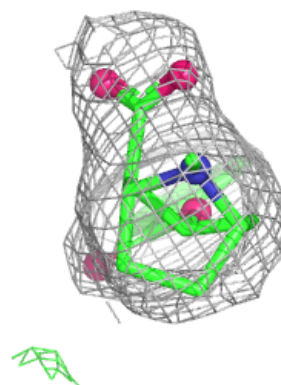
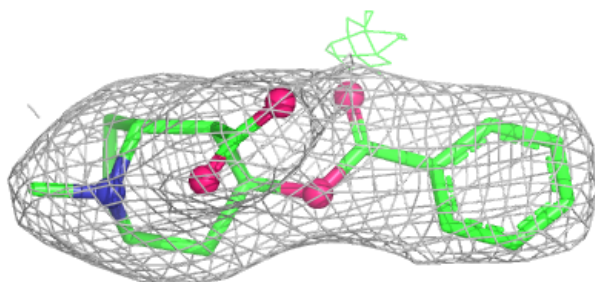
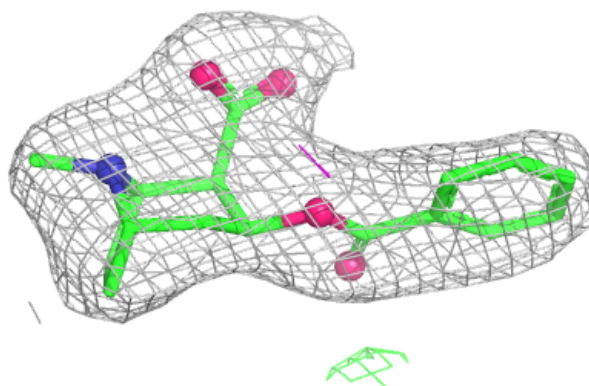


Electron density around BCG O 301:

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

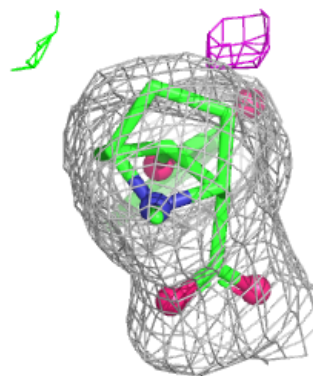
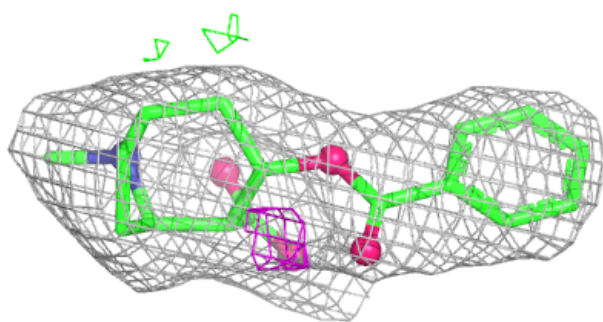
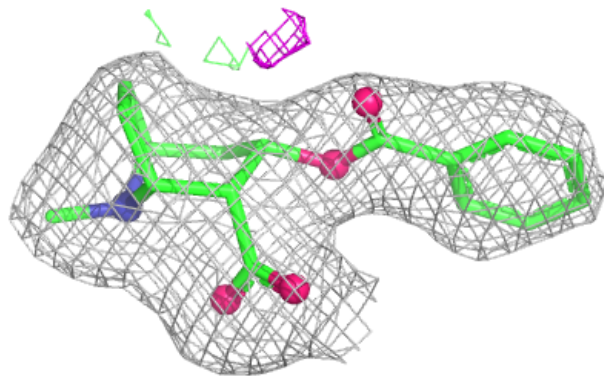
**Electron density around BCG E 301:**

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

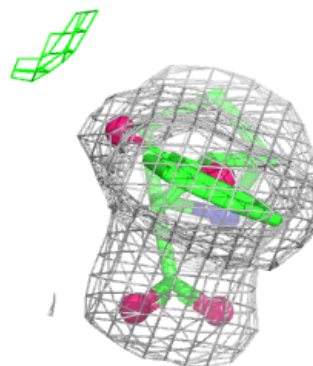
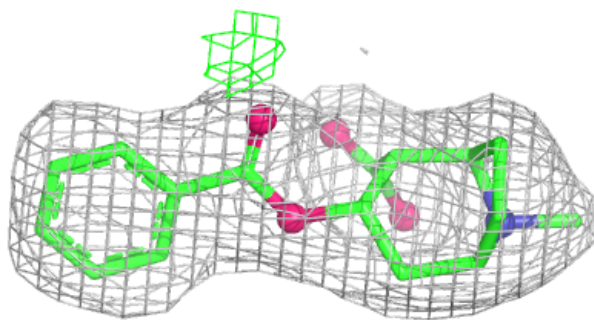
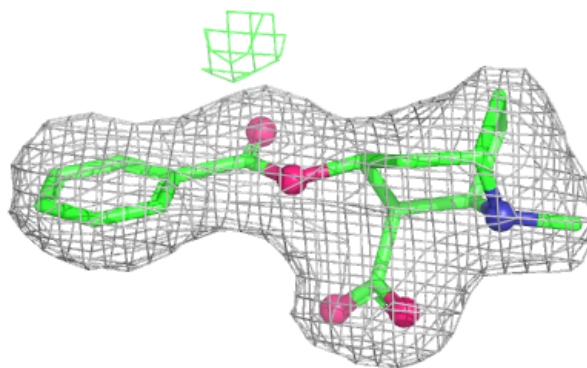


Electron density around BCG B 301:

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

**Electron density around BCG J 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.