



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:26 am BST

PDB ID : 6NFN
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 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 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 : 2.11
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) : 2.11

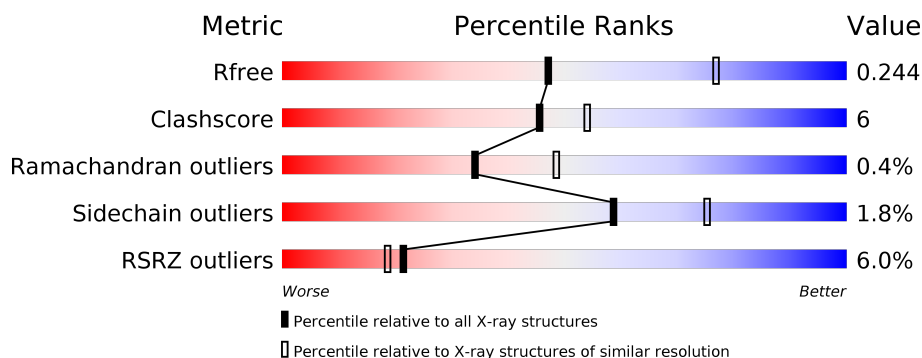
1 Overall quality at a glance

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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (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 on 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	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> <div></div> </div>
1	C	215	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> <div></div> </div>
1	E	215	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> </div> <div></div> </div>
1	I	215	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> <div></div> </div>
1	L	215	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> <div></div> </div>
1	M	215	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>22%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
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

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.

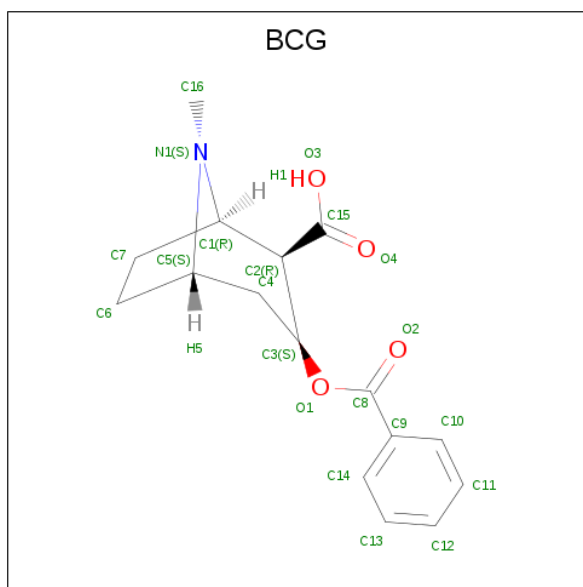
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	204	Total	C	N	O	S	0	0	0
			1507	953	252	296	6			
2	B	206	Total	C	N	O	S	0	0	0
			1533	968	258	301	6			
2	D	209	Total	C	N	O	S	0	0	0
			1556	982	261	307	6			
2	F	212	Total	C	N	O	S	0	0	0
			1585	999	267	312	7			
2	J	219	Total	C	N	O	S	0	0	0
			1624	1021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

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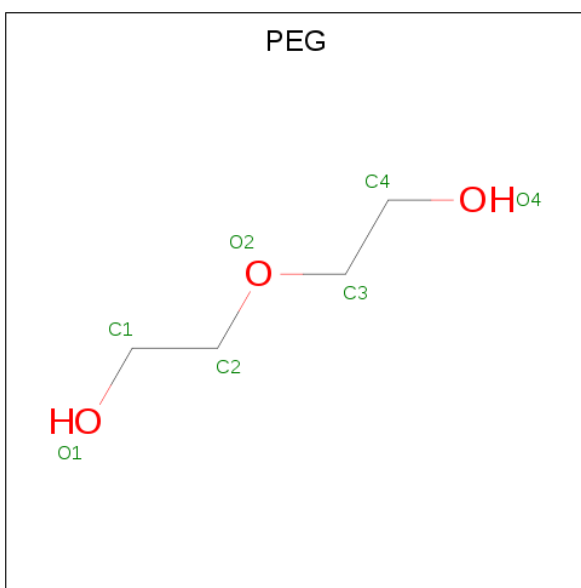
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	201	Total	C	N	O	S	0	0	0
			1492	939	252	295	6			
2	N	214	Total	C	N	O	S	0	0	0
			1597	1007	277	306	7			

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



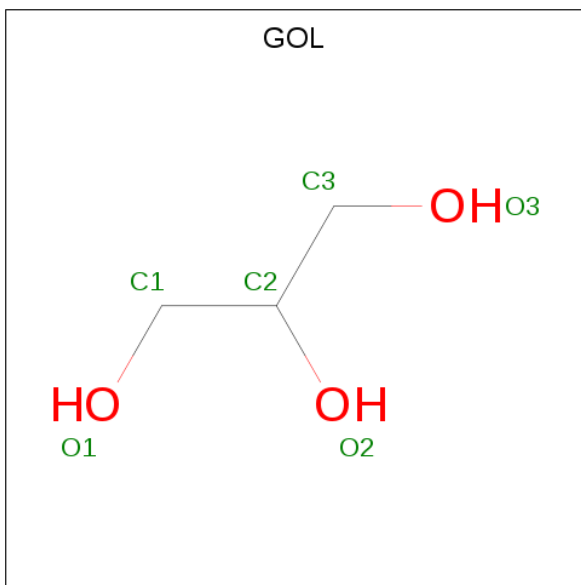
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			21	16	1	4		
3	B	1	Total	C	N	O	0	0
			21	16	1	4		
3	C	1	Total	C	N	O	0	0
			21	16	1	4		
3	E	1	Total	C	N	O	0	0
			21	16	1	4		
3	J	1	Total	C	N	O	0	0
			21	16	1	4		
3	O	1	Total	C	N	O	0	0
			21	16	1	4		
3	Q	1	Total	C	N	O	0	0
			21	16	1	4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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



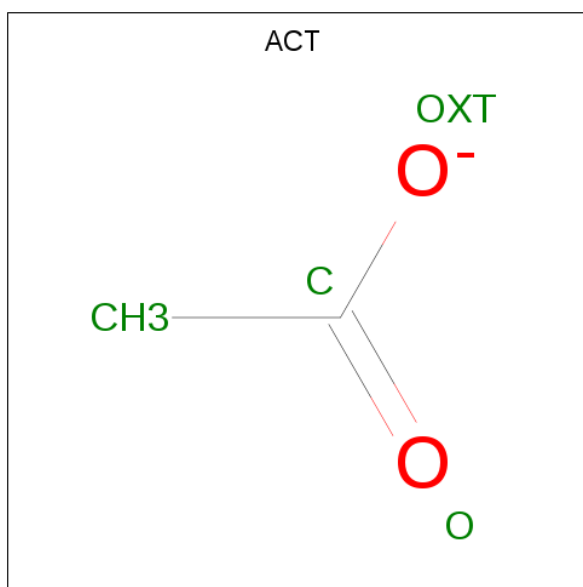
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



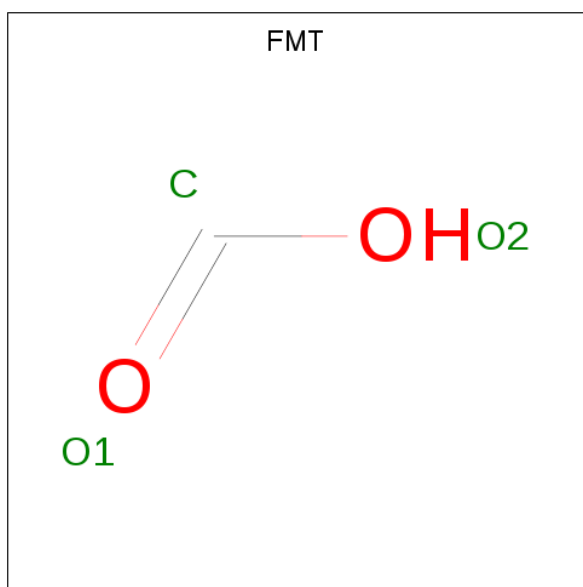
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (three-letter code: 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 (three-letter code: 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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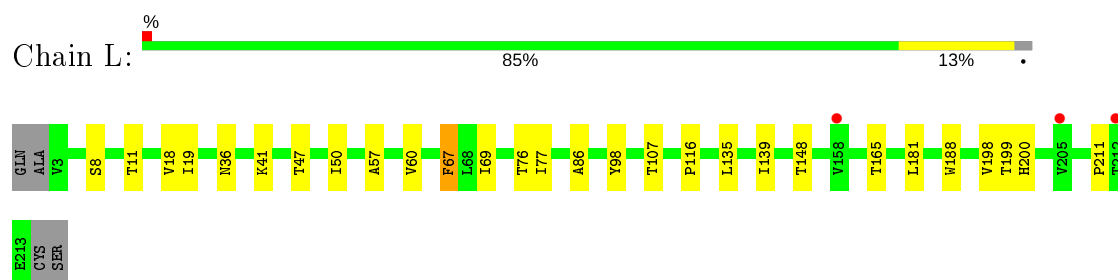
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	17	Total 17	O 17	0	0
8	Q	4	Total 4	O 4	0	0
8	R	6	Total 6	O 6	0	0
8	M	6	Total 6	O 6	0	0
8	N	6	Total 6	O 6	0	0

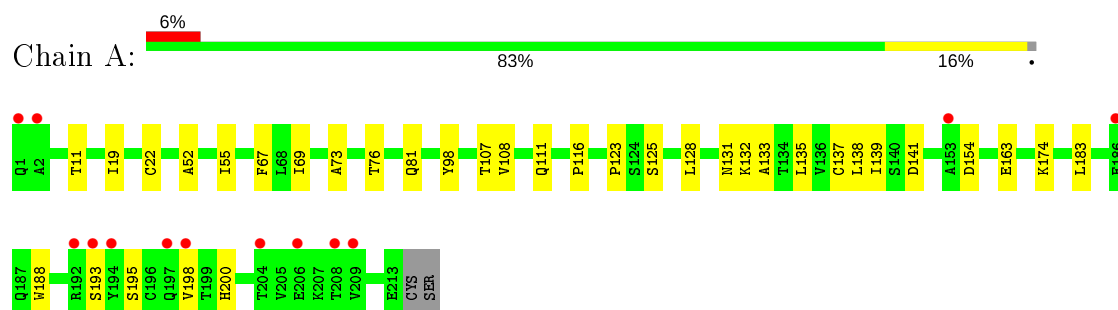
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

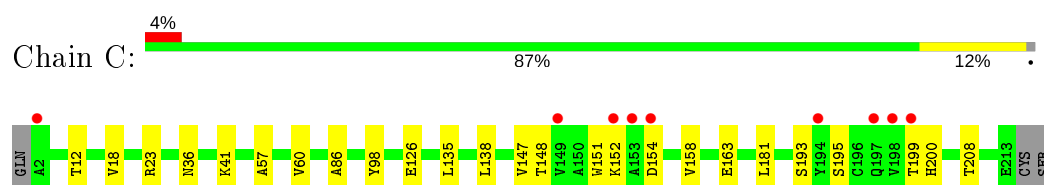
- Molecule 1: Fab h2E2 light chain



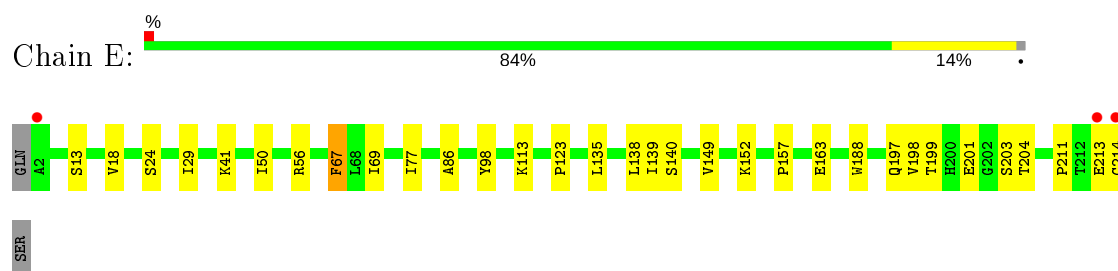
- Molecule 1: Fab h2E2 light chain



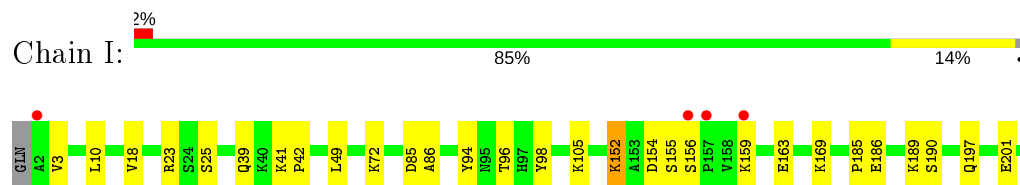
- Molecule 1: Fab h2E2 light chain



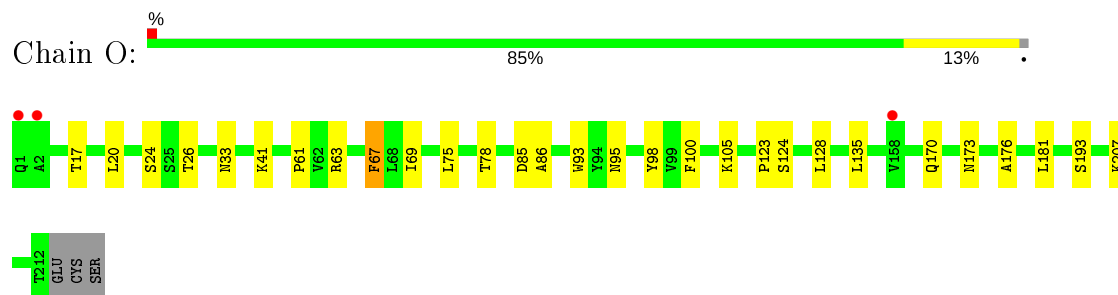
- Molecule 1: Fab h2E2 light chain



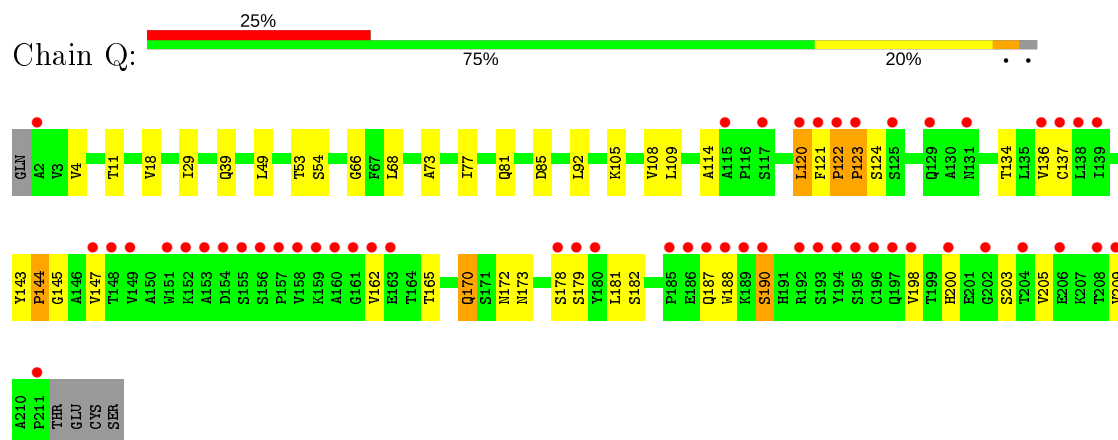
- Molecule 1: Fab h2E2 light chain



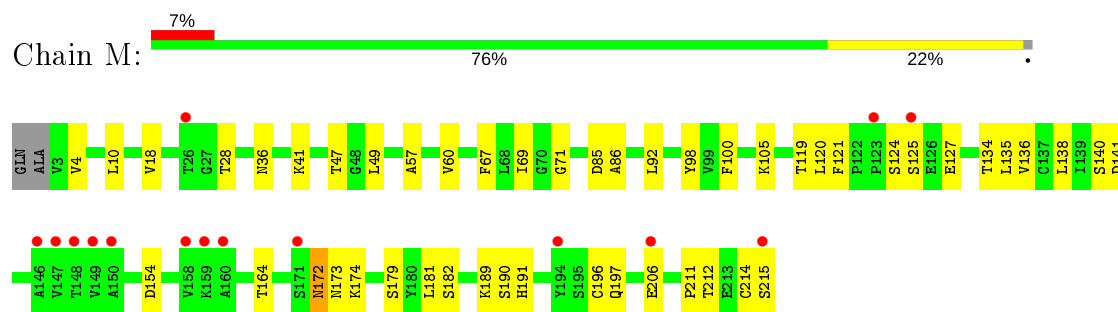
- Molecule 1: Fab h2E2 light chain



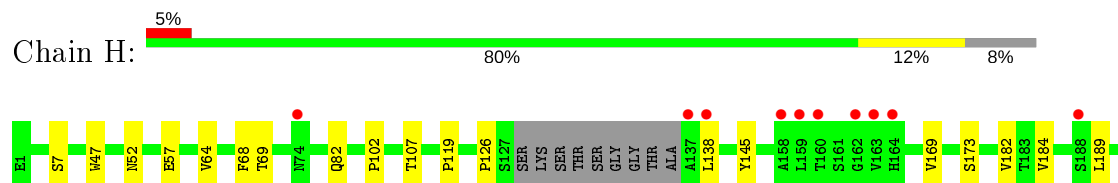
- Molecule 1: Fab h2E2 light chain



- Molecule 1: Fab h2E2 light chain

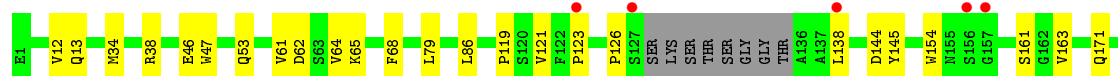
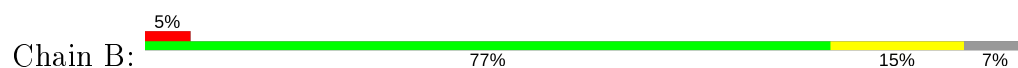


- Molecule 2: Fab h2E2 heavy chain

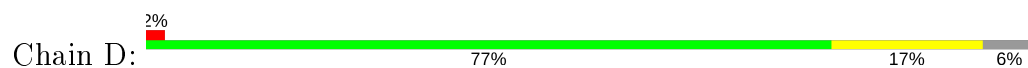




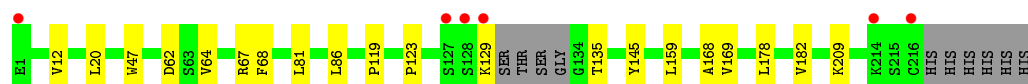
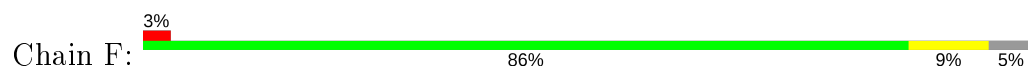
- Molecule 2: Fab h2E2 heavy chain



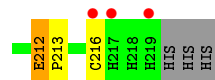
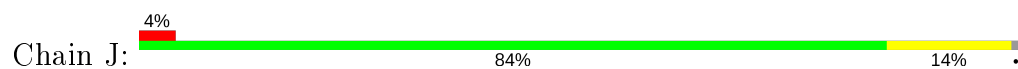
- Molecule 2: Fab h2E2 heavy chain



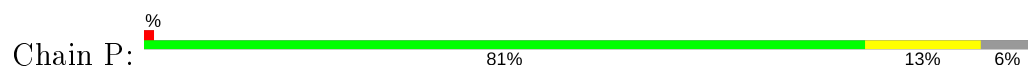
- Molecule 2: Fab h2E2 heavy chain

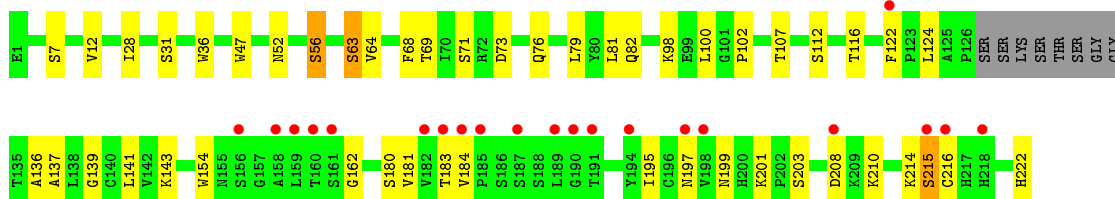


- Molecule 2: Fab h2E2 heavy chain



- 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 48.60 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.67-2.63) 92.1 (48.60-2.63)	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 0.185 , 0.244	Depositor DCC
R_{free} test set	5131 reflections (4.93%)	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 , 51.8	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, GOL, FMT, BCG, ACT

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	0.28	0/1593	0.53	0/2185
1	C	0.29	0/1609	0.49	0/2204
1	E	0.29	0/1621	0.49	0/2218
1	I	0.28	0/1625	0.48	0/2223
1	L	0.30	0/1598	0.50	0/2189
1	M	0.33	0/1584	0.54	1/2172 (0.0%)
1	O	0.32	0/1613	0.52	0/2208
1	Q	0.34	0/1480	0.54	0/2037
2	B	0.28	0/1569	0.49	0/2140
2	D	0.29	0/1592	0.49	0/2170
2	F	0.28	0/1621	0.49	0/2206
2	H	0.34	0/1543	0.55	0/2108
2	J	0.28	0/1662	0.50	0/2264
2	N	0.31	0/1639	0.53	0/2237
2	P	0.29	0/1593	0.49	0/2172
2	R	0.28	0/1527	0.49	0/2083
All	All	0.30	0/25469	0.51	1/34816 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	212	THR	C-N-CA	5.91	136.47	121.70

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	19	0
1	C	1570	0	1537	16	0
1	E	1582	0	1559	21	0
1	I	1586	0	1563	17	0
1	L	1559	0	1531	17	0
1	M	1546	0	1495	31	0
1	O	1574	0	1553	16	0
1	Q	1447	0	1317	28	0
2	B	1533	0	1483	20	0
2	D	1556	0	1514	25	0
2	F	1585	0	1553	15	0
2	H	1507	0	1438	23	0
2	J	1624	0	1581	20	0
2	N	1597	0	1523	38	0
2	P	1557	0	1515	19	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	317	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 6.

All (317) 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
1:Q:147:VAL:HG21	1:Q:198:VAL:HG23	1.56	0.85
1:E:163:GLU:HG2	2:F:169:VAL:CG1	2.09	0.83
2:R:121:VAL:HG21	2:R:198:VAL:HG11	1.61	0.83
1:E:24:SER:H	1:E:29:ILE:HD11	1.45	0.81
2:B:61:VAL:O	2:B:64:VAL:HG12	1.82	0.79
2:D:121:VAL:HG21	2:D:207:VAL:HG21	1.66	0.78
1:Q:187:GLN:HA	1:Q:190:SER:HB3	1.66	0.77
2:H:199:ASN:HD22	2:H:206:LYS:CG	2.02	0.73
1:I:163:GLU:HB3	2:J:169:VAL:HG11	1.71	0.72
2:H:199:ASN:HD22	2:H:206:LYS:HG3	1.55	0.71
1:I:39:GLN:HB2	1:I:49:LEU:HD11	1.70	0.71
2:H:199:ASN:ND2	2:H:206:LYS:HG3	2.06	0.71
2:J:212:GLU:HG2	2:J:213:PRO:HD2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:123:PRO:HB2	1:O:128:LEU:HD11	1.75	0.69
1:O:67:PHE:CE1	1:O:69:ILE:HD11	2.29	0.67
2:D:201:LYS:NZ	2:P:173:SER:O	2.28	0.66
2:H:195:ILE:HD12	2:H:210:LYS:HA	1.78	0.66
1:Q:165:THR:HB	1:Q:178:SER:H	1.61	0.66
2:B:154:TRP:CD1	2:B:163:VAL:HG21	2.32	0.65
1:E:152:LYS:HE3	1:E:157:PRO:HB3	1.79	0.65
1:I:185:PRO:O	1:I:189:LYS:HD2	1.97	0.64
1:M:67:PHE:HE1	1:M:69:ILE:HD13	1.63	0.64
2:P:210:LYS:HD3	2:P:212:GLU:HG3	1.81	0.63
1:A:139:ILE:HD12	1:A:198:VAL:HG21	1.81	0.63
2:D:198:VAL:HB	2:D:207:VAL:HG23	1.81	0.62
2:B:126:PRO:HD3	2:B:138:LEU:HB3	1.81	0.62
1:C:195:SER:HB3	1:C:208:THR:HG22	1.82	0.62
1:M:215:SER:HB2	2:N:216:CYS:HA	1.81	0.62
1:O:17:THR:HG22	1:O:78:THR:HA	1.81	0.62
1:M:121:PHE:HB2	1:M:136:VAL:HB	1.81	0.62
2:R:138:LEU:HD13	2:R:154:TRP:CH2	2.34	0.61
1:C:41:LYS:HG2	1:C:86:ALA:HB2	1.81	0.61
2:P:123:PRO:HD3	2:P:209:LYS:HE2	1.83	0.61
2:N:139:GLY:HA2	2:N:154:TRP:CH2	2.36	0.61
2:N:124:LEU:HD12	2:N:139:GLY:HA3	1.83	0.61
2:R:62:ASP:HA	2:R:65:LYS:HG3	1.82	0.61
1:Q:147:VAL:CG2	1:Q:198:VAL:HG23	2.31	0.60
1:C:151:TRP:O	1:C:152:LYS:HE2	2.02	0.60
2:J:69:THR:HG23	2:J:82:GLN:HB3	1.82	0.60
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.82	0.60
1:C:138:LEU:HD22	2:D:181:VAL:HG11	1.83	0.60
1:Q:134:THR:HG23	1:Q:182:SER:HA	1.84	0.60
1:Q:114:ALA:HB3	1:Q:143:TYR:H	1.66	0.59
2:J:9:GLY:H	2:J:107:THR:HG21	1.68	0.59
1:O:85:ASP:OD1	1:O:105:LYS:NZ	2.36	0.59
1:M:135:LEU:HD12	1:M:181:LEU:HD13	1.85	0.59
1:L:41:LYS:HG2	1:L:86:ALA:HB2	1.84	0.59
2:R:9:GLY:H	2:R:107:THR:HG21	1.67	0.59
1:A:116:PRO:HD3	1:A:200:HIS:CD2	2.38	0.58
1:Q:124:SER:HB3	2:R:122:PHE:HB3	1.86	0.58
1:I:85:ASP:OD1	1:I:105:LYS:NZ	2.37	0.58
2:J:126:PRO:HD2	2:J:213:PRO:HA	1.85	0.58
1:A:52:ALA:HB3	1:A:55:ILE:HD12	1.86	0.57
1:O:33:ASN:HA	1:O:93:TRP:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD21	1:A:188:TRP:CZ3	2.39	0.57
2:F:123:PRO:HD3	2:F:209:LYS:HE2	1.85	0.57
1:M:47:THR:HA	2:N:102:PRO:HA	1.87	0.57
2:F:168:ALA:HA	2:F:178:LEU:HB3	1.87	0.57
1:L:67:PHE:CE1	1:L:69:ILE:HD11	2.40	0.57
1:Q:170:GLN:HB3	2:R:164:HIS:CE1	2.40	0.57
1:M:10:LEU:HD13	1:M:18:VAL:HG12	1.87	0.57
2:R:83:MET:HB3	2:R:86:LEU:HD21	1.86	0.56
2:F:12:VAL:HG11	2:F:86:LEU:HD13	1.88	0.56
1:Q:85:ASP:OD1	1:Q:105:LYS:NZ	2.36	0.56
1:Q:39:GLN:HB2	1:Q:49:LEU:HD11	1.88	0.55
2:N:197:ASN:ND2	2:N:208:ASP:OD1	2.32	0.55
2:D:12:VAL:HG21	2:D:86:LEU:HD13	1.89	0.55
2:H:173:SER:HB2	2:B:204:ASN:HB3	1.89	0.55
2:N:124:LEU:HB2	2:N:139:GLY:H	1.71	0.55
2:H:64:VAL:HG13	2:H:68:PHE:HB2	1.88	0.55
1:M:138:LEU:HD12	2:N:181:VAL:HG11	1.87	0.55
1:Q:162:VAL:HG13	1:Q:181:LEU:HD23	1.89	0.55
2:N:124:LEU:HD21	2:N:141:LEU:HB2	1.89	0.55
1:A:11:THR:HG22	1:A:107:THR:HB	1.88	0.54
2:D:126:PRO:HD2	2:D:213:PRO:HA	1.88	0.54
2:N:69:THR:HG23	2:N:82:GLN:HB3	1.88	0.54
1:L:11:THR:HG22	1:L:107:THR:HB	1.90	0.54
1:L:67:PHE:HE1	1:L:69:ILE:HD11	1.71	0.54
1:M:4:VAL:HG22	1:M:92:LEU:HD12	1.90	0.54
1:M:127:GLU:HG2	2:N:122:PHE:CG	2.42	0.54
1:C:57:ALA:HB3	1:C:60:VAL:HG23	1.88	0.54
2:R:152:VAL:HG11	2:R:165:THR:HG21	1.90	0.54
2:B:64:VAL:HG22	2:B:68:PHE:CG	2.42	0.54
1:Q:53:THR:HG21	1:Q:68:LEU:HG	1.89	0.54
1:L:57:ALA:HB3	1:L:60:VAL:HG13	1.91	0.53
1:M:100:PHE:CZ	6:M:302:ACT:H3	2.44	0.53
1:M:28:THR:HG23	1:M:71:GLY:HA2	1.89	0.53
1:E:41:LYS:HG2	1:E:86:ALA:HB2	1.90	0.53
1:A:163:GLU:OE1	2:B:171:GLN:HA	2.09	0.53
1:M:138:LEU:C	1:M:138:LEU:HD23	2.29	0.53
2:R:186:SER:HA	2:R:189:LEU:HD11	1.91	0.53
1:O:61:PRO:HB2	1:O:63:ARG:HG2	1.90	0.53
2:N:116:THR:HG22	2:N:203:SER:HB3	1.89	0.53
1:E:67:PHE:HE1	1:E:69:ILE:HD11	1.74	0.52
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:4:VAL:HG22	1:Q:92:LEU:HD12	1.92	0.52
1:C:36:ASN:ND2	6:C:302:ACT:OXT	2.42	0.52
1:O:24:SER:HG	1:O:26:THR:HG1	1.50	0.52
2:H:52:ASN:HB2	2:H:57:GLU:H	1.75	0.52
2:H:7:SER:HA	2:H:107:THR:HG21	1.92	0.52
1:M:138:LEU:HD21	1:M:140:SER:OG	2.09	0.52
1:Q:198:VAL:HG13	1:Q:205:VAL:HB	1.91	0.52
1:A:123:PRO:HD3	1:A:135:LEU:HD23	1.93	0.51
1:E:24:SER:N	1:E:29:ILE:HD11	2.18	0.51
1:I:41:LYS:HG2	1:I:86:ALA:HB2	1.91	0.51
1:E:152:LYS:HD3	1:E:157:PRO:HA	1.92	0.51
1:L:19:ILE:HG23	1:L:76:THR:HG22	1.92	0.51
2:N:98:LYS:NZ	2:N:100:LEU:O	2.38	0.50
1:I:186:GLU:O	1:I:190:SER:HB3	2.10	0.50
1:O:41:LYS:HG2	1:O:86:ALA:HB2	1.93	0.50
1:L:135:LEU:HD12	1:L:181:LEU:HD23	1.93	0.50
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.47	0.50
2:N:28:ILE:HB	2:N:31:SER:OG	2.12	0.50
2:R:138:LEU:HD11	2:R:182:VAL:HB	1.93	0.50
2:F:129:LYS:HD3	2:F:135:THR:OG1	2.12	0.50
2:N:52:ASN:HD21	2:N:56:SER:HB3	1.76	0.50
2:H:184:VAL:HG11	2:H:194:TYR:CZ	2.47	0.49
1:C:148:THR:HG23	1:C:199:THR:OG1	2.13	0.49
2:R:198:VAL:HG13	2:R:207:VAL:HB	1.93	0.49
2:B:188:SER:HB3	2:B:192:GLN:OE1	2.12	0.49
1:I:10:LEU:HD13	1:I:18:VAL:HG13	1.94	0.49
2:R:198:VAL:CG1	2:R:207:VAL:HB	2.43	0.49
1:C:163:GLU:HG2	2:D:169:VAL:CG1	2.42	0.49
2:R:186:SER:HA	2:R:189:LEU:CD1	2.42	0.49
1:A:98:TYR:HB2	2:B:47:TRP:CG	2.47	0.49
2:H:69:THR:OG1	2:H:82:GLN:HB3	2.12	0.49
1:E:98:TYR:HB2	2:F:47:TRP:CG	2.47	0.48
1:M:189:LYS:HB3	2:N:222:HIS:HB2	1.93	0.48
1:E:213:GLU:O	1:E:214:CYS:HB2	2.13	0.48
1:E:18:VAL:HG12	1:E:77:ILE:HB	1.95	0.48
1:A:138:LEU:HD13	2:B:181:VAL:HG11	1.95	0.48
1:C:23:ARG:HG2	1:C:23:ARG:HH11	1.78	0.48
2:F:20:LEU:HD12	2:F:81:LEU:HD23	1.94	0.48
1:Q:137:CYS:HB3	1:Q:179:SER:OG	2.13	0.48
1:M:134:THR:HG21	2:N:143:LYS:HE3	1.96	0.48
2:B:62:ASP:HA	2:B:65:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:LEU:HD12	1:M:136:VAL:O	2.14	0.48
2:J:119:PRO:HD2	2:J:205:THR:HG21	1.96	0.48
2:P:119:PRO:HB3	2:P:145:TYR:HB3	1.95	0.48
2:R:52:ASN:HB2	2:R:57:GLU:H	1.78	0.48
2:B:121:VAL:CG2	2:B:198:VAL:HG11	2.35	0.48
2:F:67:ARG:HG3	2:J:19:ARG:HD3	1.95	0.48
1:C:98:TYR:HB2	2:D:47:TRP:CG	2.49	0.47
1:M:85:ASP:OD1	1:M:105:LYS:NZ	2.35	0.47
2:N:64:VAL:HG13	2:N:68:PHE:HB2	1.96	0.47
1:A:67:PHE:HE1	1:A:69:ILE:HD11	1.78	0.47
2:J:142:VAL:HG11	2:J:150:VAL:HG11	1.95	0.47
2:N:201:LYS:HE3	2:N:201:LYS:HB3	1.62	0.47
1:M:119:THR:HG21	2:N:137:ALA:HB3	1.96	0.47
1:M:57:ALA:HB3	1:M:60:VAL:HG23	1.96	0.47
1:M:191:HIS:O	1:M:211:PRO:HG2	2.14	0.47
2:B:138:LEU:HD13	2:B:211:VAL:HG21	1.96	0.47
2:N:73:ASP:OD2	2:N:76:GLN:HB2	2.14	0.47
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.95	0.47
2:N:162:GLY:HA3	2:N:183:THR:OG1	2.14	0.47
1:I:98:TYR:HB2	2:J:47:TRP:CG	2.50	0.47
1:I:39:GLN:HB2	1:I:49:LEU:CD1	2.44	0.47
1:Q:11:THR:HB	1:Q:109:LEU:HD11	1.96	0.47
2:D:201:LYS:HD2	2:D:201:LYS:HA	1.64	0.46
2:J:9:GLY:N	2:J:107:THR:HG21	2.30	0.46
1:M:41:LYS:HG2	1:M:86:ALA:HB2	1.96	0.46
1:M:164:THR:HG23	1:M:179:SER:HB2	1.96	0.46
2:F:64:VAL:HG13	2:F:68:PHE:CG	2.50	0.46
1:I:152:LYS:HE3	1:I:155:SER:O	2.15	0.46
1:L:98:TYR:HB2	2:H:47:TRP:CG	2.51	0.46
1:M:67:PHE:CE1	1:M:69:ILE:HD13	2.48	0.46
2:P:210:LYS:HD3	2:P:212:GLU:CG	2.45	0.46
2:R:28:ILE:O	2:R:31:SER:OG	2.28	0.46
2:N:64:VAL:CG1	2:N:68:PHE:HB2	2.46	0.46
2:F:159:LEU:HD21	2:F:182:VAL:HG21	1.98	0.46
2:N:136:ALA:HB3	2:N:184:VAL:HG13	1.98	0.46
1:Q:124:SER:HB3	2:R:122:PHE:CB	2.46	0.46
2:B:123:PRO:HD3	2:B:209:LYS:HE2	1.98	0.46
2:B:38:ARG:HD2	2:B:46:GLU:OE1	2.15	0.46
1:C:135:LEU:HD12	1:C:181:LEU:HD23	1.98	0.45
2:J:129:LYS:HD2	2:J:137:ALA:HB2	1.97	0.45
1:E:139:ILE:HG12	1:E:198:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:HB	1:C:18:VAL:CG1	2.47	0.45
1:I:197:GLN:HG2	1:I:206:GLU:HB3	1.97	0.45
1:L:116:PRO:HD3	1:L:200:HIS:CD2	2.50	0.45
1:M:120:LEU:HD22	1:M:196:CYS:HB2	1.97	0.45
2:D:12:VAL:HG11	2:D:18:LEU:HD13	1.99	0.45
2:D:2:VAL:HB	2:D:102:PRO:HD2	1.97	0.45
2:F:64:VAL:CG1	2:F:68:PHE:HB2	2.47	0.45
1:I:3:VAL:HG12	1:I:25:SER:HB3	1.97	0.45
1:L:36:ASN:ND2	1:L:50:ILE:O	2.50	0.45
1:M:98:TYR:HB2	2:N:47:TRP:CG	2.51	0.45
2:P:135:THR:HA	8:P:402:HOH:O	2.16	0.45
2:P:135:THR:HG22	2:P:184:VAL:O	2.16	0.45
2:P:64:VAL:HG13	2:P:68:PHE:CG	2.51	0.45
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.98	0.45
2:D:121:VAL:CG2	2:D:207:VAL:HG21	2.44	0.45
2:P:52:ASN:HB2	2:P:57:GLU:HB2	1.98	0.45
1:A:116:PRO:HD3	1:A:200:HIS:HD2	1.81	0.45
1:C:147:VAL:HG22	1:C:200:HIS:HB2	1.98	0.45
2:D:52:ASN:HB2	2:D:57:GLU:HB2	1.98	0.45
2:H:199:ASN:HD22	2:H:206:LYS:HG2	1.81	0.45
1:I:42:PRO:HG2	1:I:169:LYS:NZ	2.32	0.45
1:A:137:CYS:SG	1:A:139:ILE:HD11	2.56	0.45
2:N:215:SER:O	2:N:216:CYS:SG	2.75	0.45
2:N:64:VAL:HG13	2:N:68:PHE:CG	2.52	0.45
1:O:124:SER:O	1:O:128:LEU:HD12	2.17	0.45
1:I:94:TYR:O	1:I:96:THR:N	2.44	0.44
2:F:64:VAL:HG13	2:F:68:PHE:HB2	1.98	0.44
2:J:69:THR:CG2	2:J:82:GLN:HB3	2.45	0.44
2:N:63:SER:OG	2:N:63:SER:O	2.35	0.44
1:Q:165:THR:OG1	1:Q:178:SER:HB2	2.18	0.44
2:H:138:LEU:O	2:H:182:VAL:HG12	2.18	0.44
2:N:139:GLY:C	2:N:154:TRP:HH2	2.20	0.44
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.00	0.44
2:P:87:ARG:HB2	2:P:89:GLU:HG2	2.00	0.44
1:M:36:ASN:OD1	6:M:302:ACT:H2	2.17	0.44
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.99	0.44
1:L:57:ALA:O	1:L:60:VAL:HG22	2.17	0.44
2:N:154:TRP:HE1	2:N:180:SER:HG	1.61	0.44
1:A:19:ILE:HG23	1:A:76:THR:HG22	2.00	0.44
1:L:18:VAL:HG12	1:L:77:ILE:HB	2.00	0.44
1:O:100:PHE:HZ	6:O:302:ACT:H3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:172:ASN:C	1:M:174:LYS:H	2.19	0.43
2:P:34:MET:HB3	2:P:79:LEU:HD22	2.00	0.43
1:A:81:GLN:O	1:A:108:VAL:HG21	2.18	0.43
1:O:170:GLN:OE1	1:O:176:ALA:HB2	2.18	0.43
1:Q:121:PHE:C	1:Q:123:PRO:HD3	2.37	0.43
2:R:138:LEU:C	2:R:138:LEU:HD12	2.39	0.43
1:E:188:TRP:CE2	1:E:211:PRO:HB3	2.54	0.43
2:J:39:GLN:HB2	2:J:45:LEU:HD23	2.01	0.43
2:J:64:VAL:HG13	2:J:68:PHE:CG	2.54	0.43
1:M:134:THR:HG22	1:M:182:SER:HA	2.01	0.43
2:P:98:LYS:HE2	2:P:98:LYS:HB3	1.81	0.43
2:R:62:ASP:C	2:R:64:VAL:H	2.21	0.43
1:E:123:PRO:HD3	1:E:135:LEU:HD23	2.01	0.43
1:C:126:GLU:OE1	1:C:126:GLU:N	2.51	0.43
2:F:119:PRO:HB3	2:F:145:TYR:HB3	2.01	0.43
1:L:165:THR:HG22	2:H:169:VAL:HB	2.01	0.43
2:P:119:PRO:HD2	2:P:205:THR:HG21	2.01	0.43
1:E:149:VAL:HG22	1:E:198:VAL:HG22	2.01	0.42
1:E:113:LYS:HD2	1:E:201:GLU:HG3	2.01	0.42
1:E:50:ILE:HD13	1:E:56:ARG:HA	2.00	0.42
2:N:195:ILE:HG12	2:N:210:LYS:HA	1.99	0.42
1:O:98:TYR:HB2	2:P:47:TRP:CG	2.54	0.42
2:H:195:ILE:CD1	2:H:210:LYS:HA	2.49	0.42
2:N:71:SER:O	2:N:79:LEU:HD12	2.19	0.42
1:Q:120:LEU:HA	1:Q:136:VAL:O	2.20	0.42
2:R:170:LEU:HD13	2:R:176:TYR:CZ	2.54	0.42
2:B:12:VAL:HG11	2:B:86:LEU:HD13	2.01	0.42
1:C:154:ASP:OD1	1:C:193:SER:HB3	2.18	0.42
1:I:154:ASP:O	1:I:156:SER:N	2.45	0.42
1:M:214:CYS:C	2:N:216:CYS:SG	2.97	0.42
1:O:20:LEU:HB2	1:O:75:LEU:HB3	2.01	0.42
1:Q:18:VAL:HG12	1:Q:77:ILE:HB	2.01	0.42
2:D:168:ALA:HA	2:D:178:LEU:HB3	2.01	0.42
2:D:62:ASP:C	2:D:64:VAL:H	2.23	0.42
2:R:98:LYS:HE2	2:R:100:LEU:O	2.20	0.42
1:O:100:PHE:CZ	6:O:302:ACT:H3	2.54	0.42
1:C:151:TRP:O	1:C:158:VAL:HG22	2.20	0.42
2:F:62:ASP:C	2:F:64:VAL:H	2.23	0.42
2:H:126:PRO:HG3	2:H:189:LEU:HD11	2.01	0.42
1:A:133:ALA:HB3	1:A:183:LEU:HB2	2.01	0.42
2:H:138:LEU:HD13	2:H:211:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:LEU:HD22	1:M:60:VAL:HG22	2.02	0.42
1:Q:188:TRP:HH2	1:Q:209:VAL:HG22	1.82	0.42
2:H:64:VAL:CG1	2:H:68:PHE:HB2	2.49	0.42
2:N:7:SER:HA	2:N:107:THR:HG21	2.02	0.42
2:P:71:SER:O	2:P:79:LEU:HD12	2.19	0.42
1:Q:54:SER:HB3	1:Q:66:GLY:O	2.20	0.42
1:I:23:ARG:HG2	1:I:72:LYS:HG2	2.02	0.42
2:R:209:LYS:HE3	2:R:210:LYS:H	1.85	0.42
2:D:198:VAL:HB	2:D:207:VAL:CG2	2.48	0.41
2:N:36:TRP:NE1	2:N:81:LEU:HB2	2.34	0.41
2:P:126:PRO:HD2	2:P:213:PRO:HA	2.02	0.41
1:Q:144:PRO:HD2	1:Q:200:HIS:NE2	2.35	0.41
2:D:64:VAL:HG13	2:D:68:PHE:HB2	2.03	0.41
2:J:168:ALA:HA	2:J:178:LEU:HB3	2.02	0.41
2:N:124:LEU:HB2	2:N:139:GLY:N	2.35	0.41
2:N:162:GLY:O	2:N:183:THR:HG23	2.20	0.41
1:Q:122:PRO:HD3	1:Q:209:VAL:HG21	2.02	0.41
2:B:64:VAL:CG2	2:B:68:PHE:CG	3.03	0.41
2:D:20:LEU:HD12	2:D:81:LEU:HD23	2.01	0.41
1:E:199:THR:HG22	1:E:204:THR:OG1	2.20	0.41
2:P:76:GLN:HB3	2:P:78:SER:OG	2.21	0.41
1:Q:29:ILE:HD11	1:Q:73:ALA:N	2.35	0.41
1:E:138:LEU:CD2	1:E:140:SER:OG	2.68	0.41
2:H:194:TYR:C	2:H:195:ILE:HD13	2.40	0.41
2:J:91:THR:HG23	2:J:110:THR:HA	2.01	0.41
1:L:148:THR:HB	1:L:199:THR:HB	2.02	0.41
2:J:98:LYS:HG3	2:J:100:LEU:O	2.21	0.41
1:A:22:CYS:HB3	1:A:73:ALA:HB3	2.03	0.41
2:D:50:ASN:OD1	2:D:59:TYR:HB2	2.21	0.41
2:R:14:PRO:O	2:N:12:VAL:HG12	2.20	0.41
1:A:131:ASN:O	1:A:132:LYS:HG2	2.21	0.41
1:E:152:LYS:NZ	1:E:197:GLN:HE21	2.18	0.41
1:I:154:ASP:C	1:I:156:SER:H	2.23	0.41
2:D:11:LEU:HB2	2:D:147:PRO:HG3	2.03	0.41
2:D:64:VAL:CG1	2:D:68:PHE:HB2	2.51	0.41
1:E:138:LEU:HD21	1:E:140:SER:OG	2.21	0.41
1:M:197:GLN:NE2	1:M:206:GLU:OE1	2.38	0.41
2:R:194:TYR:O	2:R:195:ILE:HD13	2.21	0.41
2:J:64:VAL:CG1	2:J:68:PHE:HB2	2.51	0.41
2:D:83:MET:HE1	2:D:109:VAL:HG21	2.03	0.41
1:L:139:ILE:HG12	1:L:198:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:135:LEU:HD12	1:O:181:LEU:HD23	2.01	0.41
2:P:83:MET:HE3	2:P:94:TYR:CZ	2.56	0.41
1:L:188:TRP:CE2	1:L:211:PRO:HG3	2.56	0.40
2:N:214:LYS:HB3	2:N:214:LYS:HE2	1.96	0.40
2:D:29:PHE:CD2	2:D:77:ASN:HA	2.56	0.40
2:J:212:GLU:CG	2:J:213:PRO:HD2	2.47	0.40
1:O:135:LEU:HB2	1:O:181:LEU:HB3	2.02	0.40
1:Q:170:GLN:HB3	2:R:164:HIS:ND1	2.36	0.40
2:B:194:TYR:O	2:B:211:VAL:HG22	2.21	0.40
2:D:116:THR:HG22	2:D:203:SER:HB3	2.03	0.40
1:L:47:THR:HA	2:H:102:PRO:HA	2.03	0.40
1:Q:81:GLN:O	1:Q:108:VAL:HG21	2.21	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	211/215 (98%)	195 (92%)	14 (7%)	2 (1%)	17	26
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%)	17	26
1	O	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
1	Q	208/215 (97%)	179 (86%)	23 (11%)	6 (3%)	4	6
2	B	202/222 (91%)	194 (96%)	7 (4%)	1 (0%)	29	43
2	D	205/222 (92%)	199 (97%)	5 (2%)	1 (0%)	29	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	43
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%)	34	48

All (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
2	J	216	CYS
1	Q	172	ASN
1	A	154	ASP
2	D	63	SER
1	Q	145	GLY
1	M	141	ASP
1	M	154	ASP
1	Q	123	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	166/177 (94%)	164 (99%)	2 (1%)	71	83
1	C	172/177 (97%)	172 (100%)	0	100	100
1	E	174/177 (98%)	171 (98%)	3 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	175/177 (99%)	171 (98%)	4 (2%)	50	68
1	L	170/177 (96%)	168 (99%)	2 (1%)	71	83
1	M	165/177 (93%)	160 (97%)	5 (3%)	41	59
1	O	173/177 (98%)	168 (97%)	5 (3%)	42	60
1	Q	141/177 (80%)	137 (97%)	4 (3%)	43	61
2	B	169/187 (90%)	165 (98%)	4 (2%)	49	67
2	D	173/187 (92%)	169 (98%)	4 (2%)	50	68
2	F	178/187 (95%)	178 (100%)	0	100	100
2	H	164/187 (88%)	163 (99%)	1 (1%)	86	93
2	J	181/187 (97%)	176 (97%)	5 (3%)	43	61
2	N	174/187 (93%)	169 (97%)	5 (3%)	42	60
2	P	173/187 (92%)	171 (99%)	2 (1%)	71	83
2	R	163/187 (87%)	160 (98%)	3 (2%)	59	75
All	All	2711/2912 (93%)	2662 (98%)	49 (2%)	59	75

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	8	SER
1	L	67	PHE
2	H	196	CYS
1	A	193	SER
1	A	195	SER
2	B	13	GLN
2	B	53	GLN
2	B	161	SER
2	B	201	LYS
2	D	25	SER
2	D	63	SER
2	D	112	SER
2	D	115	SER
1	E	13	SER
1	E	67	PHE
1	E	203	SER
1	I	152	LYS
1	I	159	LYS
1	I	201	GLU

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Mol	Chain	Res	Type
1	I	214	CYS
2	J	62	ASP
2	J	132	SER
2	J	201	LYS
2	J	209	LYS
2	J	212	GLU
1	O	67	PHE
1	O	95	ASN
1	O	173	ASN
1	O	193	SER
1	O	207	LYS
2	P	53	GLN
2	P	161	SER
1	Q	120	LEU
1	Q	170	GLN
1	Q	190	SER
1	Q	203	SER
2	R	115	SER
2	R	197	ASN
2	R	209	LYS
1	M	124	SER
1	M	125	SER
1	M	172	ASN
1	M	173	ASN
1	M	190	SER
2	N	56	SER
2	N	63	SER
2	N	112	SER
2	N	199	ASN
2	N	215	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	200	HIS
2	H	199	ASN
1	A	111	GLN
1	A	173	ASN
1	A	200	HIS
2	B	53	GLN
1	C	187	GLN
2	D	105	GLN

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Mol	Chain	Res	Type
1	E	197	GLN
1	I	197	GLN
2	P	53	GLN
1	M	173	ASN
2	N	199	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 carbohydrates 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	$\# Z > 2$
6	ACT	C	302	-	1,3,3	6.38	1 (100%)	0,3,3	0.00	-
3	BCG	J	301	-	20,23,23	0.43	0	26,33,33	1.00	2 (7%)
6	ACT	E	302	-	1,3,3	6.20	1 (100%)	0,3,3	0.00	-
3	BCG	Q	301	-	20,23,23	0.47	0	26,33,33	0.90	2 (7%)
3	BCG	L	301	-	20,23,23	0.47	0	26,33,33	0.93	2 (7%)
6	ACT	J	302	-	1,3,3	6.83	1 (100%)	0,3,3	0.00	-
3	BCG	E	301	-	20,23,23	0.47	0	26,33,33	0.93	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FMT	O	303	-	0,2,2	0.00	-	0,1,1	0.00	-
3	BCG	C	301	-	20,23,23	0.45	0	26,33,33	0.92	2 (7%)
5	GOL	L	303	-	5,5,5	0.95	0	5,5,5	0.98	0
6	ACT	B	302	-	1,3,3	5.68	1 (100%)	0,3,3	0.00	-
3	BCG	O	301	-	20,23,23	0.46	0	26,33,33	0.97	2 (7%)
6	ACT	P	301	-	1,3,3	6.74	1 (100%)	0,3,3	0.00	-
3	BCG	M	301	-	20,23,23	0.48	0	26,33,33	0.92	2 (7%)
6	ACT	M	302	-	1,3,3	5.74	1 (100%)	0,3,3	0.00	-
3	BCG	B	301	-	20,23,23	0.48	0	26,33,33	0.89	2 (7%)
6	ACT	O	302	-	1,3,3	5.55	1 (100%)	0,3,3	0.00	-
6	ACT	Q	302	-	1,3,3	5.74	1 (100%)	0,3,3	0.00	-
4	PEG	L	302	-	6,6,6	0.14	0	5,5,5	0.07	0
6	ACT	H	301	-	1,3,3	5.16	1 (100%)	0,3,3	0.00	-

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	J	301	-	-	0/8/37/37	0/4/3/3
3	BCG	Q	301	-	-	0/8/37/37	0/4/3/3
3	BCG	L	301	-	-	0/8/37/37	0/4/3/3
3	BCG	E	301	-	-	0/8/37/37	0/4/3/3
3	BCG	C	301	-	-	0/8/37/37	0/4/3/3
5	GOL	L	303	-	-	2/4/4/4	-
3	BCG	O	301	-	-	0/8/37/37	0/4/3/3
3	BCG	M	301	-	-	0/8/37/37	0/4/3/3
3	BCG	B	301	-	-	0/8/37/37	0/4/3/3
4	PEG	L	302	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	302	ACT	CH3-C	6.83	1.57	1.48
6	P	301	ACT	CH3-C	6.74	1.57	1.48
6	C	302	ACT	CH3-C	6.38	1.56	1.48
6	E	302	ACT	CH3-C	6.20	1.56	1.48
6	Q	302	ACT	CH3-C	5.74	1.56	1.48
6	M	302	ACT	CH3-C	5.74	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	302	ACT	CH3-C	5.68	1.56	1.48
6	O	302	ACT	CH3-C	5.55	1.55	1.48
6	H	301	ACT	CH3-C	5.16	1.55	1.48

All (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
3	M	301	BCG	C7-C1-N1	-3.07	102.02	105.18
3	C	301	BCG	C7-C1-C2	3.05	116.78	112.28
3	L	301	BCG	C7-C1-N1	-3.04	102.06	105.18
3	Q	301	BCG	C7-C1-N1	-3.03	102.07	105.18
3	E	301	BCG	C7-C1-N1	-3.02	102.07	105.18
3	E	301	BCG	C7-C1-C2	3.01	116.71	112.28
3	B	301	BCG	C7-C1-N1	-2.95	102.14	105.18
3	M	301	BCG	C7-C1-C2	2.94	116.60	112.28
3	C	301	BCG	C7-C1-N1	-2.92	102.17	105.18
3	Q	301	BCG	C7-C1-C2	2.87	116.51	112.28
3	B	301	BCG	C7-C1-C2	2.84	116.46	112.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	303	GOL	C1-C2-C3-O3
5	L	303	GOL	O2-C2-C3-O3

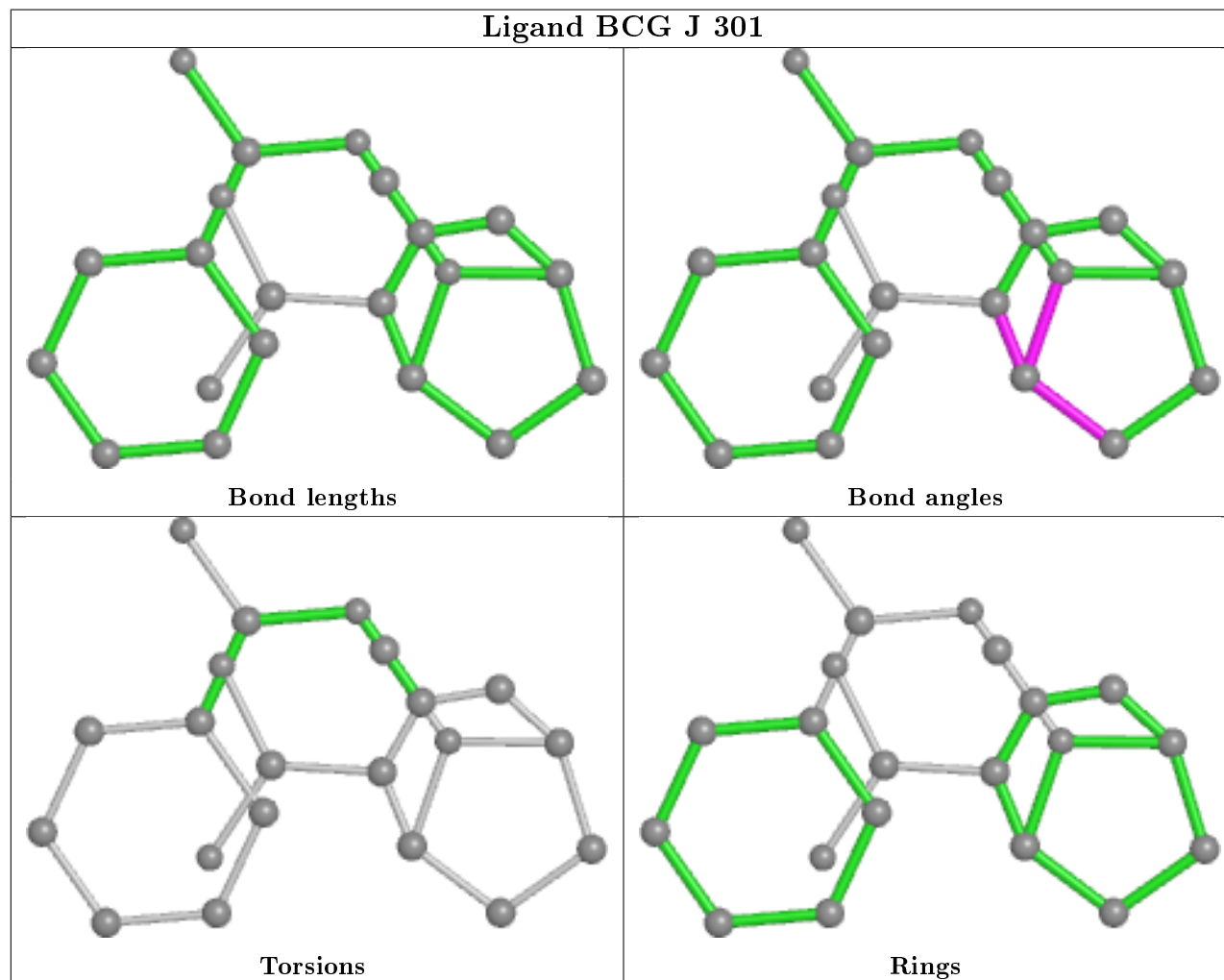
There are no ring outliers.

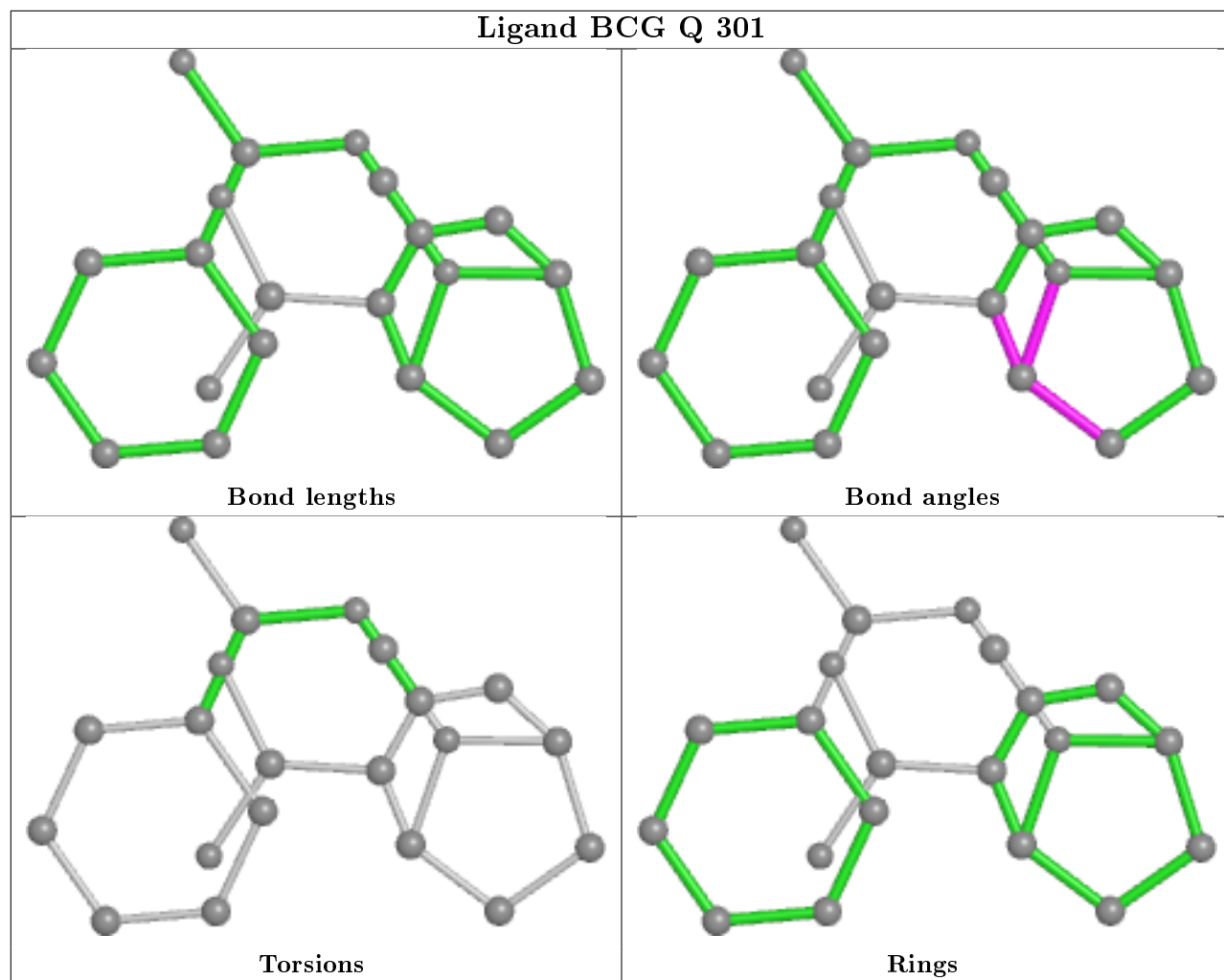
3 monomers are involved in 5 short contacts:

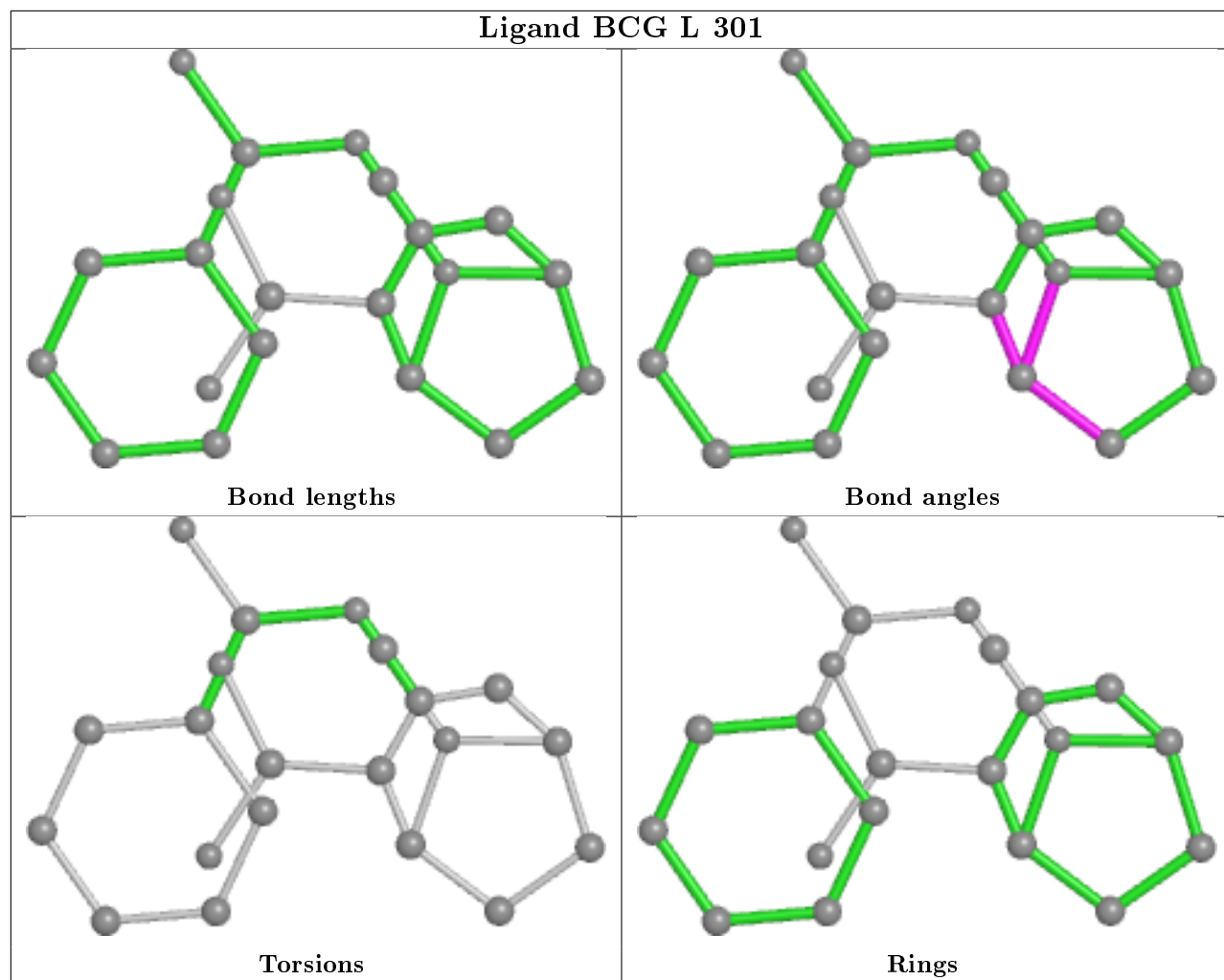
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	302	ACT	1	0
6	M	302	ACT	2	0
6	O	302	ACT	2	0

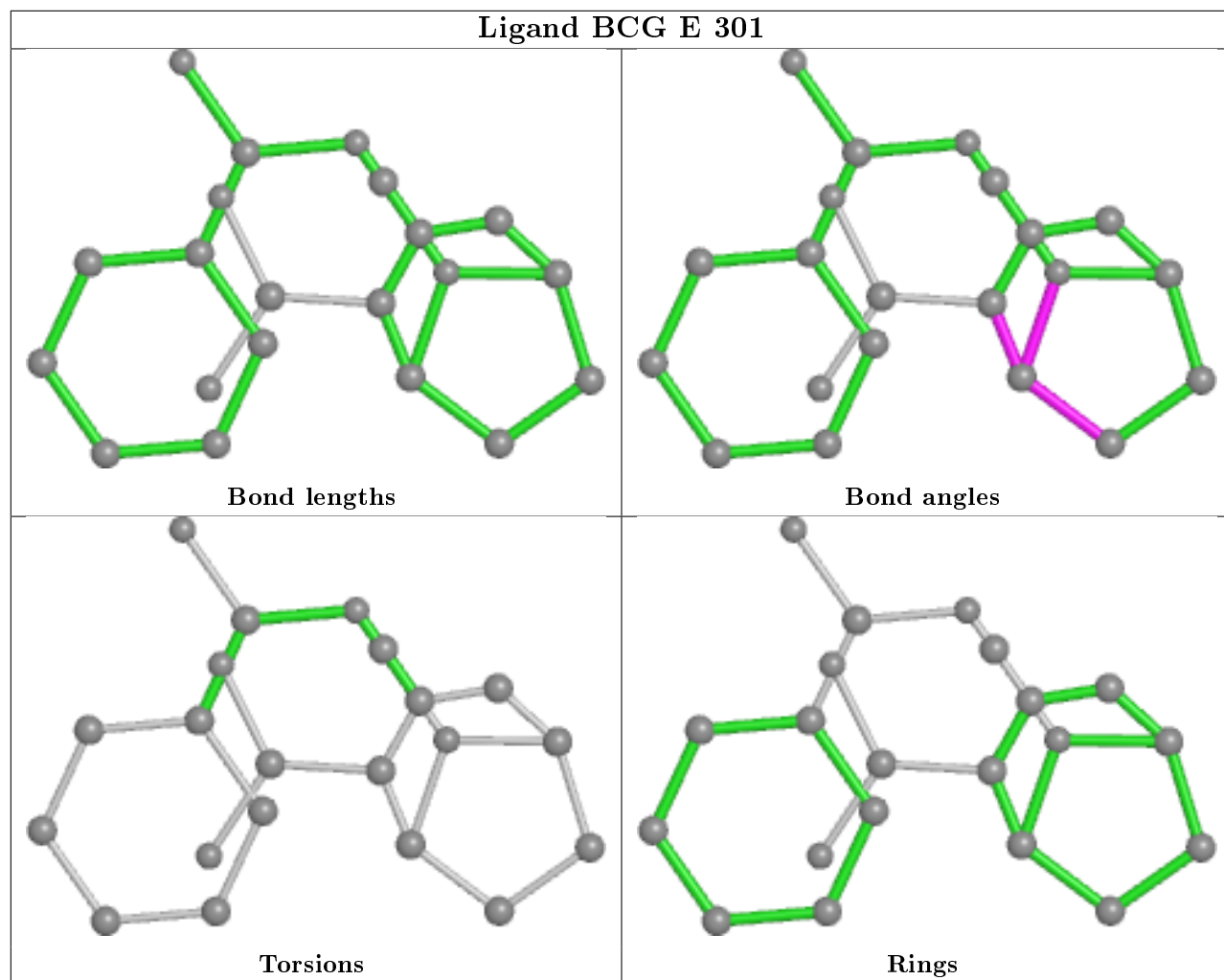
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

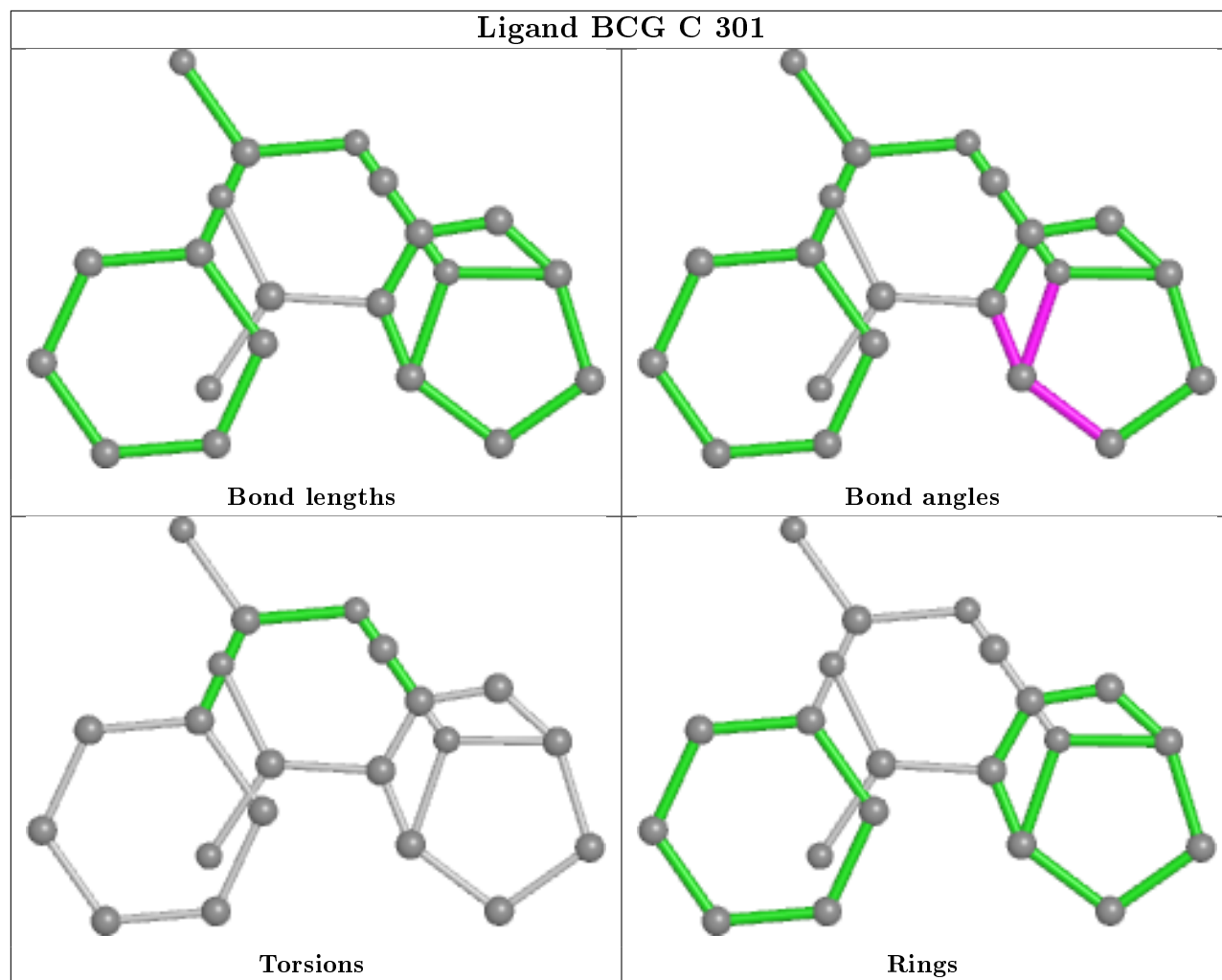
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

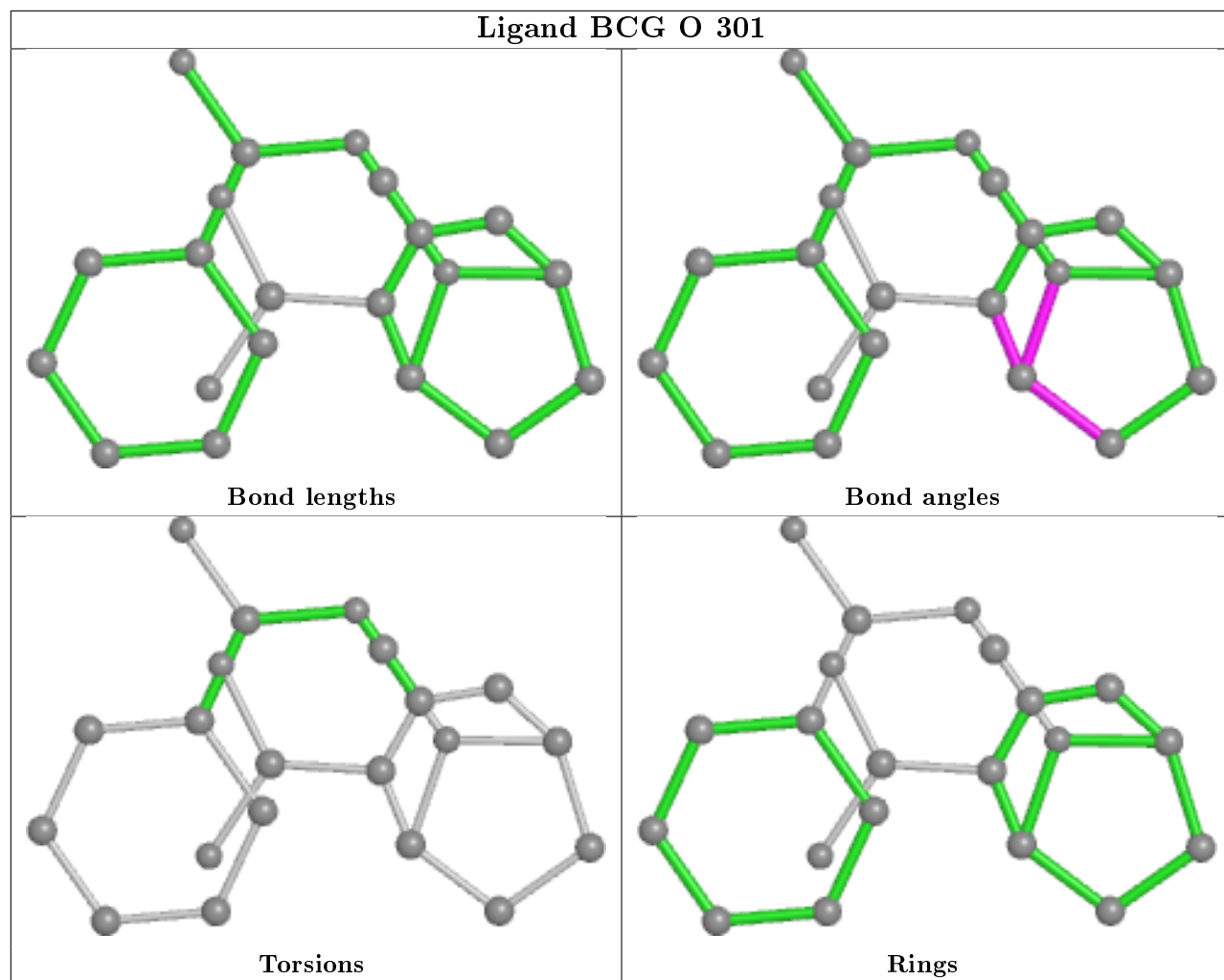


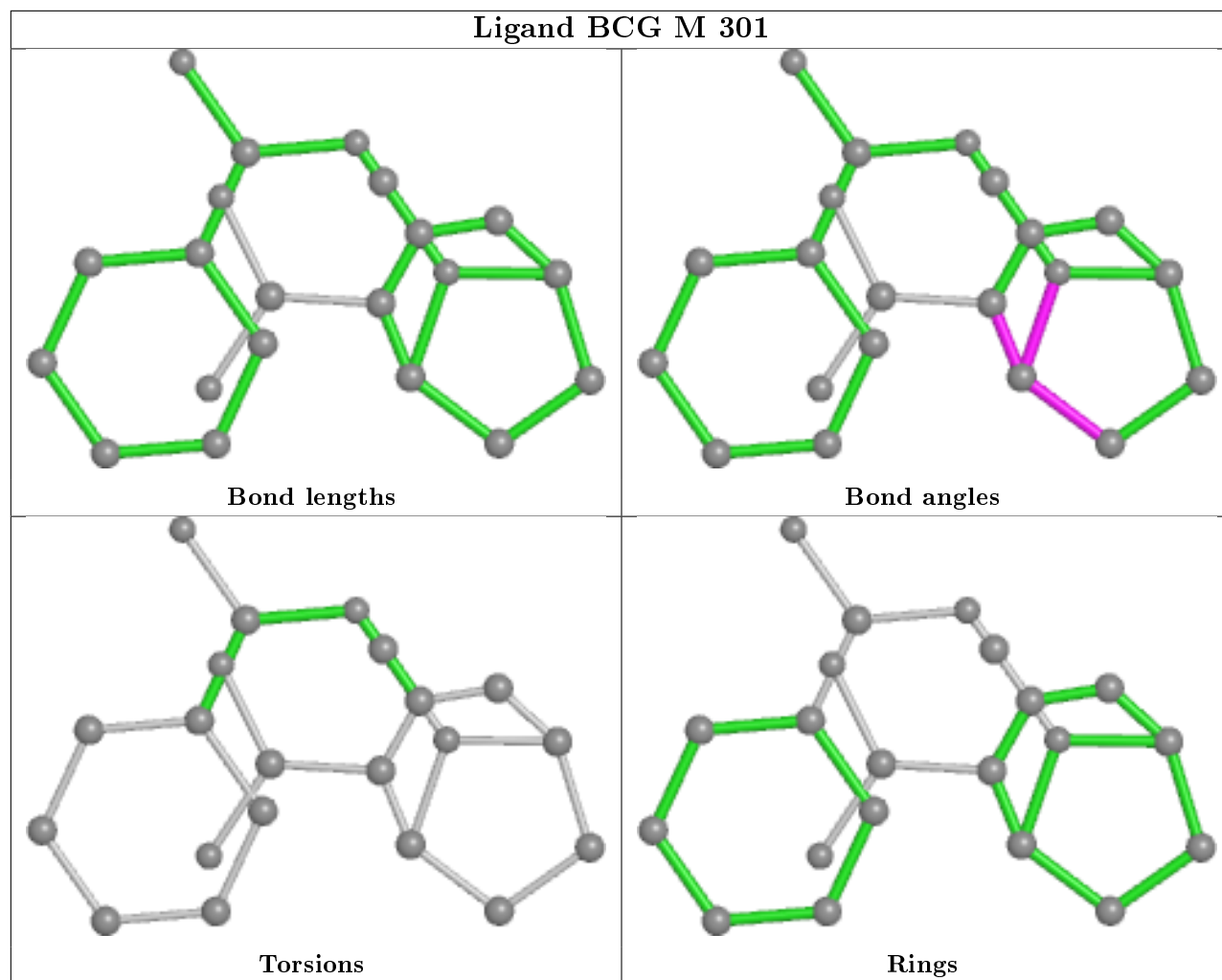


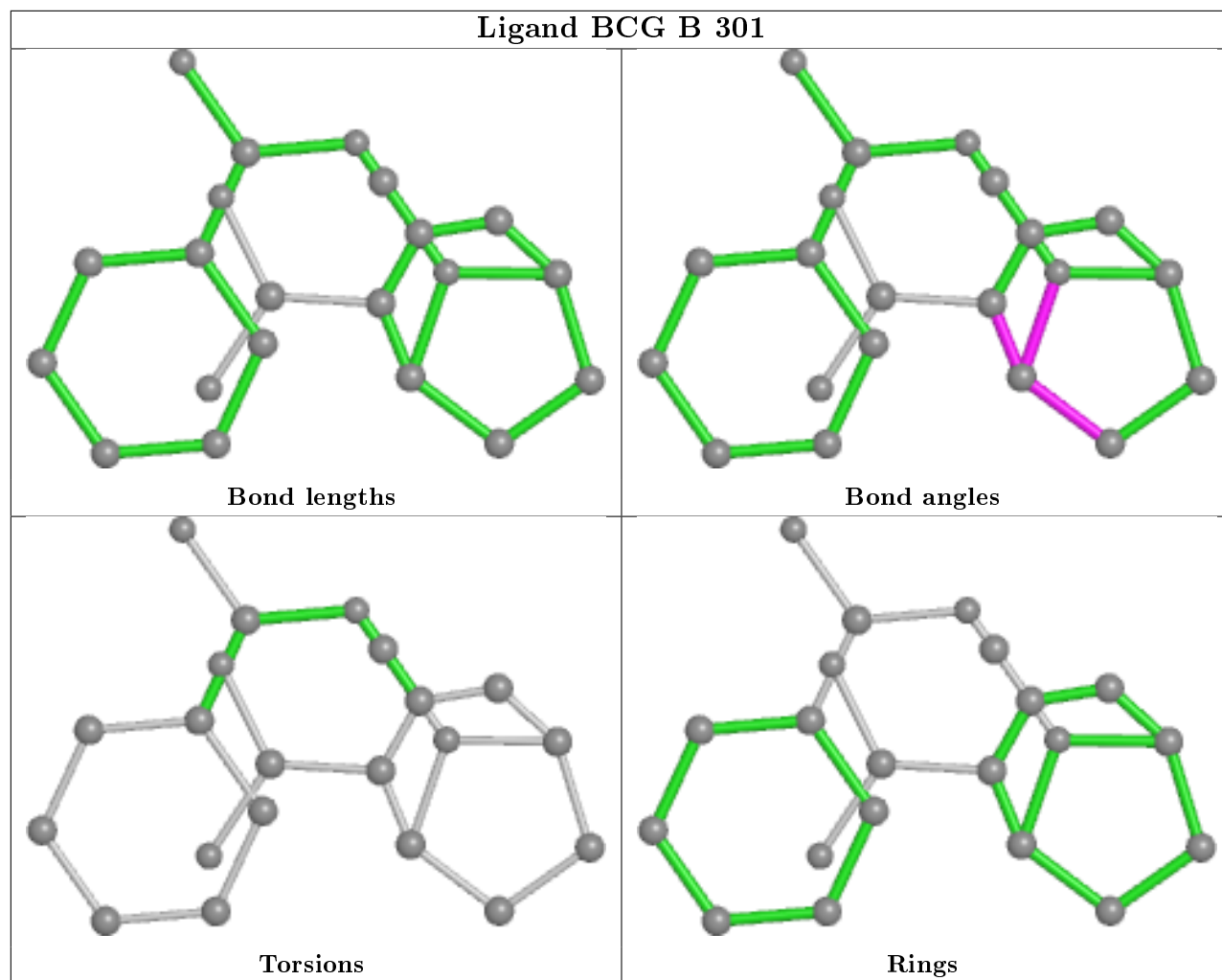












5.7 Other polymers [i](#)

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	213/215 (99%)	0.21	13 (6%) 21 18	30, 62, 121, 147	0
1	C	212/215 (98%)	0.06	9 (4%) 36 33	34, 62, 101, 117	0
1	E	213/215 (99%)	-0.17	3 (1%) 75 73	30, 52, 76, 130	0
1	I	213/215 (99%)	-0.09	4 (1%) 66 64	27, 51, 97, 137	0
1	L	211/215 (98%)	-0.06	3 (1%) 75 73	26, 46, 71, 94	0
1	M	213/215 (99%)	0.23	15 (7%) 16 13	36, 66, 135, 155	0
1	O	212/215 (98%)	-0.00	3 (1%) 75 73	31, 53, 79, 99	0
1	Q	210/215 (97%)	0.98	53 (25%) 0 0	36, 77, 174, 186	0
2	B	206/222 (92%)	0.09	10 (4%) 29 25	35, 63, 116, 148	0
2	D	209/222 (94%)	-0.11	4 (1%) 66 64	34, 52, 89, 118	0
2	F	212/222 (95%)	-0.15	6 (2%) 53 49	31, 47, 99, 133	0
2	H	204/222 (91%)	0.11	12 (5%) 22 19	30, 52, 112, 143	0
2	J	219/222 (98%)	-0.16	8 (3%) 41 38	22, 43, 98, 139	0
2	N	214/222 (96%)	0.34	21 (9%) 7 5	32, 66, 134, 184	0
2	P	209/222 (94%)	-0.10	2 (0%) 82 81	24, 46, 75, 99	0
2	R	201/222 (90%)	0.68	36 (17%) 1 1	37, 62, 140, 161	0
All	All	3371/3496 (96%)	0.11	202 (5%) 21 19	22, 53, 125, 186	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	187	SER	9.9
2	R	194	TYR	9.4
1	A	1	GLN	9.2
2	N	187	SER	8.3
1	Q	211	PRO	8.2

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Mol	Chain	Res	Type	RSRZ
1	Q	123	PRO	8.1
2	R	137	ALA	8.0
1	Q	158	VAL	7.2
1	Q	147	VAL	6.9
1	I	2	ALA	6.9
2	R	181	VAL	6.5
2	R	138	LEU	6.5
2	R	179	SER	6.0
1	O	2	ALA	5.7
2	R	183	THR	5.3
1	Q	137	CYS	5.2
1	A	194	TYR	5.2
1	A	2	ALA	5.2
1	Q	125	SER	5.1
1	Q	209	VAL	5.1
1	Q	121	PHE	5.0
2	N	159	LEU	5.0
2	N	160	THR	5.0
1	M	194	TYR	4.8
2	N	158	ALA	4.7
1	Q	120	LEU	4.7
2	R	123	PRO	4.7
2	R	125	ALA	4.7
2	R	193	THR	4.6
1	Q	198	VAL	4.6
1	Q	149	VAL	4.6
1	O	1	GLN	4.5
1	Q	153	ALA	4.5
2	N	182	VAL	4.5
2	B	184	VAL	4.5
2	R	166	PHE	4.4
2	N	191	THR	4.4
1	Q	139	ILE	4.4
2	F	127	SER	4.4
2	R	122	PHE	4.3
1	Q	155	SER	4.3
1	Q	136	VAL	4.2
2	N	194	TYR	4.1
1	C	2	ALA	4.1
2	N	190	GLY	4.1
1	Q	193	SER	4.1
1	Q	189	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	159	LYS	4.0
1	Q	204	THR	4.0
2	D	189	LEU	4.0
2	F	128	SER	4.0
2	N	184	VAL	4.0
1	Q	157	PRO	3.9
2	R	158	ALA	3.9
1	E	214	CYS	3.8
2	R	184	VAL	3.8
1	Q	188	TRP	3.7
1	Q	152	LYS	3.7
2	D	128	SER	3.7
2	N	216	CYS	3.6
1	Q	151	TRP	3.6
2	R	142	VAL	3.6
2	R	124	LEU	3.6
2	J	219	HIS	3.6
2	R	154	TRP	3.5
1	Q	202	GLY	3.5
2	B	157	GLY	3.5
2	F	214	LYS	3.5
1	A	198	VAL	3.5
1	E	2	ALA	3.5
1	Q	154	ASP	3.4
2	J	130	SER	3.4
1	A	193	SER	3.4
2	P	128	SER	3.4
1	L	205	VAL	3.3
1	Q	200	HIS	3.3
2	B	127	SER	3.3
2	H	74	ASN	3.3
1	Q	192	ARG	3.3
1	A	153	ALA	3.3
2	N	185	PRO	3.3
1	Q	162	VAL	3.2
2	B	187	SER	3.2
1	Q	117	SER	3.2
1	M	123	PRO	3.2
1	Q	187	GLN	3.2
1	Q	196	CYS	3.1
2	J	216	CYS	3.1
2	H	163	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	R	191	THR	3.1
1	A	186	GLU	3.1
1	Q	194	TYR	3.1
2	F	1	GLU	3.1
1	Q	195	SER	3.1
1	A	204	THR	3.1
1	M	147	VAL	3.1
1	C	153	ALA	3.1
1	Q	178	SER	3.1
2	R	163	VAL	3.0
2	R	161	SER	3.0
1	Q	180	TYR	3.0
1	Q	129	GLN	3.0
2	B	194	TYR	3.0
2	R	121	VAL	3.0
1	Q	115	ALA	3.0
1	M	215	SER	3.0
2	R	186	SER	2.9
2	R	182	VAL	2.9
2	F	216	CYS	2.9
1	Q	159	LYS	2.9
2	R	164	HIS	2.9
1	Q	190	SER	2.8
1	A	206	GLU	2.8
2	R	141	LEU	2.8
2	N	156	SER	2.7
1	I	157	PRO	2.7
1	M	149	VAL	2.7
2	P	127	SER	2.7
2	N	215	SER	2.7
2	B	185	PRO	2.7
2	R	210	LYS	2.7
2	N	183	THR	2.7
2	J	217	HIS	2.7
2	R	139	GLY	2.7
2	R	196	CYS	2.7
2	B	123	PRO	2.6
2	H	159	LEU	2.6
2	F	129	LYS	2.6
1	Q	197	GLN	2.6
1	Q	122	PRO	2.6
1	Q	138	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	186	GLU	2.6
2	R	195	ILE	2.6
2	N	218	HIS	2.6
2	J	131	THR	2.5
2	D	1	GLU	2.5
2	J	133	GLY	2.5
1	M	125	SER	2.5
1	A	208	THR	2.5
1	E	213	GLU	2.5
1	I	159	LYS	2.5
1	M	158	VAL	2.5
2	B	138	LEU	2.5
1	Q	179	SER	2.5
1	M	148	THR	2.5
1	C	197	GLN	2.5
1	C	198	VAL	2.5
2	H	162	GLY	2.5
2	B	189	LEU	2.5
2	R	180	SER	2.5
1	Q	148	THR	2.4
2	H	193	THR	2.4
1	Q	185	PRO	2.4
2	H	160	THR	2.4
2	J	132	SER	2.4
1	Q	161	GLY	2.4
1	C	149	VAL	2.4
1	Q	208	THR	2.4
1	M	160	ALA	2.4
2	H	138	LEU	2.4
1	I	156	SER	2.4
2	R	162	GLY	2.4
1	Q	160	ALA	2.4
1	M	26	THR	2.4
2	N	161	SER	2.4
2	N	208	ASP	2.4
2	H	137	ALA	2.3
2	B	156	SER	2.3
2	R	188	SER	2.3
1	A	209	VAL	2.3
1	O	158	VAL	2.3
1	Q	2	ALA	2.3
2	N	198	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	199	THR	2.3
1	M	150	ALA	2.3
1	Q	206	GLU	2.3
2	R	160	THR	2.3
1	C	154	ASP	2.3
2	J	134	GLY	2.2
2	R	192	GLN	2.2
2	N	122	PHE	2.2
1	M	146	ALA	2.2
1	A	192	ARG	2.2
2	H	195	ILE	2.1
2	N	189	LEU	2.1
1	Q	163	GLU	2.1
2	H	188	SER	2.1
1	L	212	THR	2.1
1	Q	156	SER	2.1
1	Q	131	ASN	2.1
2	N	197	ASN	2.1
2	H	158	ALA	2.1
1	M	171	SER	2.1
2	R	152	VAL	2.1
1	C	152	LYS	2.0
1	L	158	VAL	2.0
1	A	197	GLN	2.0
2	H	164	HIS	2.0
1	M	206	GLU	2.0
2	D	184	VAL	2.0
1	C	194	TYR	2.0
2	R	170	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands

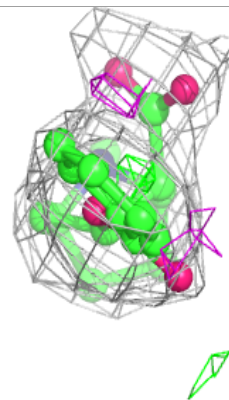
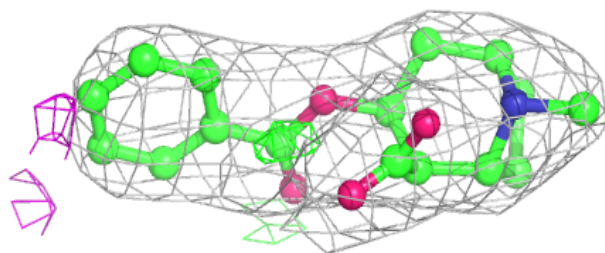
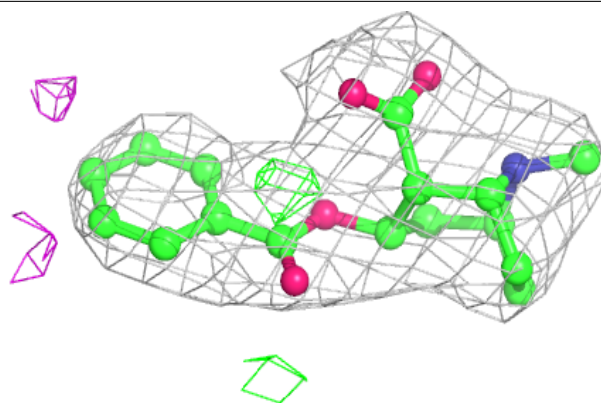
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	Q	302	4/4	0.76	0.31	67,79,80,89	0
4	PEG	L	302	7/7	0.77	0.23	50,59,71,72	0
6	ACT	M	302	4/4	0.86	0.30	73,75,79,81	0
5	GOL	L	303	6/6	0.88	0.18	51,67,77,77	0
7	FMT	O	303	3/3	0.91	0.24	56,56,61,66	0
6	ACT	J	302	4/4	0.92	0.21	41,66,72,75	0
6	ACT	E	302	4/4	0.92	0.21	53,60,65,75	0
6	ACT	P	301	4/4	0.93	0.21	56,58,61,62	0
6	ACT	C	302	4/4	0.93	0.25	49,60,60,60	0
6	ACT	H	301	4/4	0.94	0.23	50,69,73,73	0
3	BCG	Q	301	21/21	0.95	0.18	36,54,69,73	0
3	BCG	M	301	21/21	0.96	0.19	42,50,57,60	0
3	BCG	C	301	21/21	0.96	0.19	42,54,60,65	0
3	BCG	E	301	21/21	0.96	0.17	28,44,61,65	0
3	BCG	O	301	21/21	0.96	0.17	37,47,60,66	0
6	ACT	O	302	4/4	0.96	0.25	55,62,63,70	0
3	BCG	L	301	21/21	0.97	0.20	27,36,51,61	0
3	BCG	B	301	21/21	0.97	0.17	28,43,52,55	0
6	ACT	B	302	4/4	0.97	0.23	55,66,68,77	0
3	BCG	J	301	21/21	0.98	0.15	29,38,49,55	0

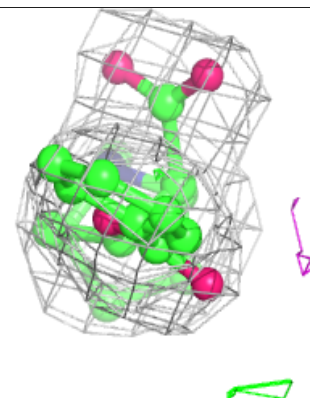
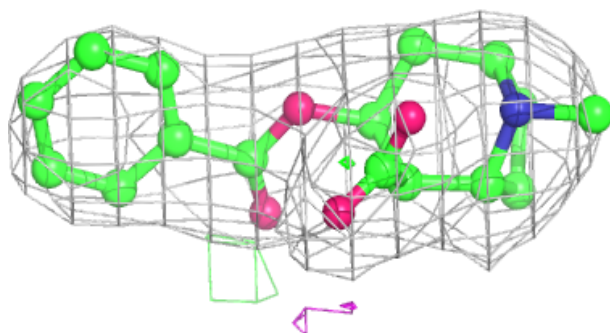
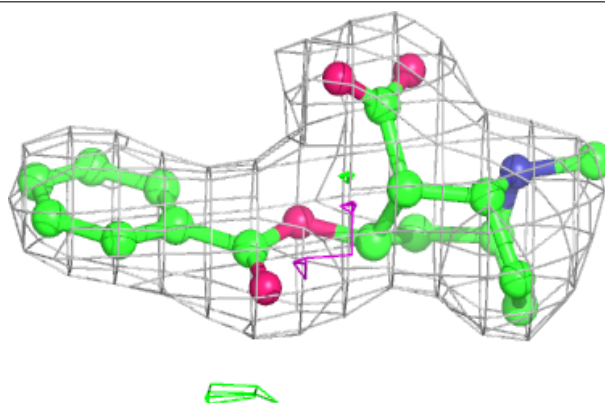
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

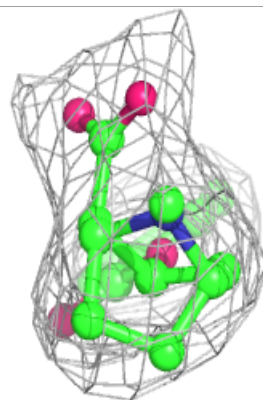
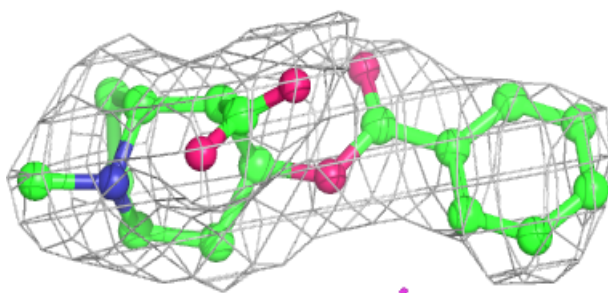
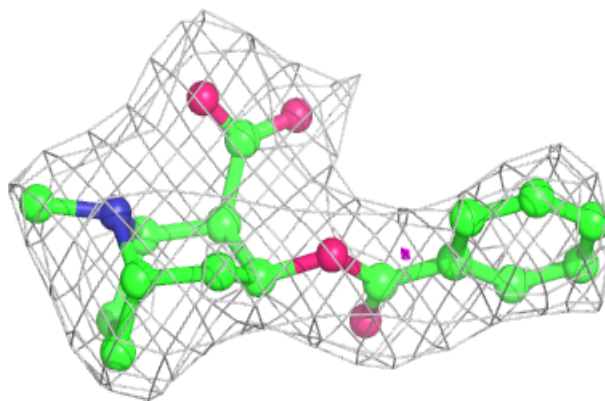
**Electron density around BCG M 301:**

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

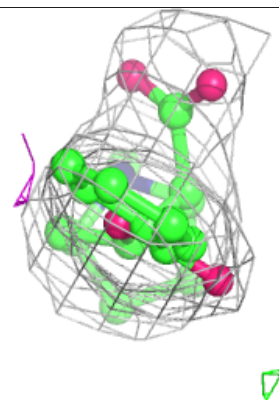
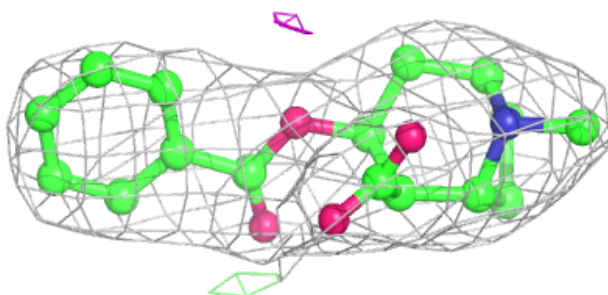
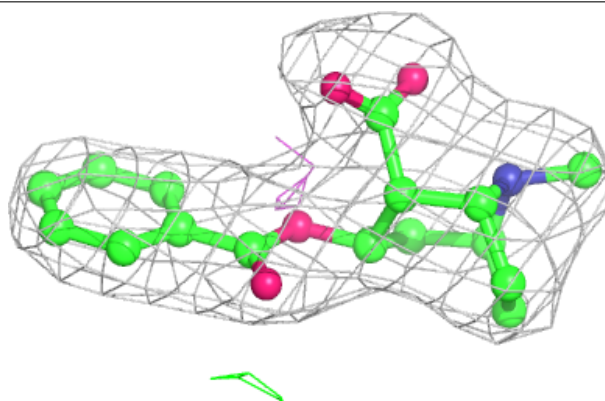


Electron density around BCG C 301:

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

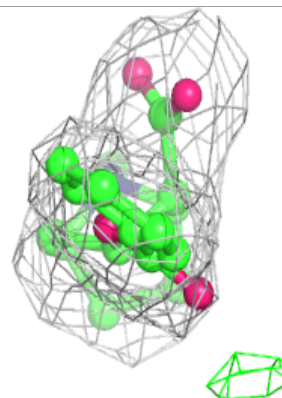
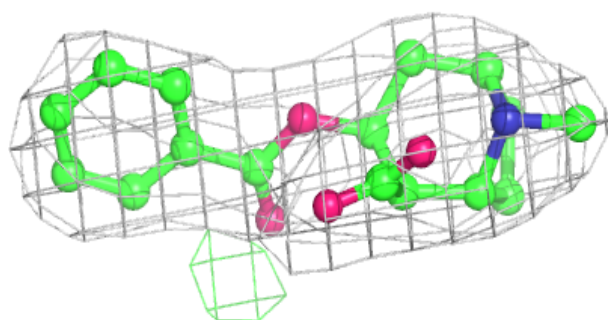
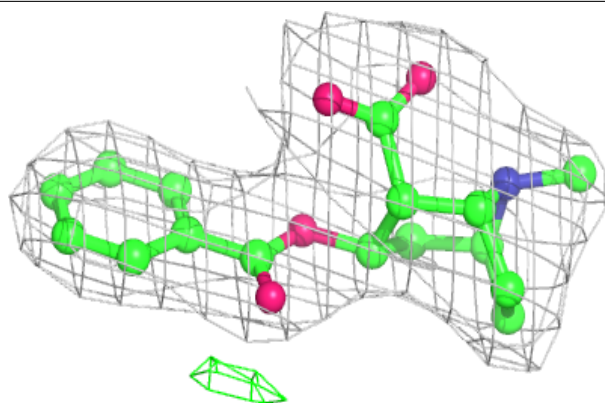
**Electron density around BCG E 301:**

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

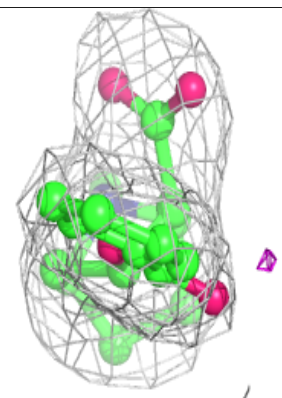
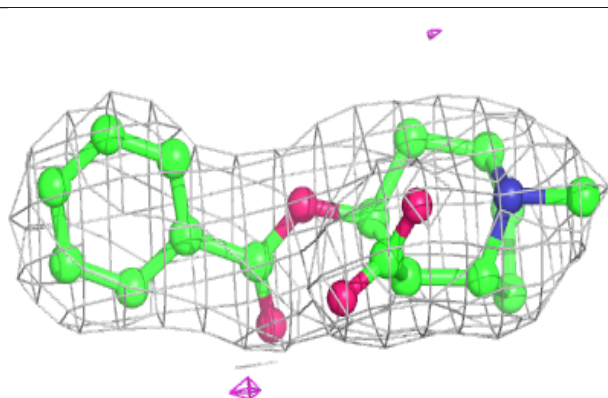
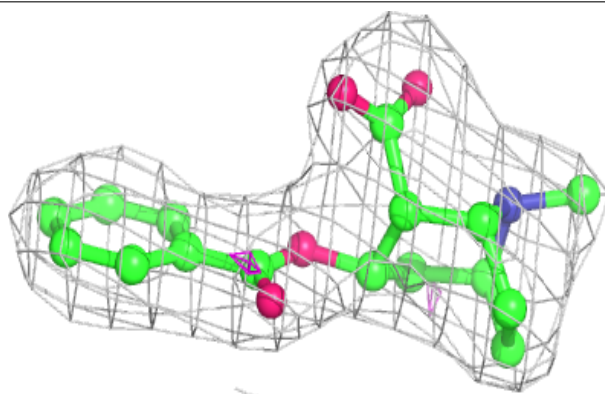


Electron density around BCG O 301:

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

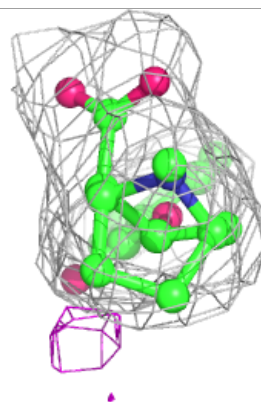
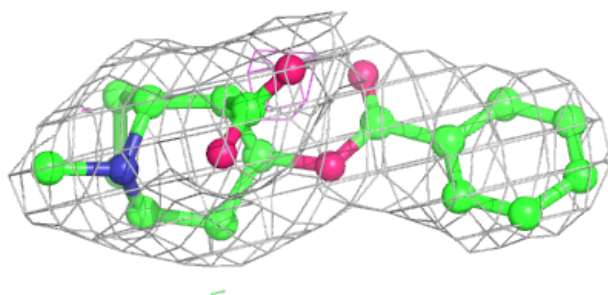
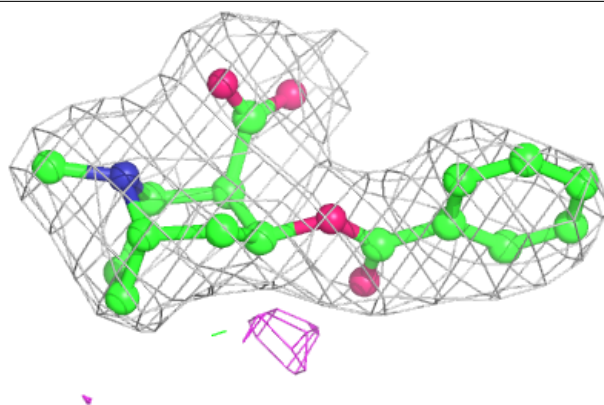
**Electron density around BCG L 301:**

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

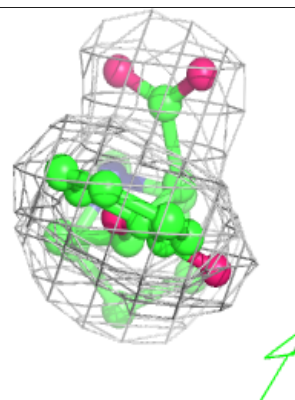
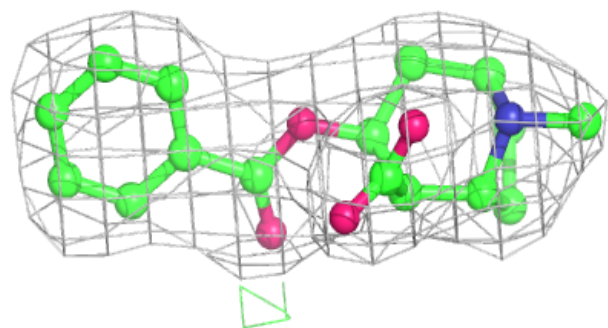
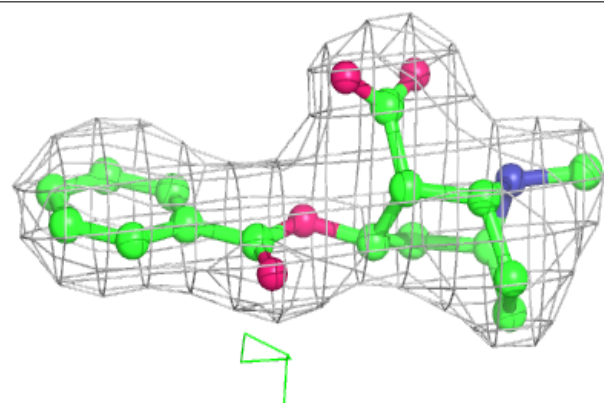


Electron density around BCG B 301:

$2mF_o-DF_c$ (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.