



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 11, 2019 – 03:22 AM EST

PDB ID : 6D6T
EMDB ID: : EMD-7816
Title : Human GABA-A receptor alpha1-beta2-gamma2 subtype in complex with
GABA and flumazenil, conformation B
Authors : Zhu, S.; Noviello, C.M.; Teng, J.; Walsh Jr, R.M.; Kim, J.J.; Hibbs, R.E.
Deposited on : 2018-04-22
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

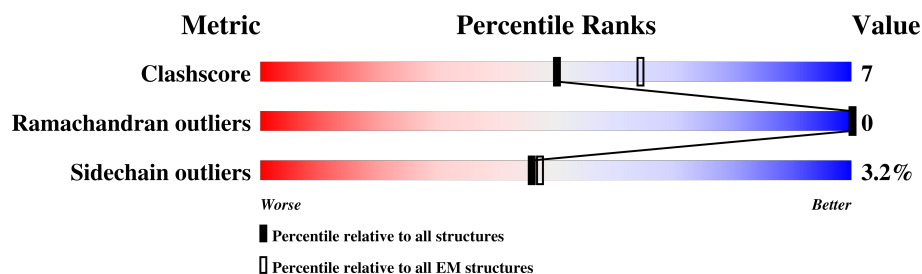
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	341	81% 16% ..
1	C	341	76% 21% ..
2	B	358	73% 18% • 7%
2	D	358	76% 18% • 6%
3	E	366	69% 13% • 17%
4	I	213	46% • 50%
4	L	213	46% • 50%
5	J	454	19% 6% 74%
5	K	454	21% • 74%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17197 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Gamma-aminobutyric acid receptor subunit beta-2, Gamma-aminobutyric acid receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2726	1788	439	483	16		
1	C	333	Total	C	N	O	S	0	0
			2726	1788	439	483	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	SER	-	linker	UNP P47870
A	309	GLN	-	linker	UNP P47870
A	310	PRO	-	linker	UNP P47870
A	311	ALA	-	linker	UNP P47870
A	312	ARG	-	linker	UNP P47870
A	313	ALA	-	linker	UNP P47870
A	314	ALA	-	linker	UNP P47870
C	308	SER	-	linker	UNP P47870
C	309	GLN	-	linker	UNP P47870
C	310	PRO	-	linker	UNP P47870
C	311	ALA	-	linker	UNP P47870
C	312	ARG	-	linker	UNP P47870
C	313	ALA	-	linker	UNP P47870
C	314	ALA	-	linker	UNP P47870

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1, Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	333	Total	C	N	O	S	0	0
			2688	1741	451	480	16		
2	D	337	Total	C	N	O	S	0	0
			2722	1759	460	487	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	313	SER	-	linker	UNP P14867
B	314	GLN	-	linker	UNP P14867
B	315	PRO	-	linker	UNP P14867
B	316	ALA	-	linker	UNP P14867
B	317	ARG	-	linker	UNP P14867
B	318	ALA	-	linker	UNP P14867
B	319	ALA	-	linker	UNP P14867
D	313	SER	-	linker	UNP P14867
D	314	GLN	-	linker	UNP P14867
D	315	PRO	-	linker	UNP P14867
D	316	ALA	-	linker	UNP P14867
D	317	ARG	-	linker	UNP P14867
D	318	ALA	-	linker	UNP P14867
D	319	ALA	-	linker	UNP P14867

- Molecule 3 is a protein called Human GABA-A receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	302	Total	C	N	O	S	0	0
			2336	1493	404	429	10		

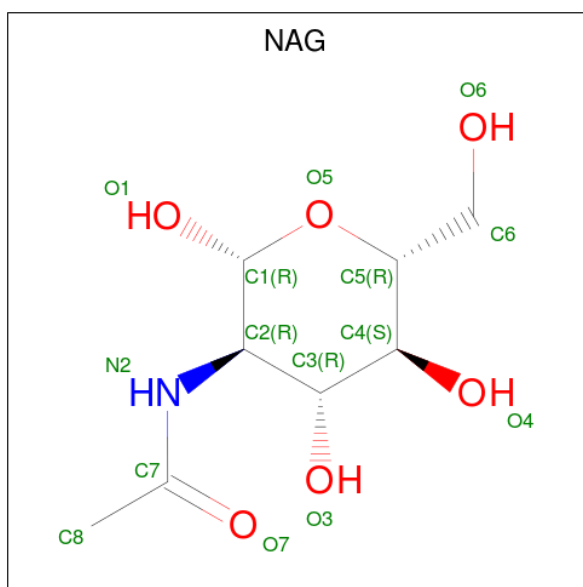
- Molecule 4 is a protein called Kappa Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	106	Total	C	N	O	S	0	0
			811	510	132	164	5		
4	L	106	Total	C	N	O	S	0	0
			811	510	132	164	5		

- Molecule 5 is a protein called IgG2b Fab Heavy Chain.

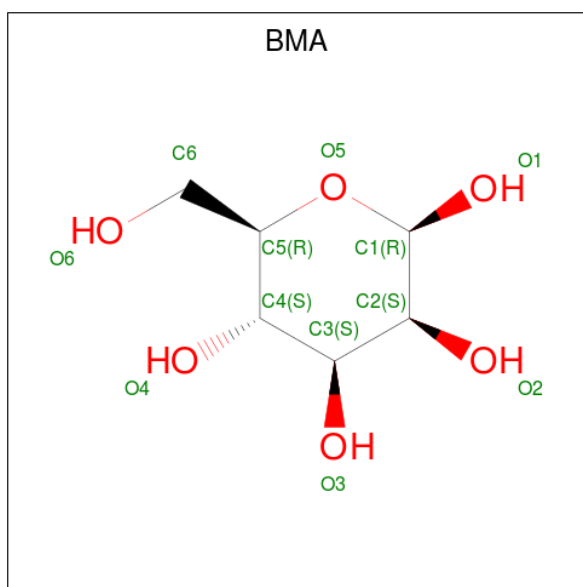
Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	116	Total	C	N	O	S	0	0
			907	574	151	178	4		
5	K	116	Total	C	N	O	S	0	0
			907	573	151	179	4		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



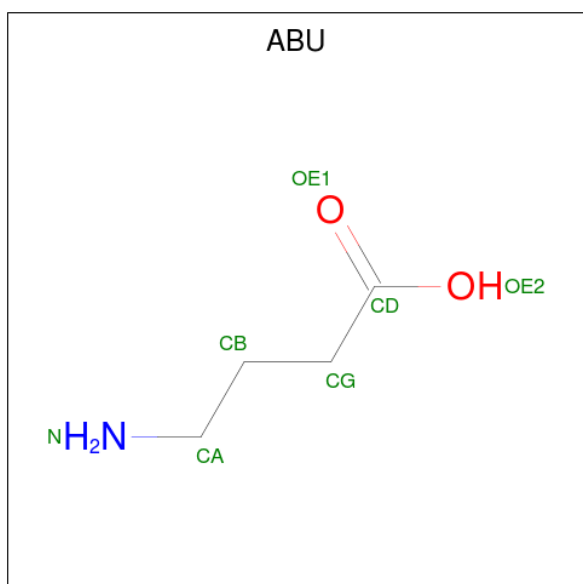
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	D	1	Total	C	N	O	0
			28	16	2	10	
6	D	1	Total	C	N	O	0
			28	16	2	10	
6	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



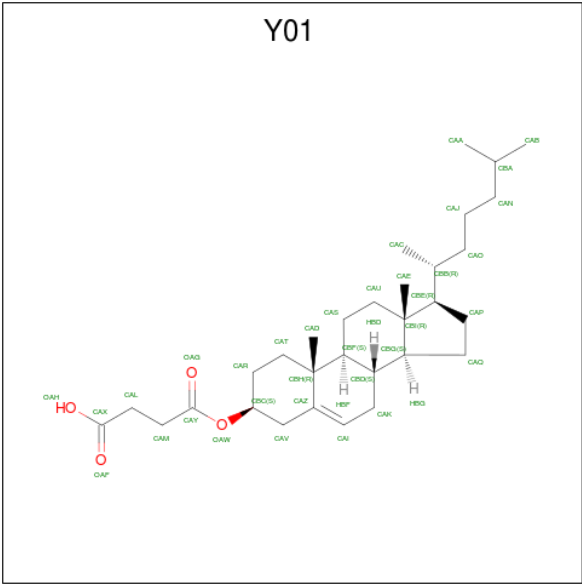
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	6	5	
7	B	1	Total	C	O	0
			11	6	5	
7	C	1	Total	C	O	0
			11	6	5	
7	D	1	Total	C	O	0
			11	6	5	

- Molecule 8 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			7	4	1	2	
8	C	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



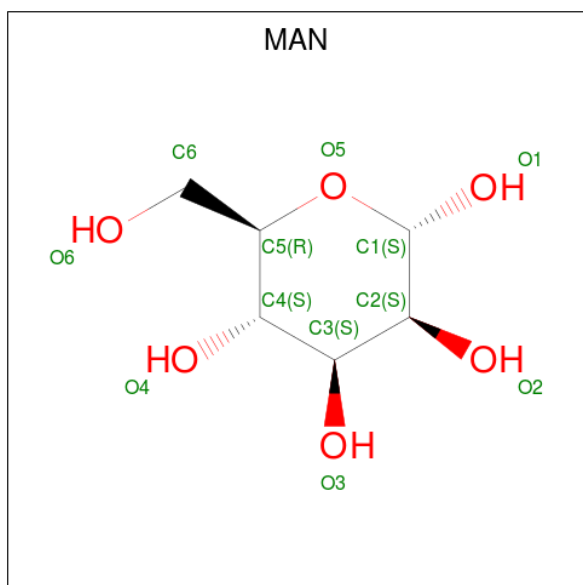
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			105	100	5	
9	A	1	Total	C	O	0
			105	100	5	
9	A	1	Total	C	O	0
			105	100	5	
9	A	1	Total	C	O	0
			105	100	5	
9	A	1	Total	C	O	0
			105	100	5	
9	B	1	Total	C	O	0
			84	80	4	
9	B	1	Total	C	O	0
			84	80	4	
9	B	1	Total	C	O	0
			84	80	4	
9	B	1	Total	C	O	0
			84	80	4	
9	D	1	Total	C	O	0
			63	60	3	

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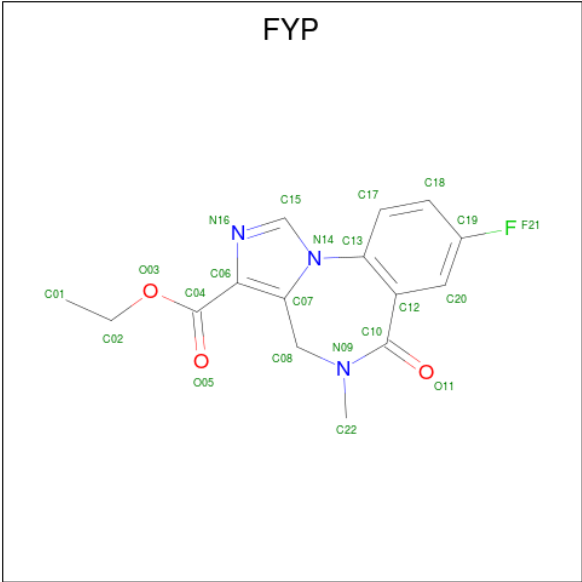
Mol	Chain	Residues	Atoms			AltConf
9	D	1	Total	C	O	0
			63	60	3	
9	D	1	Total	C	O	0
			63	60	3	

- Molecule 10 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	C	O	0
			55	30	25	
10	B	1	Total	C	O	0
			55	30	25	
10	B	1	Total	C	O	0
			55	30	25	
10	B	1	Total	C	O	0
			55	30	25	
10	B	1	Total	C	O	0
			55	30	25	
10	D	1	Total	C	O	0
			22	12	10	
10	D	1	Total	C	O	0
			22	12	10	

- Molecule 11 is ethyl 8-fluoro-5-methyl-6-oxo-5,6-dihydro-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylate (three-letter code: FYP) (formula: C₁₅H₁₄FN₃O₃).

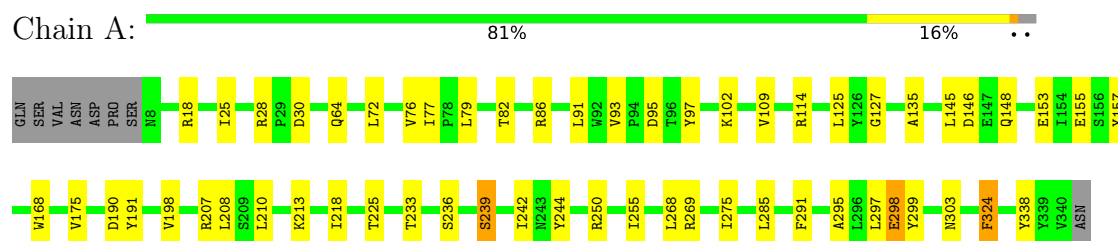


Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	F	N	O	0
			22	15	1	3	3	

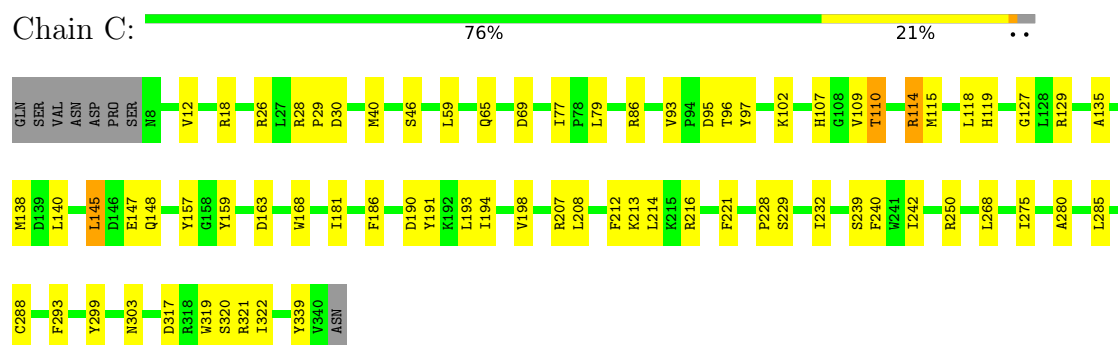
3 Residue-property plots

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. 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. 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.

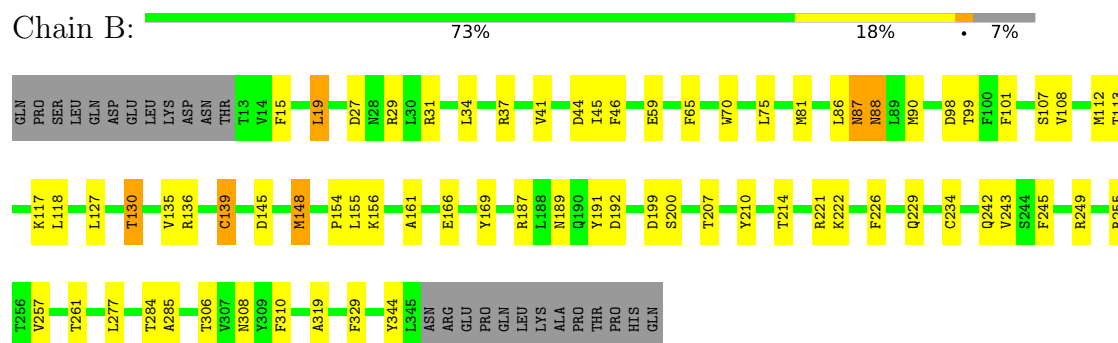
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2, Gamma-aminobutyric acid receptor subunit beta-2



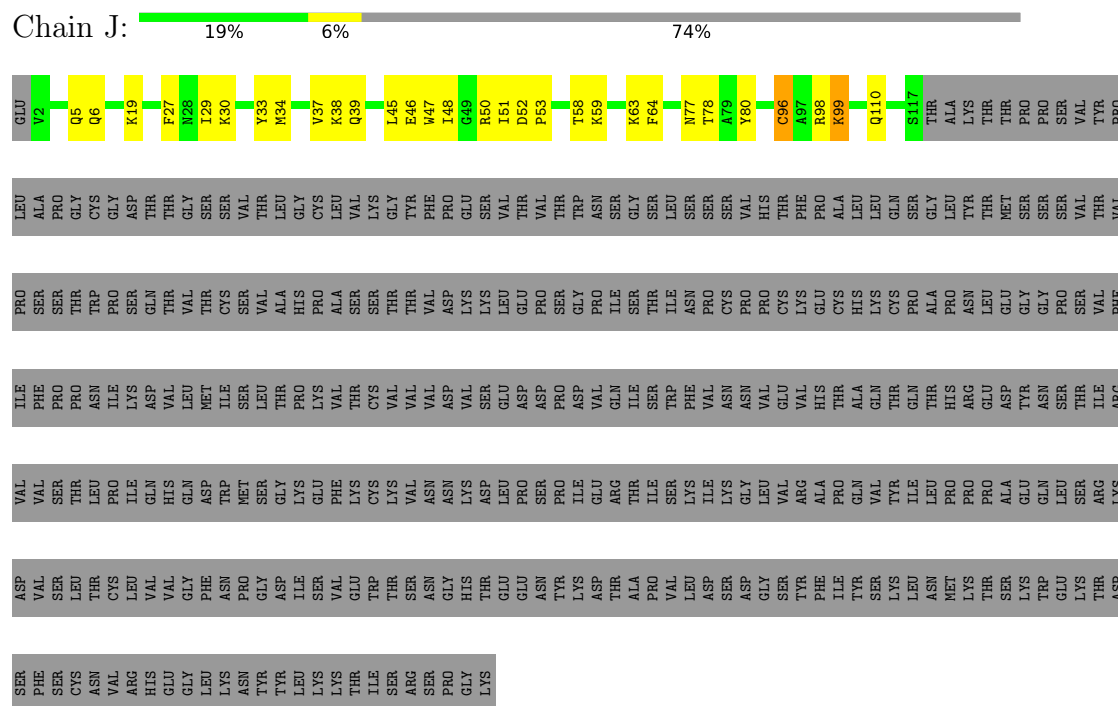
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2, Gamma-aminobutyric acid receptor subunit beta-2



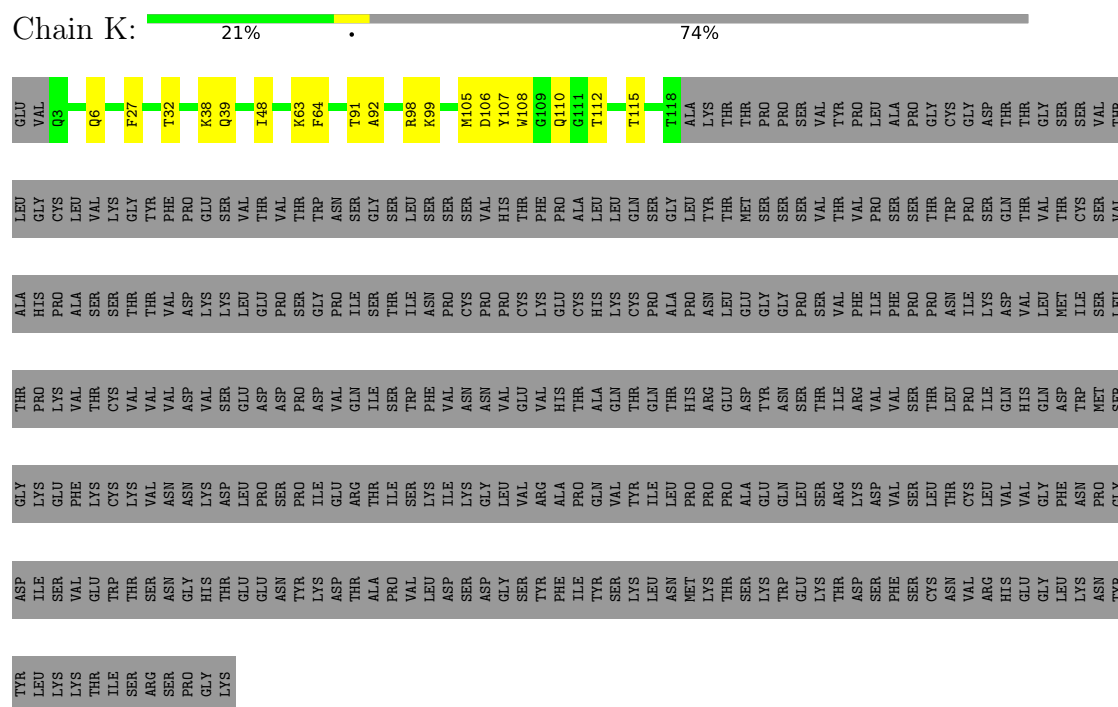
- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1, Gamma-aminobutyric acid receptor subunit alpha-1



- Molecule 5: IgG2b Fab Heavy Chain



- Molecule 5: IgG2b Fab Heavy Chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NAG, FYP, BMA, ABU, MAN

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 >2	RMSZ	# Z >2
1	A	0.32	0/2798	0.44	0/3810
1	C	0.29	0/2798	0.42	0/3810
2	B	0.30	0/2757	0.43	0/3748
2	D	0.32	0/2791	0.44	0/3794
3	E	0.31	0/2177	0.45	0/2962
4	I	0.32	0/829	0.45	0/1123
4	L	0.31	0/829	0.46	0/1123
5	J	0.29	0/928	0.47	0/1260
5	K	0.29	0/928	0.44	0/1260
All	All	0.31	0/16835	0.44	0/22890

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2726	0	2736	38	0
1	C	2726	0	2736	41	0
2	B	2688	0	2686	43	0
2	D	2722	0	2718	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2336	0	2163	34	0
4	I	811	0	784	4	0
4	L	811	0	784	4	0
5	J	907	0	877	22	0
5	K	907	0	875	10	0
6	A	42	0	37	1	0
6	B	28	0	24	0	0
6	C	42	0	37	3	0
6	D	28	0	24	0	0
6	E	14	0	13	0	0
7	A	11	0	10	0	0
7	B	11	0	8	0	0
7	C	11	0	10	0	0
7	D	11	0	8	0	0
8	A	7	0	5	0	0
8	C	7	0	5	1	0
9	A	105	0	140	5	0
9	B	84	0	112	2	0
9	D	63	0	84	1	0
10	B	55	0	47	0	0
10	D	22	0	20	0	0
11	D	22	0	0	0	0
All	All	17197	0	16943	223	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.

All (223) 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)
5:J:29:ILE:HG13	5:J:77:ASN:OD1	1.43	1.16
3:E:130:MET:HB3	3:E:142:THR:HG22	1.29	1.10
3:E:130:MET:HB3	3:E:142:THR:CG2	1.81	1.08
2:B:249:ARG:HH12	2:B:319:ALA:HA	1.53	0.73
1:A:146:ASP:OD2	1:A:148:GLN:NE2	2.21	0.73
1:A:239:SER:O	1:A:250:ARG:NH1	2.22	0.72
5:J:110:GLN:N	5:J:110:GLN:OE1	2.17	0.72
5:K:38:LYS:HB3	5:K:48:ILE:HD11	1.73	0.70
2:D:139:CYS:HB3	2:D:154:PRO:HD2	1.76	0.68
2:B:139:CYS:HB3	2:B:154:PRO:HD2	1.74	0.67
5:J:6:GLN:HE21	5:J:96:CYS:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:253:VAL:HA	3:E:257:ILE:HD13	1.74	0.67
1:A:242:ILE:O	1:A:250:ARG:NH2	2.28	0.66
2:B:88:ASN:ND2	2:B:117:LYS:O	2.29	0.65
1:A:213:LYS:HG3	6:A:401:NAG:H83	1.77	0.65
2:D:88:ASN:ND2	2:D:117:LYS:O	2.30	0.65
5:J:33:TYR:HE1	5:J:52:ASP:CG	2.00	0.64
2:B:277:LEU:HD21	2:B:284:THR:HG21	1.78	0.64
2:B:87:ASN:HD22	2:B:88:ASN:H	1.45	0.64
2:D:275:ASN:HB2	3:E:286:SER:HB2	1.79	0.64
2:B:99:THR:HG1	2:B:169:TYR:HH	1.43	0.64
1:A:77:ILE:HG22	1:A:79:LEU:H	1.63	0.64
2:D:164:ARG:NH1	2:D:209:GLU:OE1	2.31	0.64
5:J:29:ILE:CG1	5:J:77:ASN:OD1	2.34	0.63
1:C:138:MET:SD	1:C:148:GLN:NE2	2.73	0.62
5:J:5:GLN:HA	5:J:5:GLN:OE1	1.99	0.62
2:D:75:LEU:HD12	2:D:127:LEU:HD11	1.80	0.62
1:A:155:GLU:HG2	1:A:207:ARG:HB2	1.82	0.62
1:C:242:ILE:O	1:C:250:ARG:NH2	2.33	0.61
1:C:28:ARG:NH1	1:C:30:ASP:O	2.34	0.61
1:C:213:LYS:HG3	6:C:401:NAG:H83	1.82	0.60
1:A:225:THR:HG22	1:A:268:LEU:HD11	1.83	0.60
3:E:132:ARG:HD2	3:E:140:LEU:HD23	1.83	0.60
3:E:130:MET:CE	3:E:142:THR:HG21	2.30	0.59
1:C:40:MET:HG2	1:C:65:GLN:HG2	1.84	0.59
1:A:268:LEU:HD23	1:A:285:LEU:HD11	1.85	0.59
3:E:98:LEU:HD13	3:E:102:MET:HG2	1.84	0.59
1:C:118:LEU:O	1:C:119:HIS:ND1	2.34	0.59
2:B:107:SER:HB2	1:C:109:VAL:HG22	1.86	0.58
1:C:12:VAL:HG22	1:C:77:ILE:HG12	1.86	0.56
1:C:102:LYS:HD2	1:C:135:ALA:HB2	1.88	0.56
1:C:145:LEU:H	1:C:145:LEU:HD12	1.70	0.56
5:J:39:GLN:HB2	5:J:45:LEU:HD23	1.88	0.55
2:D:112:MET:HG3	2:D:113:THR:HG23	1.87	0.55
5:J:37:VAL:HG13	5:J:46:GLU:O	2.07	0.55
2:B:41:VAL:HG22	2:B:70:TRP:HB3	1.89	0.55
5:K:91:THR:HG23	5:K:115:THR:HA	1.89	0.55
2:D:266:MET:HG2	2:D:294:TYR:HD1	1.72	0.54
1:A:269:ARG:CZ	2:B:229:GLN:HE22	2.20	0.54
1:C:114:ARG:HA	1:C:127:GLY:O	2.08	0.54
1:A:297:LEU:HD21	2:B:243:VAL:HG21	1.89	0.54
1:A:95:ASP:OD1	1:A:95:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:33:TYR:CE1	5:J:52:ASP:CG	2.81	0.54
1:A:28:ARG:NH1	1:A:30:ASP:O	2.41	0.54
1:A:153:GLU:OE1	1:A:207:ARG:NH2	2.42	0.53
1:C:147:GLU:OE1	1:C:213:LYS:NZ	2.38	0.53
2:D:181:VAL:HB	2:D:196:GLN:HE22	1.73	0.53
6:C:402:NAG:H3	6:C:402:NAG:H83	1.90	0.53
5:J:37:VAL:HG22	5:J:47:TRP:HA	1.91	0.53
2:B:161:ALA:HB2	1:C:115:MET:HB2	1.91	0.52
5:J:51:ILE:HG13	5:J:58:THR:HG22	1.91	0.52
2:B:226:PHE:HA	2:B:229:GLN:HB3	1.92	0.52
2:D:161:ALA:HA	3:E:130:MET:SD	2.50	0.52
1:A:338:TYR:CE2	9:A:409:Y01:HAD2	2.44	0.52
2:B:199:ASP:OD1	2:B:200:SER:N	2.42	0.52
2:B:34:LEU:HD23	1:C:12:VAL:HG11	1.92	0.52
5:J:30:LYS:HA	5:J:53:PRO:HB2	1.92	0.52
1:C:194:ILE:HD13	6:C:402:NAG:H2	1.92	0.52
5:J:99:LYS:C	5:J:99:LYS:HD2	2.31	0.52
1:A:198:VAL:CG2	1:A:207:ARG:HD2	2.40	0.51
2:B:31:ARG:HH21	2:B:166:GLU:HG2	1.76	0.51
2:D:86:LEU:HD13	2:D:90:MET:SD	2.50	0.51
3:E:176:ARG:N	3:E:219:ASP:O	2.43	0.51
4:L:29:VAL:HG12	4:L:92:TYR:HB3	1.93	0.51
2:B:98:ASP:N	2:B:98:ASP:OD1	2.40	0.51
1:A:109:VAL:HG22	3:E:119:ALA:HB3	1.92	0.51
1:C:96:THR:O	2:D:113:THR:OG1	2.24	0.50
1:A:295:ALA:O	1:A:298:GLU:HG3	2.12	0.50
2:D:98:ASP:N	2:D:98:ASP:OD1	2.43	0.50
3:E:130:MET:HE1	3:E:142:THR:HG21	1.93	0.50
1:A:114:ARG:HA	1:A:127:GLY:O	2.11	0.49
1:C:198:VAL:HG21	1:C:207:ARG:CZ	2.42	0.49
5:J:19:LYS:HE2	5:J:80:TYR:CD1	2.48	0.49
1:A:97:TYR:CD1	1:A:157:TYR:HB2	2.47	0.49
5:J:27:PHE:CZ	5:J:98:ARG:HD3	2.47	0.49
4:L:14:SER:OG	4:L:106:LYS:NZ	2.36	0.49
1:C:168:TRP:CE2	1:C:208:LEU:HD13	2.47	0.49
2:D:44:ASP:OD2	2:D:173:ARG:NH1	2.43	0.49
1:C:186:PHE:HD2	1:C:214:LEU:HB3	1.78	0.49
3:E:53:ILE:HG13	3:E:82:TRP:HB3	1.95	0.49
1:C:28:ARG:HB2	1:C:29:PRO:HD2	1.95	0.48
3:E:97:ARG:HE	3:E:132:ARG:HH12	1.61	0.48
2:B:242:GLN:HE22	2:B:329:PHE:HB3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:40:ASN:N	3:E:40:ASN:OD1	2.44	0.48
1:C:293:PHE:HE1	2:D:240:LEU:HD13	1.78	0.48
5:J:34:MET:HB2	5:J:51:ILE:CG2	2.43	0.48
1:C:95:ASP:OD1	1:C:95:ASP:N	2.39	0.48
5:K:106:ASP:OD1	5:K:107:TYR:N	2.46	0.48
3:E:84:ASP:OD1	3:E:85:ARG:N	2.47	0.48
5:K:105:MET:O	5:K:108:TRP:NE1	2.38	0.48
2:B:242:GLN:HE22	2:B:329:PHE:HD2	1.63	0.47
3:E:260:ASP:OD1	3:E:260:ASP:N	2.38	0.47
2:B:245:PHE:HA	2:B:255:ARG:HH22	1.78	0.47
2:B:44:ASP:OD1	2:B:45:ILE:N	2.47	0.47
2:D:44:ASP:OD1	2:D:45:ILE:N	2.47	0.47
5:J:33:TYR:CE1	5:J:52:ASP:HB2	2.50	0.47
1:A:76:VAL:HB	1:A:77:ILE:HD12	1.96	0.47
2:D:296:PHE:HE2	2:D:333:PHE:HA	1.79	0.47
2:B:101:PHE:CE2	2:B:135:VAL:HG21	2.49	0.47
5:K:6:GLN:H	5:K:110:GLN:HE22	1.61	0.47
2:D:156:LYS:HG2	2:D:214:THR:HG23	1.95	0.47
3:E:45:ASP:HB3	3:E:48:VAL:HG23	1.96	0.47
2:D:242:GLN:NE2	2:D:329:PHE:HB3	2.30	0.47
2:B:112:MET:HG3	2:B:113:THR:HG23	1.96	0.47
2:B:191:TYR:OH	2:B:221:ARG:NH2	2.49	0.46
1:C:77:ILE:HG22	1:C:79:LEU:H	1.80	0.46
3:E:63:GLY:N	3:E:73:THR:O	2.38	0.46
1:A:175:VAL:HG21	1:A:210:LEU:HD13	1.98	0.46
1:A:324:PHE:HE1	9:A:406:Y01:HAE3	1.80	0.46
3:E:34:LEU:HD21	3:E:89:PHE:HB3	1.97	0.46
4:I:61:ARG:HD2	4:I:77:SER:O	2.16	0.46
4:L:105:LEU:HD22	4:L:106:LYS:H	1.80	0.46
1:A:198:VAL:HG23	1:A:207:ARG:HD2	1.98	0.46
2:B:86:LEU:HD13	2:B:90:MET:SD	2.56	0.46
1:C:229:SER:HB3	1:C:288:CYS:SG	2.56	0.46
2:D:240:LEU:HG	2:D:258:PHE:CE1	2.51	0.45
3:E:264:ALA:HB3	3:E:266:THR:HG22	1.97	0.45
1:A:145:LEU:HD12	1:A:145:LEU:H	1.80	0.45
2:D:100:PHE:O	2:D:100:PHE:CD1	2.70	0.45
3:E:145:LEU:HB3	3:E:147:ILE:HD11	1.99	0.45
1:A:168:TRP:CE2	1:A:208:LEU:HD13	2.52	0.45
5:K:32:THR:HB	5:K:99:LYS:HG2	1.98	0.45
2:D:191:TYR:OH	2:D:221:ARG:NH2	2.50	0.45
1:A:244:TYR:HA	1:A:250:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:PHE:O	2:D:100:PHE:CG	2.70	0.45
2:D:161:ALA:CB	3:E:130:MET:HG3	2.47	0.45
5:J:34:MET:HB2	5:J:51:ILE:HG22	1.98	0.45
2:B:75:LEU:HD12	2:B:127:LEU:HD11	1.99	0.44
3:E:114:ARG:NH1	3:E:220:TYR:HD2	2.15	0.44
2:B:285:ALA:HB1	2:B:344:TYR:CE2	2.52	0.44
1:C:280:ALA:HB1	1:C:339:TYR:CE2	2.52	0.44
2:B:207:THR:OG1	2:B:210:TYR:OH	2.34	0.44
1:C:140:LEU:HD12	1:C:275:ILE:HG21	1.99	0.44
3:E:115:ASN:ND2	3:E:150:GLU:H	2.16	0.44
2:B:156:LYS:HG2	2:B:214:THR:HG23	1.99	0.44
1:C:319:TRP:CE3	1:C:322:ILE:HD11	2.53	0.44
5:K:63:LYS:HG3	5:K:64:PHE:CD1	2.52	0.44
2:B:192:ASP:HB2	2:B:222:LYS:HE2	1.99	0.44
2:D:29:ARG:HE	3:E:31:LEU:HD13	1.82	0.44
1:A:64:GLN:HE21	1:A:125:LEU:HD11	1.83	0.44
2:D:259:GLY:HA3	2:D:301:LEU:HD13	2.00	0.44
1:C:317:ASP:HB3	1:C:321:ARG:NH2	2.32	0.43
1:A:72:LEU:HD11	1:A:91:LEU:HD22	2.00	0.43
2:B:118:LEU:HB3	2:B:130:THR:HG23	2.00	0.43
1:A:255:ILE:HD13	2:B:257:VAL:HG12	2.00	0.43
2:B:99:THR:O	1:C:110:THR:OG1	2.28	0.43
3:E:252:TRP:CZ2	3:E:257:ILE:HD11	2.53	0.43
1:A:190:ASP:OD1	1:A:191:TYR:N	2.49	0.43
9:A:406:Y01:HAS2	9:A:406:Y01:HAE1	1.81	0.43
2:B:27:ASP:OD2	2:B:29:ARG:NH2	2.52	0.43
2:D:274:ARG:CZ	3:E:239:GLN:HA	2.48	0.43
2:D:143:LEU:HD13	2:D:277:LEU:HD11	2.01	0.43
1:C:46:SER:HA	1:C:181:ILE:HD12	2.00	0.43
4:I:105:LEU:HD22	4:I:106:LYS:H	1.84	0.43
2:B:145:ASP:O	2:B:148:MET:N	2.51	0.43
1:C:268:LEU:HD23	1:C:285:LEU:HD11	2.01	0.43
3:E:155:LEU:HD21	3:E:231:ARG:HH21	1.83	0.43
2:B:46:PHE:HB3	2:B:65:PHE:HB2	2.01	0.43
1:C:216:ARG:HD2	1:C:221:PHE:HE2	1.84	0.42
5:J:50:ARG:HH21	5:J:59:LYS:HE3	1.84	0.42
2:B:15:PHE:HE1	2:B:81:MET:HG2	1.84	0.42
1:C:107:HIS:HD2	1:C:129:ARG:HG2	1.85	0.42
8:C:405:ABU:OE2	2:D:67:ARG:NE	2.50	0.42
2:D:226:PHE:HA	2:D:229:GLN:HB3	2.00	0.42
9:A:407:Y01:HAE1	9:A:407:Y01:HAS2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:PHE:HD1	2:D:157:PHE:HB3	1.84	0.42
1:A:82:THR:HG21	3:E:173:GLY:O	2.20	0.42
1:C:250:ARG:HD2	1:C:299:TYR:CG	2.54	0.42
4:L:46:LEU:HD21	4:L:49:TYR:HB3	2.00	0.42
1:A:145:LEU:HG	1:A:218:ILE:HD13	2.02	0.42
1:A:64:GLN:NE2	1:A:125:LEU:HD11	2.35	0.42
1:C:97:TYR:CD1	1:C:157:TYR:HB2	2.55	0.42
2:B:19:LEU:HA	2:B:19:LEU:HD12	1.82	0.42
2:D:199:ASP:OD1	2:D:200:SER:N	2.52	0.42
1:A:157:TYR:HH	2:B:130:THR:HG1	1.66	0.42
2:B:101:PHE:CD2	2:B:155:LEU:HD11	2.54	0.42
5:J:29:ILE:O	5:J:53:PRO:HG2	2.19	0.42
9:A:409:Y01:HAE1	9:A:409:Y01:HAS2	1.81	0.42
2:D:232:LEU:HA	2:D:232:LEU:HD23	1.87	0.42
1:C:29:PRO:HB3	1:C:69:ASP:OD1	2.19	0.41
5:J:38:LYS:HB3	5:J:48:ILE:HD11	2.01	0.41
3:E:252:TRP:CH2	3:E:257:ILE:HD11	2.55	0.41
9:B:409:Y01:HAE1	9:B:409:Y01:HAS2	1.81	0.41
1:C:190:ASP:OD1	1:C:191:TYR:N	2.53	0.41
3:E:170:SER:HB3	3:E:222:VAL:HA	2.01	0.41
2:D:28:ASN:HB3	2:D:93:LYS:O	2.20	0.41
5:K:39:GLN:O	5:K:92:ALA:HB1	2.20	0.41
1:C:159:TYR:HB3	1:C:163:ASP:HB2	2.02	0.41
2:D:91:ALA:HB1	2:D:129:TYR:HE1	1.85	0.41
2:D:310:PHE:CZ	2:D:317:ARG:HD2	2.56	0.41
1:C:250:ARG:HD2	1:C:299:TYR:CD1	2.55	0.41
5:J:63:LYS:HG3	5:J:64:PHE:CD1	2.56	0.41
1:C:240:PHE:CE2	1:C:320:SER:HB3	2.56	0.41
2:D:277:LEU:HD12	2:D:278:PRO:HD2	2.01	0.41
3:E:58:TYR:CD1	3:E:58:TYR:C	2.94	0.41
5:K:63:LYS:HG3	5:K:64:PHE:HD1	1.86	0.41
9:B:411:Y01:HAE1	9:B:411:Y01:HAS2	1.81	0.41
3:E:267:SER:HA	3:E:270:ILE:HG12	2.03	0.41
2:B:59:GLU:CD	2:B:136:ARG:HH21	2.23	0.41
1:C:228:PRO:O	1:C:232:ILE:HG12	2.21	0.41
9:D:407:Y01:HAS2	9:D:407:Y01:HAE1	1.81	0.41
4:I:65:SER:OG	4:I:72:THR:HB	2.20	0.41
1:A:102:LYS:HD2	1:A:135:ALA:HB2	2.02	0.40
1:A:255:ILE:HG23	2:B:261:THR:HG21	2.03	0.40
1:A:250:ARG:HD2	1:A:299:TYR:CZ	2.57	0.40
2:B:31:ARG:NH2	2:B:166:GLU:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ASN:HD22	2:B:88:ASN:N	2.16	0.40
3:E:153:LEU:HA	3:E:163:HIS:HD2	1.85	0.40
4:I:13:MET:HG3	4:I:19:VAL:HG22	2.03	0.40
5:K:27:PHE:CZ	5:K:98:ARG:HD3	2.56	0.40
2:D:204:GLN:HG3	2:D:209:GLU:HG2	2.03	0.40
2:D:230:THR:HG21	2:D:290:ILE:HD11	2.03	0.40
1:A:233:THR:O	1:A:236:SER:OG	2.26	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	331/341 (97%)	320 (97%)	11 (3%)	0	100	100
1	C	331/341 (97%)	325 (98%)	6 (2%)	0	100	100
2	B	331/358 (92%)	317 (96%)	14 (4%)	0	100	100
2	D	335/358 (94%)	322 (96%)	13 (4%)	0	100	100
3	E	256/366 (70%)	239 (93%)	17 (7%)	0	100	100
4	I	104/213 (49%)	100 (96%)	4 (4%)	0	100	100
4	L	104/213 (49%)	100 (96%)	4 (4%)	0	100	100
5	J	114/454 (25%)	112 (98%)	2 (2%)	0	100	100
5	K	114/454 (25%)	110 (96%)	4 (4%)	0	100	100
All	All	2020/3098 (65%)	1945 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	301/309 (97%)	291 (97%)	10 (3%)	41	72
1	C	301/309 (97%)	289 (96%)	12 (4%)	34	66
2	B	295/319 (92%)	281 (95%)	14 (5%)	29	64
2	D	299/319 (94%)	287 (96%)	12 (4%)	34	66
3	E	239/293 (82%)	233 (98%)	6 (2%)	50	77
4	I	90/188 (48%)	90 (100%)	0	100	100
4	L	90/188 (48%)	90 (100%)	0	100	100
5	J	97/407 (24%)	94 (97%)	3 (3%)	43	72
5	K	97/407 (24%)	96 (99%)	1 (1%)	78	89
All	All	1809/2739 (66%)	1751 (97%)	58 (3%)	46	72

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	25	ILE
1	A	86	ARG
1	A	93	VAL
1	A	239	SER
1	A	275	ILE
1	A	291	PHE
1	A	298	GLU
1	A	303	ASN
1	A	324	PHE
2	B	19	LEU
2	B	37	ARG
2	B	87	ASN
2	B	88	ASN
2	B	108	VAL
2	B	130	THR
2	B	139	CYS
2	B	148	MET

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Mol	Chain	Res	Type
2	B	187	ARG
2	B	189	ASN
2	B	234	CYS
2	B	306	THR
2	B	308	ASN
2	B	310	PHE
1	C	18	ARG
1	C	26	ARG
1	C	59	LEU
1	C	86	ARG
1	C	93	VAL
1	C	110	THR
1	C	114	ARG
1	C	145	LEU
1	C	193	LEU
1	C	212	PHE
1	C	239	SER
1	C	303	ASN
2	D	37	ARG
2	D	85	ARG
2	D	114	MET
2	D	118	LEU
2	D	130	THR
2	D	139	CYS
2	D	234	CYS
2	D	249	ARG
2	D	258	PHE
2	D	288	TRP
2	D	308	ASN
2	D	329	PHE
3	E	40	ASN
3	E	83	TYR
3	E	115	ASN
3	E	206	LEU
3	E	221	VAL
3	E	266	THR
5	J	78	THR
5	J	96	CYS
5	J	99	LYS
5	K	112	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	267	HIS
2	B	87	ASN
2	B	189	ASN
2	B	229	GLN
2	B	337	ASN
2	D	196	GLN
2	D	216	HIS
2	D	337	ASN
3	E	115	ASN
4	I	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

37 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	NAG	A	401	1,6	14,14,15	0.25	0	17,19,21	0.56	0
6	NAG	A	402	7,6	14,14,15	0.26	0	17,19,21	0.45	0
7	BMA	A	403	6	11,11,12	0.58	0	15,15,17	0.77	0
6	NAG	A	404	1	14,14,15	0.17	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ABU	A	405	-	3,6,6	0.20	0	2,6,6	0.37	0
9	Y01	A	406	-	24,24,38	0.81	1 (4%)	38,39,57	1.67	8 (21%)
9	Y01	A	407	-	24,24,38	0.81	1 (4%)	38,39,57	1.67	8 (21%)
9	Y01	A	408	-	24,24,38	0.82	1 (4%)	38,39,57	1.67	8 (21%)
9	Y01	A	409	-	24,24,38	0.81	1 (4%)	38,39,57	1.69	9 (23%)
9	Y01	A	410	-	24,24,38	0.82	1 (4%)	38,39,57	1.67	9 (23%)
6	NAG	B	401	2,6	14,14,15	0.21	0	17,19,21	0.51	0
6	NAG	B	402	7,6	14,14,15	0.26	0	17,19,21	0.38	0
7	BMA	B	403	10,6	11,11,12	0.58	0	15,15,17	0.89	0
10	MAN	B	404	10,7	11,11,12	0.88	1 (9%)	15,15,17	1.14	1 (6%)
10	MAN	B	405	10	11,11,12	0.67	1 (9%)	15,15,17	1.24	2 (13%)
10	MAN	B	406	10	11,11,12	0.91	1 (9%)	15,15,17	1.41	2 (13%)
10	MAN	B	407	10,7	11,11,12	0.81	0	15,15,17	1.52	2 (13%)
10	MAN	B	408	10	11,11,12	0.73	0	15,15,17	0.83	0
9	Y01	B	409	-	24,24,38	0.81	1 (4%)	38,39,57	1.66	9 (23%)
9	Y01	B	410	-	24,24,38	0.82	1 (4%)	38,39,57	1.66	8 (21%)
9	Y01	B	411	-	24,24,38	0.81	1 (4%)	38,39,57	1.65	8 (21%)
9	Y01	B	412	-	24,24,38	0.82	1 (4%)	38,39,57	1.65	9 (23%)
6	NAG	C	401	1,6	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	C	402	7,6	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
7	BMA	C	403	6	11,11,12	0.89	0	15,15,17	0.94	0
6	NAG	C	404	1	14,14,15	0.15	0	17,19,21	0.45	0
8	ABU	C	405	-	3,6,6	0.21	0	2,6,6	0.37	0
6	NAG	D	401	2,6	14,14,15	0.37	0	17,19,21	0.41	0
6	NAG	D	402	7,6	14,14,15	0.26	0	17,19,21	0.43	0
7	BMA	D	403	10,6	11,11,12	0.51	0	15,15,17	0.77	0
10	MAN	D	404	7	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
10	MAN	D	405	7	11,11,12	0.59	0	15,15,17	1.17	2 (13%)
11	FYP	D	406	-	21,24,24	1.31	3 (14%)	26,35,35	1.20	3 (11%)
9	Y01	D	407	-	24,24,38	0.82	1 (4%)	38,39,57	1.66	8 (21%)
9	Y01	D	408	-	24,24,38	0.81	1 (4%)	38,39,57	1.67	8 (21%)
9	Y01	D	409	-	24,24,38	0.82	1 (4%)	38,39,57	1.67	8 (21%)
6	NAG	E	401	3	14,14,15	0.22	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	401	1,6	-	3/6/23/26	0/1/1/1
6	NAG	A	402	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	403	6	-	1/2/19/22	0/1/1/1
6	NAG	A	404	1	-	1/6/23/26	0/1/1/1
8	ABU	A	405	-	-	0/2/4/4	-
9	Y01	A	406	-	-	-	0/4/4/4
9	Y01	A	407	-	-	-	0/4/4/4
9	Y01	A	408	-	-	-	0/4/4/4
9	Y01	A	409	-	-	-	0/4/4/4
9	Y01	A	410	-	-	-	0/4/4/4
6	NAG	B	401	2,6	-	2/6/23/26	0/1/1/1
6	NAG	B	402	7,6	-	1/6/23/26	0/1/1/1
7	BMA	B	403	10,6	-	2/2/19/22	0/1/1/1
10	MAN	B	404	10,7	-	1/2/19/22	0/1/1/1
10	MAN	B	405	10	-	2/2/19/22	0/1/1/1
10	MAN	B	406	10	-	2/2/19/22	1/1/1/1
10	MAN	B	407	10,7	-	2/2/19/22	0/1/1/1
10	MAN	B	408	10	-	0/2/19/22	0/1/1/1
9	Y01	B	409	-	-	-	0/4/4/4
9	Y01	B	410	-	-	-	0/4/4/4
9	Y01	B	411	-	-	-	0/4/4/4
9	Y01	B	412	-	-	-	0/4/4/4
6	NAG	C	401	1,6	-	3/6/23/26	0/1/1/1
6	NAG	C	402	7,6	-	4/6/23/26	0/1/1/1
7	BMA	C	403	6	-	1/2/19/22	0/1/1/1
6	NAG	C	404	1	-	2/6/23/26	0/1/1/1
8	ABU	C	405	-	-	0/2/4/4	-
6	NAG	D	401	2,6	-	1/6/23/26	0/1/1/1
6	NAG	D	402	7,6	-	0/6/23/26	0/1/1/1
7	BMA	D	403	10,6	-	2/2/19/22	0/1/1/1
10	MAN	D	404	7	-	2/2/19/22	0/1/1/1
10	MAN	D	405	7	-	2/2/19/22	0/1/1/1
11	FYP	D	406	-	-	0/7/23/23	0/2/3/3
9	Y01	D	407	-	-	-	0/4/4/4
9	Y01	D	408	-	-	-	0/4/4/4
9	Y01	D	409	-	-	-	0/4/4/4
6	NAG	E	401	3	-	4/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	406	FYP	C08-C07	-2.90	1.47	1.51
11	D	406	FYP	C15-N16	-2.65	1.30	1.35
10	B	406	MAN	C1-C2	2.49	1.58	1.52
11	D	406	FYP	C10-N09	-2.43	1.33	1.35
9	B	410	Y01	CBH-CBF	-2.27	1.52	1.56
9	A	408	Y01	CBH-CBF	-2.26	1.52	1.56
9	D	407	Y01	CBH-CBF	-2.25	1.52	1.56
9	D	409	Y01	CBH-CBF	-2.25	1.52	1.56
9	B	411	Y01	CBH-CBF	-2.24	1.52	1.56
9	A	410	Y01	CBH-CBF	-2.24	1.52	1.56
10	B	404	MAN	O5-C1	-2.23	1.40	1.43
9	D	408	Y01	CBH-CBF	-2.23	1.52	1.56
9	B	409	Y01	CBH-CBF	-2.22	1.52	1.56
9	B	412	Y01	CBH-CBF	-2.21	1.52	1.56
9	A	406	Y01	CBH-CBF	-2.20	1.52	1.56
9	A	409	Y01	CBH-CBF	-2.19	1.52	1.56
9	A	407	Y01	CBH-CBF	-2.19	1.52	1.56
10	B	405	MAN	C1-C2	2.01	1.56	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	409	Y01	CBI-CBG-CBD	-4.81	107.17	114.39
9	D	409	Y01	CBI-CBG-CBD	-4.74	107.27	114.39
9	A	406	Y01	CBI-CBG-CBD	-4.71	107.31	114.39
9	D	408	Y01	CBI-CBG-CBD	-4.69	107.34	114.39
9	A	408	Y01	CBI-CBG-CBD	-4.68	107.35	114.39
9	A	407	Y01	CBI-CBG-CBD	-4.68	107.36	114.39
9	B	410	Y01	CBI-CBG-CBD	-4.66	107.38	114.39
9	B	409	Y01	CBI-CBG-CBD	-4.65	107.40	114.39
9	D	407	Y01	CBI-CBG-CBD	-4.63	107.43	114.39
9	A	410	Y01	CBI-CBG-CBD	-4.61	107.46	114.39
9	B	411	Y01	CBI-CBG-CBD	-4.61	107.46	114.39
9	B	412	Y01	CBI-CBG-CBD	-4.58	107.51	114.39
10	B	407	MAN	C1-O5-C5	4.56	118.40	112.20
6	C	402	NAG	C2-N2-C7	4.26	129.02	122.92
10	B	406	MAN	C1-O5-C5	3.61	117.11	112.20
11	D	406	FYP	C07-C08-N09	-3.42	107.45	111.85
9	D	408	Y01	CAS-CAU-CBI	-3.37	106.97	112.80
9	B	411	Y01	CAS-CAU-CBI	-3.36	106.98	112.80
9	B	410	Y01	CAS-CAU-CBI	-3.36	106.98	112.80
9	A	410	Y01	CAS-CAU-CBI	-3.35	107.00	112.80
9	A	407	Y01	CAS-CAU-CBI	-3.34	107.01	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	412	Y01	CAS-CAU-CBI	-3.34	107.02	112.80
9	B	409	Y01	CAS-CAU-CBI	-3.33	107.03	112.80
9	A	406	Y01	CAS-CAU-CBI	-3.33	107.03	112.80
9	A	408	Y01	CAS-CAU-CBI	-3.33	107.03	112.80
9	D	407	Y01	CAS-CAU-CBI	-3.32	107.05	112.80
9	A	409	Y01	CAS-CAU-CBI	-3.32	107.05	112.80
9	D	409	Y01	CAS-CAU-CBI	-3.30	107.08	112.80
11	D	406	FYP	C08-N09-C10	3.30	123.61	120.94
10	B	405	MAN	C1-O5-C5	3.18	116.52	112.20
10	B	404	MAN	O2-C2-C3	-3.01	104.29	110.16
9	D	407	Y01	CBB-CBE-CBI	-2.98	110.21	115.94
9	B	410	Y01	CBB-CBE-CBI	-2.97	110.22	115.94
9	B	411	Y01	CBB-CBE-CBI	-2.96	110.24	115.94
10	D	405	MAN	C1-O5-C5	2.96	116.23	112.20
9	D	409	Y01	CBB-CBE-CBI	-2.95	110.26	115.94
9	D	408	Y01	CBB-CBE-CBI	-2.95	110.26	115.94
9	A	409	Y01	CBB-CBE-CBI	-2.95	110.27	115.94
9	A	407	Y01	CBB-CBE-CBI	-2.95	110.27	115.94
9	A	406	Y01	CBB-CBE-CBI	-2.94	110.28	115.94
9	A	406	Y01	CAD-CBH-CBF	-2.94	108.13	111.67
9	A	408	Y01	CBB-CBE-CBI	-2.93	110.30	115.94
9	A	407	Y01	CAD-CBH-CBF	-2.92	108.15	111.67
9	A	409	Y01	CAD-CBH-CBF	-2.92	108.16	111.67
9	A	410	Y01	CBB-CBE-CBI	-2.92	110.33	115.94
9	A	408	Y01	CAD-CBH-CBF	-2.91	108.17	111.67
9	B	409	Y01	CBB-CBE-CBI	-2.90	110.35	115.94
9	B	412	Y01	CBB-CBE-CBI	-2.90	110.36	115.94
9	A	410	Y01	CAD-CBH-CBF	-2.89	108.19	111.67
9	D	409	Y01	CAD-CBH-CBF	-2.89	108.19	111.67
9	D	408	Y01	CAD-CBH-CBF	-2.89	108.19	111.67
9	D	407	Y01	CAD-CBH-CBF	-2.89	108.19	111.67
9	B	409	Y01	CAD-CBH-CBF	-2.89	108.19	111.67
9	B	411	Y01	CAD-CBH-CBF	-2.86	108.22	111.67
9	B	412	Y01	CAD-CBH-CBF	-2.86	108.23	111.67
9	B	410	Y01	CAD-CBH-CBF	-2.85	108.24	111.67
10	B	407	MAN	O2-C2-C3	-2.83	104.64	110.16
9	A	409	Y01	CAS-CBF-CBH	-2.55	109.67	113.10
9	A	407	Y01	CAS-CBF-CBH	-2.52	109.71	113.10
9	A	408	Y01	CAS-CBF-CBH	-2.51	109.73	113.10
9	B	409	Y01	CAS-CBF-CBH	-2.51	109.73	113.10
9	A	409	Y01	CBD-CAK-CAI	-2.49	109.08	112.73
9	D	407	Y01	CAS-CBF-CBH	-2.49	109.76	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	408	Y01	CAS-CBF-CBH	-2.47	109.78	113.10
9	D	409	Y01	CAS-CBF-CBH	-2.47	109.78	113.10
9	B	412	Y01	CAS-CBF-CBH	-2.47	109.78	113.10
9	A	406	Y01	CAS-CBF-CBH	-2.46	109.80	113.10
10	B	405	MAN	O2-C2-C3	-2.45	105.37	110.16
9	A	410	Y01	CAS-CBF-CBH	-2.45	109.81	113.10
9	B	411	Y01	CAS-CBF-CBH	-2.44	109.81	113.10
10	B	406	MAN	O2-C2-C3	-2.44	105.39	110.16
9	D	409	Y01	CBD-CAK-CAI	-2.44	109.15	112.73
9	B	410	Y01	CAS-CBF-CBH	-2.41	109.86	113.10
10	D	404	MAN	O2-C2-C3	-2.40	105.47	110.16
9	A	409	Y01	CBF-CBH-CAZ	2.40	113.39	109.65
10	D	405	MAN	O2-C2-C3	-2.39	105.49	110.16
9	A	410	Y01	CBD-CAK-CAI	-2.38	109.24	112.73
9	D	408	Y01	CBD-CAK-CAI	-2.37	109.26	112.73
9	A	407	Y01	CBD-CAK-CAI	-2.36	109.27	112.73
9	B	409	Y01	CBD-CAK-CAI	-2.36	109.27	112.73
9	A	406	Y01	CBD-CAK-CAI	-2.36	109.28	112.73
9	D	409	Y01	CBF-CBH-CAZ	2.35	113.31	109.65
9	B	412	Y01	CBD-CAK-CAI	-2.34	109.30	112.73
9	A	408	Y01	CBD-CAK-CAI	-2.33	109.31	112.73
9	A	406	Y01	CBF-CBH-CAZ	2.30	113.25	109.65
9	A	410	Y01	CBF-CBH-CAZ	2.30	113.25	109.65
9	A	407	Y01	CBF-CBH-CAZ	2.27	113.19	109.65
9	B	409	Y01	CBF-CBH-CAZ	2.27	113.19	109.65
9	B	410	Y01	CBD-CAK-CAI	-2.27	109.40	112.73
9	D	408	Y01	CBF-CBH-CAZ	2.27	113.19	109.65
9	D	407	Y01	CBD-CAK-CAI	-2.27	109.41	112.73
9	B	411	Y01	CBD-CAK-CAI	-2.26	109.41	112.73
9	B	411	Y01	CBF-CBH-CAZ	2.23	113.14	109.65
9	A	408	Y01	CBF-CBH-CAZ	2.23	113.12	109.65
9	B	410	Y01	CBF-CBH-CAZ	2.22	113.12	109.65
9	B	412	Y01	CBF-CBH-CAZ	2.21	113.10	109.65
9	D	407	Y01	CBF-CBH-CAZ	2.20	113.08	109.65
10	D	404	MAN	C1-O5-C5	2.14	115.11	112.20
9	A	409	Y01	CBC-CAV-CAZ	-2.11	108.37	112.02
9	A	406	Y01	CBC-CAV-CAZ	-2.10	108.38	112.02
9	D	407	Y01	CBC-CAV-CAZ	-2.10	108.38	112.02
9	A	408	Y01	CBC-CAV-CAZ	-2.10	108.39	112.02
9	B	411	Y01	CBC-CAV-CAZ	-2.09	108.41	112.02
9	A	410	Y01	CBC-CAV-CAZ	-2.08	108.42	112.02
9	B	412	Y01	CBC-CAV-CAZ	-2.07	108.43	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	406	FYP	C17-C13-C12	-2.07	121.02	122.95
9	B	409	Y01	CBC-CAV-CAZ	-2.07	108.44	112.02
9	B	412	Y01	CAQ-CBG-CBD	-2.06	115.63	119.06
9	D	409	Y01	CBC-CAV-CAZ	-2.05	108.47	112.02
9	A	410	Y01	CAQ-CBG-CBD	-2.04	115.65	119.06
9	B	409	Y01	CAQ-CBG-CBD	-2.03	115.67	119.06
9	A	407	Y01	CBC-CAV-CAZ	-2.03	108.50	112.02
9	B	410	Y01	CBC-CAV-CAZ	-2.03	108.51	112.02
9	A	409	Y01	CAQ-CBG-CBD	-2.03	115.68	119.06
9	D	408	Y01	CAQ-CBG-CBD	-2.00	115.71	119.06

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	404	NAG	C4-C5-C6-O6
6	C	404	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	E	401	NAG	O5-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
7	B	403	BMA	O5-C5-C6-O6
10	B	406	MAN	O5-C5-C6-O6
7	D	403	BMA	C4-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6
10	B	406	MAN	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
10	D	404	MAN	O5-C5-C6-O6
10	D	405	MAN	O5-C5-C6-O6
10	D	404	MAN	C4-C5-C6-O6
6	E	401	NAG	C4-C5-C6-O6
6	E	401	NAG	C8-C7-N2-C2
6	E	401	NAG	O7-C7-N2-C2
6	C	402	NAG	C8-C7-N2-C2
6	C	402	NAG	O7-C7-N2-C2
7	B	403	BMA	C4-C5-C6-O6
7	D	403	BMA	O5-C5-C6-O6
6	B	401	NAG	O5-C5-C6-O6
7	C	403	BMA	O5-C5-C6-O6
6	B	401	NAG	C4-C5-C6-O6
6	D	401	NAG	O5-C5-C6-O6
7	A	403	BMA	O5-C5-C6-O6
6	A	404	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	B	407	MAN	C4-C5-C6-O6
10	B	407	MAN	O5-C5-C6-O6
10	B	405	MAN	O5-C5-C6-O6
10	B	405	MAN	C4-C5-C6-O6
10	D	405	MAN	C4-C5-C6-O6
6	A	401	NAG	C3-C2-N2-C7
6	C	402	NAG	C3-C2-N2-C7
6	C	401	NAG	C3-C2-N2-C7
10	B	404	MAN	C4-C5-C6-O6
6	B	402	NAG	C4-C5-C6-O6
6	C	402	NAG	C4-C5-C6-O6

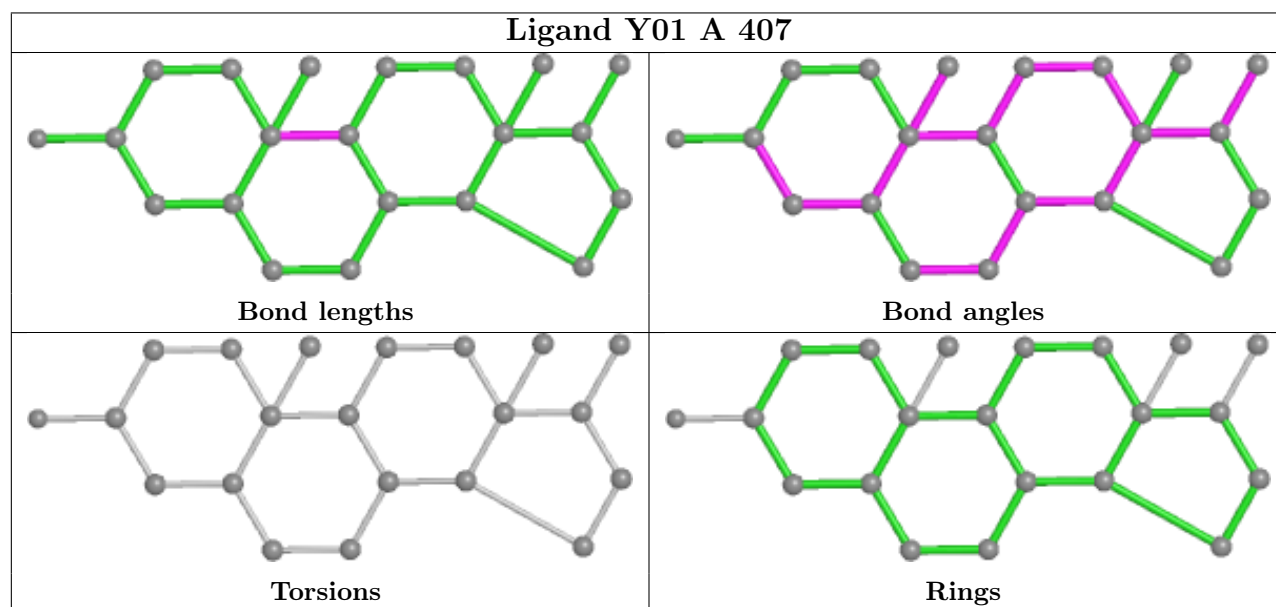
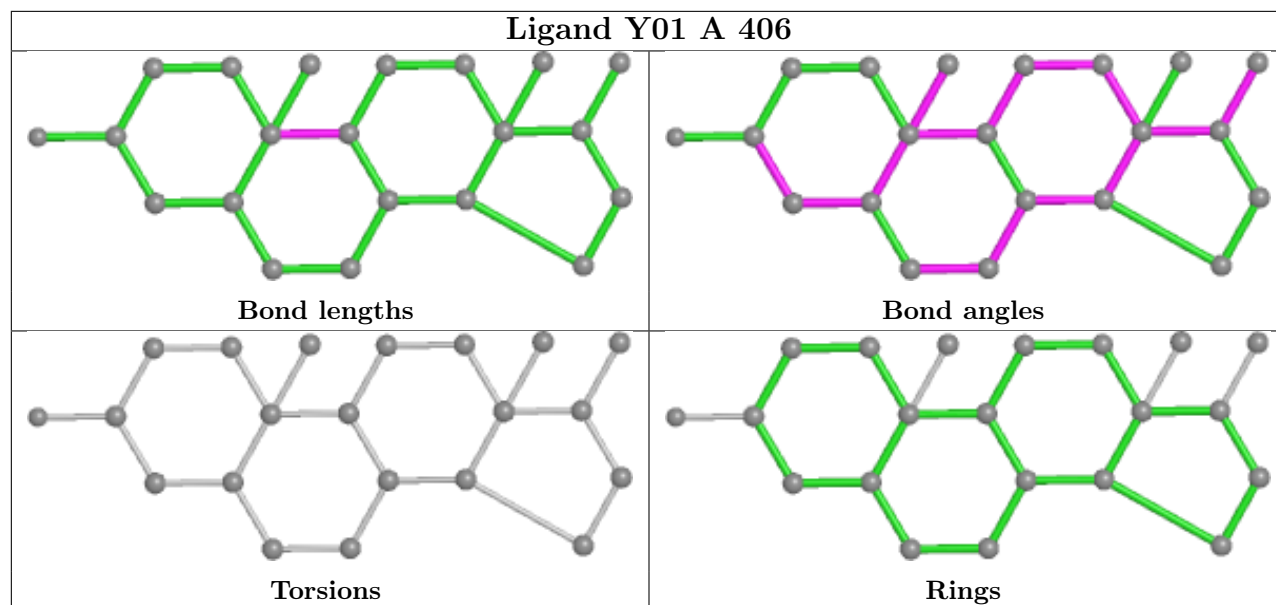
All (1) ring outliers are listed below:

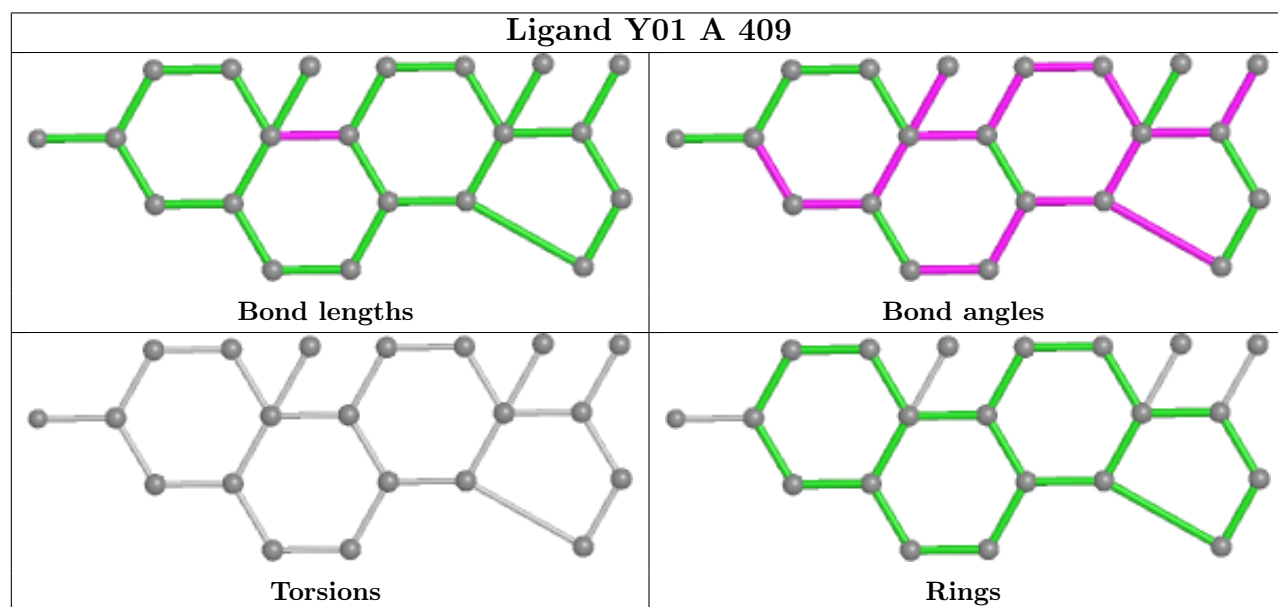
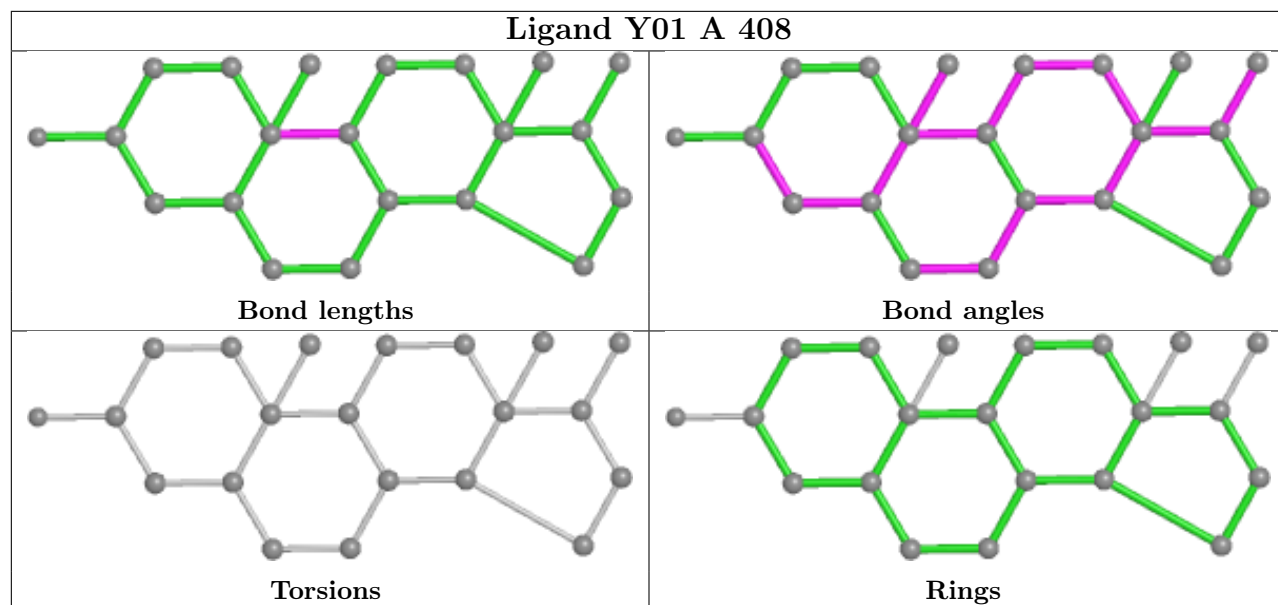
Mol	Chain	Res	Type	Atoms
10	B	406	MAN	C1-C2-C3-C4-C5-O5

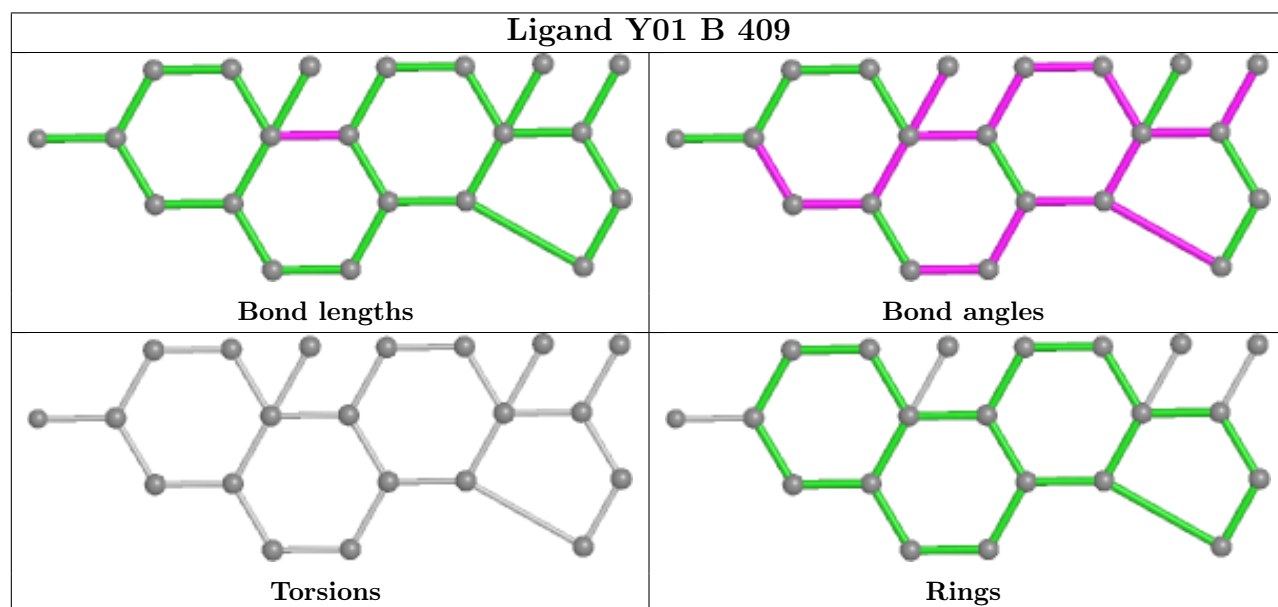
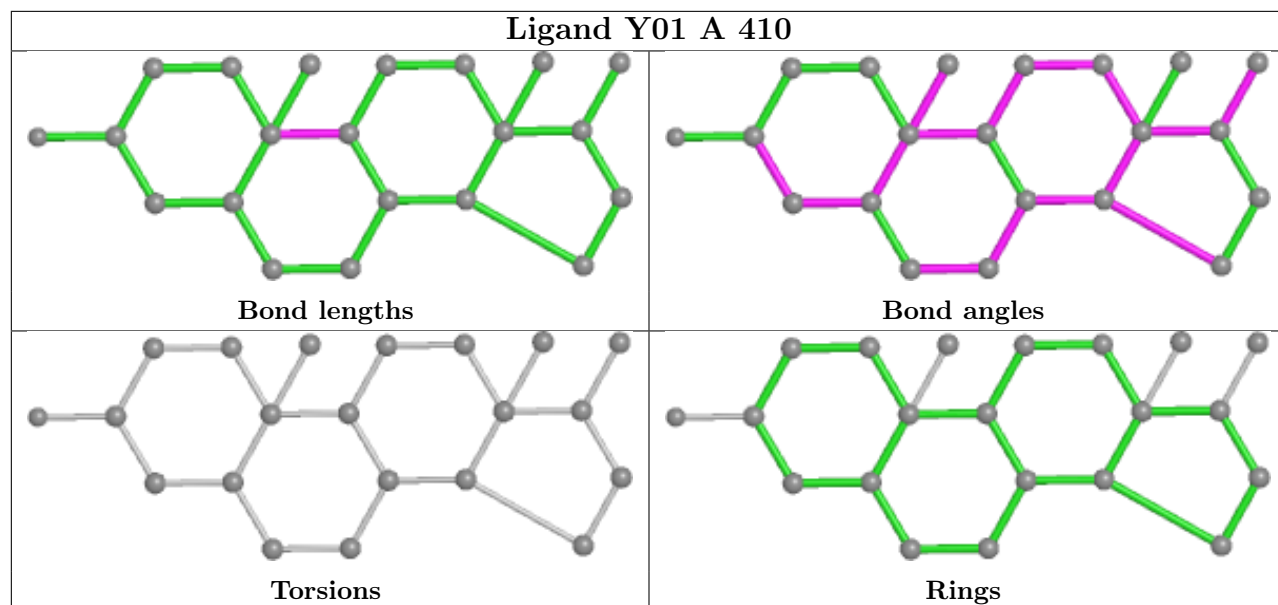
10 monomers are involved in 13 short contacts:

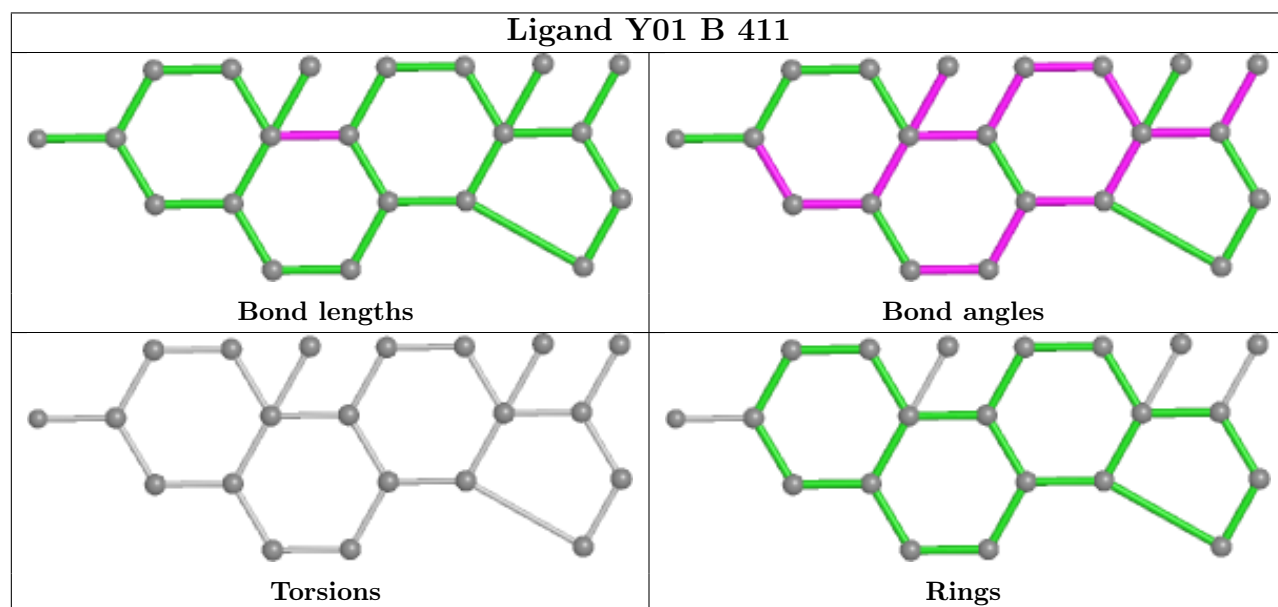
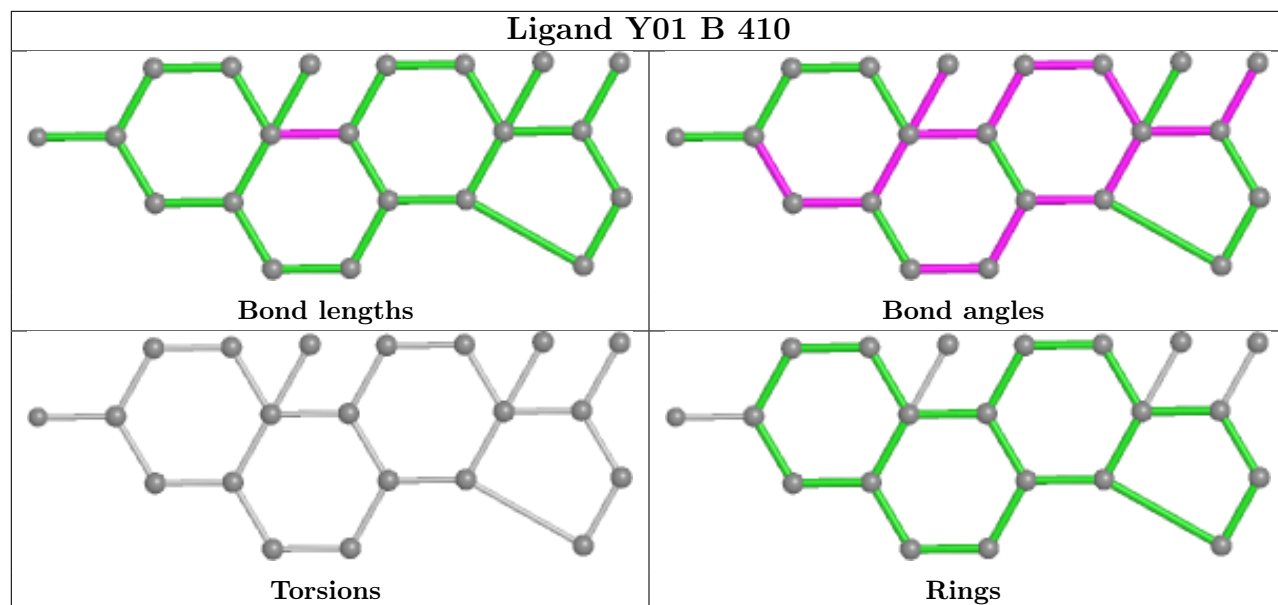
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	NAG	1	0
9	A	406	Y01	2	0
9	A	407	Y01	1	0
9	A	409	Y01	2	0
9	B	409	Y01	1	0
9	B	411	Y01	1	0
6	C	401	NAG	1	0
6	C	402	NAG	2	0
8	C	405	ABU	1	0
9	D	407	Y01	1	0

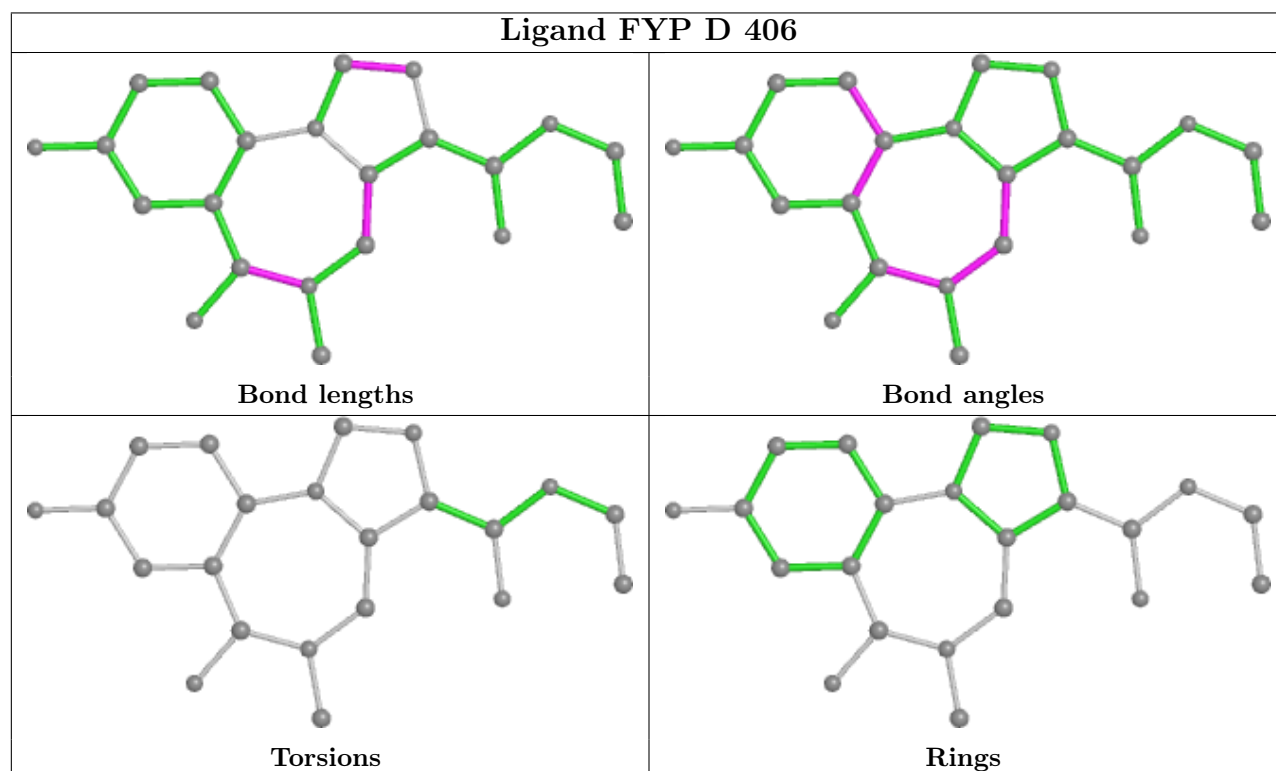
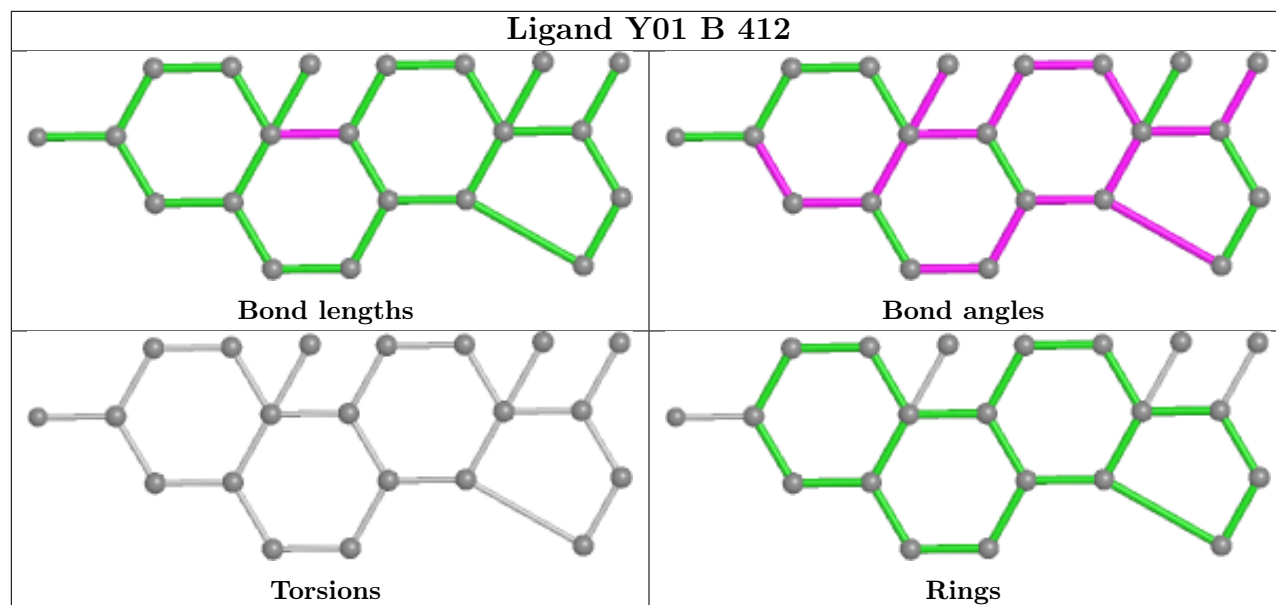
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

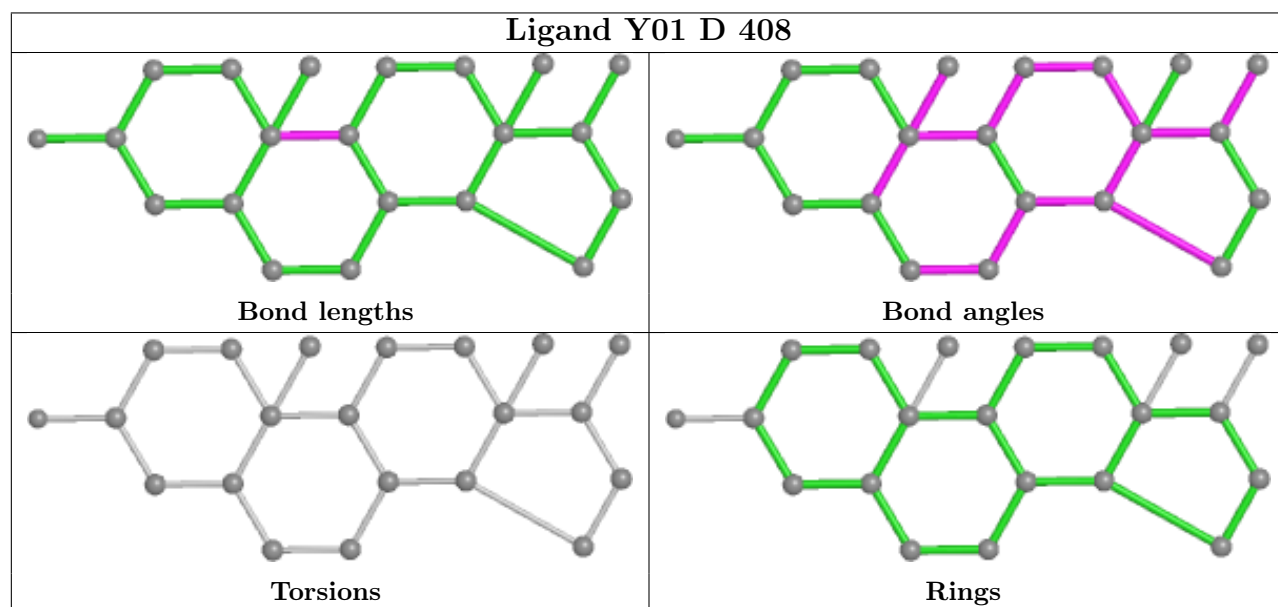
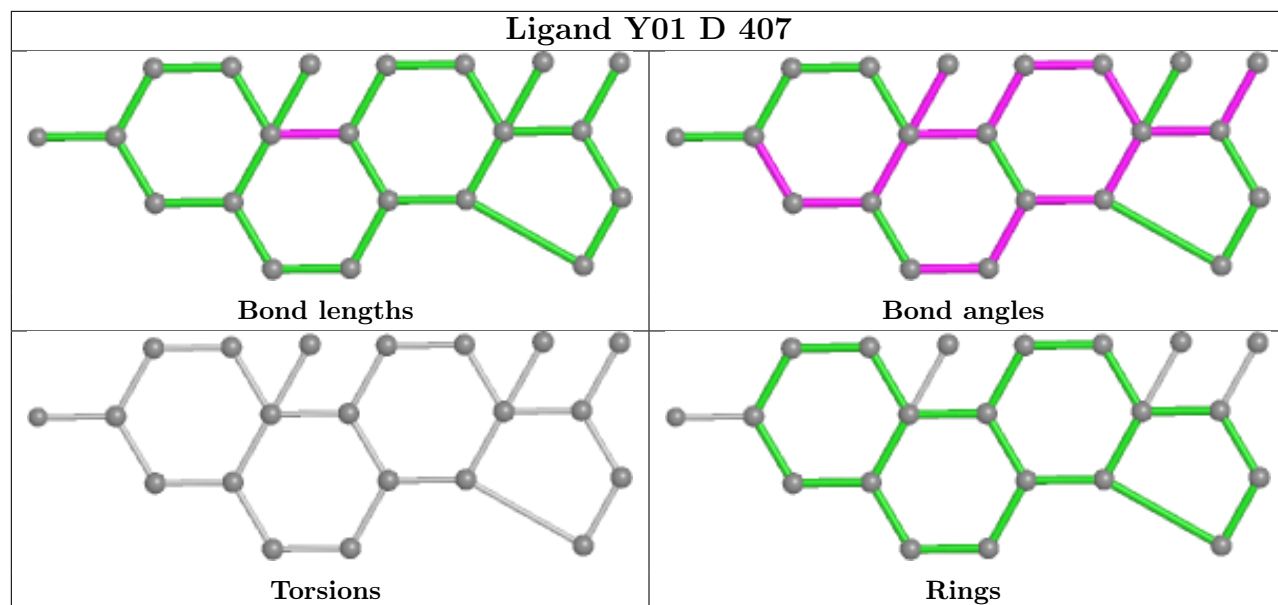


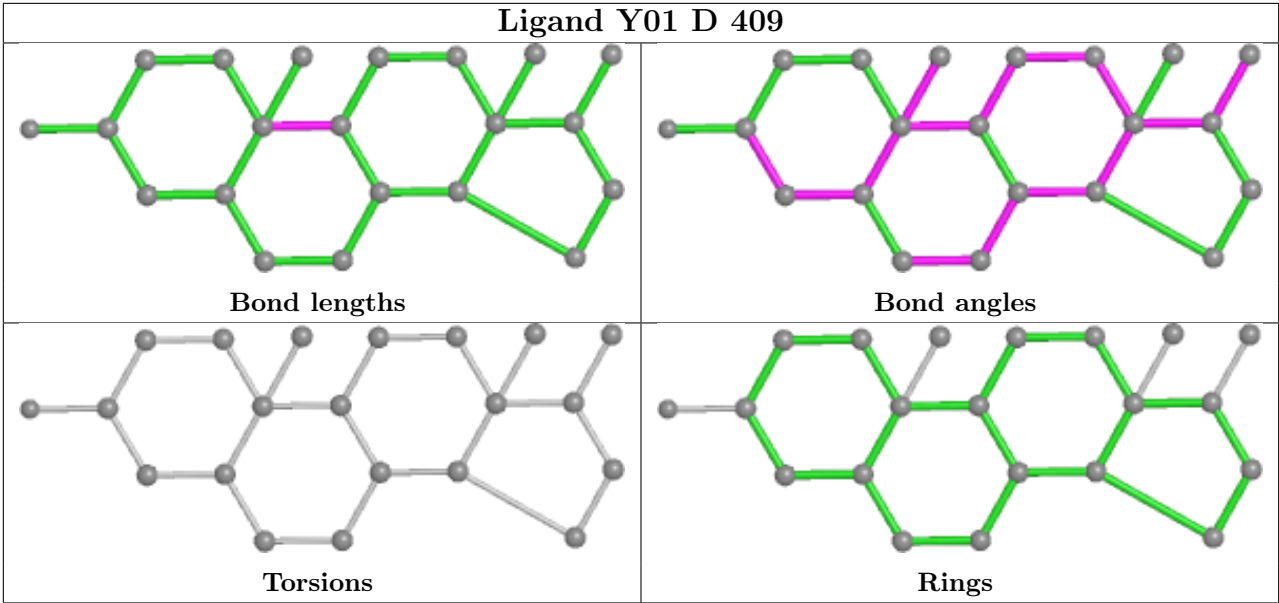












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	318:UNK	C	327:UNK	N	16.64
1	E	287:LEU	C	297:UNK	N	10.85