



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:30 PM UTC

PDB ID : 9LFQ / pdb_00009lfq
Title : Complex crystal structure of transaldolase AprG with GlcNAc from *Streptococcus tenebrarius*
Authors : Xie, Z.Z.; Li, Q.R.; Zhang, L.L.; Huang, J.-W.; He, Y.T.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2025-01-08
Resolution : 2.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

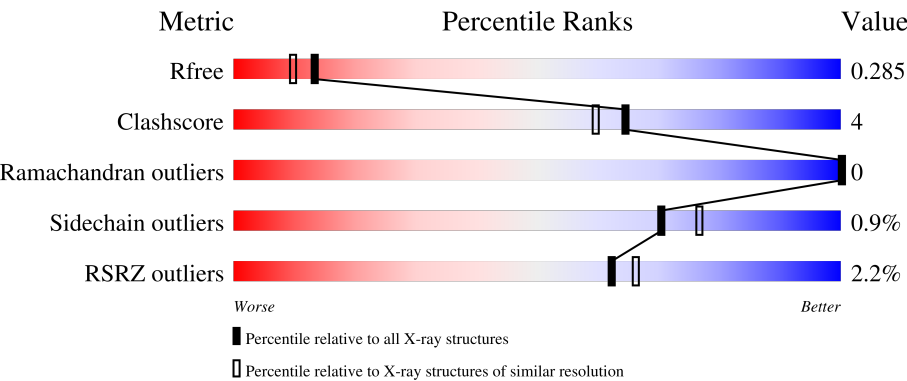
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	345	4% 86% 11% .
1	D	345	2% 88% 9% ..
1	E	345	% 87% 9% .
2	B	345	% 85% 12% .

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Mol	Chain	Length	Quality of chain
2	C	345	% 86% 12% ••
3	F	345	2% 90% 7% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16121 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 AprG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2575	1621	446	497	11			
1	D	335	Total	C	N	O	S	0	0	0
			2584	1627	448	498	11			
1	E	332	Total	C	N	O	S	0	0	0
			2563	1615	443	494	11			

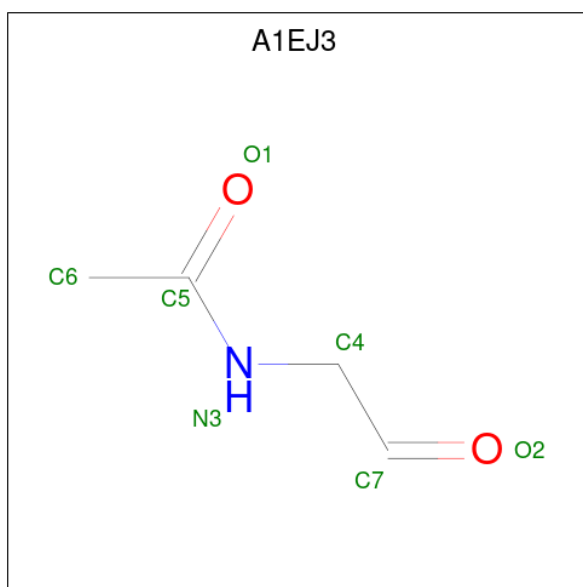
- Molecule 2 is a protein called AprG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	335	Total	C	N	O	S	0	0	0
			2587	1628	448	500	11			
2	C	339	Total	C	N	O	S	0	0	0
			2613	1645	453	504	11			

- Molecule 3 is a protein called AprG.

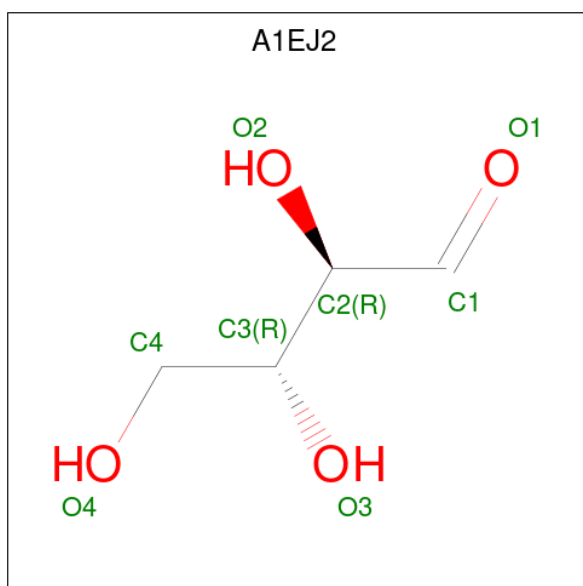
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	336	Total	C	N	O	S	0	0	0
			2602	1637	450	504	11			

- Molecule 4 is {N}-(2-oxidanylideneethyl)ethanamide (CCD ID: A1EJ3) (formula: C₄H₇NO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is D-Erythrose (CCD ID: A1EJ2) (formula: $C_4H_8O_4$) (labeled as "Ligand of Interest" by depositor).



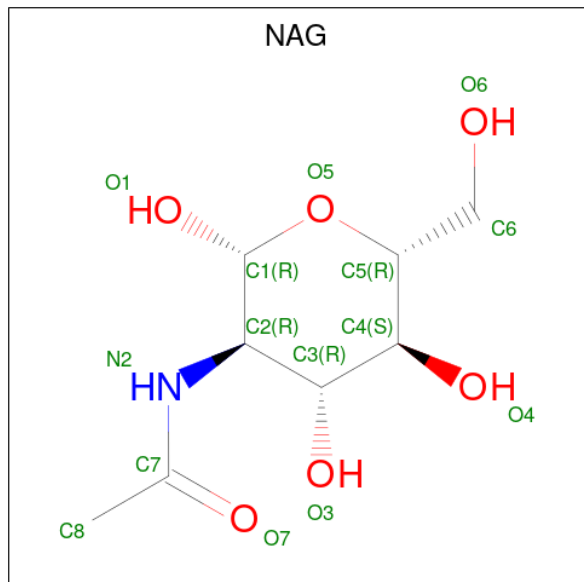
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	E	1	Total C O 8 4 4	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



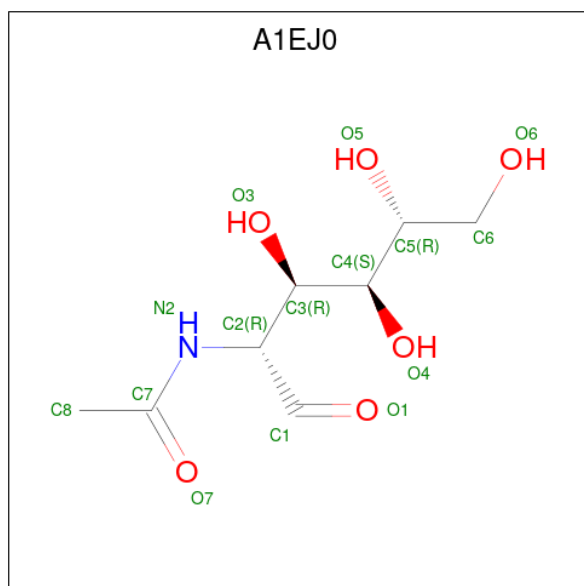
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 8 is N-Acetylglucosamine (CCD ID: A1EJ0) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			15	8	1	6		

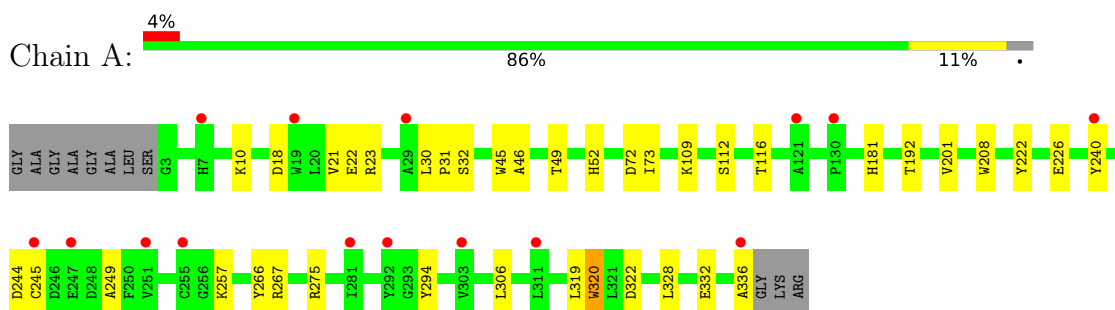
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	64	Total 64	O 64	0	0
9	B	73	Total 73	O 73	0	0
9	C	94	Total 94	O 94	0	0
9	D	86	Total 86	O 86	0	0
9	E	80	Total 80	O 80	0	0
9	F	66	Total 66	O 66	0	0

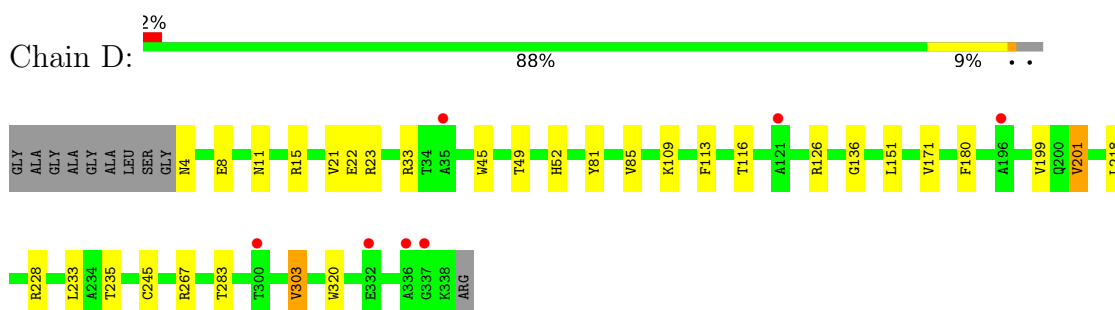
3 Residue-property plots [i](#)

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

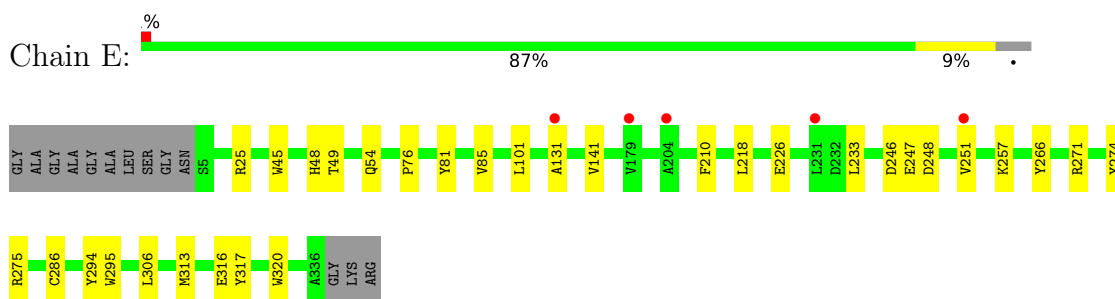
- Molecule 1: AprG



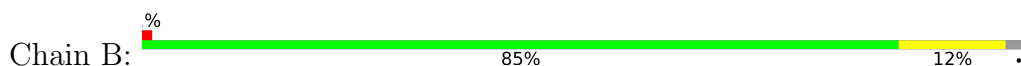
- Molecule 1: AprG

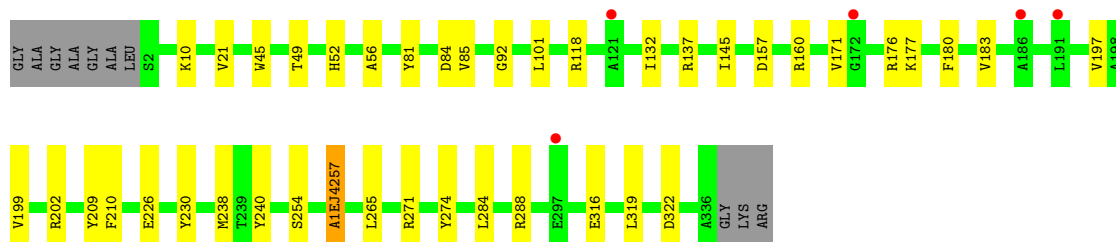


- Molecule 1: AprG

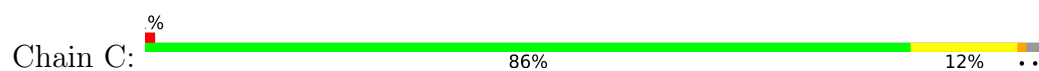


- Molecule 2: AprG

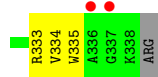
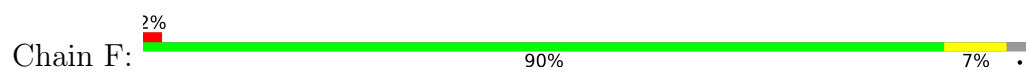




• Molecule 2: AprG



• Molecule 3: AprG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.89Å 140.72Å 130.78Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	36.87 – 2.13 36.87 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.87-2.13) 99.7 (36.87-2.13)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.228 , 0.263 (Not available) , 0.285	Depositor DCC
R_{free} test set	5275 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.256 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16121	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, A1EJ3, A1EJ1, A1EJ0, PEG, A1EJ4, A1EJ2

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	0.09	0/2637	0.25	0/3589
1	D	0.09	0/2646	0.25	0/3600
1	E	0.10	0/2625	0.24	0/3573
2	B	0.08	0/2633	0.26	0/3583
2	C	0.09	0/2659	0.27	0/3617
3	F	0.09	0/2640	0.25	0/3591
All	All	0.09	0/15840	0.25	0/21553

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	257	A1EJ1	Mainchain

5.2 Too-close contacts [i](#)

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	2575	0	2454	24	0
1	D	2584	0	2467	18	0
1	E	2563	0	2445	18	1
2	B	2587	0	2446	22	0
2	C	2613	0	2481	26	0
3	F	2602	0	2457	17	0
4	A	7	0	0	0	0
4	C	7	0	0	0	1
4	D	7	0	0	0	0
5	A	8	0	0	0	0
5	B	8	0	0	1	0
5	C	24	0	0	0	0
5	E	8	0	0	0	0
6	A	14	0	20	0	0
6	B	7	0	10	0	0
6	D	7	0	10	0	0
6	F	7	0	10	2	0
7	B	15	0	15	0	0
8	E	15	0	0	0	0
9	A	64	0	0	1	0
9	B	73	0	0	1	0
9	C	94	0	0	1	0
9	D	86	0	0	1	0
9	E	80	0	0	1	0
9	F	66	0	0	2	0
All	All	16121	0	14815	120	1

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 4.

All (120) 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)
2:C:177:LYS:HD2	2:C:177:LYS:H	1.47	0.80
2:C:118:ARG:NH2	9:C:503:HOH:O	2.28	0.67
1:D:201:VAL:HG13	1:D:245:CYS:HA	1.76	0.66
1:A:45:TRP:CE3	1:A:319:LEU:HD21	2.35	0.62
1:E:218:LEU:HD13	1:E:233:LEU:HG	1.81	0.61
2:B:157:ASP:OD2	2:B:160:ARG:NH1	2.31	0.61
2:C:269:THR:HB	1:E:131:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:ARG:NH1	2:C:161:SER:OG	2.35	0.59
1:E:54:GLN:NE2	9:E:501:HOH:O	2.30	0.59
1:A:266:TYR:OH	1:A:275:ARG:NH2	2.36	0.57
3:F:333:ARG:NH2	9:F:504:HOH:O	2.37	0.56
3:F:45:TRP:CE3	3:F:319:LEU:HD21	2.40	0.56
3:F:3:GLY:N	9:F:506:HOH:O	2.40	0.55
2:B:226:GLU:OE1	1:D:109:LYS:NZ	2.38	0.55
1:A:201:VAL:HG13	1:A:245:CYS:HA	1.89	0.54
1:A:275:ARG:HG3	1:A:328:LEU:HD22	1.88	0.53
2:C:175:ASP:OD1	2:C:177:LYS:HD3	2.09	0.53
3:F:326:ARG:HH11	6:F:401:PEG:H32	1.74	0.53
3:F:46:ALA:HA	3:F:319:LEU:HD13	1.91	0.52
1:E:294:TYR:HB2	1:E:306:LEU:HD11	1.90	0.52
1:A:10:LYS:NZ	1:A:322:ASP:OD2	2.38	0.52
1:A:267:ARG:NH1	9:A:504:HOH:O	2.43	0.52
2:B:118:ARG:NH2	5:B:401:A1EJ2:O3	2.43	0.51
1:D:81:TYR:HA	1:D:85:VAL:HB	1.92	0.51
1:E:271:ARG:HD2	1:E:274:TYR:CE2	2.46	0.51
2:B:45:TRP:O	2:B:49:THR:HG23	2.10	0.51
1:D:218:LEU:HD13	1:D:233:LEU:HG	1.93	0.51
1:A:208:TRP:CG	1:A:249:ALA:HA	2.47	0.50
1:D:33:ARG:HH21	1:D:303:VAL:HG11	1.76	0.50
1:E:45:TRP:O	1:E:49:THR:HG23	2.12	0.49
1:D:22:GLU:OE1	1:D:23:ARG:NH1	2.45	0.49
1:A:46:ALA:HA	1:A:319:LEU:HD13	1.95	0.49
1:D:21:VAL:HG21	1:D:52:HIS:CG	2.47	0.49
1:A:72:ASP:OD1	1:A:73:ILE:N	2.45	0.49
2:C:141:VAL:HG23	2:C:210:PHE:HA	1.94	0.49
1:E:248:ASP:HA	1:E:251:VAL:HB	1.95	0.49
3:F:137:ARG:HD3	3:F:183:VAL:HG11	1.93	0.49
1:E:48:HIS:HD2	1:E:101:LEU:HD13	1.77	0.49
1:A:23:ARG:HB2	1:A:31:PRO:HG3	1.94	0.48
3:F:209:TYR:HB3	3:F:254:SER:HB2	1.95	0.48
3:F:80:ARG:HD2	3:F:83:LEU:HD12	1.95	0.48
2:C:275:ARG:O	2:C:279:GLU:HG2	2.13	0.48
2:C:201:VAL:HG21	2:C:240:TYR:OH	2.13	0.48
2:B:238:MET:HG3	2:B:265:LEU:HD12	1.96	0.48
2:B:45:TRP:CE3	2:B:319:LEU:HD21	2.49	0.48
1:A:109:LYS:NZ	1:E:226:GLU:OE2	2.46	0.47
2:B:197:VAL:HG11	2:B:210:PHE:CZ	2.49	0.47
1:E:257:LYS:NZ	1:E:316:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:O	1:A:49:THR:HG23	2.15	0.47
2:C:319:LEU:HD12	2:C:320:TRP:CZ3	2.50	0.47
2:C:209:TYR:HB3	2:C:254:SER:HB2	1.97	0.47
3:F:45:TRP:O	3:F:49:THR:HG23	2.16	0.46
1:A:275:ARG:HH22	1:A:332:GLU:HB2	1.80	0.46
2:B:176:ARG:O	2:B:240:TYR:OH	2.32	0.46
1:D:113:PHE:O	1:D:116:THR:OG1	2.30	0.46
2:C:54:GLN:HG2	3:F:326:ARG:HA	1.98	0.46
2:B:177:LYS:HB3	2:B:202:ARG:HH21	1.81	0.46
1:D:126:ARG:HD2	1:D:136:GLY:HA2	1.97	0.46
1:E:246:ASP:OD1	1:E:247:GLU:N	2.49	0.46
2:B:137:ARG:HD3	2:B:183:VAL:HG11	1.98	0.45
1:E:266:TYR:CZ	1:E:275:ARG:HD2	2.51	0.45
2:C:256:GLY:HA3	2:C:320:TRP:CD1	2.52	0.45
1:D:4:ASN:ND2	1:D:8:GLU:OE1	2.48	0.45
2:B:288:ARG:NH1	9:B:505:HOH:O	2.43	0.45
2:C:338:LYS:HB3	1:E:76:PRO:HD3	1.98	0.45
1:E:81:TYR:HA	1:E:85:VAL:HB	1.97	0.45
3:F:264:LEU:HD13	6:F:401:PEG:H22	1.99	0.45
1:A:181:HIS:CD2	1:A:192:THR:HG22	2.51	0.45
2:C:45:TRP:O	2:C:49:THR:HG23	2.17	0.45
2:C:275:ARG:NH2	2:C:332:GLU:OE2	2.50	0.45
1:A:222:TYR:O	1:A:226:GLU:N	2.38	0.44
3:F:271:ARG:HE	3:F:271:ARG:HB3	1.45	0.44
1:D:180:PHE:HB3	1:D:199:VAL:HB	2.00	0.44
3:F:330:SER:O	3:F:334:VAL:HG12	2.18	0.44
2:B:81:TYR:HA	2:B:85:VAL:HB	1.99	0.44
1:D:45:TRP:O	1:D:49:THR:HG23	2.18	0.44
3:F:294:TYR:HB2	3:F:306:LEU:HD11	1.99	0.44
2:C:241:MET:HA	2:C:245:CYS:SG	2.58	0.44
2:B:10:LYS:NZ	2:B:322:ASP:OD2	2.35	0.43
2:B:180:PHE:HB3	2:B:199:VAL:HB	1.99	0.43
1:D:228:ARG:O	1:D:228:ARG:HG3	2.17	0.43
1:A:21:VAL:HG21	1:A:52:HIS:CG	2.54	0.43
3:F:81:TYR:HA	3:F:85:VAL:HB	2.00	0.43
2:B:84:ASP:HB3	2:B:132:ILE:HG21	2.00	0.43
2:B:21:VAL:HG21	2:B:52:HIS:CG	2.54	0.43
1:A:201:VAL:HG21	1:A:240:TYR:OH	2.19	0.42
2:C:88:LEU:HD21	2:C:117:MET:HG3	2.01	0.42
1:D:4:ASN:N	1:D:283:THR:OG1	2.52	0.42
2:C:81:TYR:HA	2:C:85:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:NH2	9:D:513:HOH:O	2.52	0.42
2:C:208:TRP:CG	2:C:249:ALA:HA	2.55	0.42
2:B:271:ARG:HB2	2:B:274:TYR:CD2	2.54	0.42
1:A:18:ASP:O	1:A:22:GLU:HG3	2.20	0.42
1:A:112:SER:O	1:A:116:THR:HG23	2.18	0.42
2:B:160:ARG:HG2	2:B:230:TYR:OH	2.20	0.42
2:C:21:VAL:HG21	2:C:52:HIS:CG	2.55	0.42
2:B:92:GLY:HA3	2:B:145:ILE:HG13	2.01	0.42
2:C:44:MET:HE1	2:C:98:ALA:HB2	2.01	0.42
3:F:201:VAL:HG11	3:F:240:TYR:OH	2.20	0.42
2:C:177:LYS:H	2:C:177:LYS:CD	2.19	0.42
2:C:295:TRP:CD2	2:C:317:TYR:HD2	2.37	0.41
2:B:209:TYR:HB3	2:B:254:SER:HB2	2.03	0.41
1:D:11:ASN:O	1:D:15:ARG:HG3	2.21	0.41
1:A:332:GLU:HG3	1:A:336:ALA:HB3	2.03	0.41
1:E:295:TRP:HB3	1:E:313:MET:HE3	2.03	0.41
1:A:294:TYR:HB2	1:A:306:LEU:HD11	2.02	0.41
2:B:56:ALA:HB1	2:B:101:LEU:HD11	2.03	0.41
1:E:141:VAL:HG23	1:E:210:PHE:HA	2.03	0.41
1:D:33:ARG:NH2	1:D:303:VAL:HG11	2.36	0.41
2:C:176:ARG:O	2:C:240:TYR:OH	2.35	0.40
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.97	0.40
2:B:257:A1EJ4:N8	2:B:316:GLU:OE1	2.54	0.40
2:C:126:ARG:NH2	2:C:129:GLY:O	2.54	0.40
3:F:334:VAL:HG13	3:F:335:TRP:CD1	2.56	0.40
1:A:30:LEU:O	1:A:32:SER:N	2.54	0.40
1:A:257:LYS:HD2	1:A:320:TRP:HE1	1.86	0.40
1:E:25:ARG:HE	1:E:25:ARG:HB3	1.73	0.40
1:A:244:ASP:OD1	1:A:244:ASP:N	2.54	0.40
2:C:55:ALA:O	2:C:59:VAL:HG23	2.22	0.40
1:E:295:TRP:CD2	1:E:317:TYR:HD2	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ARG:NH1	4:C:401:A1EJ3:O1[1_455]	1.31	0.89

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	332/345 (96%)	321 (97%)	11 (3%)	0	100	100
1	D	333/345 (96%)	323 (97%)	10 (3%)	0	100	100
1	E	330/345 (96%)	321 (97%)	9 (3%)	0	100	100
2	B	332/345 (96%)	325 (98%)	7 (2%)	0	100	100
2	C	336/345 (97%)	325 (97%)	11 (3%)	0	100	100
3	F	333/345 (96%)	324 (97%)	9 (3%)	0	100	100
All	All	1996/2070 (96%)	1939 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/264 (98%)	259 (100%)	1 (0%)	84	88
1	D	261/264 (99%)	256 (98%)	5 (2%)	50	55
1	E	259/264 (98%)	257 (99%)	2 (1%)	73	79
2	B	260/263 (99%)	258 (99%)	2 (1%)	73	79
2	C	262/263 (100%)	259 (99%)	3 (1%)	65	71
3	F	260/263 (99%)	259 (100%)	1 (0%)	84	88
All	All	1562/1581 (99%)	1548 (99%)	14 (1%)	70	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	TRP
2	B	171	VAL
2	B	284	LEU
2	C	141	VAL
2	C	197	VAL
2	C	319	LEU
1	D	171	VAL
1	D	201	VAL
1	D	235	THR
1	D	303	VAL
1	D	320	TRP
1	E	286	CYS
1	E	320	TRP
3	F	320	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	181	HIS
2	B	181	HIS
2	C	11	ASN
1	D	4	ASN
1	D	54	GLN
1	E	54	GLN
1	E	68	GLN
1	E	178	ASN
1	E	181	HIS
1	E	200	GLN
3	F	7	HIS
3	F	48	HIS
3	F	54	GLN
3	F	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
2	A1EJ4	C	257	2	13,14,15	0.49	0	7,15,17	0.89	1 (14%)
3	A1EJ1	F	257	3	20,22,23	0.55	0	18,27,29	0.69	1 (5%)
2	A1EJ4	B	257	2	13,14,15	0.48	0	7,15,17	0.82	1 (14%)

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
2	A1EJ4	C	257	2	-	0/10/13/15	-
3	A1EJ1	F	257	3	-	7/26/29/31	-
2	A1EJ4	B	257	2	-	2/10/13/15	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	257	A1EJ1	CE-NZ-C16	-2.78	113.83	117.18
2	C	257	A1EJ4	CE-NZ-C12	-2.34	114.36	117.18
2	B	257	A1EJ4	CE-NZ-C12	-2.16	114.57	117.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	257	A1EJ1	C14-C15-C17-C18
3	F	257	A1EJ1	C14-C15-C17-O7
3	F	257	A1EJ1	O9-C15-C17-C18

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Mol	Chain	Res	Type	Atoms
3	F	257	A1EJ1	O9-C15-C17-O7
3	F	257	A1EJ1	C13-C16-NZ-CE
3	F	257	A1EJ1	CA-CB-CG-CD
2	B	257	A1EJ4	CD-CE-NZ-C12
3	F	257	A1EJ1	CD-CE-NZ-C16
2	B	257	A1EJ4	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	257	A1EJ4	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
5	A1EJ2	A	402	-	5,7,7	0.08	0	4,8,8	0.25	0
4	A1EJ3	D	401	-	6,6,6	0.08	0	4,6,6	0.08	0
8	A1EJ0	E	401	-	13,14,14	0.08	0	14,18,18	0.20	0
6	PEG	A	403	-	6,6,6	0.26	0	5,5,5	0.26	0
6	PEG	B	403	-	6,6,6	0.25	0	5,5,5	0.28	0
5	A1EJ2	C	403	-	5,7,7	0.03	0	4,8,8	0.11	0
6	PEG	F	401	-	6,6,6	0.24	0	5,5,5	0.42	0
4	A1EJ3	C	401	-	6,6,6	0.74	0	4,6,6	0.45	0
4	A1EJ3	A	401	-	6,6,6	0.08	0	4,6,6	0.07	0
6	PEG	A	404	-	6,6,6	0.26	0	5,5,5	0.26	0
6	PEG	D	402	-	6,6,6	0.25	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1EJ2	B	401	-	5,7,7	0.04	0	4,8,8	0.13	0
7	NAG	B	402	-	15,15,15	0.57	0	21,21,21	0.62	0
5	A1EJ2	C	404	-	5,7,7	0.04	0	4,8,8	0.11	0
5	A1EJ2	C	402	-	5,7,7	0.04	0	4,8,8	0.15	0
5	A1EJ2	E	402	-	5,7,7	0.05	0	4,8,8	0.10	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
5	A1EJ2	A	402	-	-	3/7/8/8	-
4	A1EJ3	D	401	-	-	1/3/4/4	-
8	A1EJ0	E	401	-	-	5/19/20/20	-
6	PEG	A	403	-	-	2/4/4/4	-
6	PEG	B	403	-	-	1/4/4/4	-
5	A1EJ2	C	403	-	-	0/7/8/8	-
6	PEG	F	401	-	-	3/4/4/4	-
4	A1EJ3	C	401	-	-	0/3/4/4	-
4	A1EJ3	A	401	-	-	0/3/4/4	-
6	PEG	A	404	-	-	1/4/4/4	-
6	PEG	D	402	-	-	1/4/4/4	-
5	A1EJ2	B	401	-	-	1/7/8/8	-
7	NAG	B	402	-	-	4/6/26/26	0/1/1/1
5	A1EJ2	C	404	-	-	5/7/8/8	-
5	A1EJ2	C	402	-	-	5/7/8/8	-
5	A1EJ2	E	402	-	-	1/7/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	402	A1EJ2	O1-C1-C2-C3
5	B	401	A1EJ2	O1-C1-C2-C3
5	C	402	A1EJ2	C1-C2-C3-C4
5	C	402	A1EJ2	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	C	402	A1EJ2	C1-C2-C3-O3
5	C	402	A1EJ2	O2-C2-C3-O3
5	C	402	A1EJ2	O1-C1-C2-C3
5	C	404	A1EJ2	C1-C2-C3-C4
5	C	404	A1EJ2	O2-C2-C3-C4
5	C	404	A1EJ2	C1-C2-C3-O3
5	C	404	A1EJ2	O2-C2-C3-O3
5	C	404	A1EJ2	O1-C1-C2-C3
5	E	402	A1EJ2	O1-C1-C2-C3
8	E	401	A1EJ0	C1-C2-N2-C7
8	E	401	A1EJ0	C3-C2-N2-C7
7	B	402	NAG	O5-C5-C6-O6
7	B	402	NAG	C4-C5-C6-O6
7	B	402	NAG	C8-C7-N2-C2
7	B	402	NAG	O7-C7-N2-C2
6	F	401	PEG	C1-C2-O2-C3
6	D	402	PEG	O2-C3-C4-O4
6	F	401	PEG	O1-C1-C2-O2
6	A	403	PEG	O1-C1-C2-O2
5	A	402	A1EJ2	O3-C3-C4-O4
6	A	404	PEG	O1-C1-C2-O2
5	A	402	A1EJ2	C2-C3-C4-O4
8	E	401	A1EJ0	C2-C3-C4-C5
6	A	403	PEG	C4-C3-O2-C2
8	E	401	A1EJ0	O3-C3-C4-C5
6	B	403	PEG	C4-C3-O2-C2
6	F	401	PEG	O2-C3-C4-O4
4	D	401	A1EJ3	C7-C4-N3-C5
8	E	401	A1EJ0	O3-C3-C4-O4

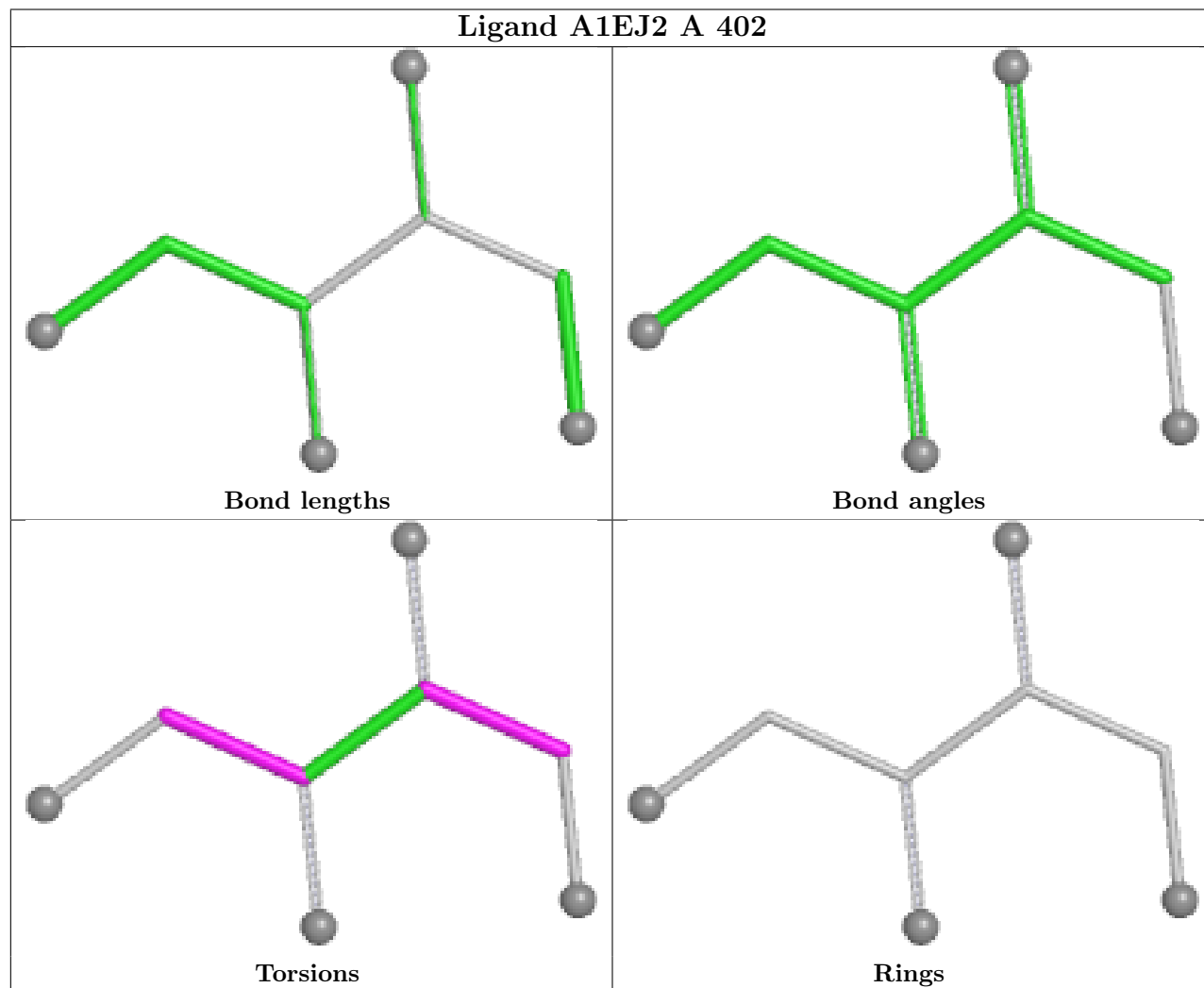
There are no ring outliers.

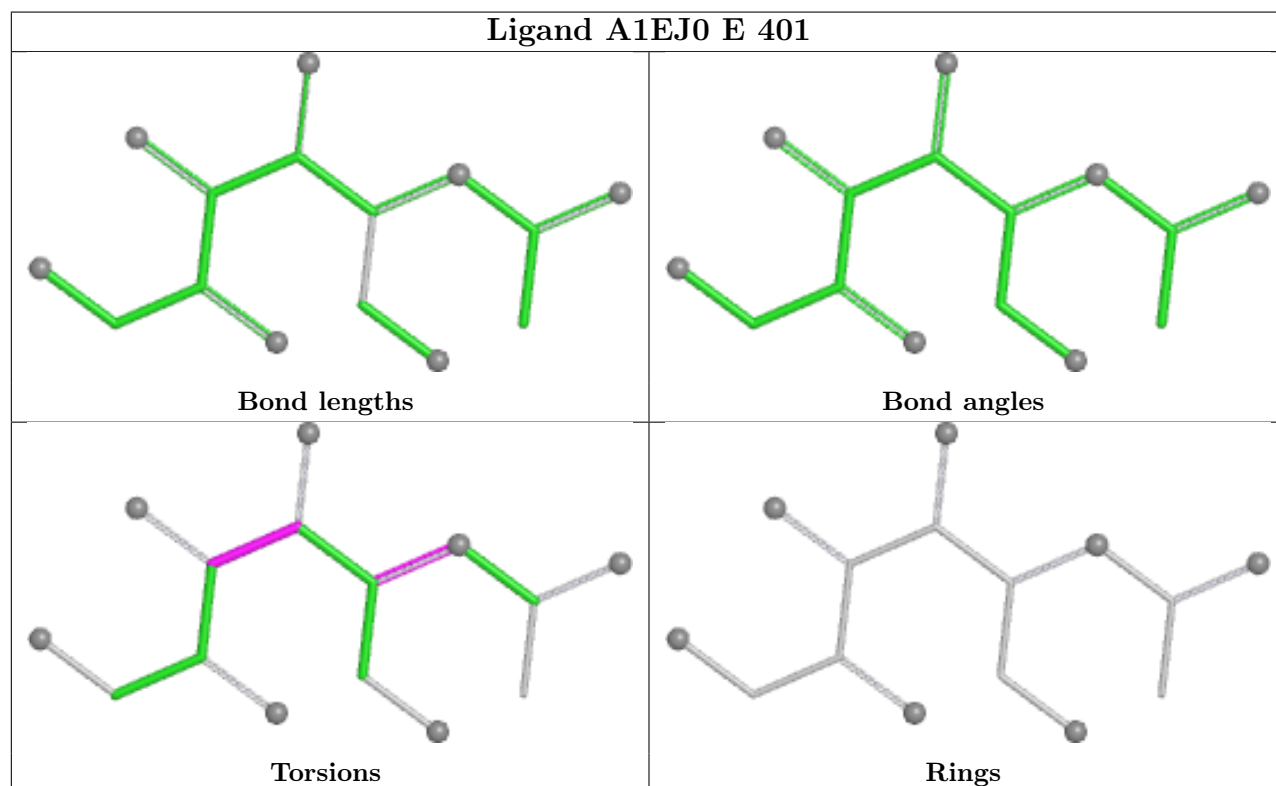
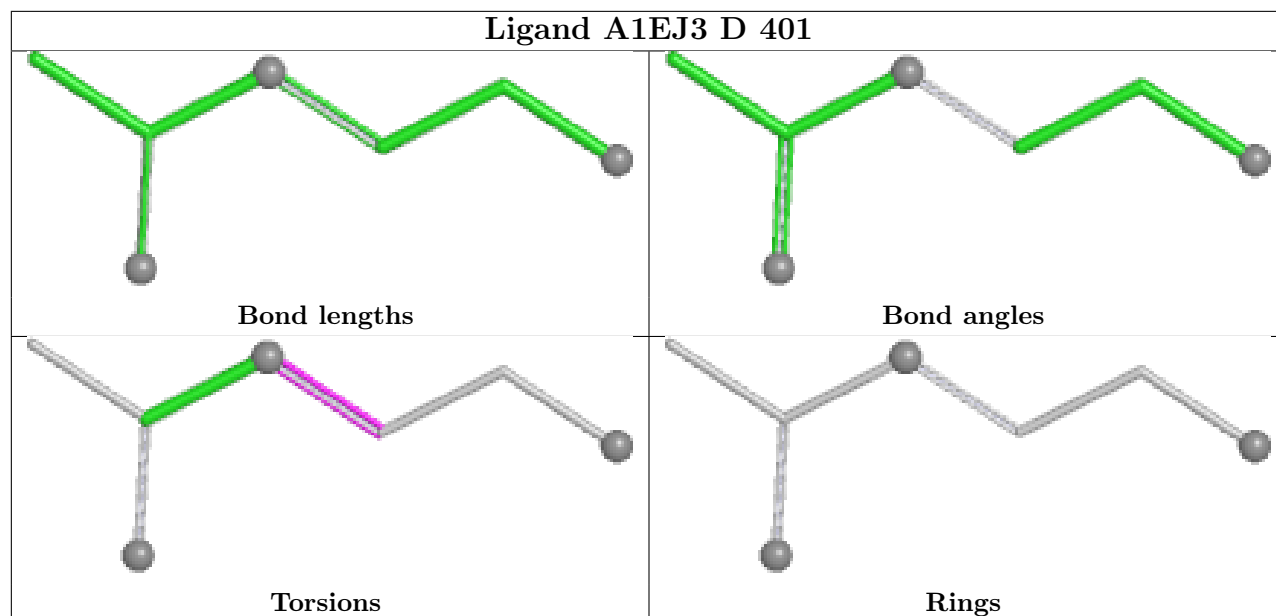
3 monomers are involved in 4 short contacts:

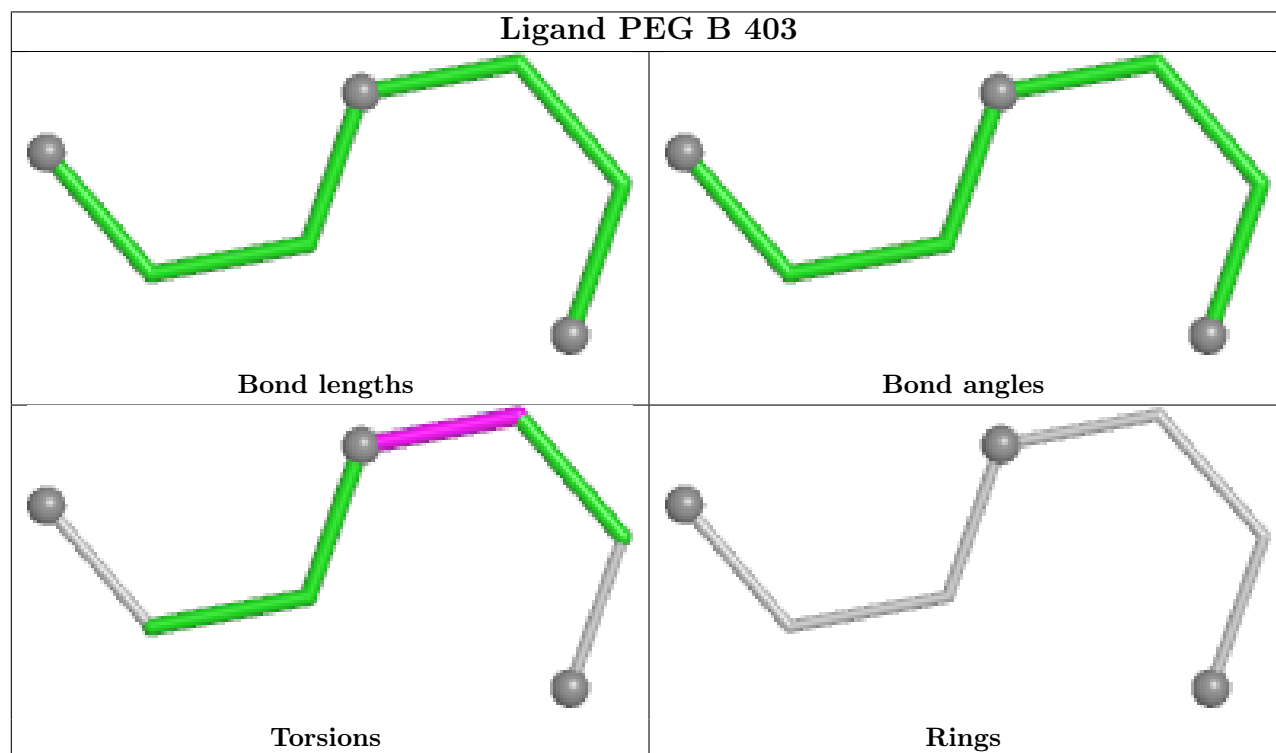
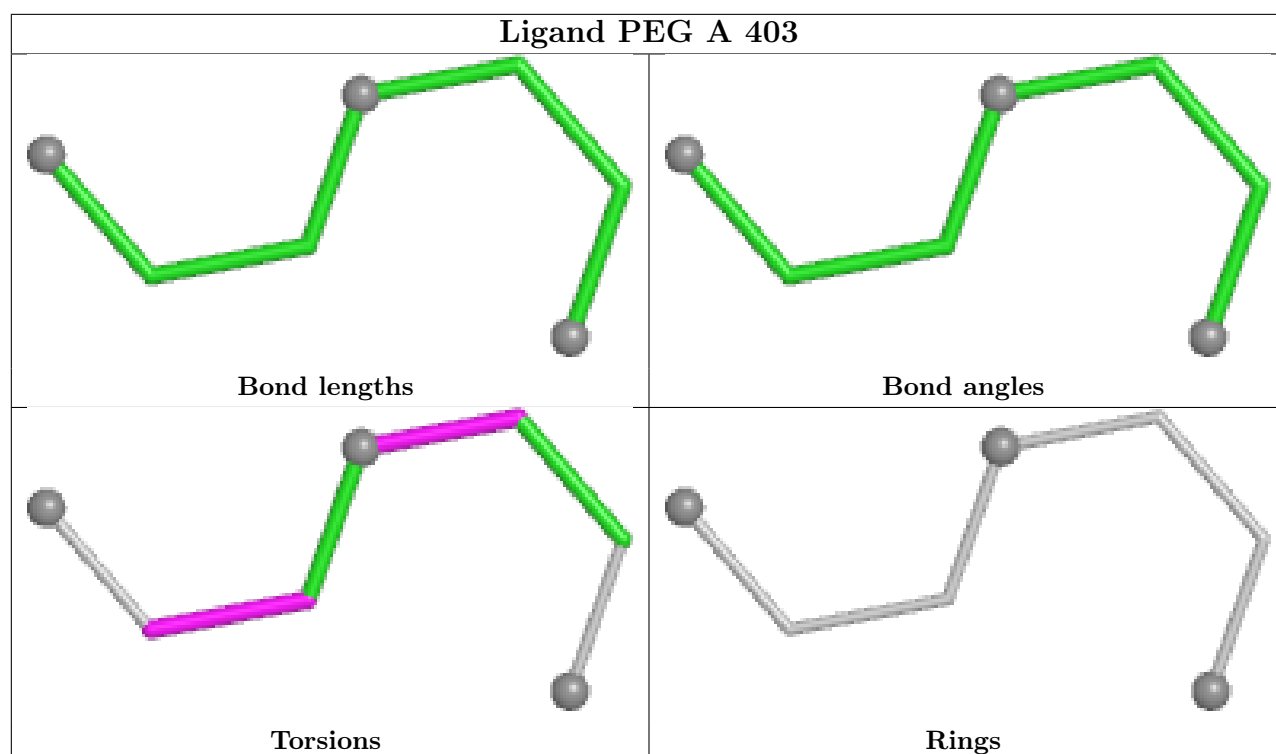
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	401	PEG	2	0
4	C	401	A1EJ3	0	1
5	B	401	A1EJ2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

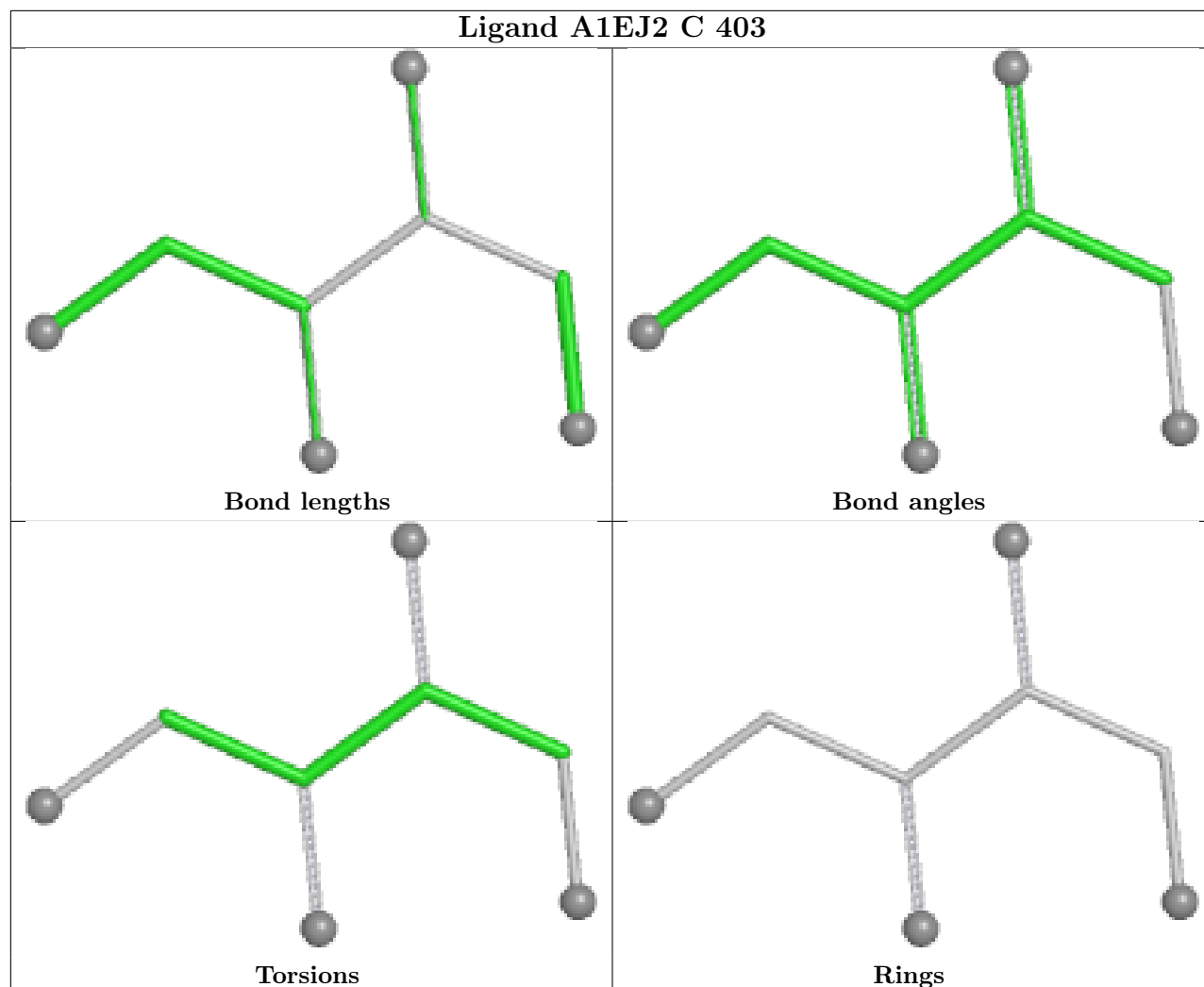
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



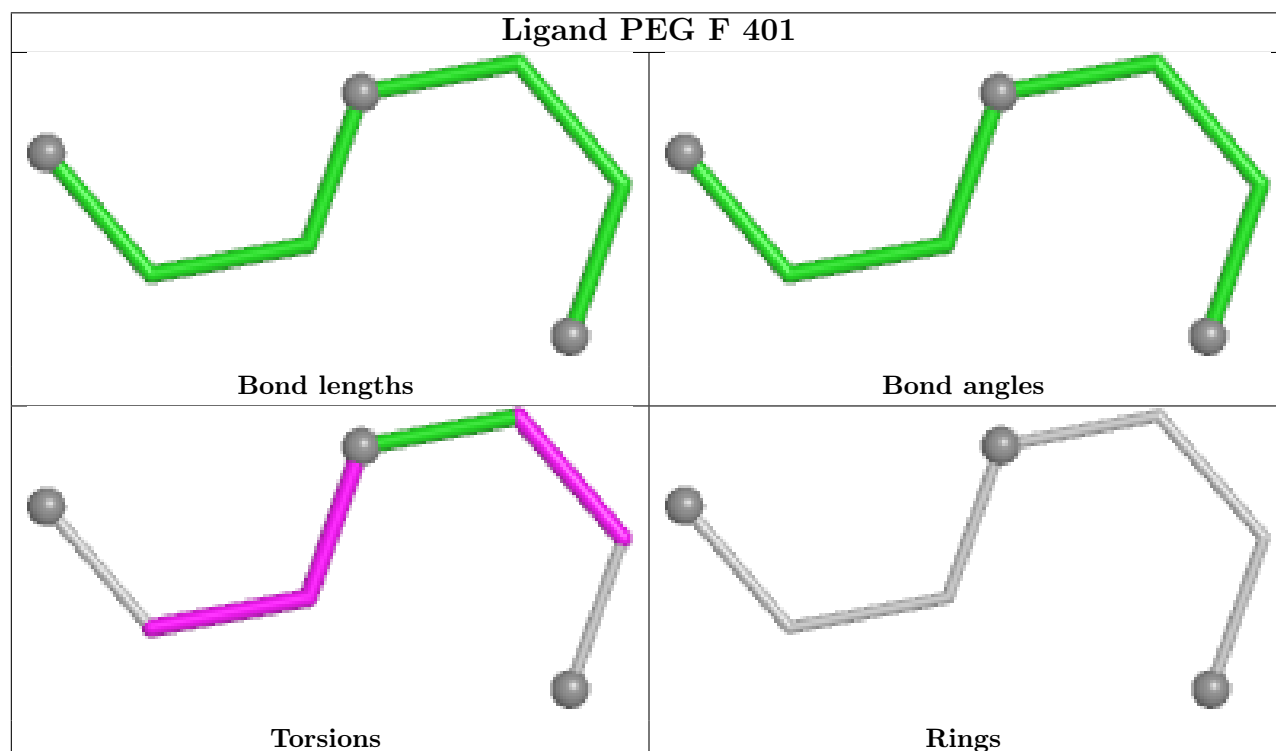


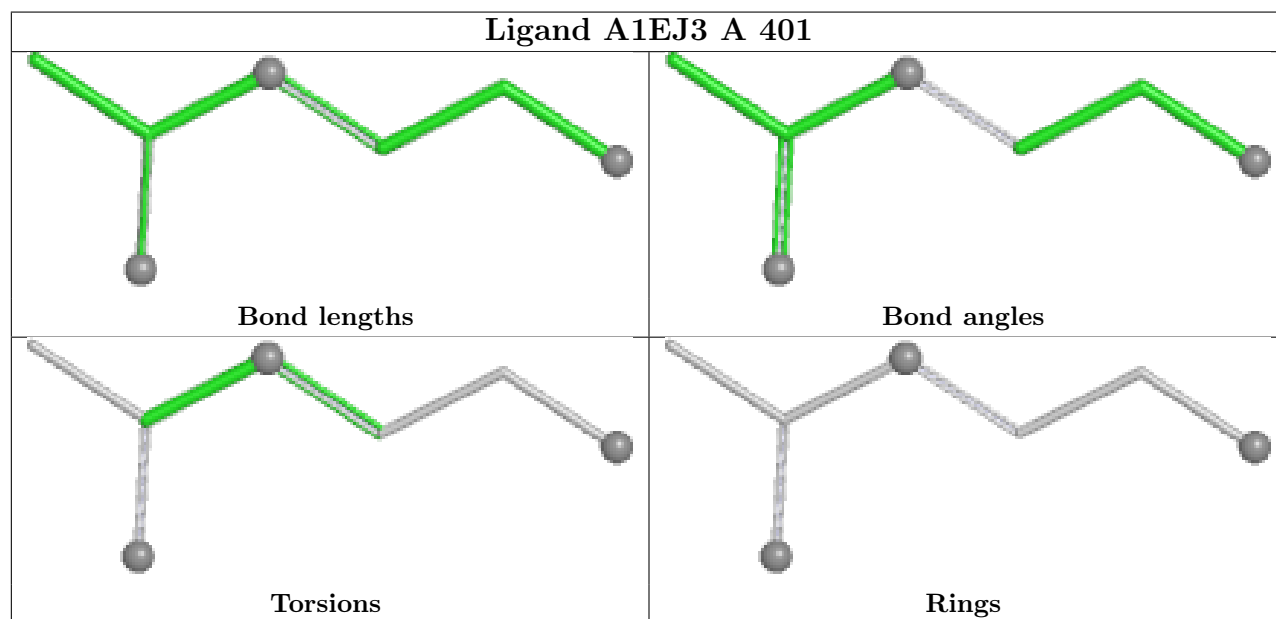
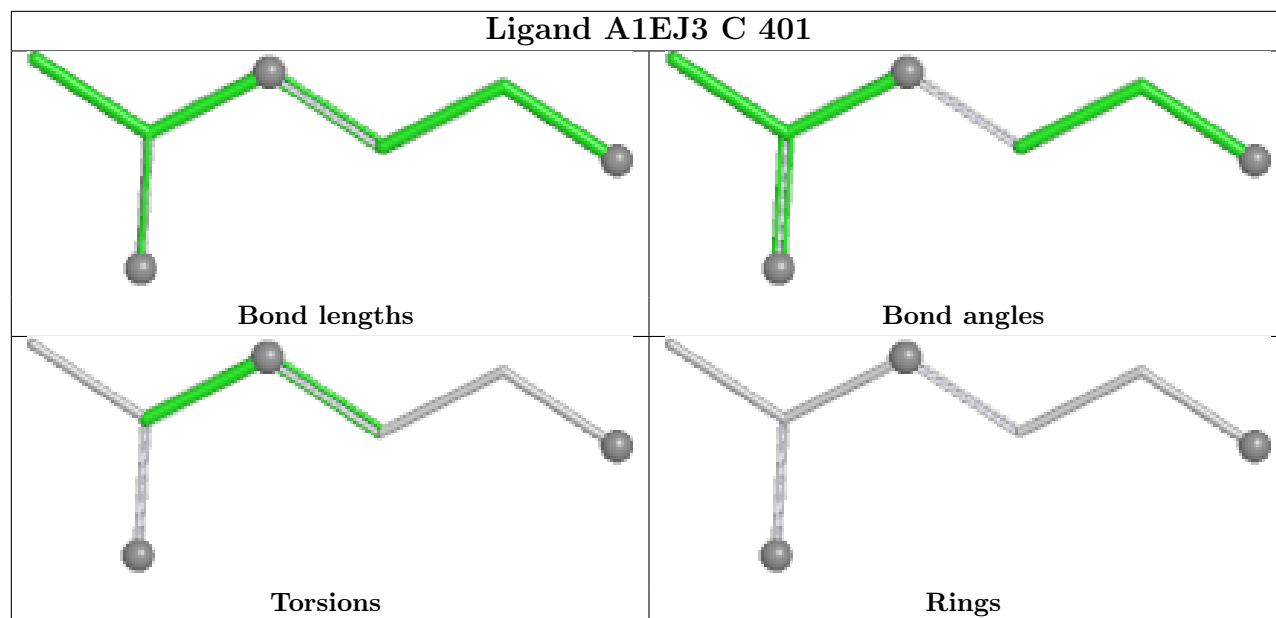


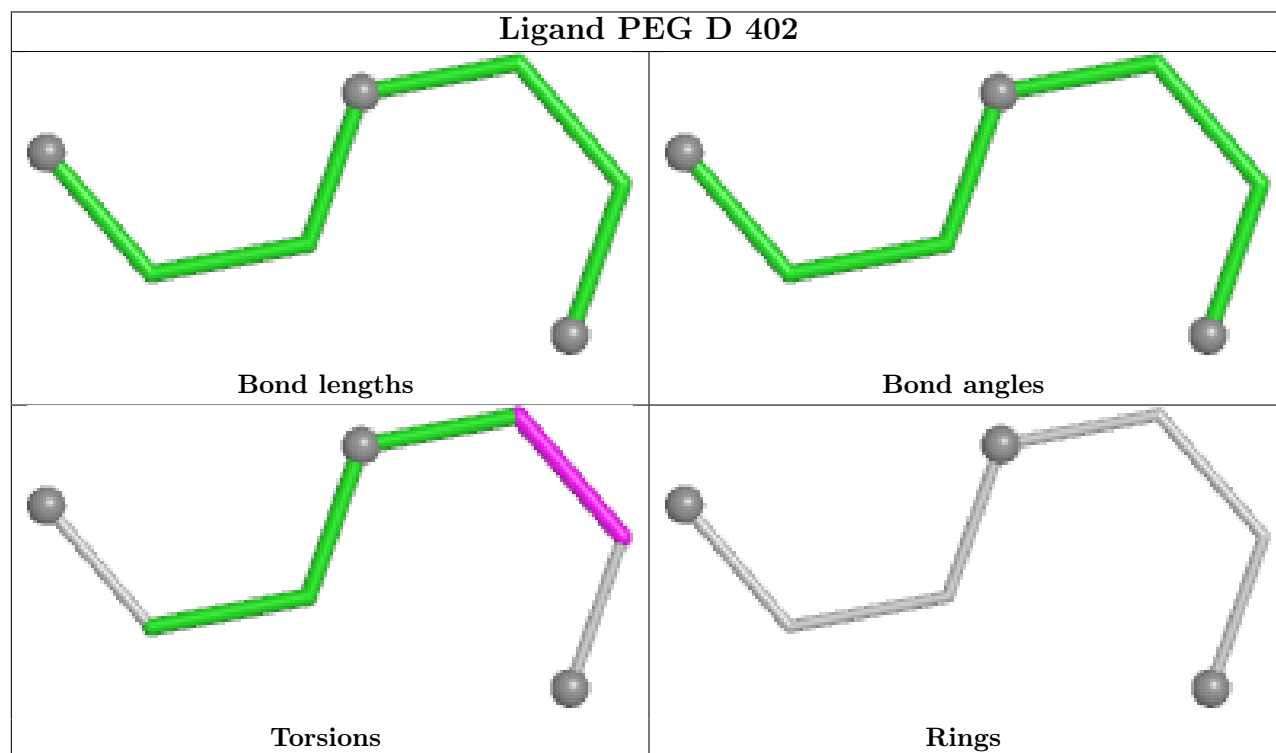
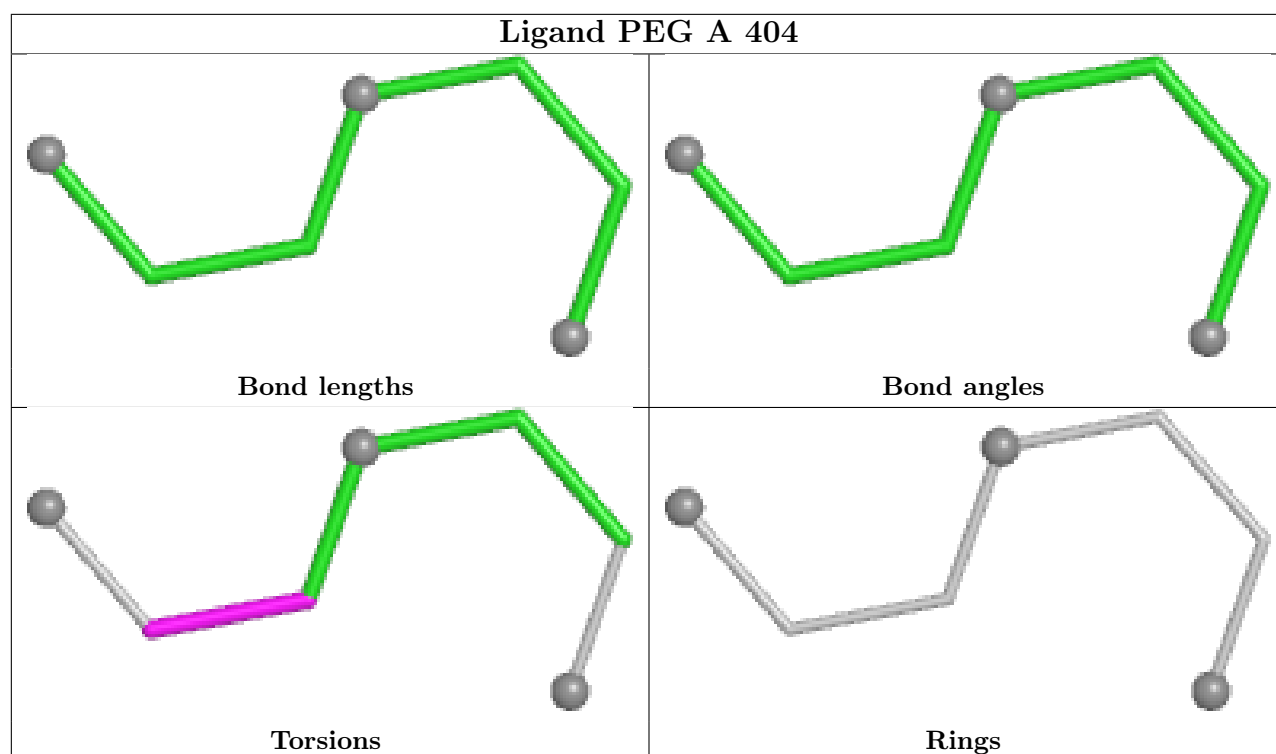
Ligand A1EJ2 C 403



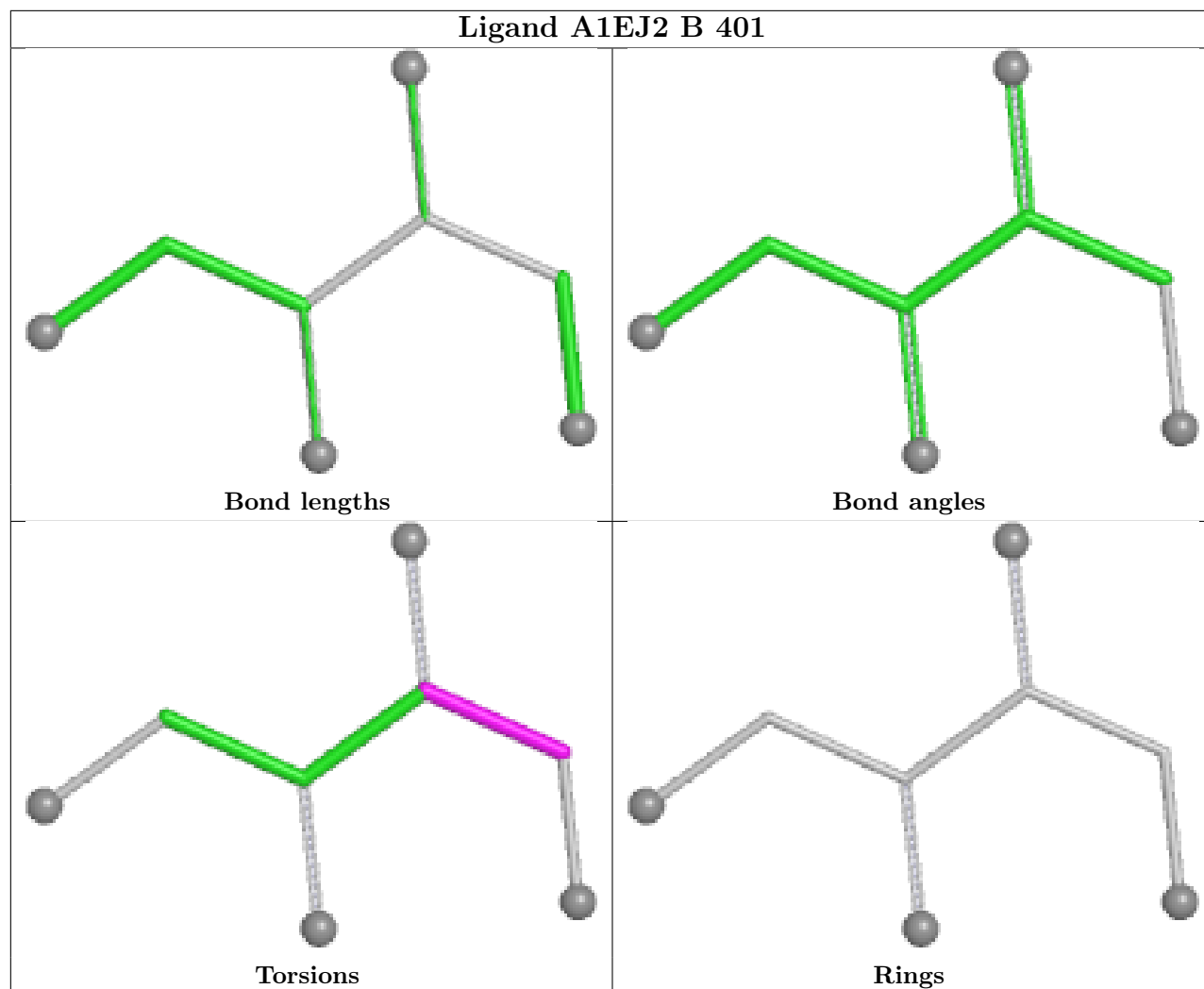
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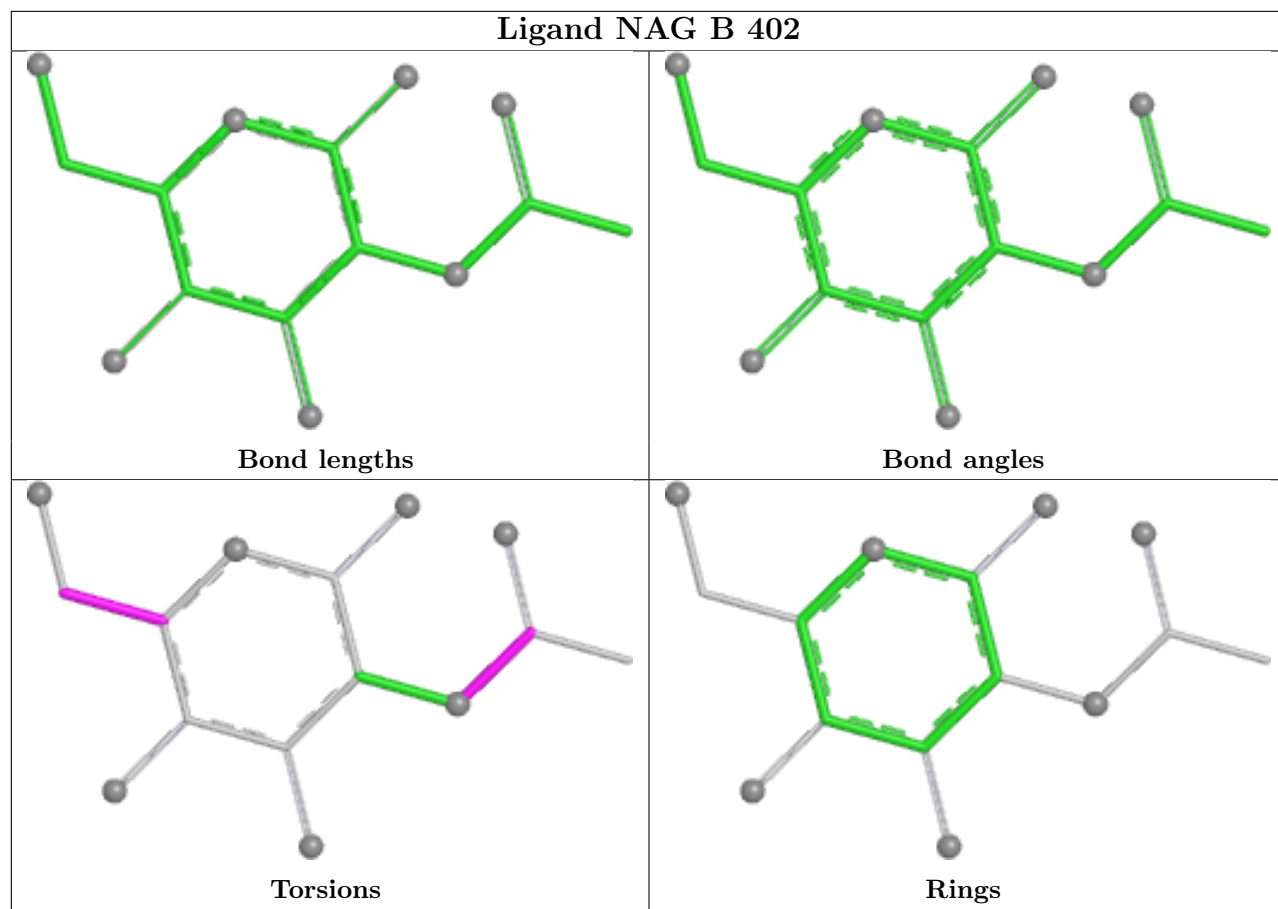




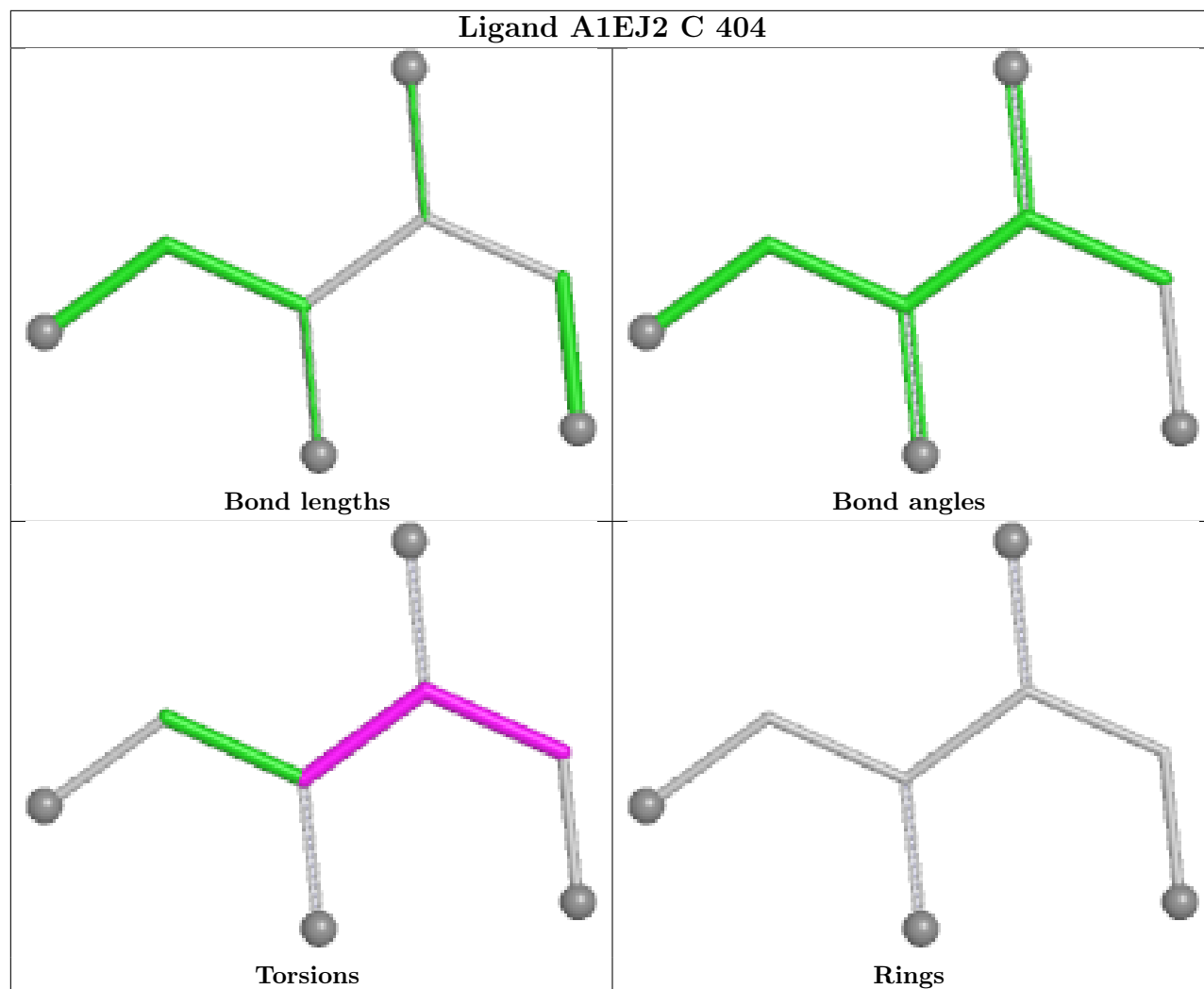


Ligand A1EJ2 B 401

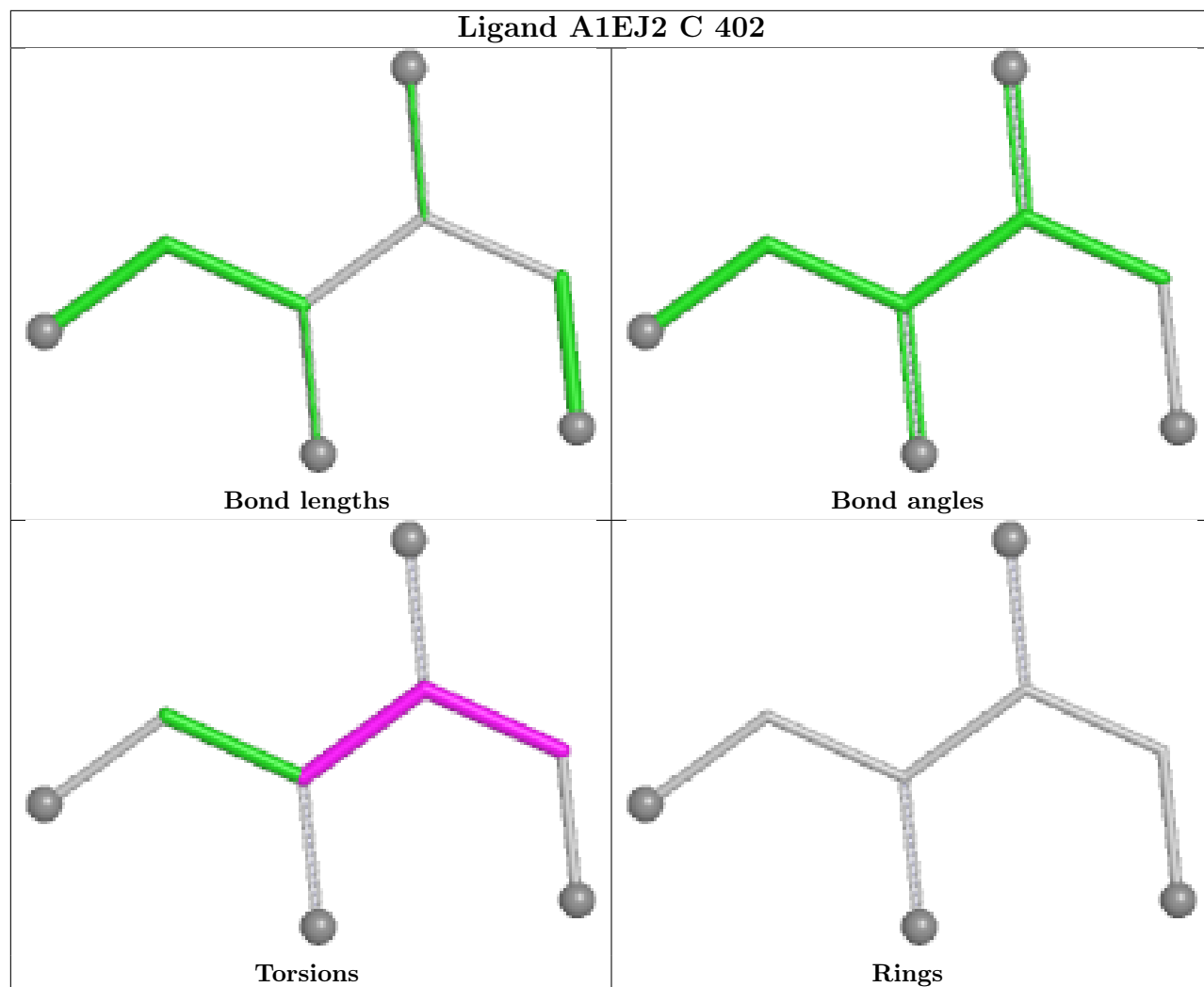


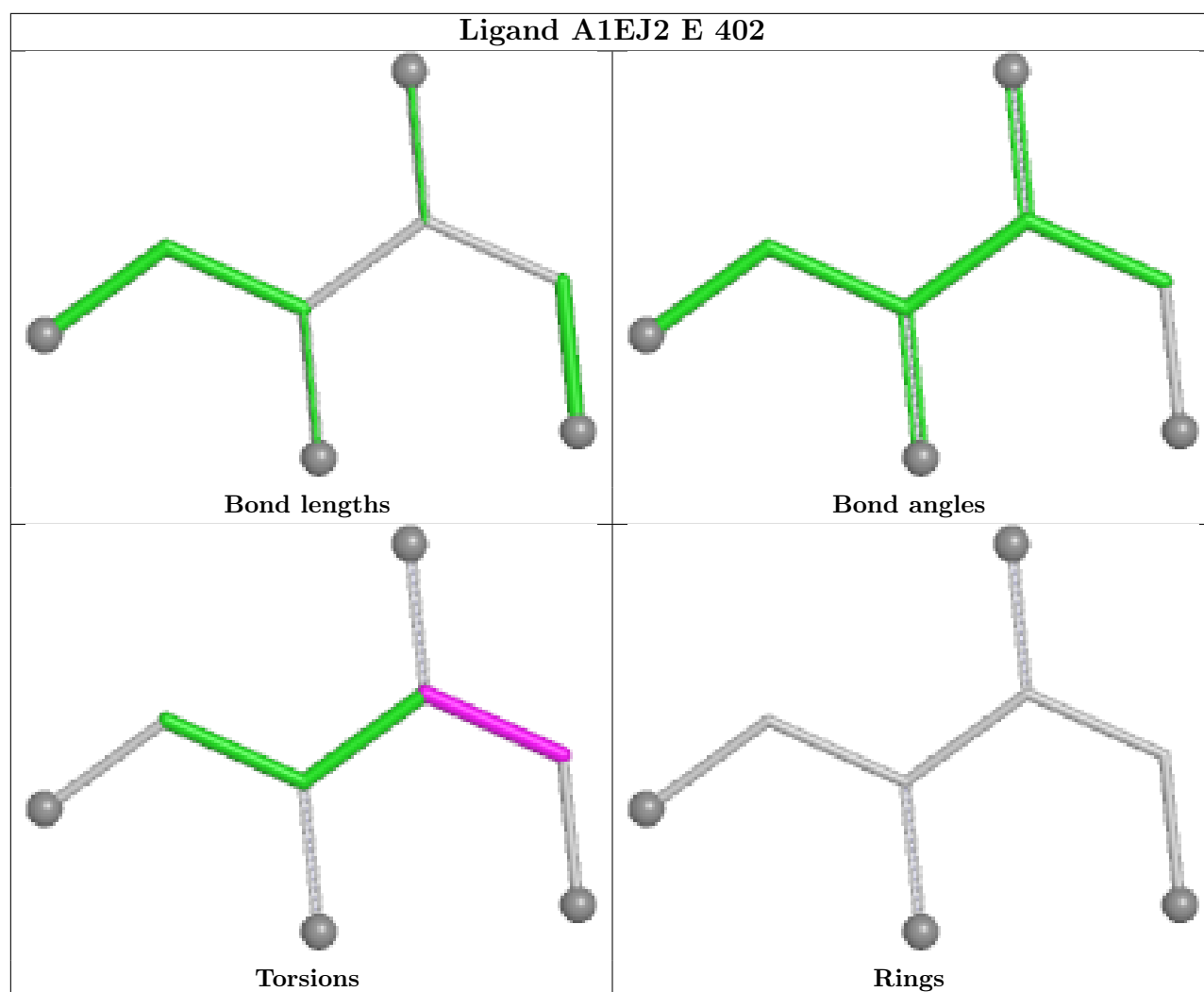


Ligand A1EJ2 C 404



Ligand A1EJ2 C 402





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	334/345 (96%)	0.69	15 (4%) 38 43	25, 36, 55, 72	0
1	D	335/345 (97%)	0.62	7 (2%) 63 67	26, 36, 50, 59	0
1	E	332/345 (96%)	0.57	5 (1%) 72 76	24, 34, 50, 65	0
2	B	334/345 (96%)	0.47	5 (1%) 72 76	24, 33, 44, 67	0
2	C	338/345 (97%)	0.46	5 (1%) 72 76	24, 32, 45, 66	0
3	F	335/345 (97%)	0.64	8 (2%) 59 63	27, 37, 48, 58	0
All	All	2008/2070 (97%)	0.57	45 (2%) 62 66	24, 35, 50, 72	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	336	ALA	6.1
3	F	337	GLY	5.1
1	A	130	PRO	3.4
1	D	336	ALA	3.1
2	B	297	GLU	2.9
1	A	19	TRP	2.8
1	D	196	ALA	2.7
2	B	121	ALA	2.7
2	C	43	GLY	2.7
1	A	281	ILE	2.7
3	F	291	PRO	2.6
1	A	303	VAL	2.5
1	E	179	VAL	2.5
1	A	245	CYS	2.5
1	A	292	TYR	2.5
1	D	300	THR	2.5
1	A	121	ALA	2.5
1	A	251	VAL	2.4
1	E	251	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	35	ALA	2.3
2	C	300	THR	2.3
1	E	131	ALA	2.3
2	C	0	ALA	2.3
2	B	172	GLY	2.2
2	B	186	ALA	2.2
1	A	247	GLU	2.2
2	C	336	ALA	2.2
3	F	308	TRP	2.2
1	D	332	GLU	2.2
1	A	336	ALA	2.2
1	A	240	TYR	2.2
1	D	337	GLY	2.1
1	D	121	ALA	2.1
1	E	204	ALA	2.1
1	A	311	LEU	2.1
1	A	255	CYS	2.1
3	F	7	HIS	2.1
1	D	35	ALA	2.1
1	E	231	LEU	2.1
2	B	191	LEU	2.1
3	F	201	VAL	2.1
2	C	204	ALA	2.1
1	A	29	ALA	2.0
3	F	204	ALA	2.0
1	A	7	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1EJ1	F	257	23/24	0.84	0.12	29,40,48,55	0
2	A1EJ4	C	257	15/16	0.87	0.10	23,29,38,38	0
2	A1EJ4	B	257	15/16	0.92	0.08	24,29,37,38	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

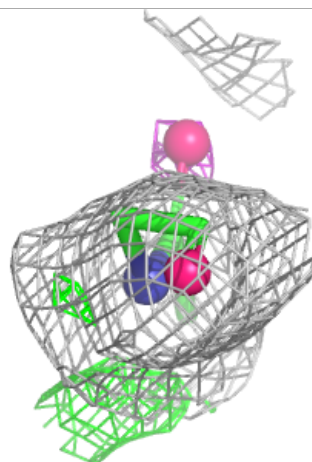
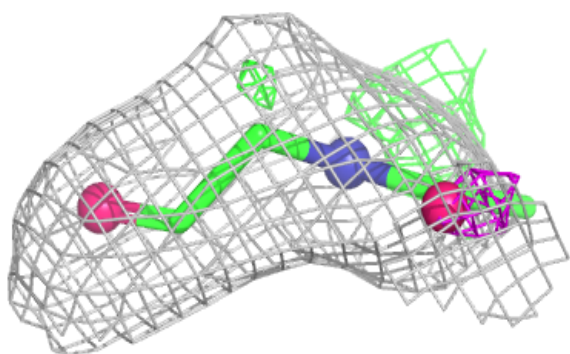
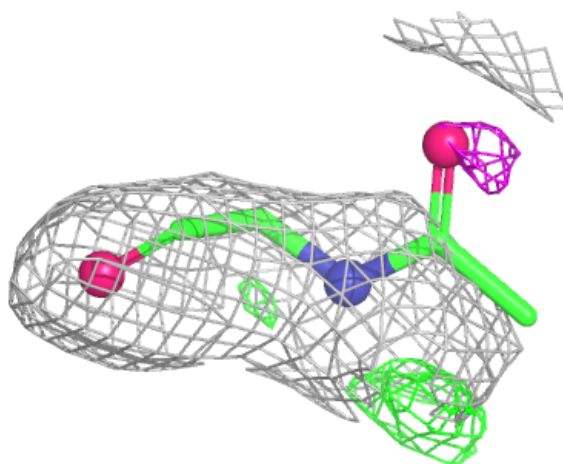
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1EJ3	C	401	7/7	0.52	0.23	47,58,67,75	0
5	A1EJ2	C	403	8/8	0.69	0.12	49,53,56,63	0
5	A1EJ2	B	401	8/8	0.70	0.14	45,47,49,50	0
8	A1EJ0	E	401	15/15	0.72	0.14	38,41,47,47	0
7	NAG	B	402	15/15	0.73	0.14	39,45,55,61	0
4	A1EJ3	A	401	7/7	0.76	0.15	37,40,42,44	0
5	A1EJ2	E	402	8/8	0.76	0.14	44,47,50,55	0
6	PEG	F	401	7/7	0.77	0.18	35,39,42,44	0
5	A1EJ2	C	402	8/8	0.80	0.11	39,42,48,52	0
5	A1EJ2	C	404	8/8	0.80	0.11	38,43,47,48	0
5	A1EJ2	A	402	8/8	0.82	0.11	46,49,52,54	0
6	PEG	B	403	7/7	0.83	0.12	41,45,48,52	0
6	PEG	A	403	7/7	0.85	0.12	36,41,42,43	0
4	A1EJ3	D	401	7/7	0.86	0.12	37,39,40,40	0
6	PEG	D	402	7/7	0.87	0.10	42,43,50,51	0
6	PEG	A	404	7/7	0.88	0.11	35,37,41,42	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.

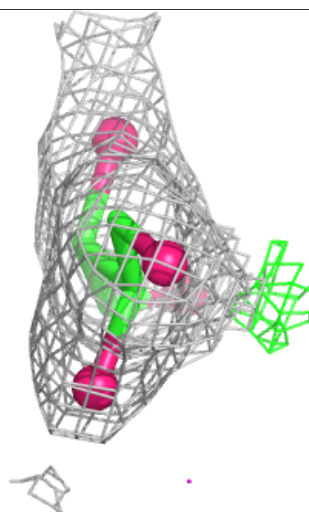
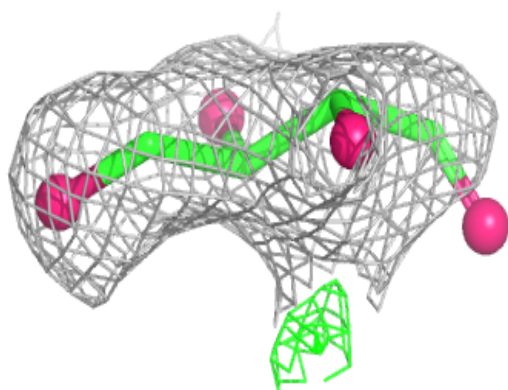
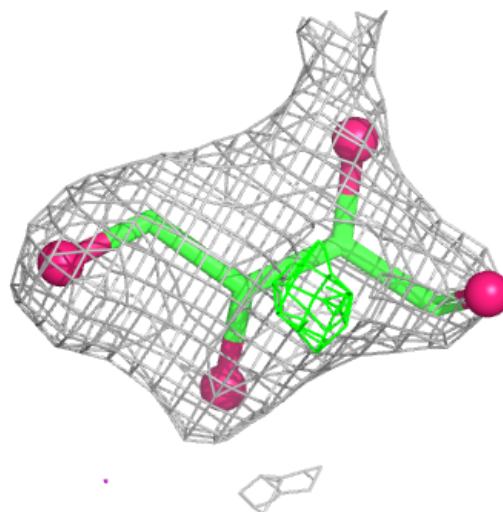
Electron density around A1EJ3 C 401:

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



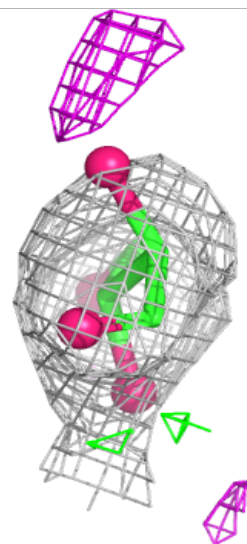
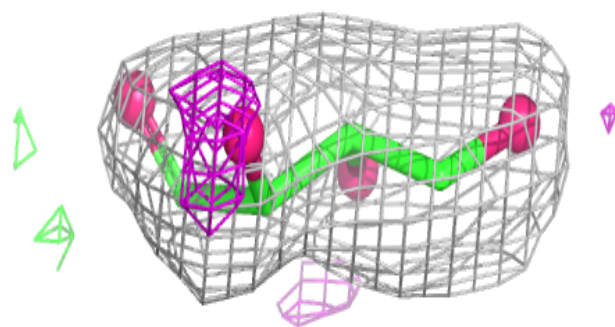
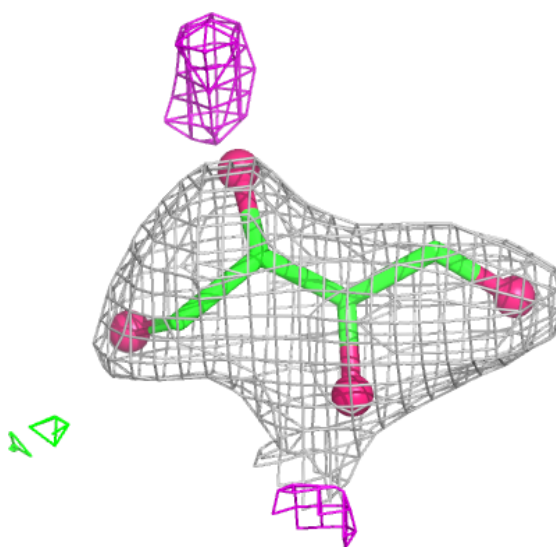
Electron density around A1EJ2 C 403:

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



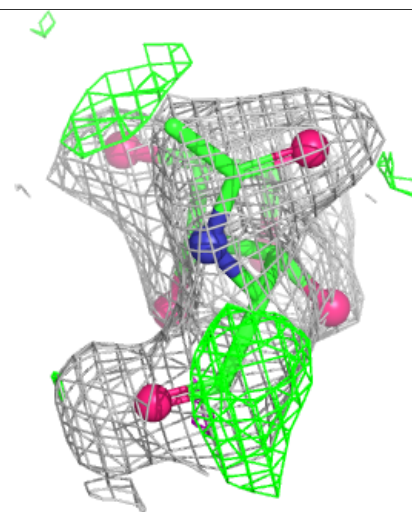
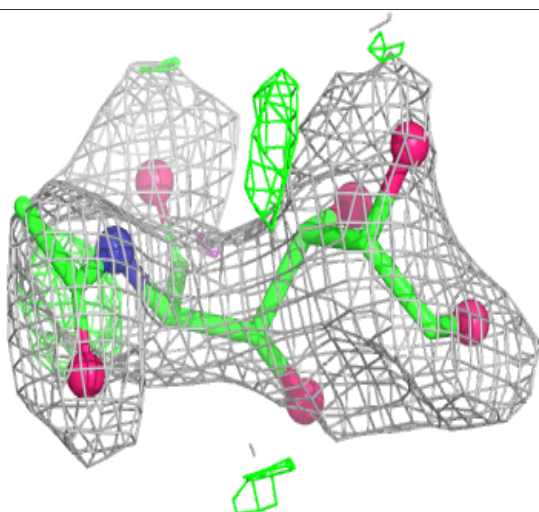
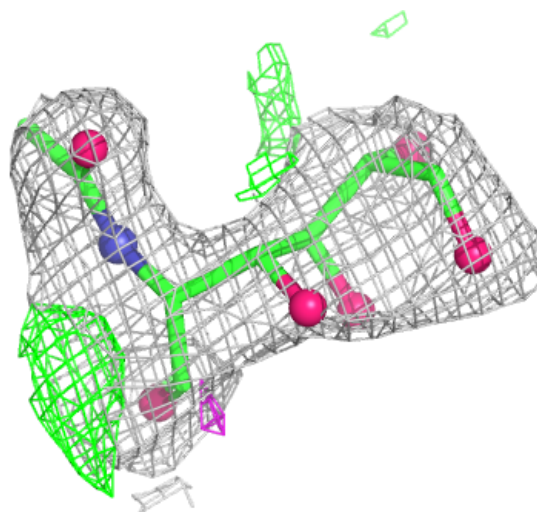
Electron density around A1EJ2 B 401:

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



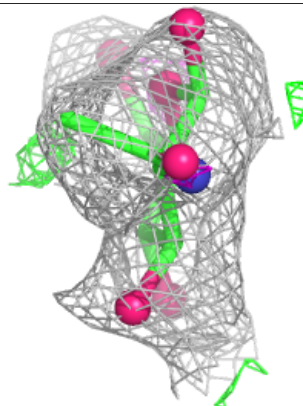
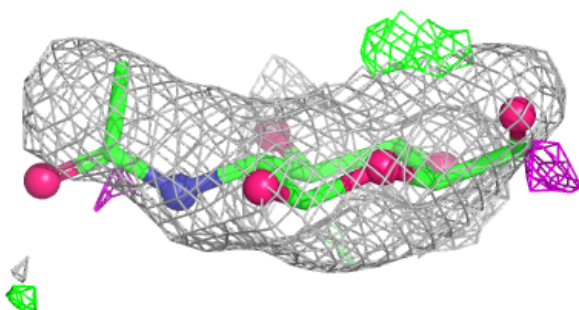
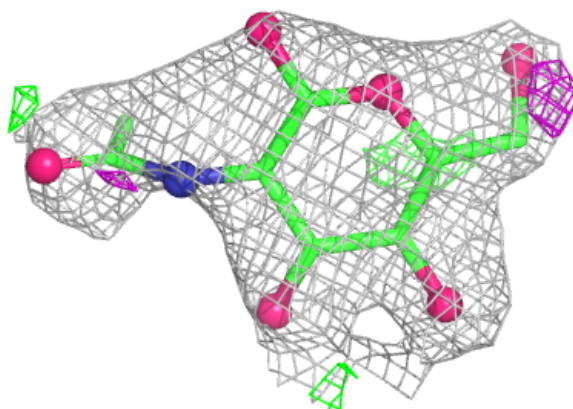
Electron density around A1EJ0 E 401:

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

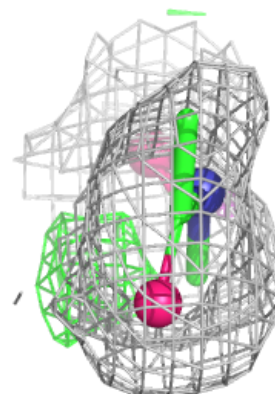
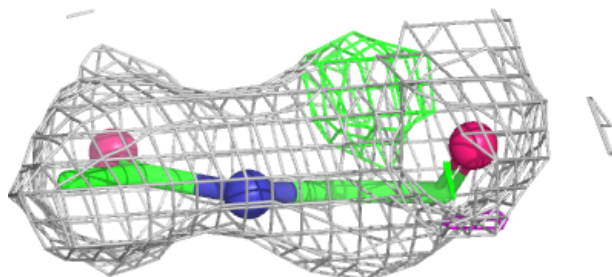
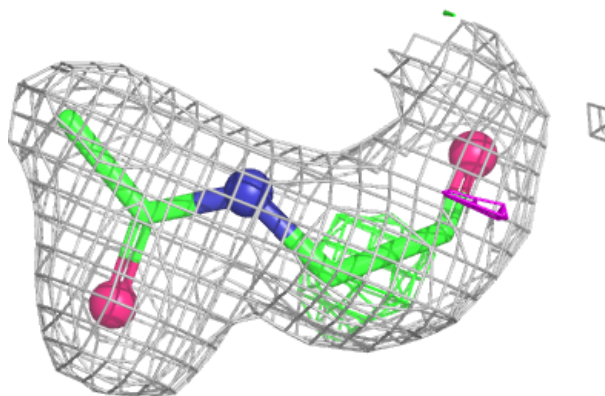


Electron density around NAG B 402:

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

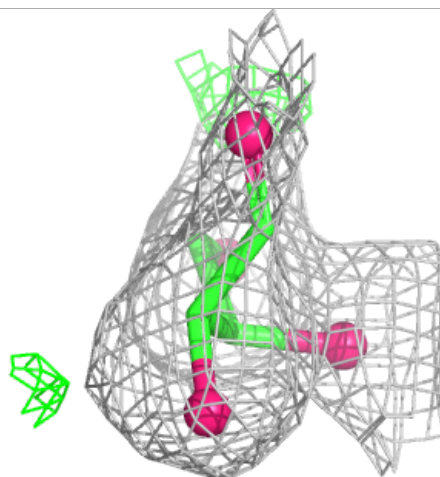
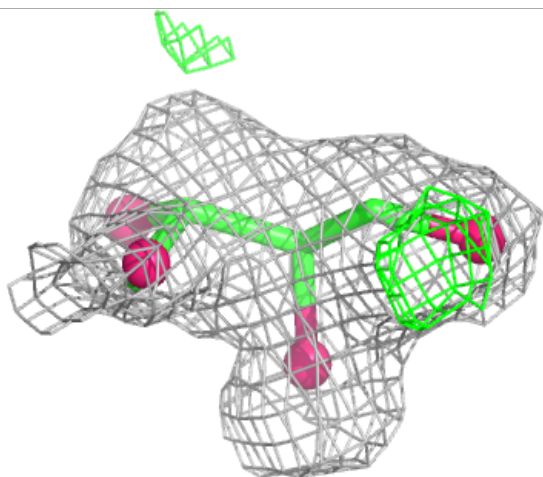
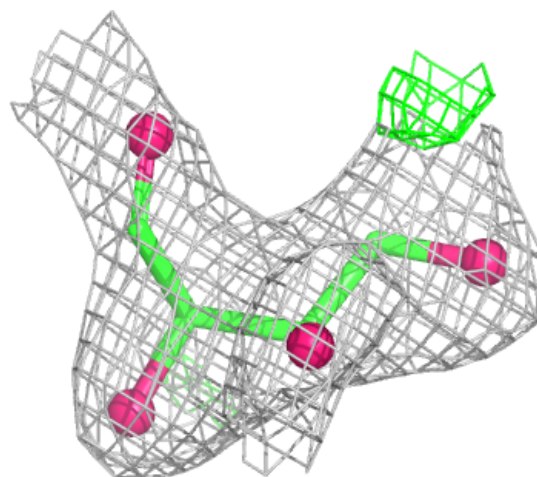
**Electron density around A1EJ3 A 401:**

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



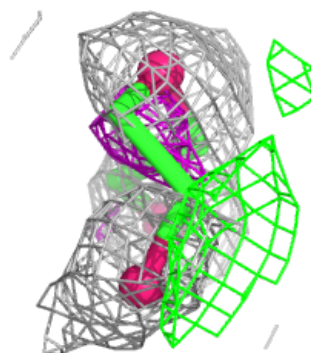
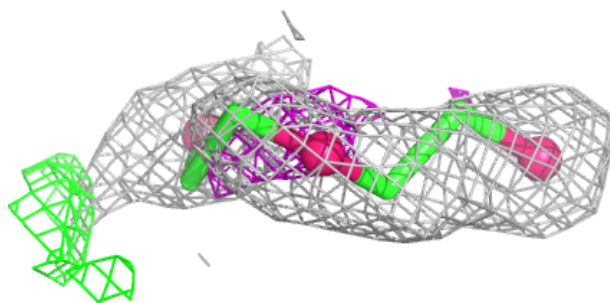
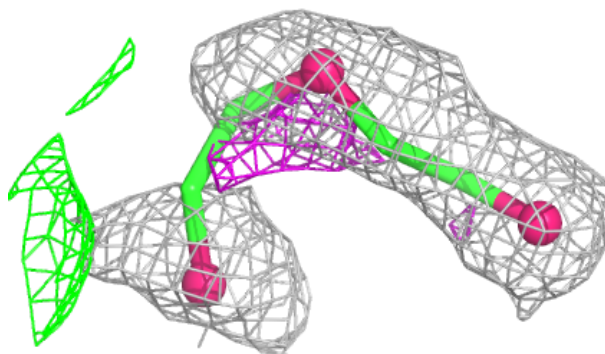
Electron density around A1EJ2 E 402:

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



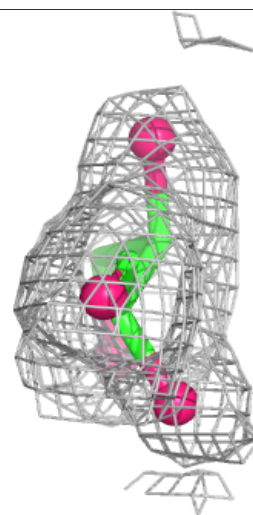
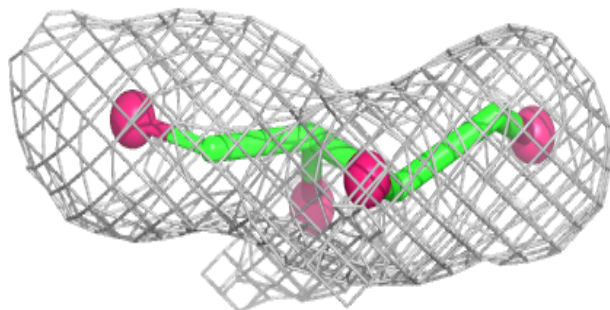
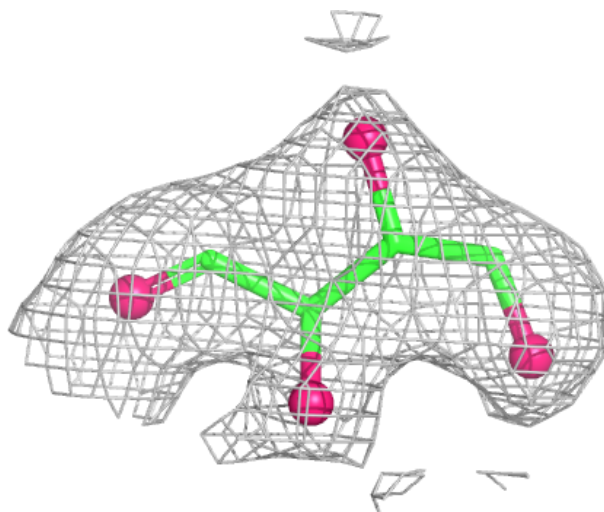
Electron density around PEG F 401:

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and green (positive)



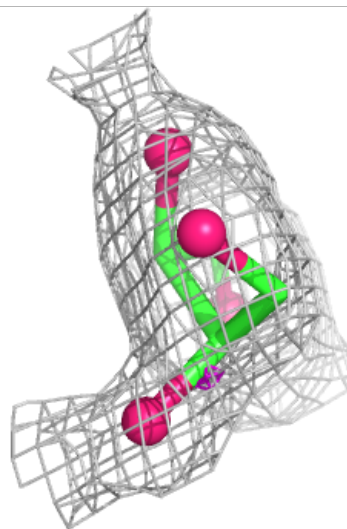
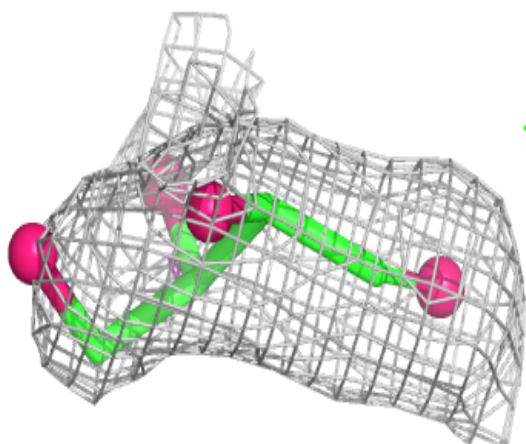
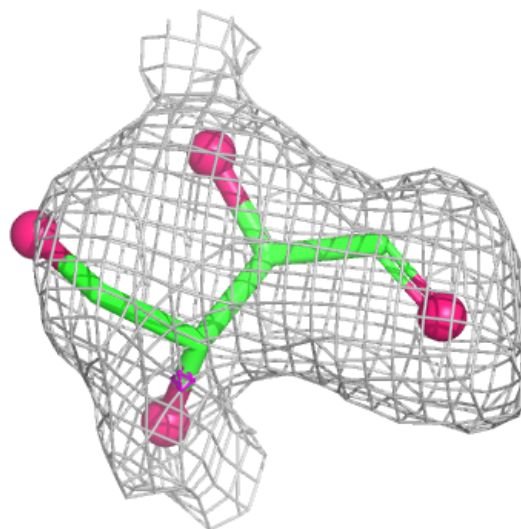
Electron density around A1EJ2 C 402:

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



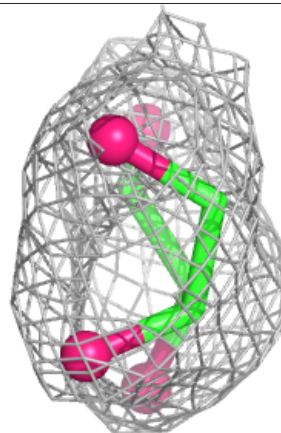
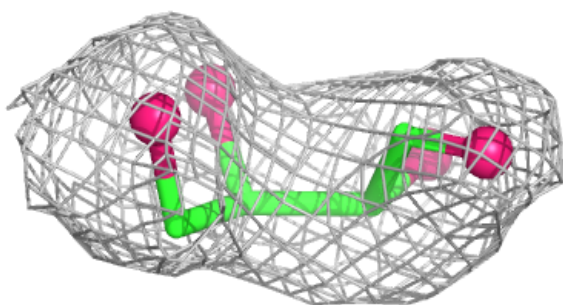
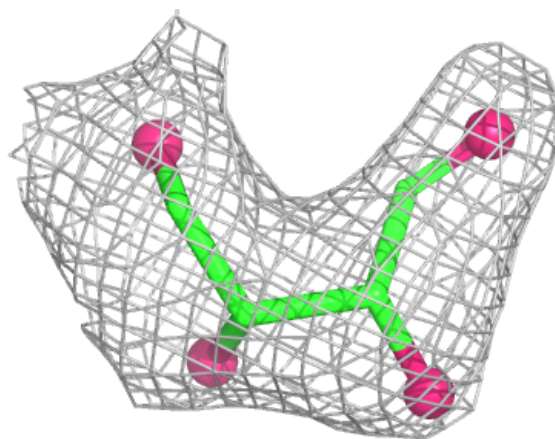
Electron density around A1EJ2 C 404:

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

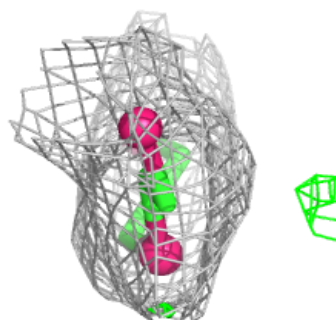
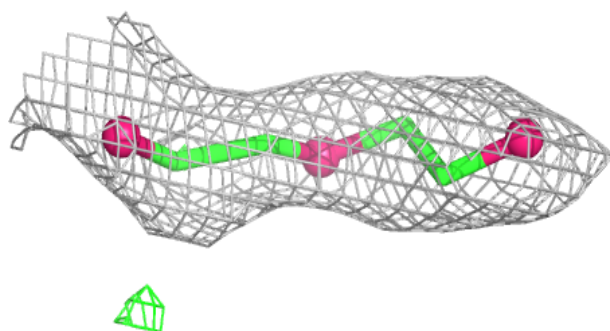
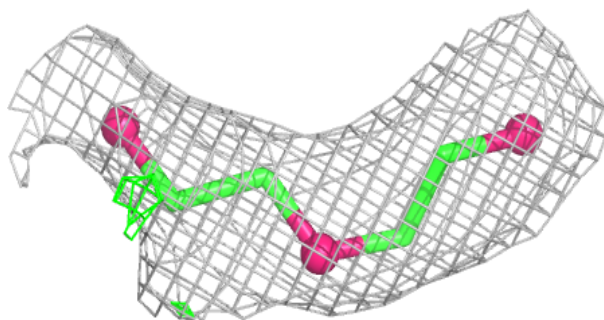


Electron density around A1EJ2 A 402:

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

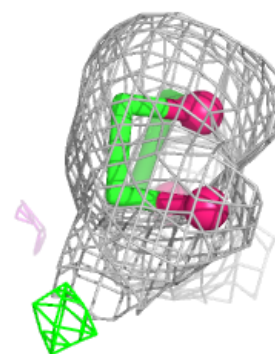
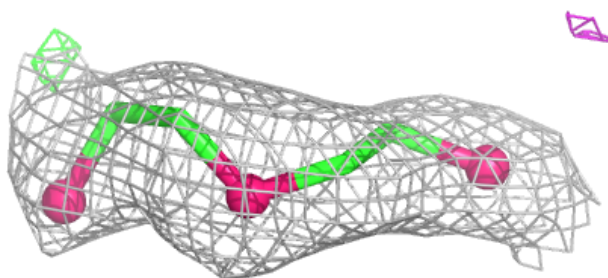
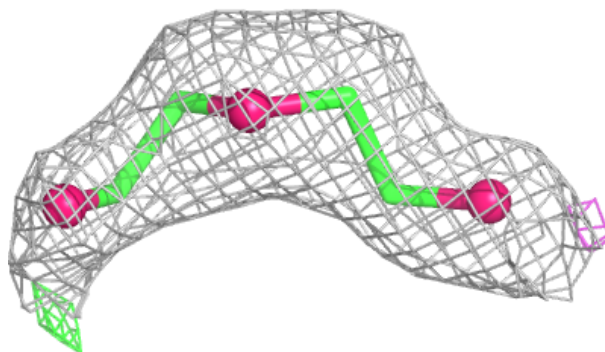
**Electron density around PEG B 403:**

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

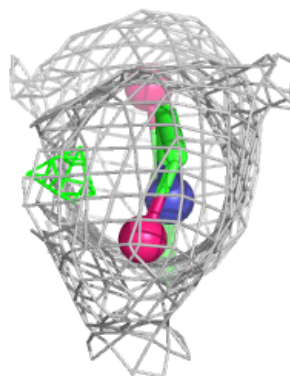
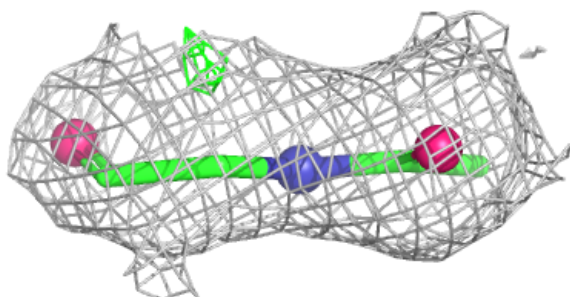
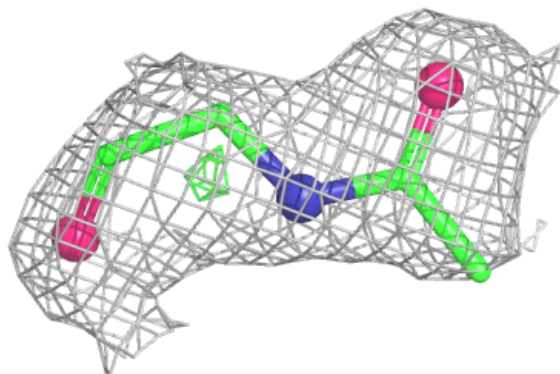


Electron density around PEG A 403:

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and green (positive)

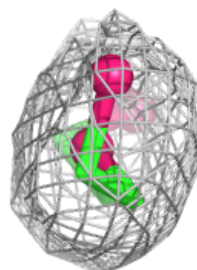
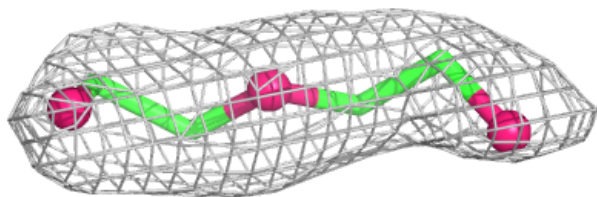
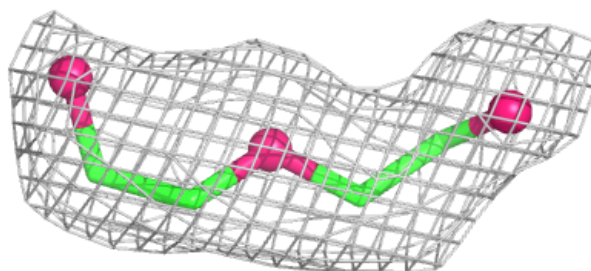
**Electron density around A1EJ3 D 401:**

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

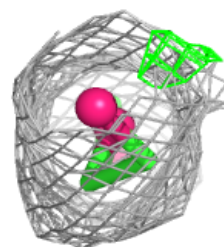
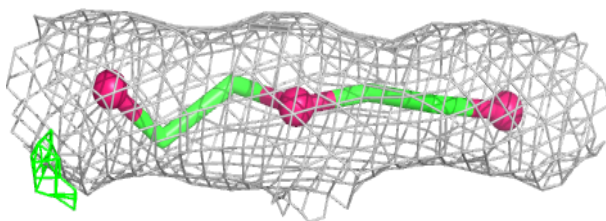
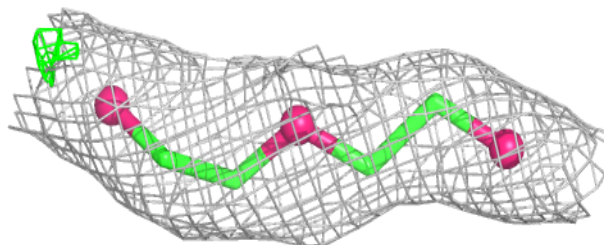


Electron density around PEG D 402:

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

**Electron density around PEG A 404:**

$2mF_o-DF_c$ (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.