



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2021 – 04:10 PM EST

PDB ID : 6X0C
Title : Tryptophan Synthase mutant beta-Q114A in complex with Cesium ion at the metal coordination site and aminoacrylate and benzimidazole at the enzyme beta site
Authors : Hilario, E.; Dunn, M.F.; Mueller, L.J.; Fan, L.
Deposited on : 2020-05-15
Resolution : 1.45 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 : 2.17.1
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) : 2.17.1

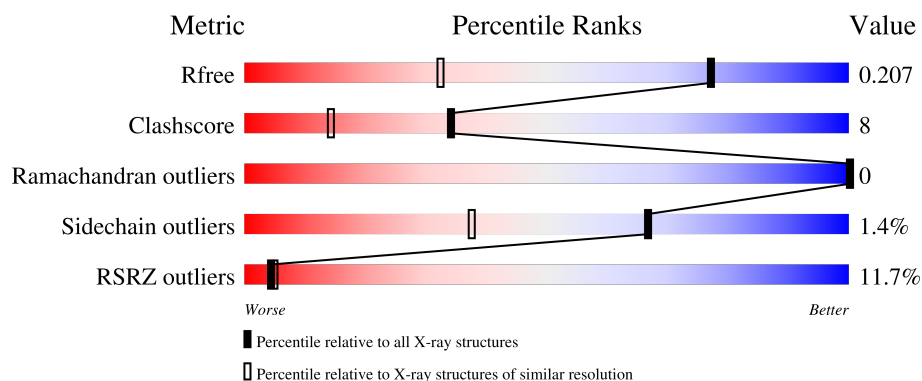
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	268	
2	B	397	

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
5	PEG	B	804	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5784 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	4	0
			1944	1237	334	365	8			

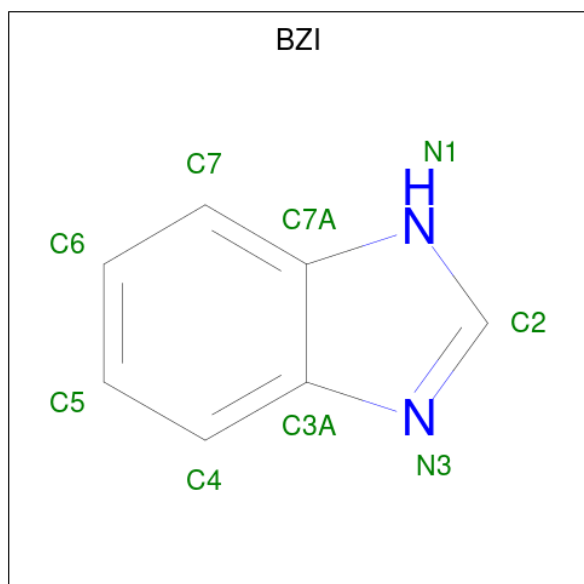
- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	19	0
			3132	1965	550	595	22			

There is a discrepancy between the modelled and reference sequences:

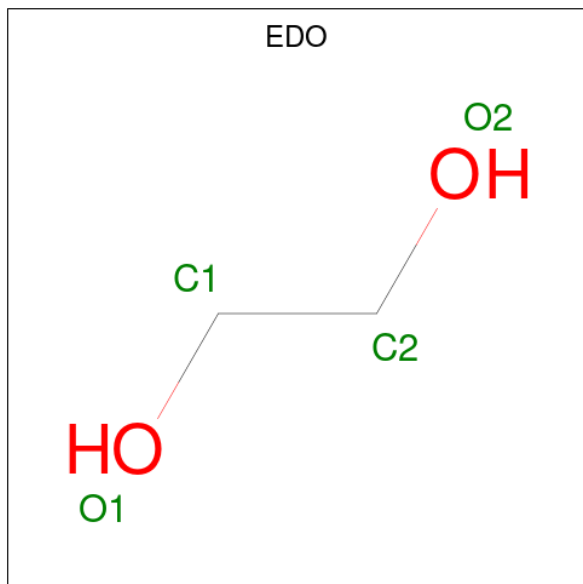
Chain	Residue	Modelled	Actual	Comment	Reference
B	114	ALA	GLN	engineered mutation	UNP P0A2K1

- Molecule 3 is BENZIMIDAZOLE (three-letter code: BZI) (formula: $C_7H_6N_2$) (labeled as "Ligand of Interest" by depositor).



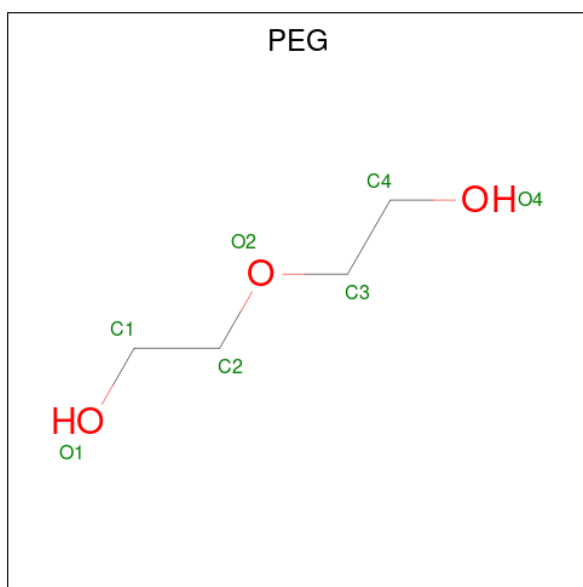
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



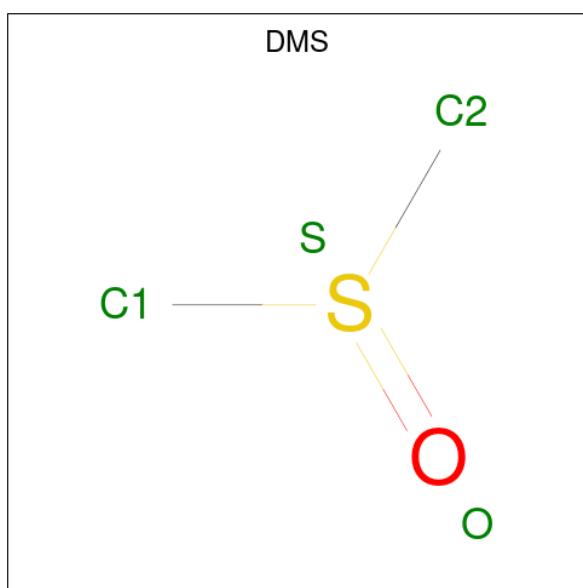
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

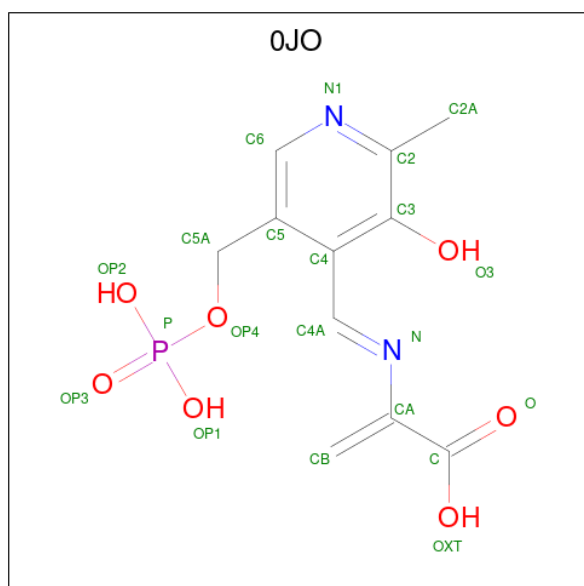
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 2-[(E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methyldene]amino}prop-2-enoic acid (three-letter code: OJO) (formula: C₁₁H₁₃N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 9 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total 3	Cs 3	0	1

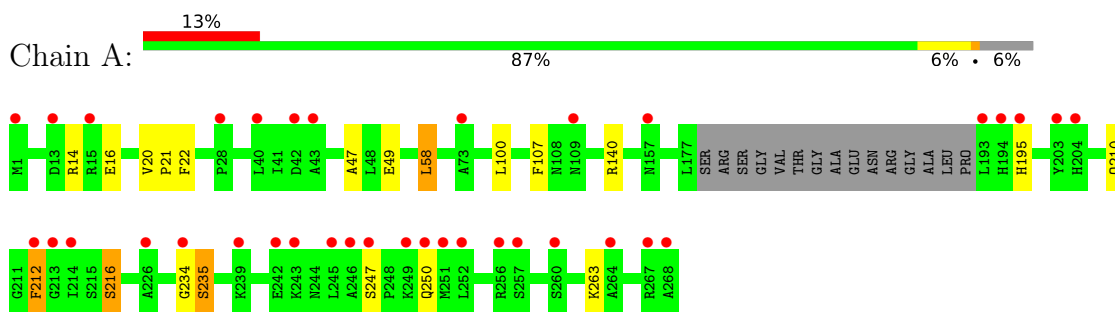
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	184	Total 188	O 188	0	4
10	B	408	Total 420	O 420	0	12

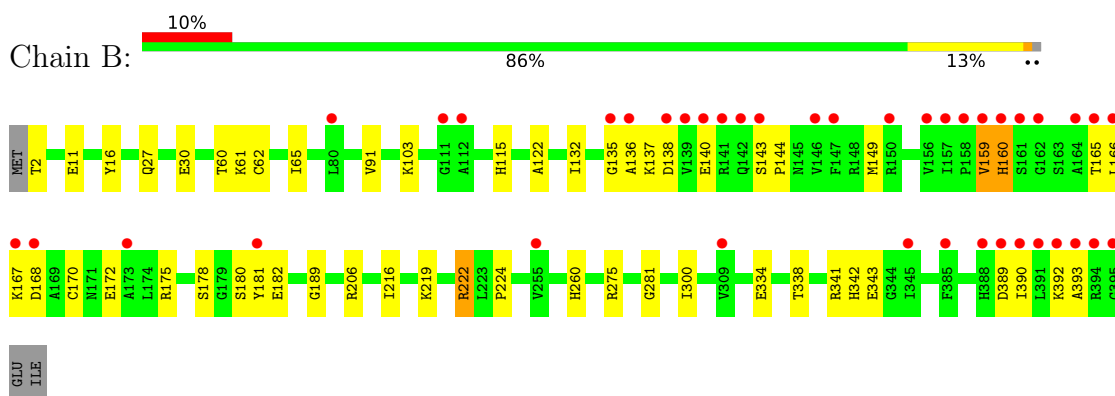
3 Residue-property plots [i](#)

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: Tryptophan synthase alpha chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.13Å 59.34Å 67.42Å 90.00° 95.11° 90.00°	Depositor
Resolution (Å)	39.39 – 1.45 39.39 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.39-1.45) 99.5 (39.39-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.164 , 0.202 0.172 , 0.207	Depositor DCC
R_{free} test set	6260 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	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	0.97	EDS
Total number of atoms	5784	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: PEG, BZI, CL, DMS, CS, EDO, OJO

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	0.74	0/1985	0.79	0/2695
2	B	0.73	2/3191 (0.1%)	0.83	1/4305 (0.0%)
All	All	0.73	2/5176 (0.0%)	0.82	1/7000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11[A]	GLU	CD-OE2	7.33	1.33	1.25
2	B	11[B]	GLU	CD-OE2	7.33	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1944	0	1948	24	0
2	B	3132	0	3095	56	0
3	A	9	0	6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	12	1	0
4	A	4	0	6	0	0
4	B	4	0	6	3	0
5	A	7	0	10	2	0
5	B	7	0	10	5	0
6	A	4	0	6	2	0
6	B	20	0	30	3	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	B	21	0	9	1	0
9	B	3	0	0	0	0
10	A	188	0	0	7	0
10	B	420	0	0	20	0
All	All	5784	0	5138	87	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 8.

All (87) 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:B:167[B]:LYS:H	2:B:167[B]:LYS:HD2	1.23	1.01
2:B:103:LYS:HE3	2:B:181:TYR:O	1.65	0.94
2:B:136:ALA:HB1	10:B:1153:HOH:O	1.66	0.93
1:A:22:PHE:HB3	1:A:234:GLY:HA2	1.50	0.91
2:B:61:LYS:H	5:B:804:PEG:H11	1.38	0.89
1:A:216[A]:SER:OG	10:A:701:HOH:O	1.90	0.88
1:A:22:PHE:HB3	1:A:234:GLY:CA	2.06	0.84
2:B:61:LYS:N	5:B:804:PEG:H11	1.92	0.83
2:B:136:ALA:CB	10:B:1153:HOH:O	2.22	0.82
1:A:107:PHE:CE2	5:A:603:PEG:H32	2.14	0.82
2:B:167[B]:LYS:H	2:B:167[B]:LYS:CD	1.89	0.82
1:A:235:SER:HB2	10:A:708:HOH:O	1.79	0.82
2:B:222:ARG:NH2	10:B:902:HOH:O	2.12	0.81
2:B:61:LYS:H	5:B:804:PEG:C1	1.97	0.77
2:B:172:GLU:O	2:B:175[B]:ARG:HG3	1.85	0.76
2:B:167[B]:LYS:HD2	2:B:167[B]:LYS:N	1.99	0.76
2:B:206:ARG:HD3	4:B:805:EDO:H12	1.69	0.74
2:B:165:THR:HG23	2:B:167[B]:LYS:HD2	1.75	0.69
1:A:58:LEU:C	1:A:58:LEU:HD12	2.16	0.66
2:B:180:SER:HA	10:B:1133:HOH:O	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:CB	10:A:708:HOH:O	2.41	0.66
6:A:604:DMS:H12	10:A:797:HOH:O	1.97	0.65
2:B:165:THR:HG23	2:B:167[B]:LYS:CD	2.27	0.65
1:A:140:ARG:NH1	10:A:702:HOH:O	2.31	0.64
2:B:160:HIS:HB3	10:B:1095:HOH:O	2.00	0.62
2:B:182:GLU:HG2	10:B:1206:HOH:O	1.98	0.61
4:B:805:EDO:H22	10:B:1022:HOH:O	2.00	0.61
6:A:604:DMS:H21	10:A:839:HOH:O	2.01	0.60
1:A:100:LEU:C	1:A:100:LEU:HD13	2.21	0.60
2:B:2:THR:HG22	10:B:1186:HOH:O	2.01	0.60
2:B:135:GLY:HA2	2:B:159:VAL:HG22	1.85	0.57
1:A:14:ARG:NH2	1:A:16:GLU:OE2	2.37	0.57
6:B:808:DMS:C2	10:B:914:HOH:O	2.53	0.57
2:B:103:LYS:CE	2:B:181:TYR:O	2.47	0.57
2:B:206:ARG:CD	4:B:805:EDO:H12	2.32	0.57
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.34	0.56
1:A:22:PHE:HB3	1:A:234:GLY:HA3	1.87	0.56
2:B:60:THR:HA	5:B:804:PEG:H12	1.88	0.56
2:B:342[B]:HIS:CD2	10:B:913:HOH:O	2.59	0.56
2:B:65:ILE:HD11	2:B:338:THR:HG22	1.88	0.55
6:B:808:DMS:H21	10:B:914:HOH:O	2.06	0.55
2:B:341:ARG:HG3	10:B:1107:HOH:O	2.07	0.54
1:A:22:PHE:CB	1:A:234:GLY:HA2	2.31	0.52
1:A:195:HIS:HB2	10:A:864:HOH:O	2.08	0.52
2:B:27:GLN:O	2:B:30[A]:GLU:HG3	2.10	0.52
2:B:62[B]:CYS:HB2	2:B:343:GLU:CD	2.30	0.51
2:B:334[B]:GLU:HG2	10:B:963:HOH:O	2.10	0.51
2:B:167[B]:LYS:O	2:B:170:CYS:HB2	2.10	0.50
2:B:216[B]:ILE:HG22	2:B:222:ARG:O	2.12	0.50
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.48	0.49
2:B:62[B]:CYS:HB2	2:B:343:GLU:OE2	2.12	0.49
2:B:137:LYS:HE2	2:B:165:THR:HB	1.95	0.49
2:B:172:GLU:HA	2:B:175[B]:ARG:HD3	1.94	0.49
2:B:168:ASP:O	2:B:172:GLU:HG2	2.13	0.48
1:A:49[A]:GLU:OE1	3:A:601:BZI:H6	2.13	0.48
1:A:58:LEU:HD23	10:B:1132:HOH:O	2.13	0.48
2:B:143:SER:N	2:B:144:PRO:CD	2.77	0.47
2:B:140:GLU:OE2	2:B:140:GLU:HA	2.15	0.47
2:B:275:ARG:HB2	10:B:1025:HOH:O	2.14	0.47
2:B:389:ASP:O	2:B:392:LYS:HG2	2.14	0.47
2:B:159:VAL:CG1	2:B:172:GLU:HG3	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LYS:H	5:B:804:PEG:C2	2.27	0.46
2:B:216[A]:ILE:HG21	2:B:224:PRO:HD3	1.97	0.46
2:B:132:ILE:HD13	2:B:149:MET:SD	2.56	0.46
1:A:107:PHE:CD2	5:A:603:PEG:H32	2.51	0.46
2:B:165:THR:HG23	2:B:167[B]:LYS:HD3	1.98	0.45
2:B:392:LYS:HG3	2:B:393:ALA:N	2.32	0.45
2:B:138:ASP:CG	10:B:905:HOH:O	2.55	0.45
2:B:219[B]:LYS:HD3	10:B:901:HOH:O	2.17	0.45
2:B:300:ILE:HD11	2:B:390:ILE:HD13	1.99	0.44
1:A:210:GLN:HE21	1:A:212:PHE:H	1.64	0.44
1:A:21:PRO:HD2	1:A:47:ALA:O	2.17	0.44
2:B:165:THR:HG21	10:B:1033:HOH:O	2.17	0.44
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.99	0.43
8:B:802:OJO:CB	3:B:803:BZI:N3	2.81	0.43
2:B:91[B]:VAL:HG12	2:B:122:ALA:HB2	1.99	0.43
2:B:166:LEU:HB3	2:B:167[B]:LYS:HE3	1.99	0.43
1:A:22:PHE:HA	1:A:49[B]:GLU:O	2.20	0.42
2:B:135:GLY:O	2:B:138:ASP:N	2.53	0.42
2:B:167[B]:LYS:CD	2:B:167[B]:LYS:N	2.67	0.42
1:A:247:SER:OG	1:A:250:GLN:HB3	2.20	0.41
1:A:58:LEU:C	1:A:58:LEU:CD1	2.85	0.41
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.94	0.41
6:B:808:DMS:H23	10:B:914:HOH:O	2.19	0.41
1:A:100:LEU:C	1:A:100:LEU:CD1	2.90	0.40
2:B:16:TYR:O	2:B:281:GLY:HA2	2.21	0.40
2:B:260:HIS:HE1	10:B:1167:HOH:O	2.05	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 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	253/268 (94%)	248 (98%)	5 (2%)	0	100	100
2	B	411/397 (104%)	401 (98%)	10 (2%)	0	100	100
All	All	664/665 (100%)	649 (98%)	15 (2%)	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	202/208 (97%)	197 (98%)	5 (2%)	47	14
2	B	325/310 (105%)	322 (99%)	3 (1%)	78	57
All	All	527/518 (102%)	519 (98%)	8 (2%)	67	35

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	212	PHE
1	A	216[A]	SER
1	A	216[B]	SER
1	A	235	SER
2	B	159	VAL
2	B	160	HIS
2	B	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	210	GLN
2	B	171	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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	DMS	B	808	-	3,3,3	0.28	0	3,3,3	0.48	0
6	DMS	B	806	-	3,3,3	0.20	0	3,3,3	0.34	0
4	EDO	A	602	-	3,3,3	0.17	0	2,2,2	0.33	0
3	BZI	A	601	-	8,10,10	0.94	0	6,13,13	1.18	1 (16%)
3	BZI	B	803	-	8,10,10	0.89	0	6,13,13	1.27	1 (16%)
3	BZI	B	801	-	8,10,10	0.96	0	6,13,13	1.43	1 (16%)
6	DMS	B	807	-	3,3,3	1.12	0	3,3,3	0.98	0
5	PEG	B	804	-	6,6,6	0.40	0	5,5,5	0.44	0
4	EDO	B	805	-	3,3,3	0.32	0	2,2,2	0.30	0
5	PEG	A	603	-	6,6,6	0.18	0	5,5,5	0.11	0
6	DMS	B	810	-	3,3,3	0.24	0	3,3,3	0.20	0
6	DMS	B	809	-	3,3,3	0.32	0	3,3,3	0.20	0
8	OJO	B	802	-	18,21,21	1.53	2 (11%)	21,30,30	1.04	1 (4%)
6	DMS	A	604	-	3,3,3	0.27	0	3,3,3	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	602	-	-	1/1/1/1	-
3	BZI	A	601	-	-	-	0/2/2/2
3	BZI	B	803	-	-	-	0/2/2/2
3	BZI	B	801	-	-	-	0/2/2/2
5	PEG	B	804	-	-	1/4/4/4	-
4	EDO	B	805	-	-	0/1/1/1	-
5	PEG	A	603	-	-	2/4/4/4	-
8	OJO	B	802	-	-	0/9/15/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	802	OJO	C-CA	-5.13	1.44	1.52
8	B	802	OJO	C3-C2	2.97	1.43	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	BZI	C6-C7-C7A	-2.70	116.20	120.08
3	B	803	BZI	C6-C7-C7A	-2.20	116.91	120.08
3	A	601	BZI	C6-C7-C7A	-2.19	116.92	120.08
8	B	802	OJO	C2A-C2-C3	2.07	123.45	120.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	603	PEG	O1-C1-C2-O2
4	A	602	EDO	O1-C1-C2-O2
5	A	603	PEG	O2-C3-C4-O4
5	B	804	PEG	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

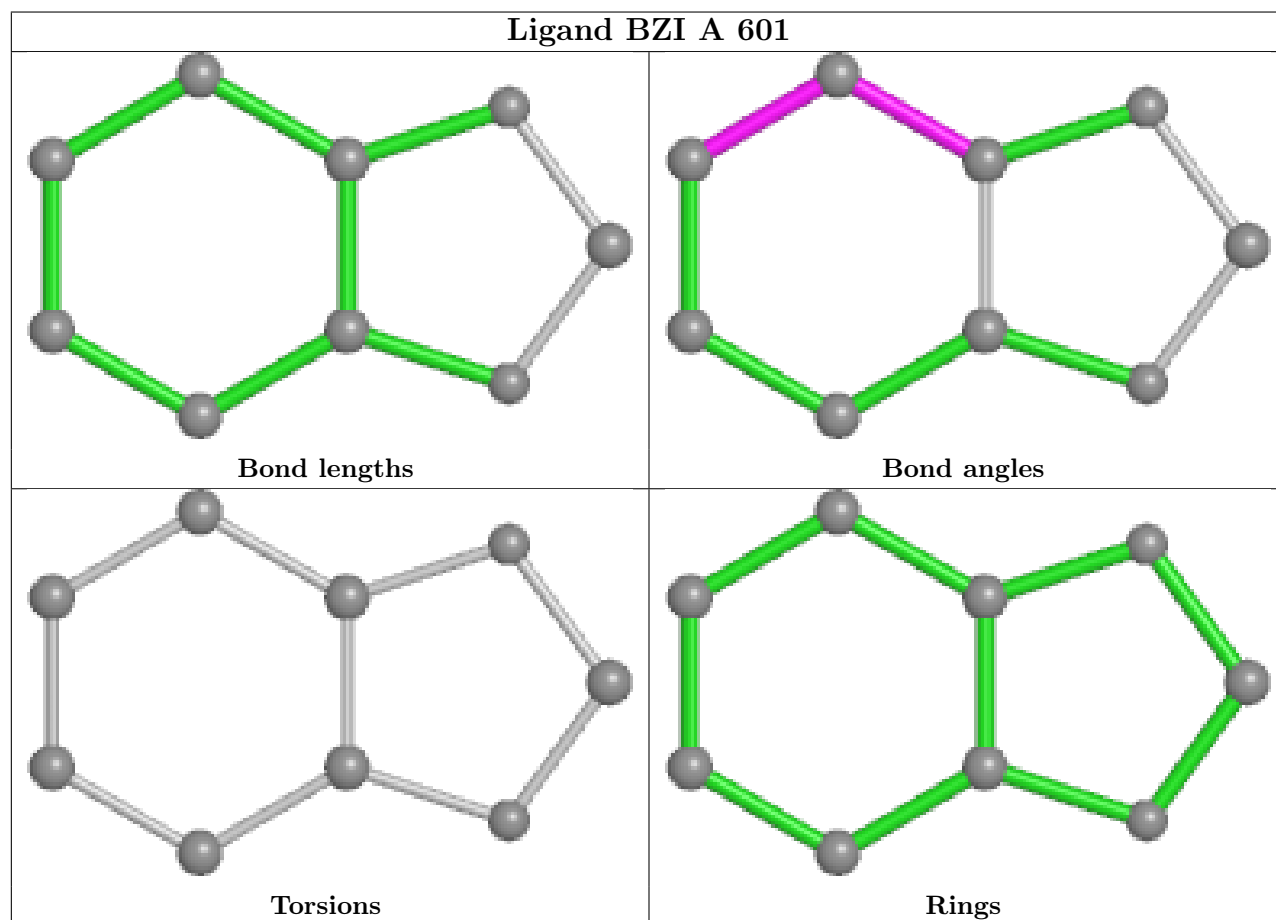
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	808	DMS	3	0
3	A	601	BZI	1	0
3	B	803	BZI	1	0

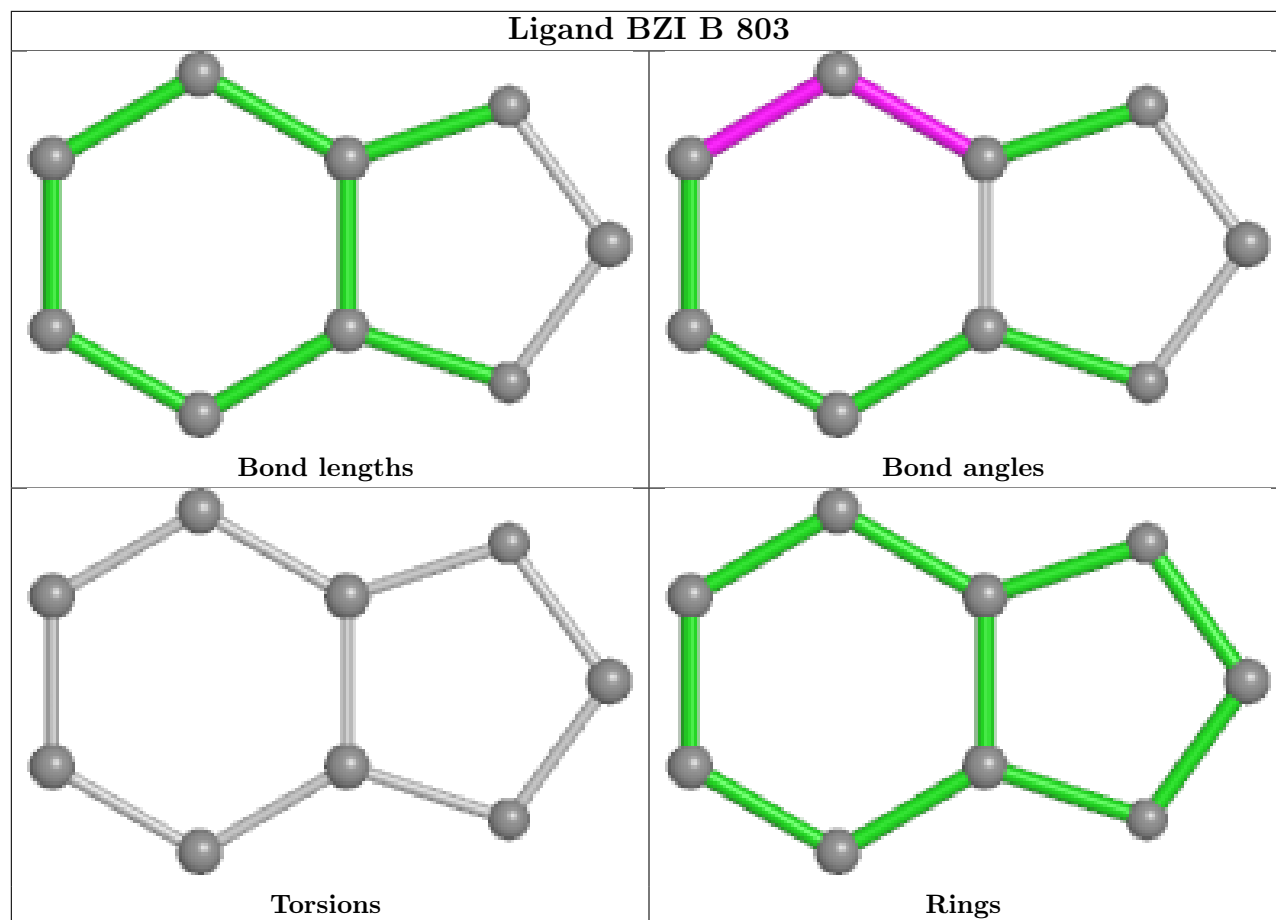
Continued on next page...

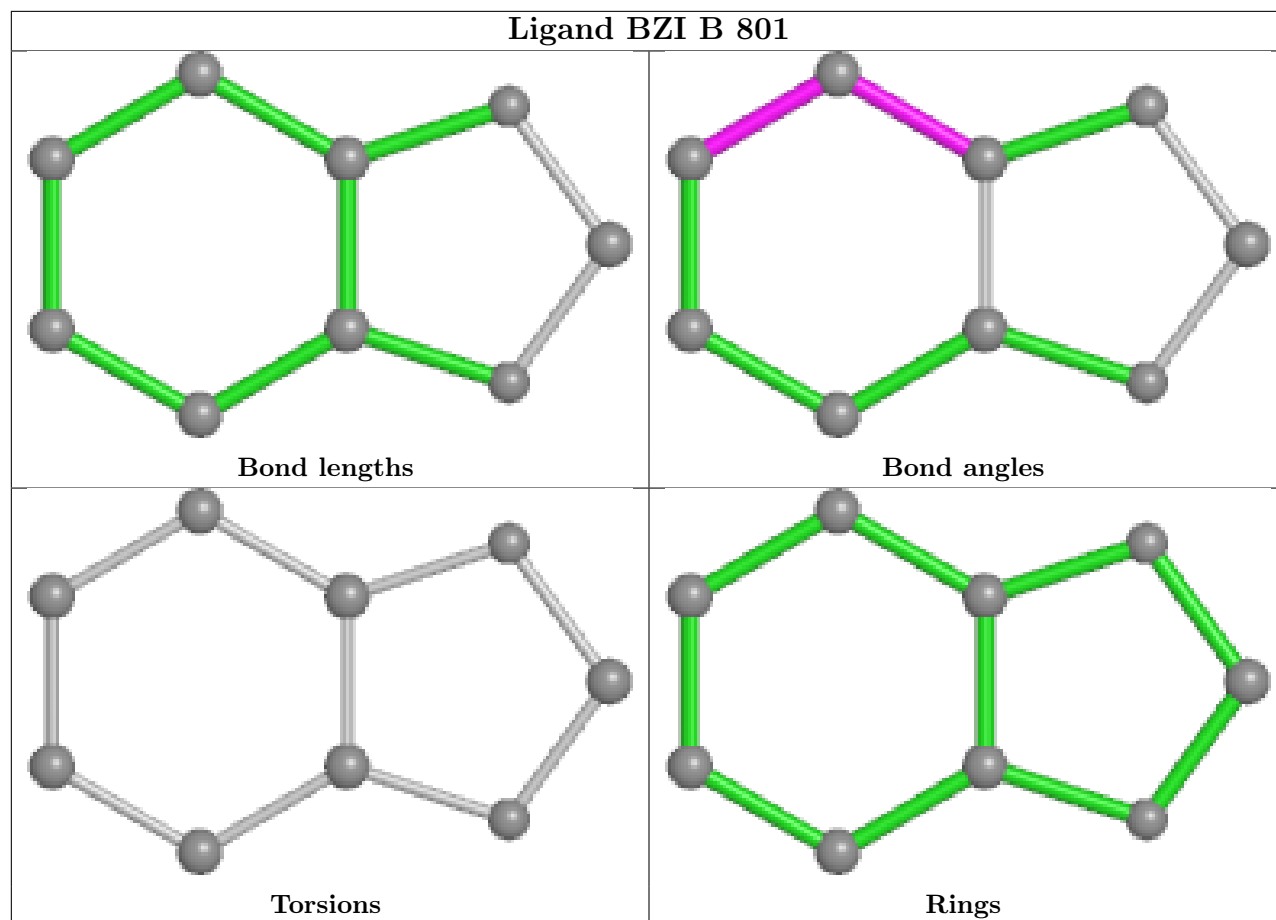
Continued from previous page...

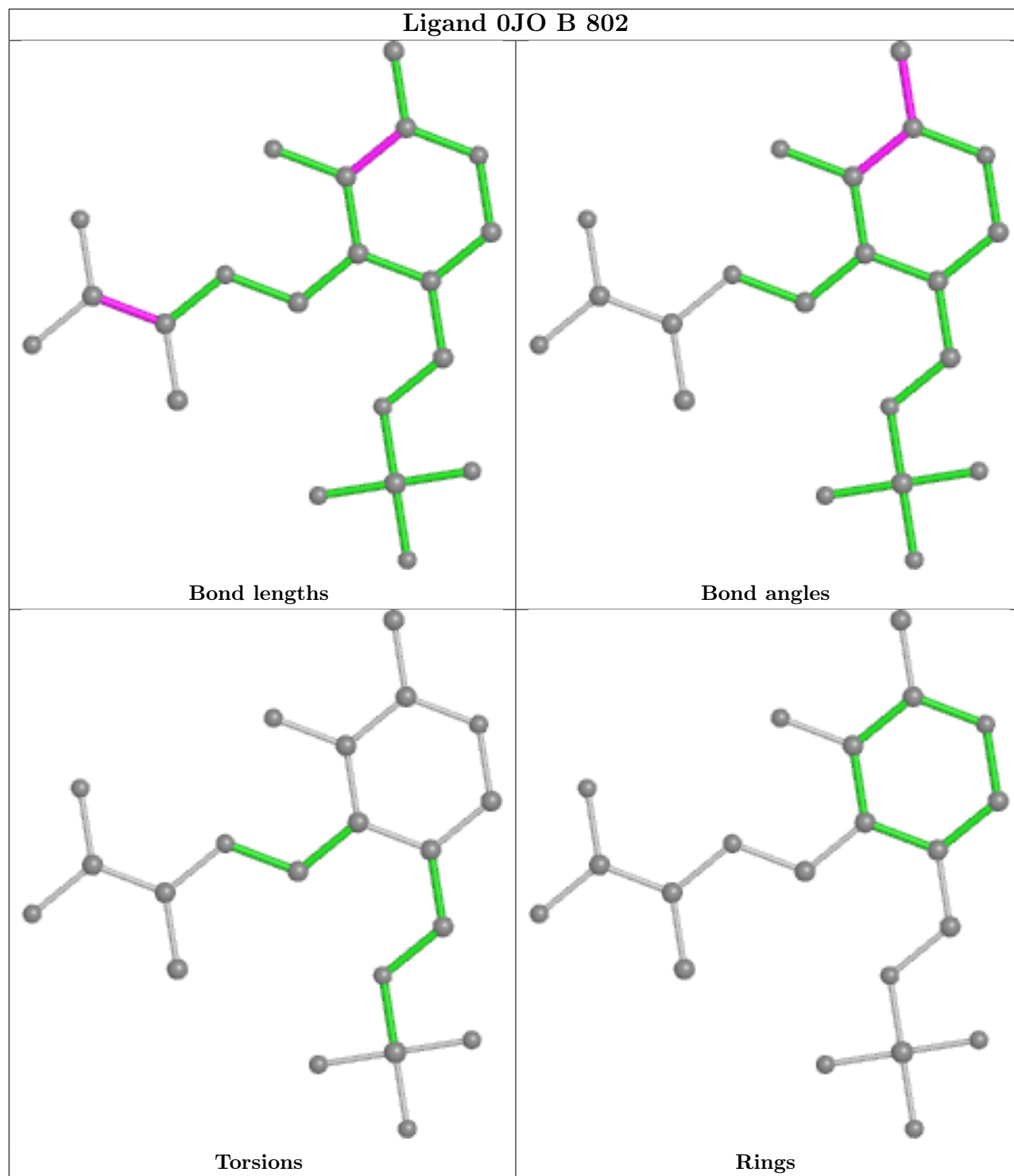
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	PEG	5	0
4	B	805	EDO	3	0
5	A	603	PEG	2	0
8	B	802	0JO	1	0
6	A	604	DMS	2	0

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 ⓘ

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	253/268 (94%)	0.66	36 (14%) 2 3	18, 33, 54, 94	0
2	B	394/397 (99%)	0.54	40 (10%) 6 7	15, 22, 54, 79	0
All	All	647/665 (97%)	0.59	76 (11%) 4 5	15, 27, 54, 94	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	9.3
2	B	159	VAL	8.5
1	A	193	LEU	7.4
1	A	212	PHE	7.0
2	B	158	PRO	6.7
2	B	164	ALA	6.4
2	B	139	VAL	6.1
2	B	385	PHE	5.4
2	B	392	LYS	5.3
2	B	135	GLY	5.2
2	B	394	ARG	5.2
2	B	160	HIS	5.1
1	A	234	GLY	5.0
2	B	141	ARG	4.8
2	B	156	VAL	4.5
1	A	247	SER	4.5
1	A	195	HIS	4.3
2	B	157	ILE	4.2
2	B	147	PHE	4.2
2	B	391	LEU	4.2
2	B	111	GLY	4.2
2	B	162	GLY	4.1
2	B	395	GLY	4.1
1	A	267	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	249	LYS	3.9
1	A	213	GLY	3.8
2	B	166	LEU	3.7
1	A	13	ASP	3.7
2	B	388	HIS	3.6
2	B	140	GLU	3.6
1	A	260	SER	3.6
2	B	143	SER	3.6
1	A	264	ALA	3.5
1	A	257	SER	3.5
1	A	203	TYR	3.4
1	A	268	ALA	3.3
1	A	214	ILE	3.3
1	A	157	ASN	3.2
2	B	136	ALA	3.2
2	B	393	ALA	3.0
1	A	243	LYS	2.9
2	B	165	THR	2.8
1	A	73	ALA	2.8
1	A	1	MET	2.8
2	B	390	ILE	2.7
1	A	250	GLN	2.7
1	A	252	LEU	2.7
2	B	112[A]	ALA	2.7
1	A	239	LYS	2.7
2	B	138	ASP	2.7
2	B	142	GLN	2.6
2	B	173	ALA	2.6
2	B	146	VAL	2.6
2	B	150	ARG	2.6
2	B	345	ILE	2.5
1	A	204	HIS	2.5
1	A	43	ALA	2.5
1	A	256	ARG	2.5
2	B	161	SER	2.4
1	A	28	PRO	2.3
2	B	167[A]	LYS	2.3
1	A	40	LEU	2.3
1	A	42	ASP	2.3
2	B	80	LEU	2.2
1	A	109	ASN	2.2
1	A	226	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	245	LEU	2.2
2	B	389	ASP	2.2
2	B	181	TYR	2.1
2	B	255	VAL	2.1
2	B	168	ASP	2.1
2	B	309	VAL	2.1
1	A	15	ARG	2.1
1	A	242	GLU	2.1
1	A	251	MET	2.1
1	A	194	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PEG	A	603	7/7	0.67	0.18	40,44,48,51	0
3	BZI	B	803	9/9	0.76	0.27	22,25,31,31	9
4	EDO	A	602	4/4	0.85	0.09	44,53,53,56	0
5	PEG	B	804	7/7	0.85	0.20	34,34,36,37	0
7	CL	A	606	1/1	0.85	0.17	65,65,65,65	0
3	BZI	A	601	9/9	0.87	0.11	37,40,47,49	0
6	DMS	A	604	4/4	0.88	0.17	50,56,56,58	0
6	DMS	B	809	4/4	0.89	0.29	45,48,57,61	0
7	CL	B	813	1/1	0.91	0.17	63,63,63,63	0
4	EDO	B	805	4/4	0.92	0.25	34,35,36,39	0
6	DMS	B	806	4/4	0.93	0.19	39,49,49,51	0
6	DMS	B	807	4/4	0.95	0.12	27,28,28,29	0
6	DMS	B	810	4/4	0.95	0.35	47,54,54,55	0

Continued on next page...

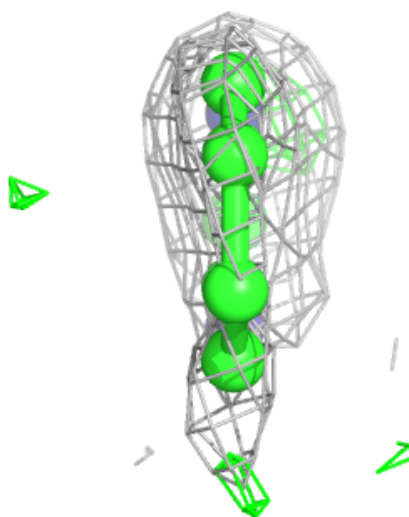
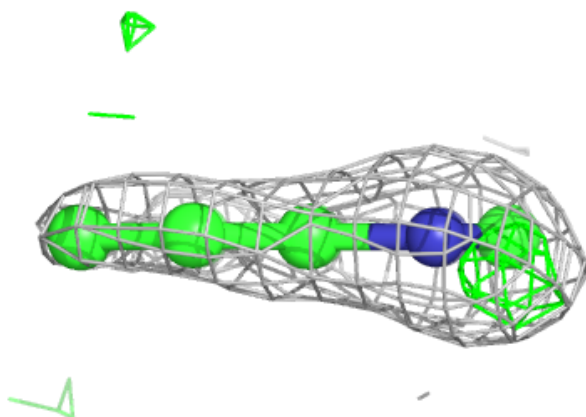
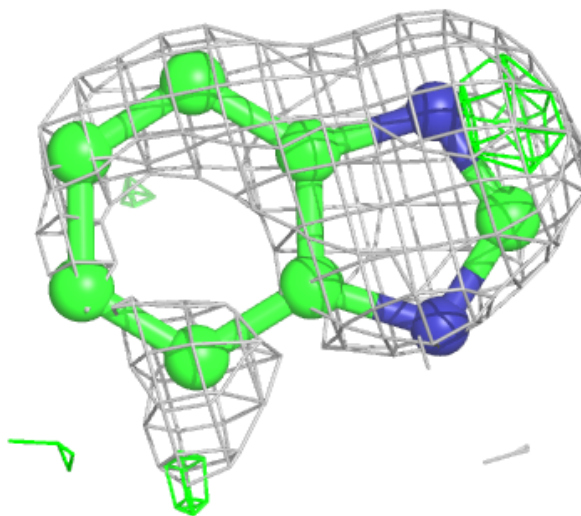
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CL	A	605	1/1	0.97	0.05	42,42,42,42	0
3	BZI	B	801	9/9	0.97	0.10	34,36,39,40	0
6	DMS	B	808	4/4	0.97	0.18	35,35,43,47	0
8	OJO	B	802	21/21	0.97	0.10	17,21,29,32	0
9	CS	B	811	1/1	1.00	0.01	26,26,26,26	1
9	CS	B	812[A]	1/1	1.00	0.03	26,26,26,26	1
9	CS	B	812[B]	1/1	1.00	0.03	27,27,27,27	1

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.

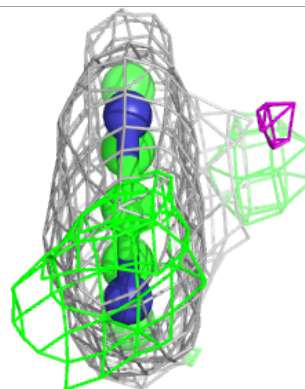
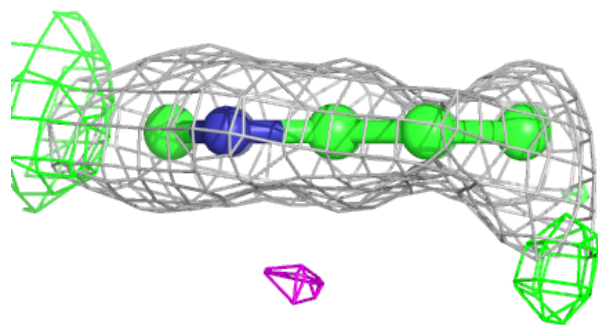
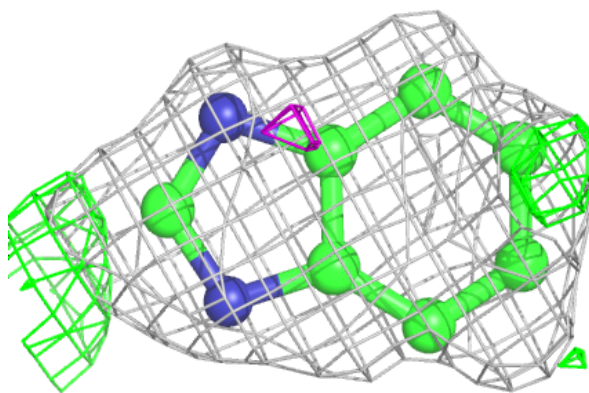
Electron density around BZI B 803:

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



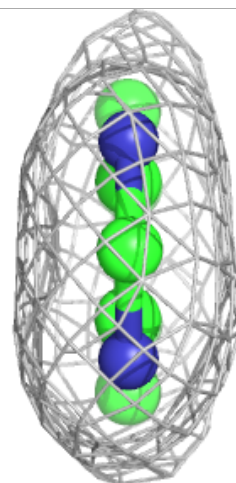
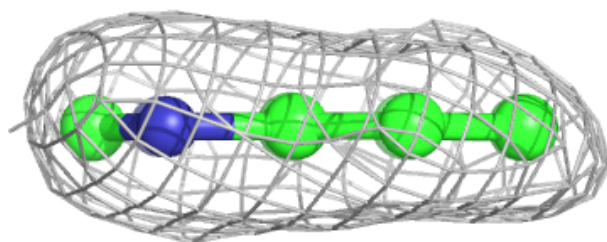
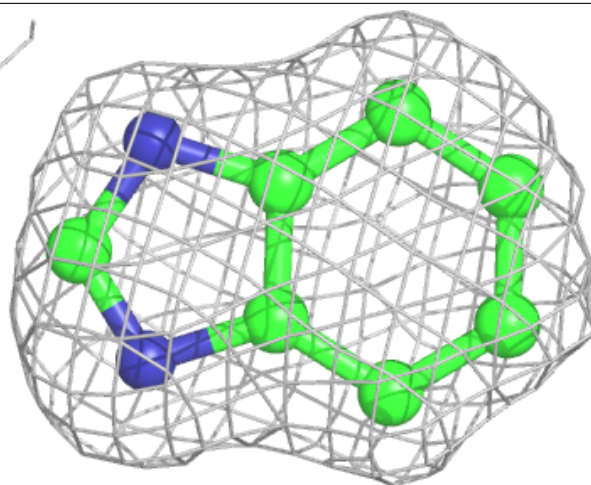
Electron density around BZI A 601:

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



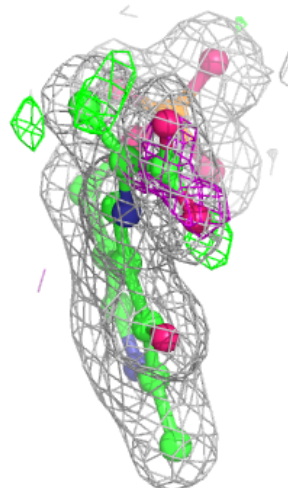
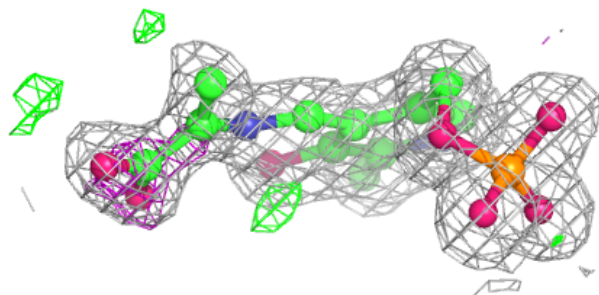
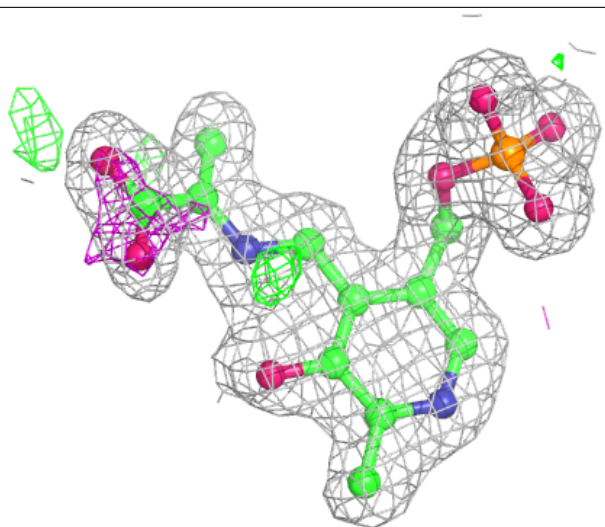
Electron density around BZI B 801:

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



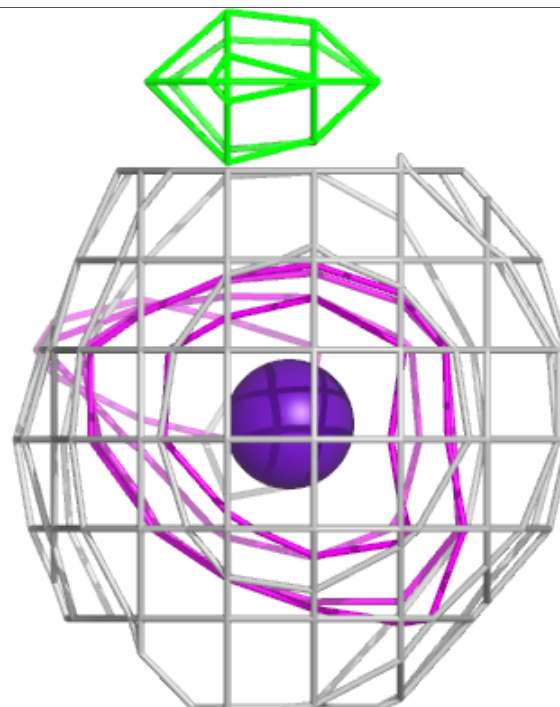
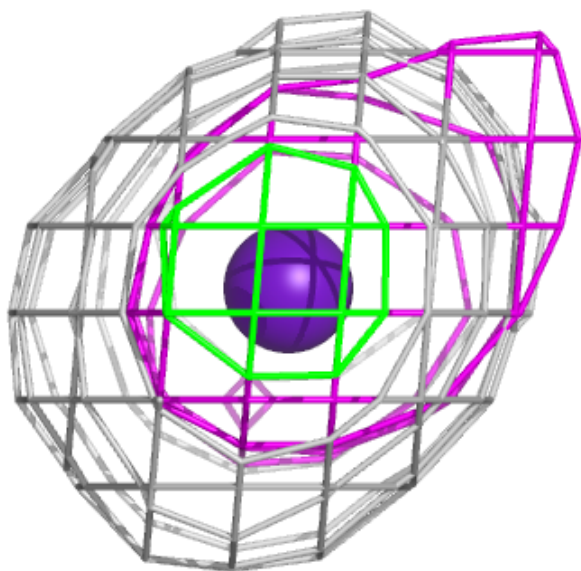
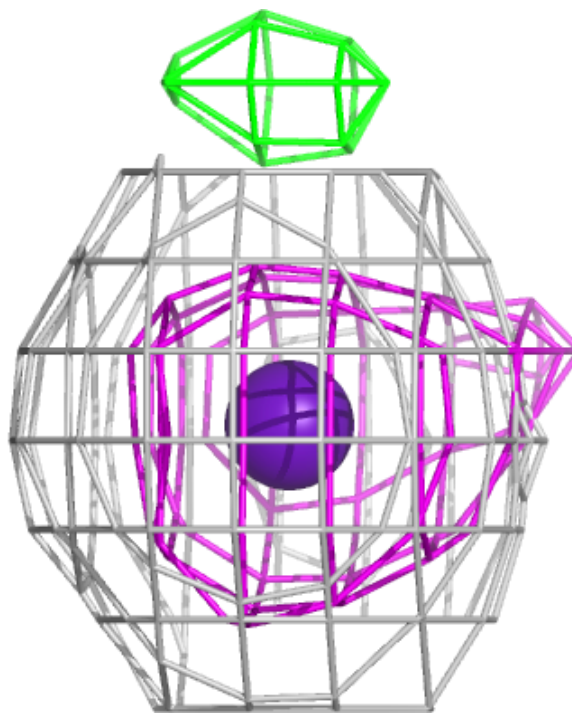
Electron density around 0JO B 802:

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



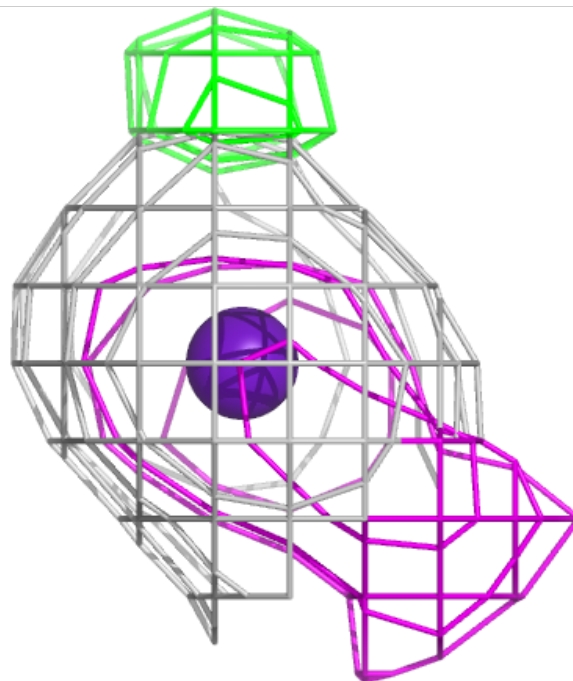
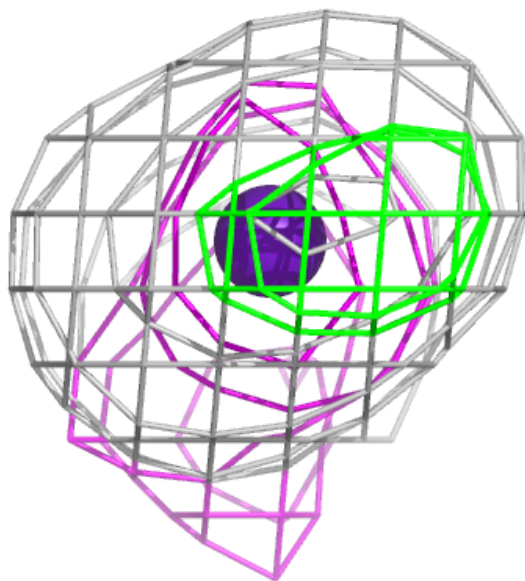
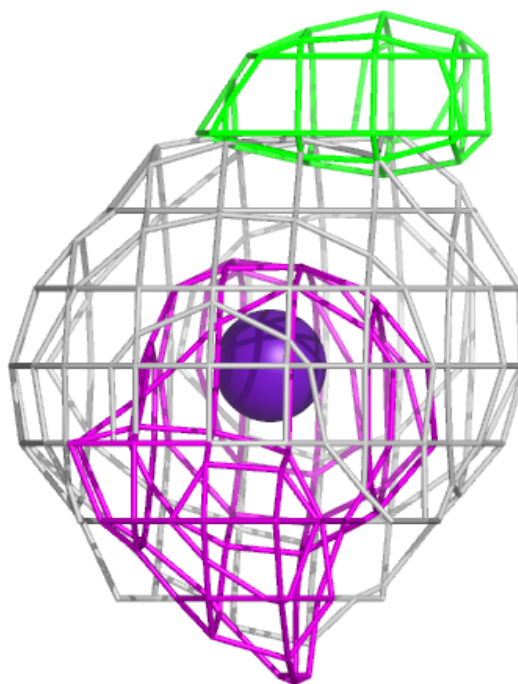
Electron density around CS B 811:

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



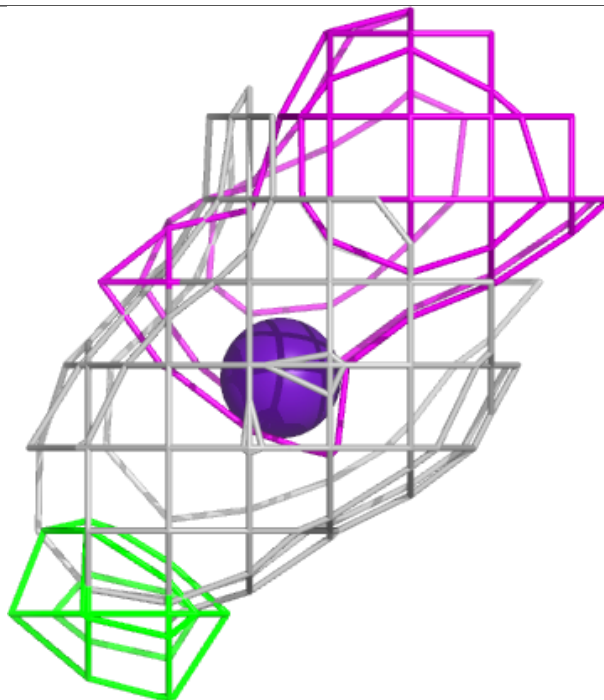
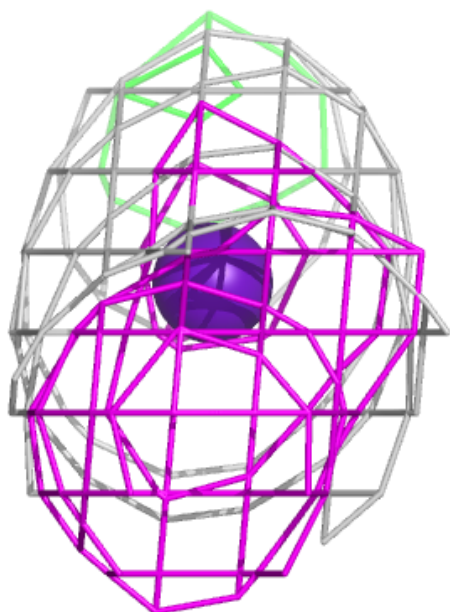
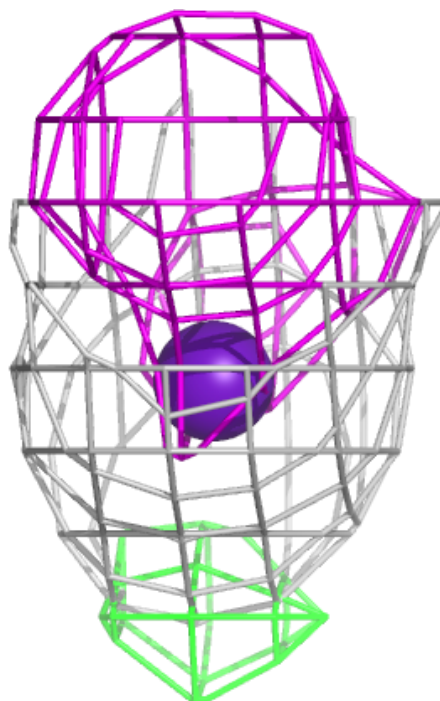
Electron density around CS B 812 (A):

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



Electron density around CS B 812 (B):

$2mF_o - DF_c$ (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.