



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:07 PM UTC

PDB ID : 6X0C / pdb_00006x0c
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 types of validation reports are described at

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

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

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

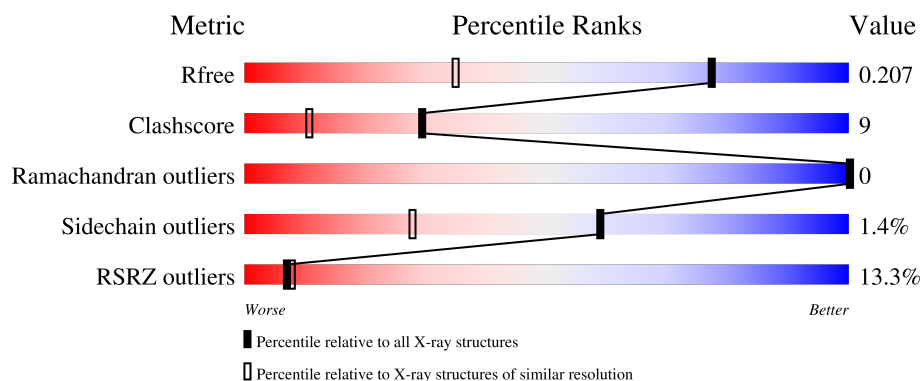
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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	16% 87% 6% • 6%
2	B	397	11% 84% 15% •

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
4	EDO	B	805	-	-	X	-
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			

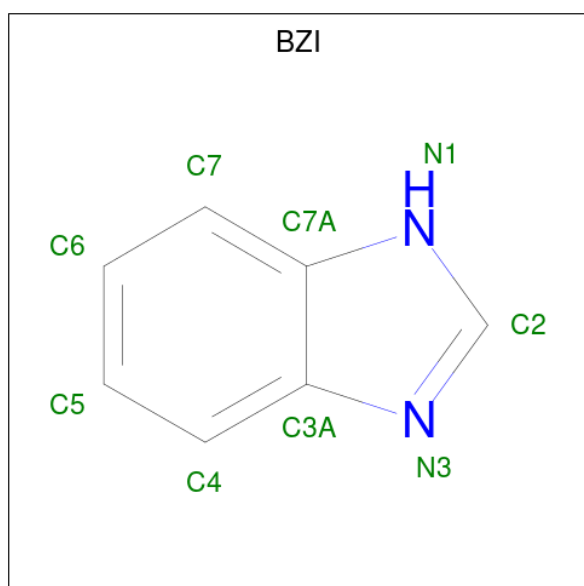
- Molecule 2 is a protein called Tryptophan synthase beta chain.

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 (CCD ID: BZI) (formula: C₇H₆N₂) (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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



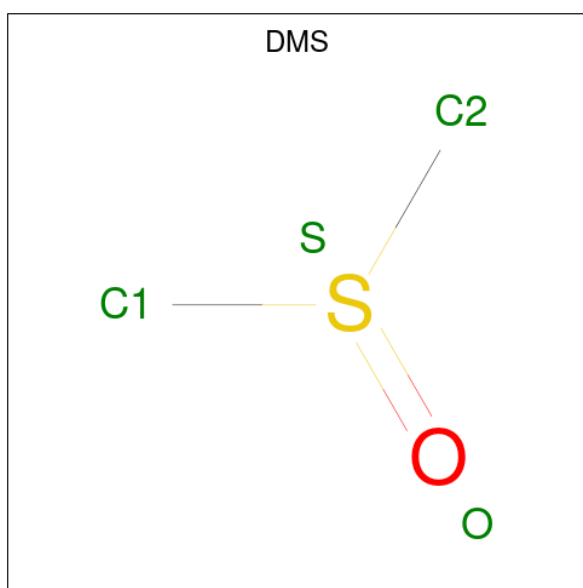
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: 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		

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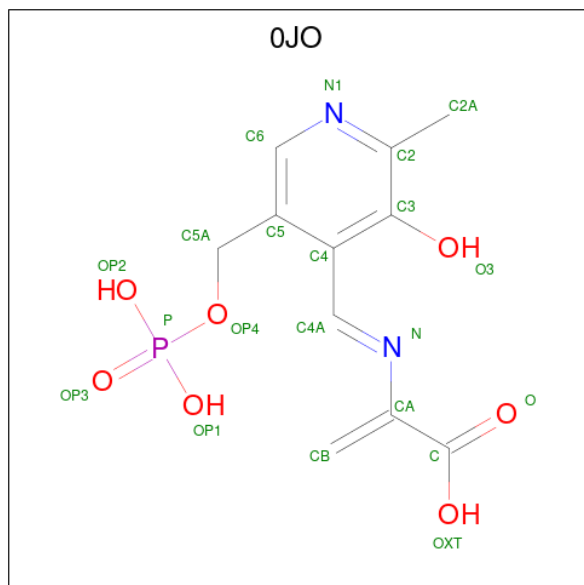
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: 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-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (CCD ID: 0JO) (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 (CCD ID: 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

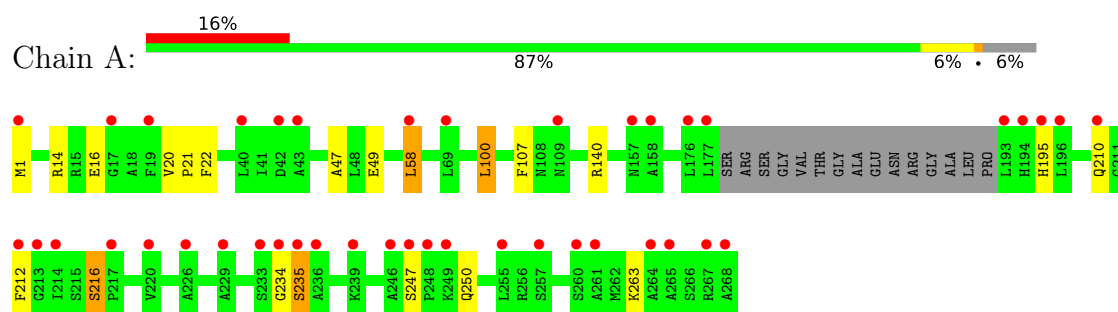
- Molecule 10 is water.

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

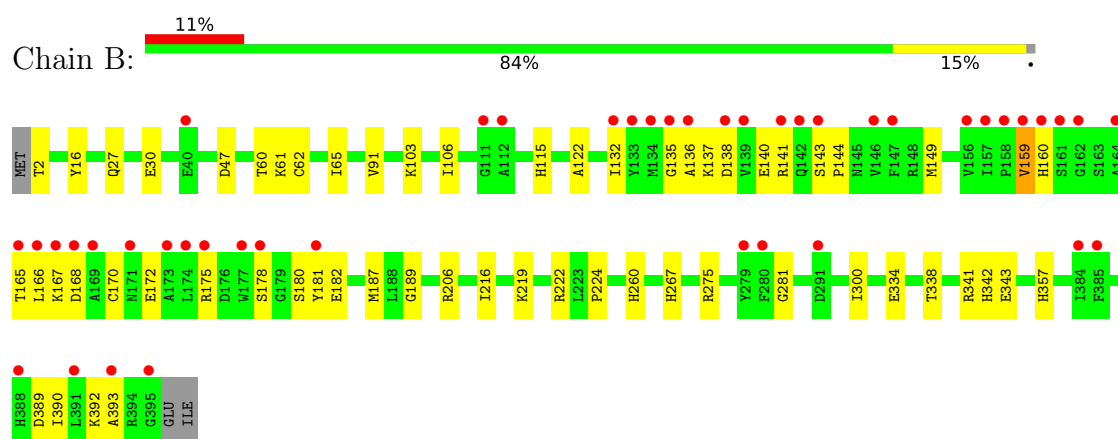
3 Residue-property plots [i](#)

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 (4.90%)	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 , 43.3	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: DMS, BZI, EDO, OJO, PEG, CL, CS

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	1.07	0/1985	1.25	0/2695
2	B	1.02	1/3191 (0.0%)	1.20	2/4305 (0.0%)
All	All	1.04	1/5176 (0.0%)	1.22	2/7000 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	267	HIS	CE1-NE2	5.05	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	ASP	CA-CB-CG	7.30	119.90	112.60
2	B	357	HIS	CA-CB-CG	-5.39	108.41	113.80

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	25	0
2	B	3132	0	3095	58	0
3	A	9	0	6	1	0

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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	4	0
5	A	7	0	10	2	0
5	B	7	0	10	6	0
6	A	4	0	6	1	0
6	B	20	0	30	2	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	6	0
10	B	420	0	0	19	0
All	All	5784	0	5138	89	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 9.

All (89) 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
6:B:808:DMS:H21	10:B:914:HOH:O	1.67	0.94
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
1:A:58:LEU:C	1:A:58:LEU:HD12	2.16	0.71
2:B:165:THR:HG23	2:B:167[B]:LYS:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:SER:HA	10:B:1133:HOH:O	1.96	0.66
1:A:235:SER:CB	10:A:708:HOH:O	2.41	0.66
1:A:100:LEU:C	1:A:100:LEU:HD13	2.21	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
2:B:2:THR:HG22	10:B:1186:HOH:O	2.01	0.60
6:A:604:DMS:H13	10:A:797:HOH:O	2.03	0.58
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
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:62[B]:CYS:HB2	2:B:343:GLU:CD	2.30	0.56
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
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: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:138:ASP:CG	10:B:905:HOH:O	2.55	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
4:B:805:EDO:H22	6:B:810:DMS:H23	1.94	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: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
1:A:58:LEU:C	1:A:58:LEU:CD1	2.85	0.47
2:B:159:VAL:CG1	2:B:172:GLU:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LYS:H	5:B:804:PEG:C2	2.27	0.46
5:B:804:PEG:O1	10:B:901:HOH:O	2.10	0.46
2:B:216[A]:ILE:HG21	2:B:224:PRO:HD3	1.97	0.46
2:B:140:GLU:OE2	2:B:140:GLU:HA	2.15	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:106:ILE:HD12	2:B:187[A]:MET:HE3	1.97	0.46
2:B:165:THR:HG23	2:B:167[B]:LYS:HD3	1.98	0.45
1:A:100:LEU:C	1:A:100:LEU:CD1	2.90	0.45
2:B:392:LYS:HG3	2:B:393:ALA:N	2.32	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
1:A:1:MET:HE3	1:A:1:MET:HB3	1.94	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
2:B:62[B]:CYS:CB	2:B:343:GLU:CD	2.93	0.42
1:A:247:SER:OG	1:A:250:GLN:HB3	2.20	0.41
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.94	0.41
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%)	42	11
2	B	325/310 (105%)	322 (99%)	3 (1%)	70	46
All	All	527/518 (102%)	519 (98%)	8 (2%)	59	25

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

Mol	Chain	Res	Type
1	A	58	LEU
1	A	100	LEU
1	A	216[A]	SER
1	A	216[B]	SER
1	A	235	SER
2	B	141	ARG
2	B	159	VAL
2	B	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	65	GLN
1	A	66	ASN
1	A	165	GLN
1	A	195	HIS

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Mol	Chain	Res	Type
1	A	210	GLN
2	B	44	GLN
2	B	51	ASN
2	B	171	ASN
2	B	365	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	EDO	A	602	-	3,3,3	0.17	0	2,2,2	0.25	0
6	DMS	B	806	-	3,3,3	0.20	0	3,3,3	0.34	0
5	PEG	B	804	-	6,6,6	0.41	0	5,5,5	0.44	0
6	DMS	A	604	-	3,3,3	0.27	0	3,3,3	0.17	0
3	BZI	B	801	-	10,10,10	0.55	0	13,13,13	0.71	0
6	DMS	B	808	-	3,3,3	0.28	0	3,3,3	0.47	0
4	EDO	B	805	-	3,3,3	0.32	0	2,2,2	0.23	0
3	BZI	A	601	-	10,10,10	0.45	0	13,13,13	0.58	0
6	DMS	B	809	-	3,3,3	0.32	0	3,3,3	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	B	810	-	3,3,3	0.24	0	3,3,3	0.19	0
6	DMS	B	807	-	3,3,3	1.14	0	3,3,3	0.99	0
8	OJO	B	802	-	20,21,21	1.28	3 (15%)	23,30,30	1.05	2 (8%)
5	PEG	A	603	-	6,6,6	0.18	0	5,5,5	0.11	0
3	BZI	B	803	-	10,10,10	0.44	0	13,13,13	0.60	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	-
5	PEG	B	804	-	-	1/4/4/4	-
3	BZI	B	801	-	-	-	0/2/2/2
4	EDO	B	805	-	-	0/1/1/1	-
3	BZI	A	601	-	-	-	0/2/2/2
8	OJO	B	802	-	-	0/11/15/15	0/1/1/1
5	PEG	A	603	-	-	2/4/4/4	-
3	BZI	B	803	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	802	OJO	CA-C	-3.22	1.44	1.50
8	B	802	OJO	OXT-C	-2.95	1.22	1.30
8	B	802	OJO	C3-C2	2.80	1.43	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	OJO	C2A-C2-C3	2.26	123.45	120.80
8	B	802	OJO	OP2-P-OP4	2.00	111.89	106.67

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

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Mol	Chain	Res	Type	Atoms
5	B	804	PEG	O1-C1-C2-O2

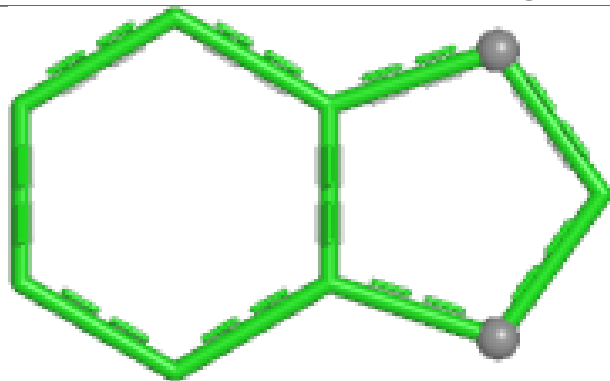
There are no ring outliers.

9 monomers are involved in 16 short contacts:

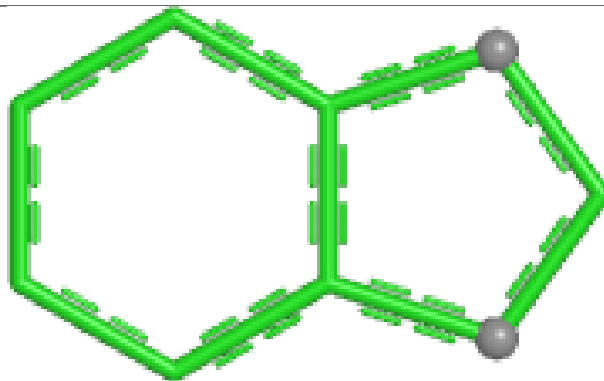
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	PEG	6	0
6	A	604	DMS	1	0
6	B	808	DMS	1	0
4	B	805	EDO	4	0
3	A	601	BZI	1	0
6	B	810	DMS	1	0
8	B	802	OJO	1	0
5	A	603	PEG	2	0
3	B	803	BZI	1	0

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.

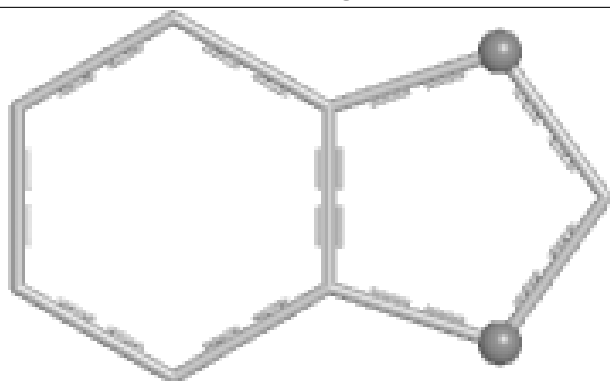
Ligand BZI B 801



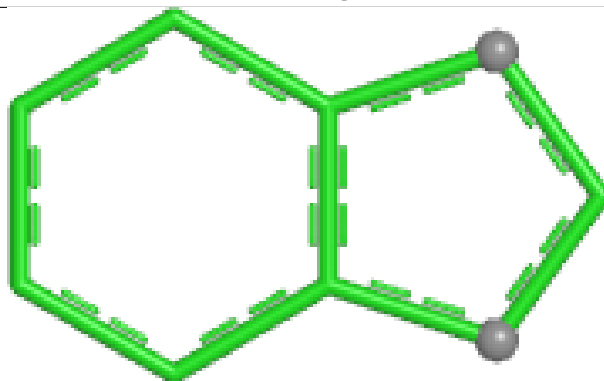
Bond lengths



Bond angles

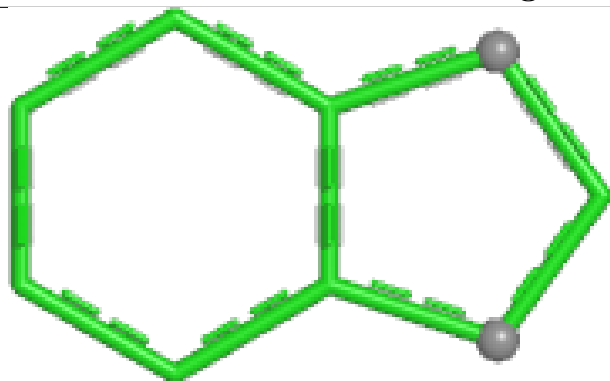


Torsions

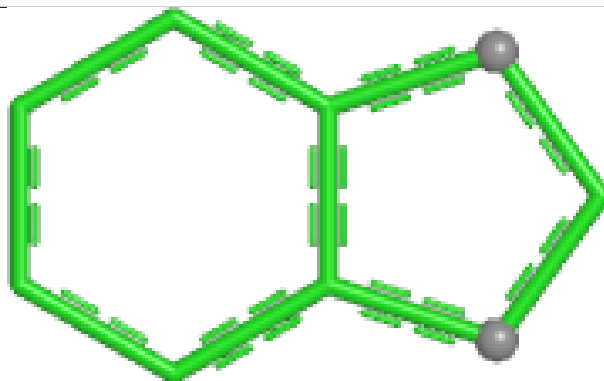


Rings

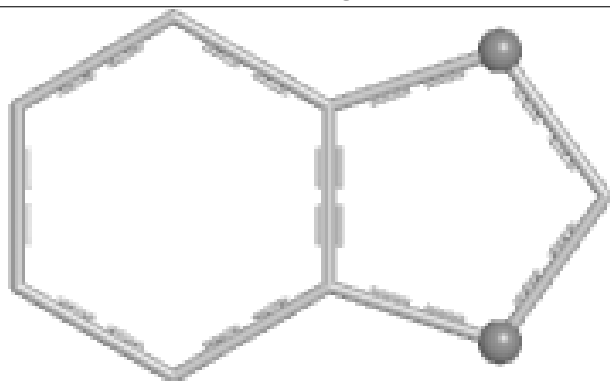
Ligand BZI A 601



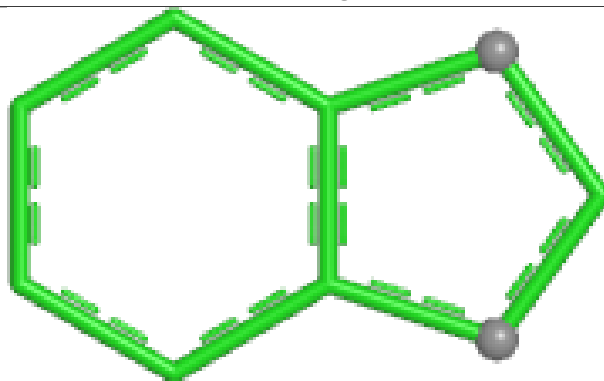
Bond lengths



Bond angles

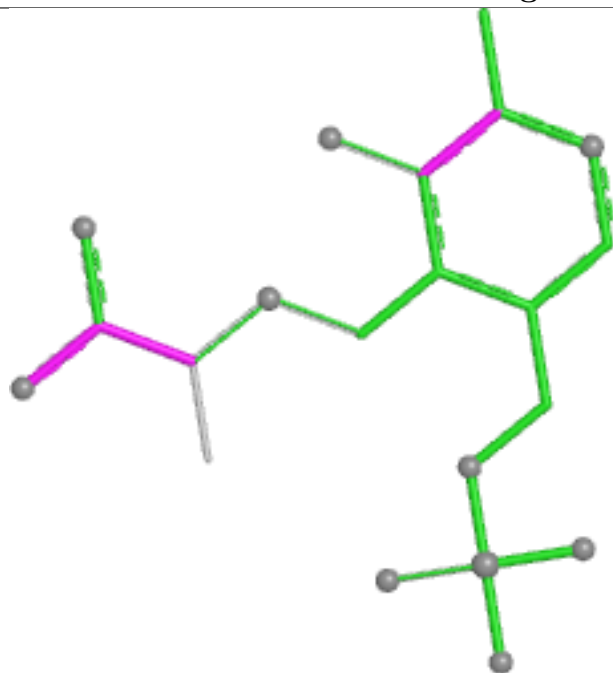


Torsions

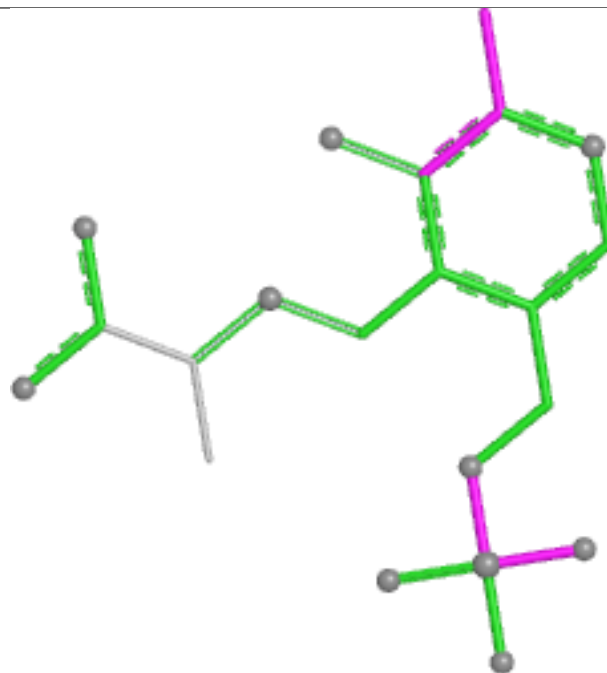


Rings

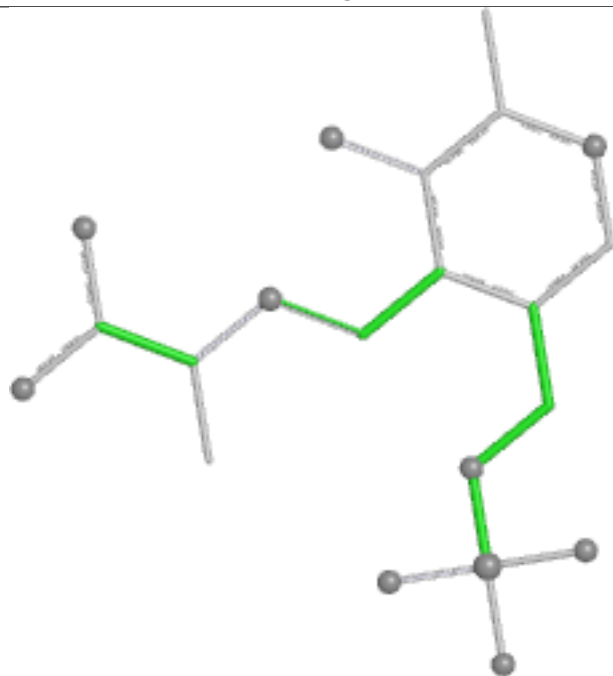
Ligand 0JO B 802



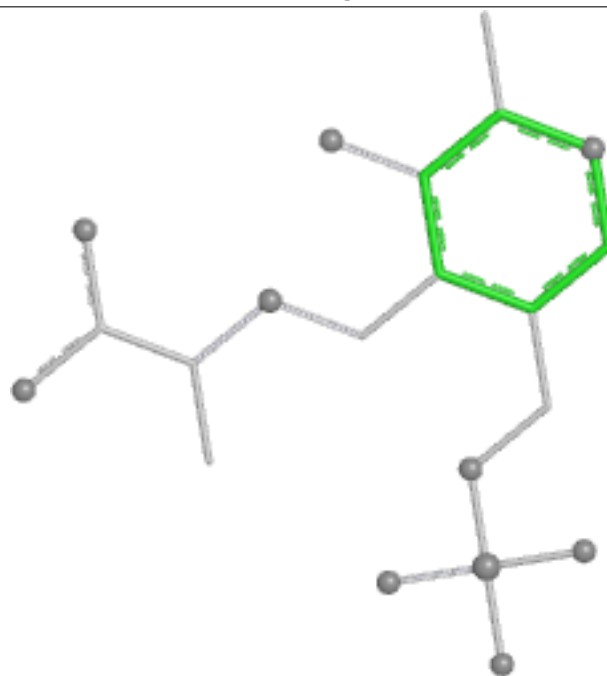
Bond lengths



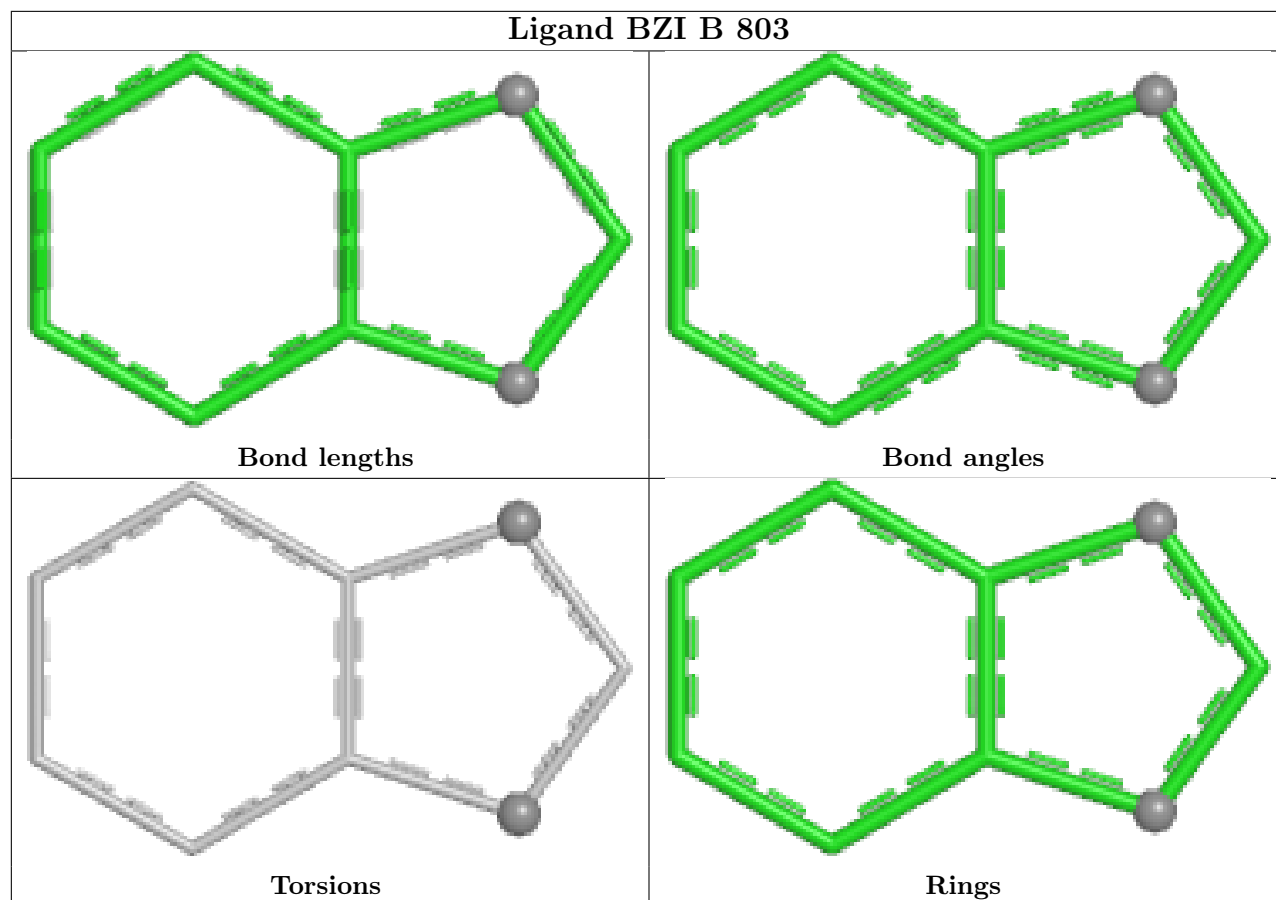
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.96	42 (16%)	4 4	14, 33, 54, 94	4 (1%)
2	B	394/397 (99%)	0.44	44 (11%)	10 10	8, 22, 54, 79	19 (4%)
All	All	647/665 (97%)	0.64	86 (13%)	7 8	8, 26, 54, 94	23 (3%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	164	ALA	6.7
1	A	212	PHE	6.4
2	B	139	VAL	5.2
1	A	234	GLY	4.9
2	B	166	LEU	4.7
2	B	173	ALA	4.6
1	A	193	LEU	4.6
2	B	167[A]	LYS	4.5
2	B	159	VAL	4.3
2	B	111	GLY	4.2
1	A	177	LEU	4.2
2	B	385	PHE	4.2
2	B	135	GLY	4.2
2	B	158	PRO	4.2
2	B	165	THR	4.1
2	B	156	VAL	4.0
2	B	162	GLY	3.9
1	A	214	ILE	3.9
1	A	194	HIS	3.8
2	B	174	LEU	3.7
2	B	112[A]	ALA	3.7
1	A	246	ALA	3.6
2	B	138	ASP	3.6
2	B	146	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	147	PHE	3.5
2	B	141	ARG	3.4
1	A	249	LYS	3.3
1	A	213	GLY	3.2
1	A	158	ALA	3.2
1	A	268	ALA	3.2
2	B	142	GLN	3.2
2	B	168	ASP	3.2
2	B	181	TYR	3.1
1	A	235	SER	2.8
2	B	279	TYR	2.8
2	B	133	TYR	2.8
2	B	160	HIS	2.8
1	A	257	SER	2.7
1	A	157	ASN	2.7
1	A	260	SER	2.6
1	A	19	PHE	2.6
1	A	43	ALA	2.6
1	A	255	LEU	2.6
1	A	58	LEU	2.5
1	A	69	LEU	2.5
2	B	175[A]	ARG	2.5
1	A	1	MET	2.5
1	A	220	VAL	2.5
2	B	132	ILE	2.4
2	B	136	ALA	2.4
2	B	143	SER	2.4
2	B	391	LEU	2.4
1	A	226	ALA	2.3
1	A	264	ALA	2.3
1	A	261	ALA	2.3
1	A	196	LEU	2.3
1	A	17	GLY	2.3
1	A	247	SER	2.3
2	B	395	GLY	2.2
2	B	134	MET	2.2
2	B	178	SER	2.2
2	B	177	TRP	2.2
2	B	384	ILE	2.2
1	A	236	ALA	2.2
2	B	169	ALA	2.2
1	A	195	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	2.2
2	B	291	ASP	2.2
2	B	388	HIS	2.2
1	A	176	LEU	2.1
1	A	217	PRO	2.1
2	B	157	ILE	2.1
1	A	42	ASP	2.1
2	B	393	ALA	2.1
1	A	267	ARG	2.1
1	A	210	GLN	2.1
1	A	233	SER	2.1
2	B	161	SER	2.1
1	A	248	PRO	2.1
2	B	280	PHE	2.0
1	A	229	ALA	2.0
1	A	265	ALA	2.0
2	B	40	GLU	2.0
1	A	109	ASN	2.0
2	B	171	ASN	2.0
1	A	40	LEU	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 oligosaccharides 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	0.69	0.18	40,44,48,51	0
6	DMS	A	604	4/4	0.76	0.24	50,56,56,58	0
3	BZI	A	601	9/9	0.78	0.13	37,40,47,49	0

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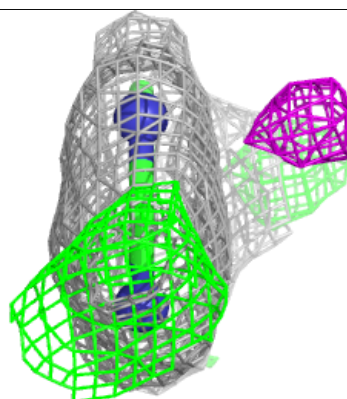
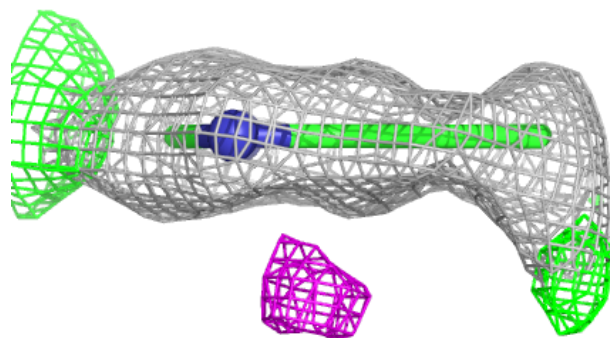
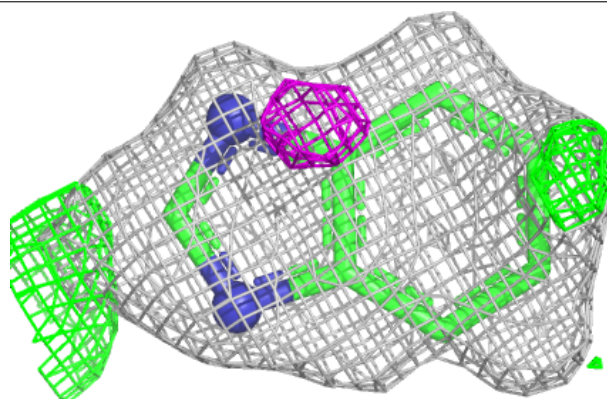
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DMS	B	809	4/4	0.79	0.22	45,48,57,61	0
3	BZI	B	803	9/9	0.80	0.20	22,25,31,31	9
5	PEG	B	804	7/7	0.80	0.14	34,34,36,37	0
6	DMS	B	806	4/4	0.85	0.17	39,49,49,51	0
6	DMS	B	810	4/4	0.85	0.17	47,54,54,55	0
7	CL	A	606	1/1	0.85	0.12	65,65,65,65	0
7	CL	B	813	1/1	0.86	0.09	63,63,63,63	0
4	EDO	B	805	4/4	0.90	0.09	34,35,36,39	0
6	DMS	B	808	4/4	0.92	0.11	35,35,43,47	0
7	CL	A	605	1/1	0.92	0.09	42,42,42,42	0
4	EDO	A	602	4/4	0.93	0.12	44,53,53,56	0
6	DMS	B	807	4/4	0.94	0.16	27,28,28,29	0
3	BZI	B	801	9/9	0.96	0.07	34,36,39,40	0
8	OJO	B	802	21/21	0.98	0.07	17,21,29,32	0
9	CS	B	811	1/1	1.00	0.04	26,26,26,26	1
9	CS	B	812[A]	1/1	1.00	0.04	26,26,26,26	1
9	CS	B	812[B]	1/1	1.00	0.04	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.

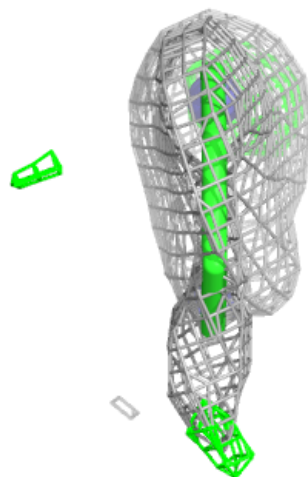
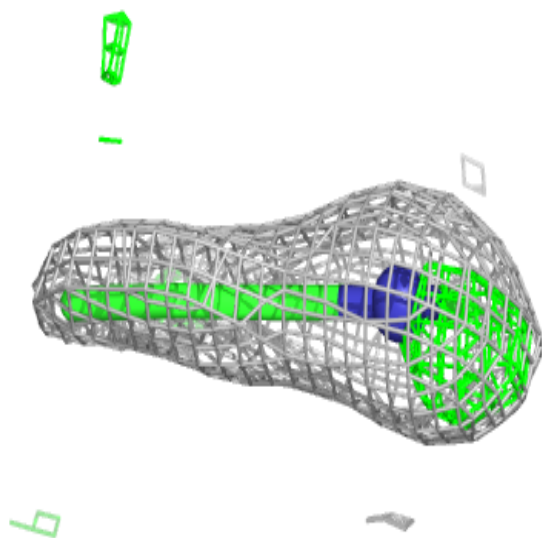
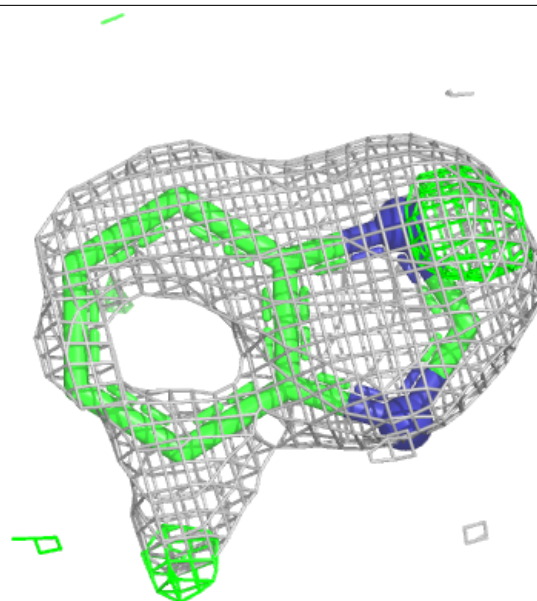
Electron density around BZI A 601:

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



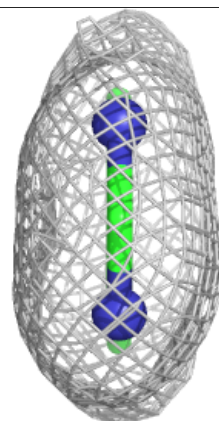
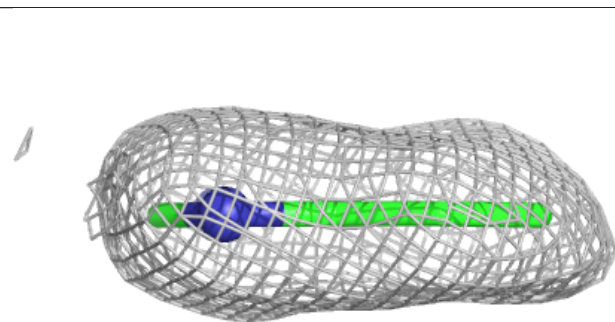
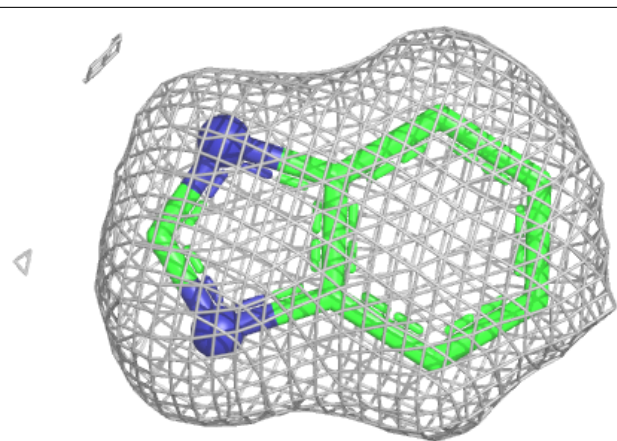
Electron density around BZI B 803:

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



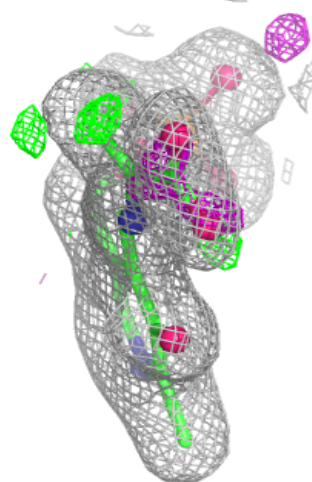
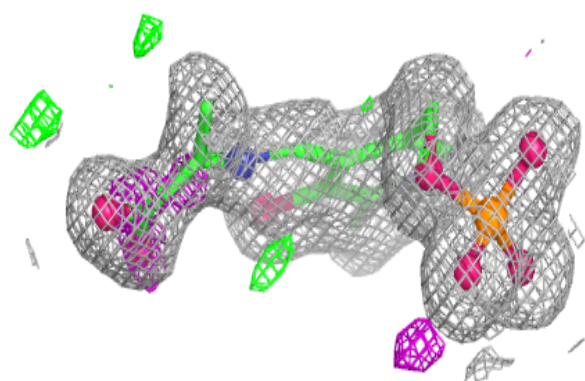
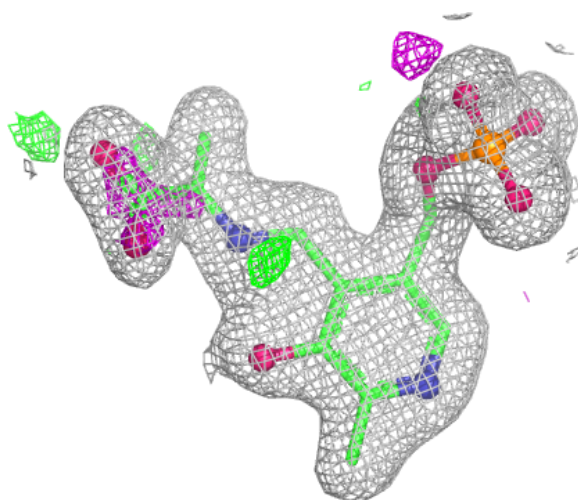
Electron density around BZI B 801:

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



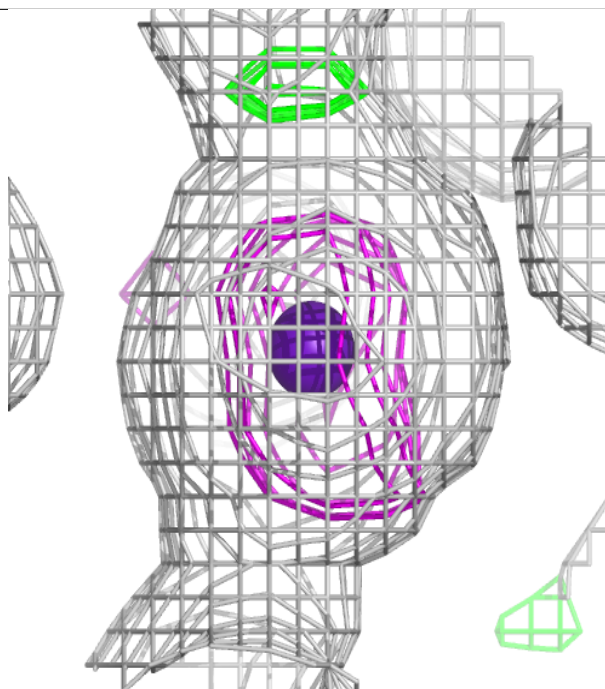
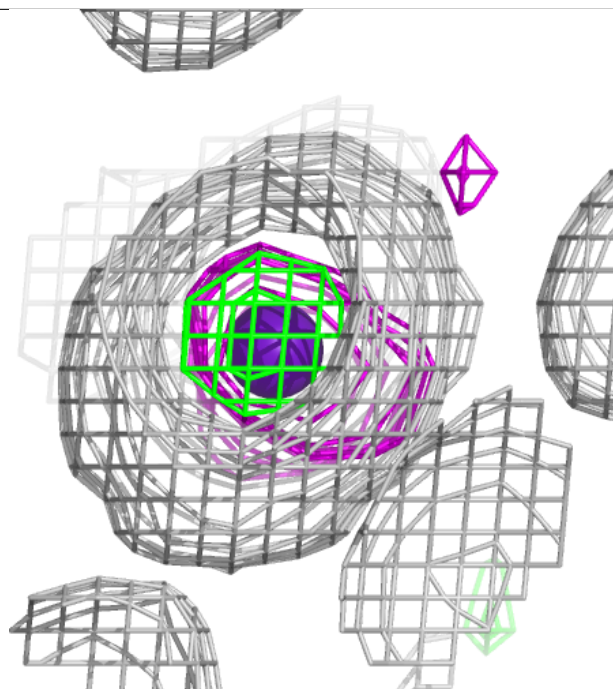
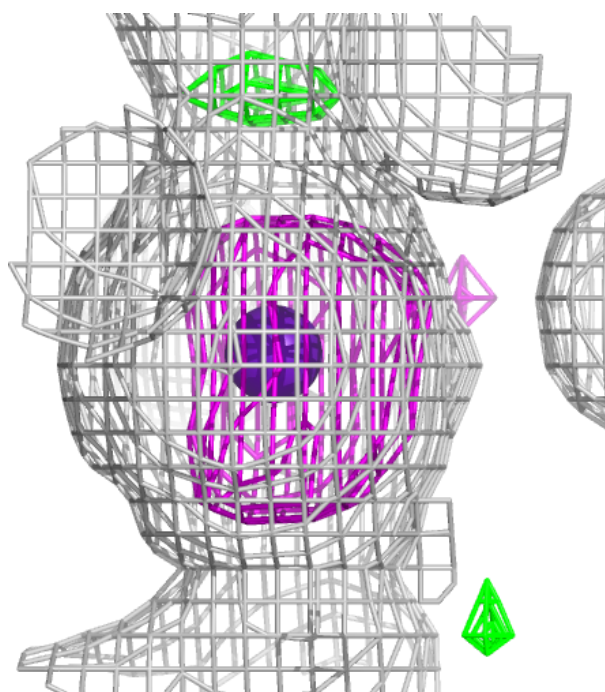
Electron density around 0JO B 802:

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



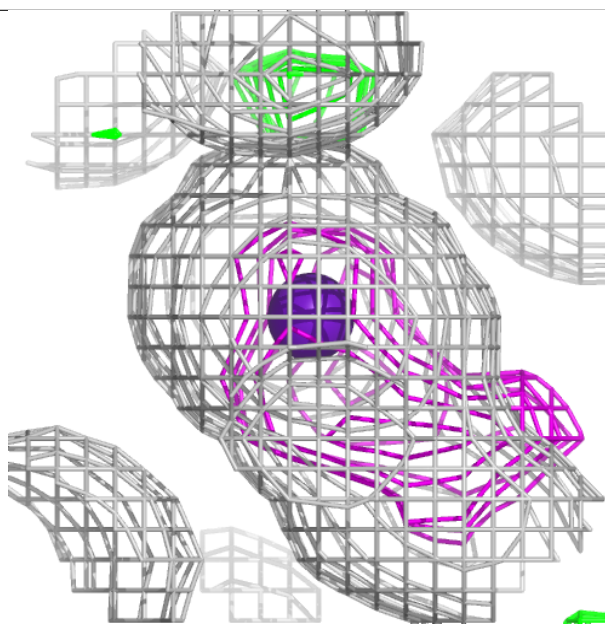
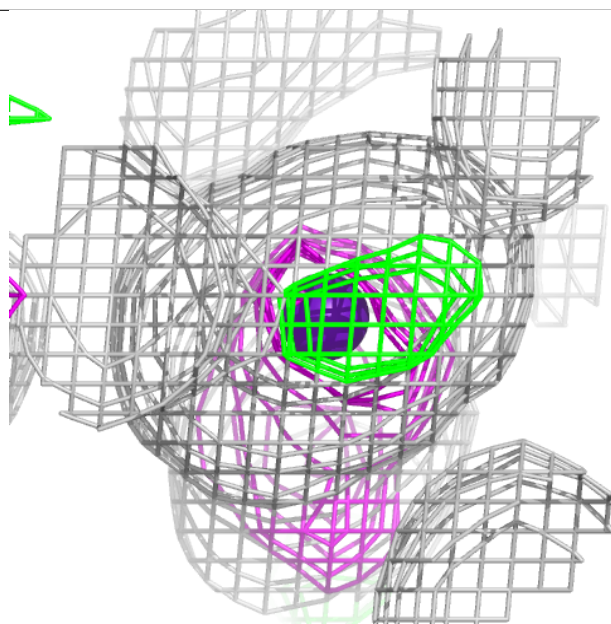
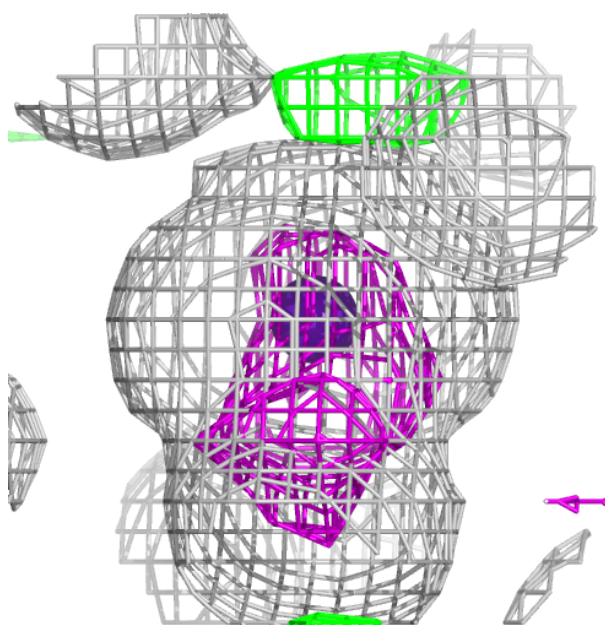
Electron density around CS B 811:

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



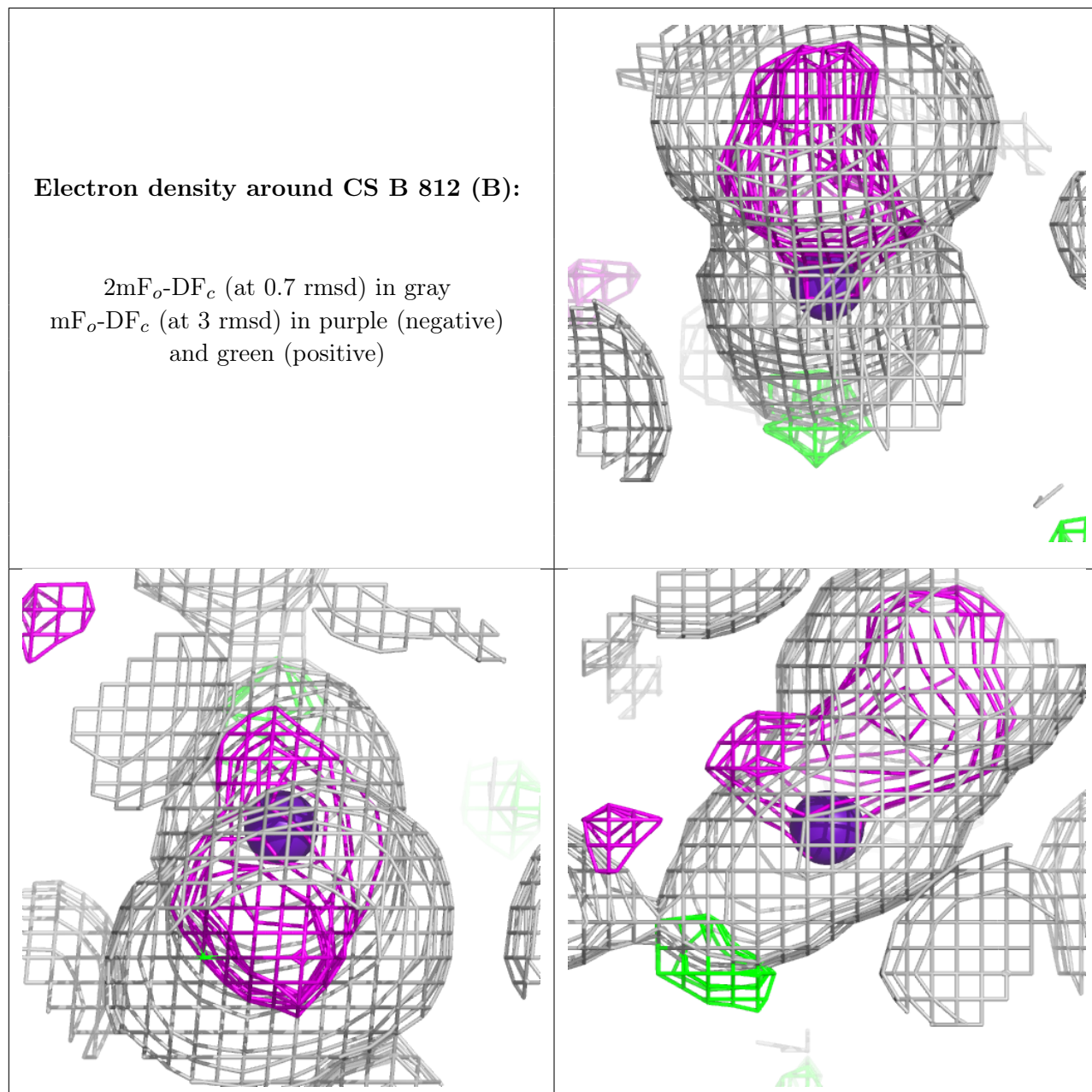
Electron density around CS B 812 (A):

$2mF_o-DF_c$ (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 ⓘ**

There are no such residues in this entry.