



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 PM UTC

PDB ID : 7LGX / pdb_00007lgx
Title : The aminoacrylate form of mutant beta-K167T Salmonella typhimurium Tryptophan Synthase in complex with with inhibitor N-(4'-trifluoromethoxybenzenesulfonyl)-2-amino-1-ethylphosphate (F9F) at the enzyme alpha-site, benzimidazole (BZI) at the enzyme beta site and cesium ion at the metal coordination site at 1.80 Angstrom resolution
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Deposited on : 2021-01-21
Resolution : 1.80 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)

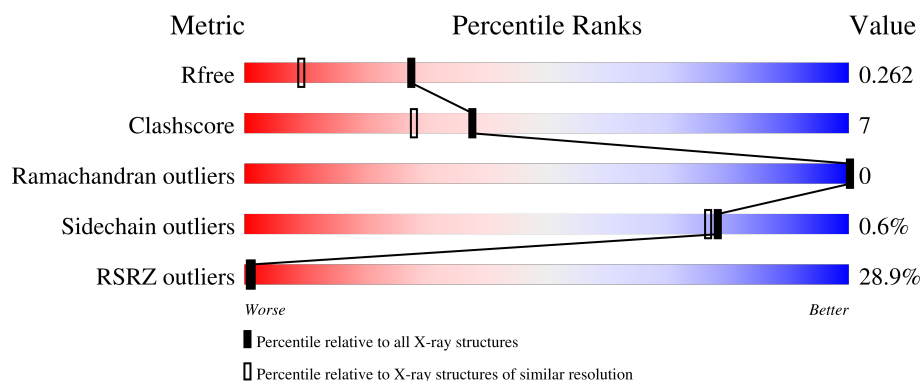
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	48% 81%15%.
2	B	397	15% 89%10%.

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5415 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	258	Total	C	N	O	S	0	0	0
			1862	1187	318	349	8			

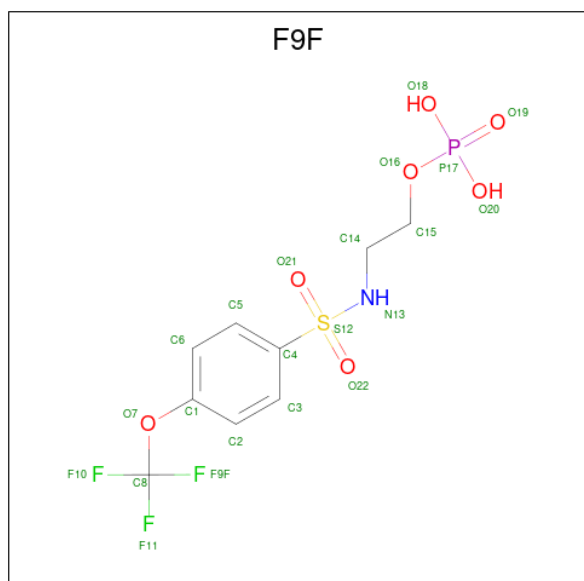
- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	5	0
			3006	1886	528	573	19			

There is a discrepancy between the modelled and reference sequences:

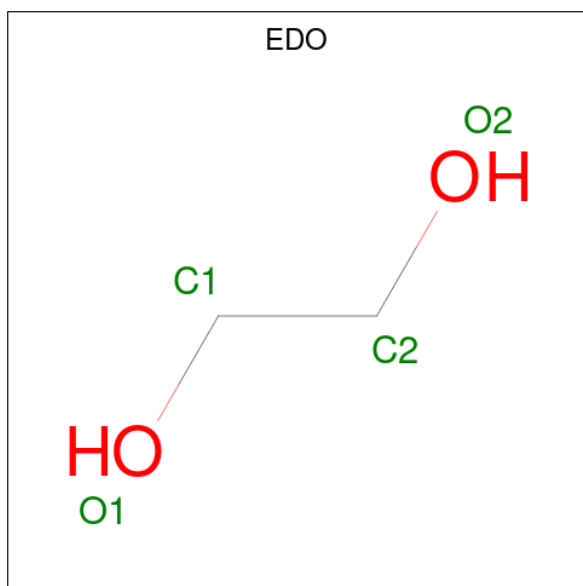
Chain	Residue	Modelled	Actual	Comment	Reference
B	167	THR	LYS	engineered mutation	UNP P0A2K1

- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F9F) (formula: C₉H₁₁F₃NO₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

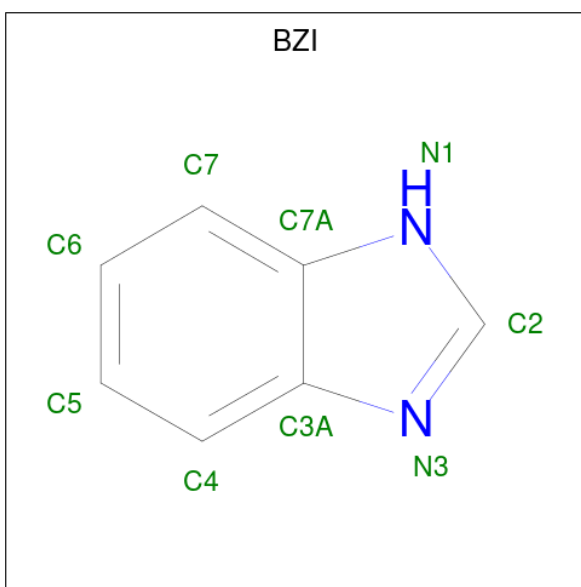


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

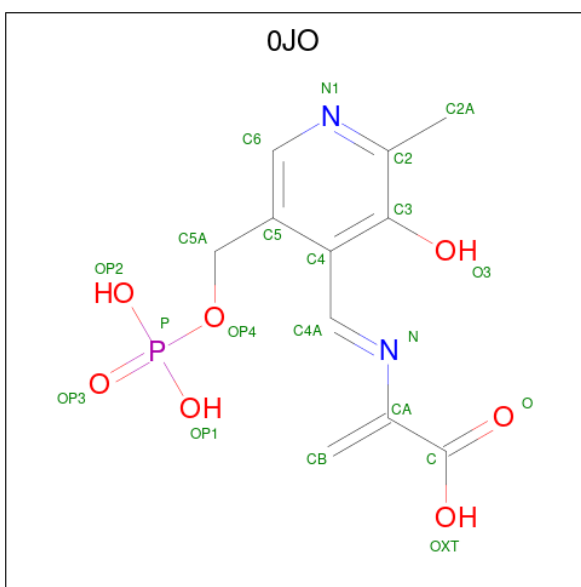
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	3	Total	Cl	0	0
			3	3		

- Molecule 6 is BENZIMIDAZOLE (CCD ID: BZI) (formula: $C_7H_6N_2$) (labeled as "Ligand of Interest" by depositor).



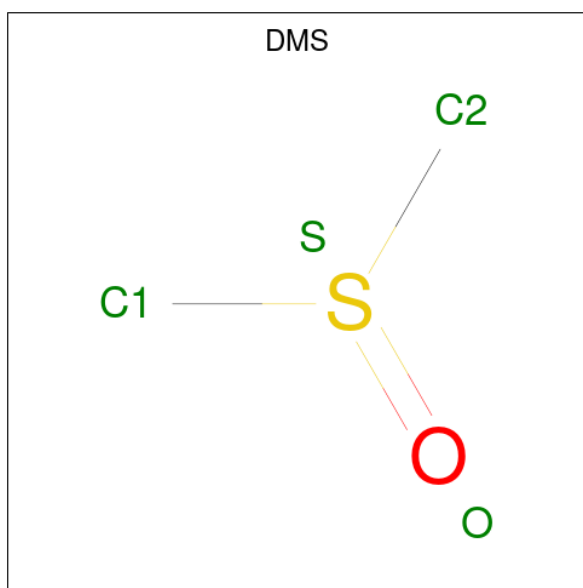
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			9	7	2		
6	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 7 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).



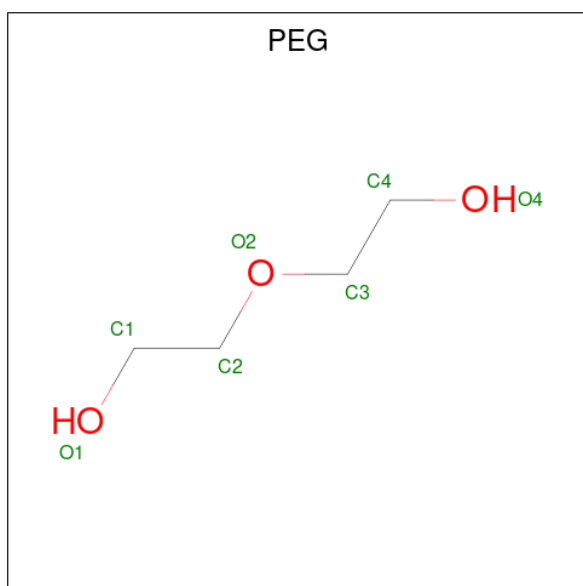
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 10 is CESIUM ION (CCD ID: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

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

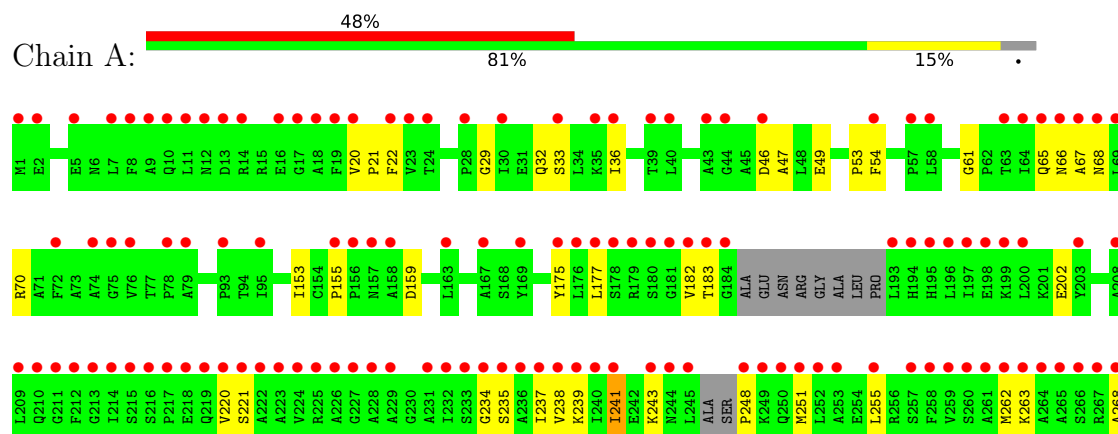
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	117	Total 122	O 122	0	5
11	B	307	Total 322	O 322	0	15

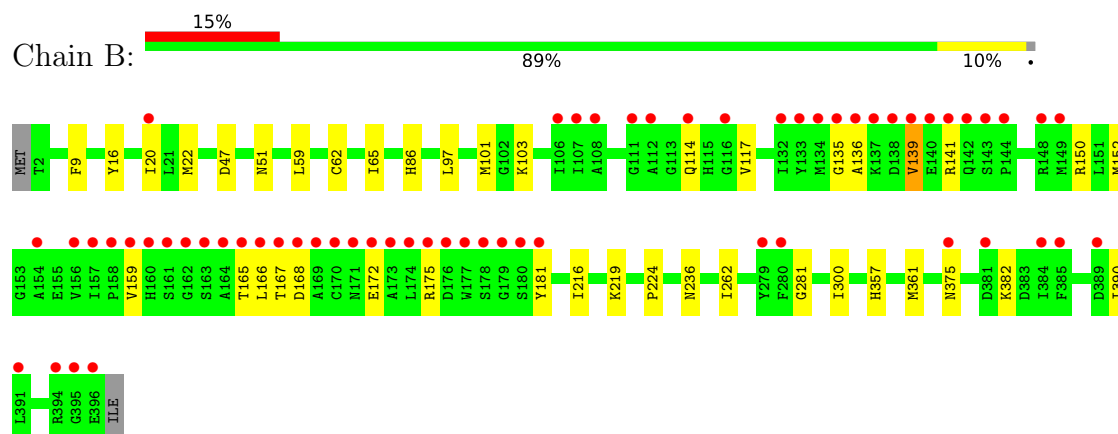
3 Residue-property plots [i](#)

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	183.33Å 60.08Å 67.27Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	39.31 – 1.80 39.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.31-1.80) 98.0 (39.31-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
R, R_{free}	0.201 , 0.237 (Not available) , 0.262	Depositor DCC
R_{free} test set	3462 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: 0JO, EDO, BZI, DMS, F9F, PEG, CS, CL

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	0.35	0/1897	0.62	1/2585 (0.0%)
2	B	0.45	0/3063	0.64	0/4141
All	All	0.41	0/4960	0.63	1/6726 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ILE	N-CA-C	-6.46	104.20	110.72

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	1862	0	1808	43	0
2	B	3006	0	2952	27	0
3	A	22	0	9	6	0
4	A	4	0	6	0	0
4	B	16	0	24	2	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	B	18	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	21	0	9	0	0
8	B	8	0	12	0	0
9	B	7	0	10	2	0
10	B	3	0	0	0	0
11	A	122	0	0	1	0
11	B	322	0	0	4	0
All	All	5415	0	4842	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLY:HA3	3:A:301:F9F:C15	1.97	0.95
1:A:182:VAL:HG11	2:B:175:ARG:HG2	1.48	0.94
1:A:234:GLY:HA3	3:A:301:F9F:H151	1.59	0.84
2:B:219:LYS:NZ	11:B:501:HOH:O	2.11	0.73
1:A:234:GLY:HA3	3:A:301:F9F:H152	1.73	0.70
1:A:53:PRO:HA	1:A:68:ASN:ND2	2.07	0.69
1:A:32:GLN:O	1:A:36:ILE:HD12	1.92	0.68
2:B:114:GLN:HE21	2:B:382:LYS:HD3	1.61	0.66
1:A:221:SER:OG	1:A:268:ALA:OXT	2.15	0.65
2:B:135:GLY:HA2	2:B:159:VAL:HB	1.77	0.65
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.80	0.64
2:B:103:LYS:NZ	2:B:181:TYR:O	2.19	0.63
2:B:141:ARG:NH1	11:B:505:HOH:O	2.33	0.61
1:A:32:GLN:HE21	1:A:32:GLN:HA	1.66	0.59
1:A:33:SER:HA	1:A:36:ILE:HD13	1.86	0.58
1:A:32:GLN:HG3	1:A:36:ILE:HD11	1.83	0.58
2:B:357:HIS:O	2:B:361:MET:HG3	2.05	0.56
2:B:117:VAL:HG13	2:B:152:MET:HE1	1.87	0.56
1:A:53:PRO:HA	1:A:68:ASN:HD22	1.71	0.54
2:B:136:ALA:O	2:B:139:VAL:HG22	2.07	0.54
1:A:251:MET:O	1:A:255:LEU:HD12	2.07	0.54
4:B:410:EDO:H12	11:B:525[B]:HOH:O	2.07	0.53
2:B:168:ASP:O	2:B:172:GLU:HG2	2.08	0.53
1:A:61:GLY:O	1:A:65:GLN:HG3	2.10	0.51
1:A:29:GLY:O	1:A:33:SER:HB2	2.10	0.51
2:B:159:VAL:HG22	2:B:172:GLU:HG3	1.93	0.51
1:A:183:THR:HB	3:A:301:F9F:O20	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.41	0.50
9:B:409:PEG:H41	11:B:681:HOH:O	2.11	0.50
1:A:153:ILE:HG21	1:A:177:LEU:HD22	1.93	0.49
1:A:239:LYS:O	1:A:243:LYS:N	2.38	0.48
2:B:236:ASN:OD1	2:B:375:ASN:ND2	2.47	0.48
1:A:22:PHE:HB3	1:A:234:GLY:HA2	1.97	0.47
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.29	0.46
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.96	0.46
1:A:220:VAL:CG2	1:A:262:MET:HE3	2.46	0.46
1:A:220:VAL:HG23	1:A:262:MET:HE3	1.98	0.46
2:B:97:LEU:O	2:B:101:MET:HG3	2.16	0.46
1:A:32:GLN:OE1	1:A:251:MET:HE3	2.17	0.45
1:A:54:PHE:H	1:A:68:ASN:ND2	2.14	0.45
2:B:375:ASN:OD1	2:B:375:ASN:C	2.59	0.45
1:A:183:THR:HG21	3:A:301:F9F:H142	1.98	0.45
2:B:47:ASP:OD1	2:B:51:ASN:ND2	2.49	0.45
2:B:62:CYS:HB3	2:B:65:ILE:HG12	1.99	0.45
1:A:235:SER:H	3:A:301:F9F:P17	2.39	0.45
2:B:165:THR:OG1	2:B:166:LEU:N	2.50	0.45
1:A:36:ILE:HD12	1:A:36:ILE:H	1.82	0.45
1:A:248:PRO:O	1:A:251:MET:HB3	2.17	0.44
1:A:21:PRO:HD2	1:A:47:ALA:O	2.18	0.43
1:A:36:ILE:HG23	1:A:255:LEU:HD22	2.00	0.43
1:A:155:PRO:HB3	2:B:20:ILE:HD13	2.01	0.43
1:A:66:ASN:O	1:A:70:ARG:HG3	2.18	0.43
1:A:159:ASP:OD1	1:A:159:ASP:C	2.61	0.43
2:B:262:ILE:O	4:B:408:EDO:H12	2.18	0.43
1:A:22:PHE:HA	1:A:49:GLU:O	2.19	0.42
1:A:67:ALA:HB2	1:A:238:VAL:HG11	2.02	0.42
2:B:86:HIS:NE2	2:B:236:ASN:HB3	2.35	0.42
1:A:202:GLU:OE2	11:A:401:HOH:O	2.22	0.42
2:B:9:PHE:HD2	9:B:409:PEG:H12	1.84	0.42
1:A:22:PHE:CD1	1:A:22:PHE:C	2.97	0.42
1:A:182:VAL:HG11	2:B:175:ARG:CG	2.35	0.41
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.93	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.54	0.41
1:A:237:ILE:O	1:A:241:ILE:HG13	2.21	0.41
2:B:59:LEU:O	2:B:219:LYS:NZ	2.52	0.41
1:A:54:PHE:H	1:A:68:ASN:HD22	1.69	0.41
2:B:16:TYR:O	2:B:281:GLY:HA2	2.22	0.40
2:B:22:MET:HE3	2:B:22:MET:HB3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HD13	1:A:175:TYR:HB3	2.03	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	252/268 (94%)	246 (98%)	6 (2%)	0	100	100
2	B	398/397 (100%)	388 (98%)	10 (2%)	0	100	100
All	All	650/665 (98%)	634 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	181/208 (87%)	181 (100%)	0	100	100
2	B	307/311 (99%)	304 (99%)	3 (1%)	68	64
All	All	488/519 (94%)	485 (99%)	3 (1%)	78	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	VAL
2	B	150	ARG
2	B	167	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	204	HIS
2	B	114	GLN
2	B	171	ASN
2	B	342	HIS
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 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	B	410	-	3,3,3	0.50	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OJO	B	403	-	20,21,21	1.42	2 (10%)	23,30,30	0.59	0
8	DMS	B	406	-	3,3,3	0.73	0	3,3,3	0.47	0
9	PEG	B	409	-	6,6,6	0.15	0	5,5,5	0.32	0
4	EDO	B	408	-	3,3,3	0.51	0	2,2,2	0.14	0
6	BZI	B	402	-	10,10,10	0.43	0	13,13,13	0.58	0
4	EDO	A	302	-	3,3,3	0.54	0	2,2,2	0.35	0
4	EDO	B	407	-	3,3,3	0.56	0	2,2,2	0.21	0
3	F9F	A	301	-	22,22,22	0.32	0	32,33,33	0.33	0
4	EDO	B	404	-	3,3,3	0.49	0	2,2,2	0.21	0
8	DMS	B	405	-	3,3,3	0.66	0	3,3,3	0.58	0
6	BZI	B	401	-	10,10,10	0.43	0	13,13,13	0.59	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	B	410	-	-	1/1/1/1	-
7	OJO	B	403	-	-	0/11/15/15	0/1/1/1
9	PEG	B	409	-	-	1/4/4/4	-
4	EDO	B	408	-	-	1/1/1/1	-
6	BZI	B	402	-	-	-	0/2/2/2
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
3	F9F	A	301	-	-	7/20/20/20	0/1/1/1
4	EDO	B	404	-	-	1/1/1/1	-
6	BZI	B	401	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	OJO	CA-C	-5.07	1.40	1.50
7	B	403	OJO	OXT-C	-3.21	1.21	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	F9F	N13-C14-C15-O16

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Mol	Chain	Res	Type	Atoms
3	A	301	F9F	C3-C4-S12-O21
3	A	301	F9F	C5-C4-S12-O21
3	A	301	F9F	C5-C4-S12-N13
4	B	404	EDO	O1-C1-C2-O2
3	A	301	F9F	C3-C4-S12-N13
4	B	407	EDO	O1-C1-C2-O2
9	B	409	PEG	O2-C3-C4-O4
4	B	408	EDO	O1-C1-C2-O2
4	B	410	EDO	O1-C1-C2-O2
3	A	301	F9F	C2-C1-O7-C8
3	A	301	F9F	C6-C1-O7-C8

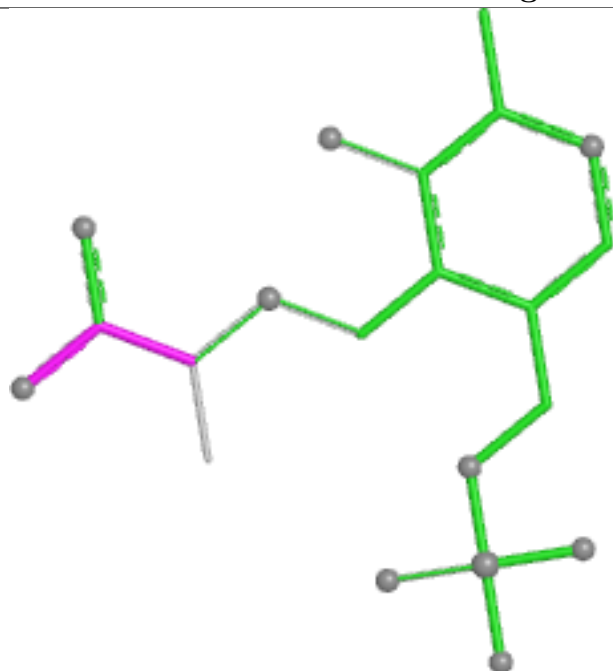
There are no ring outliers.

4 monomers are involved in 10 short contacts:

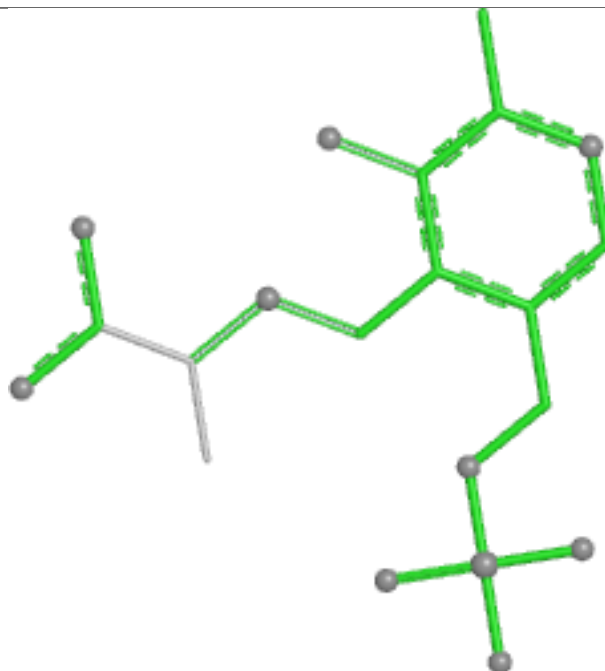
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	410	EDO	1	0
9	B	409	PEG	2	0
4	B	408	EDO	1	0
3	A	301	F9F	6	0

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.

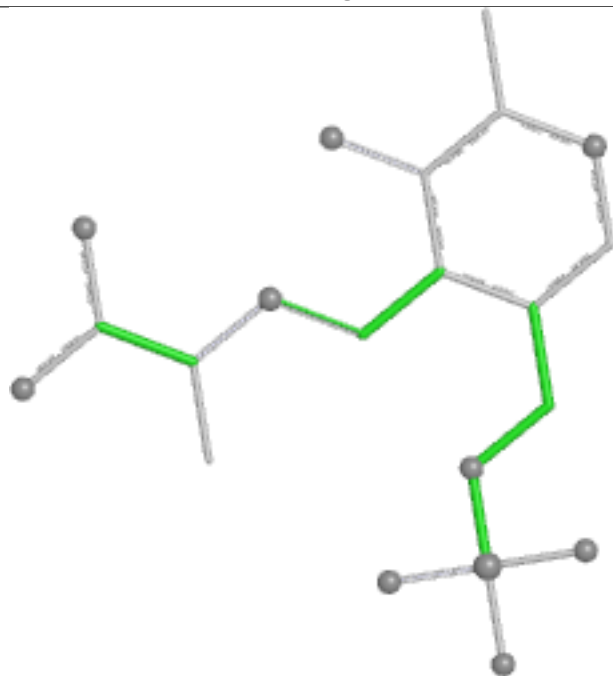
Ligand 0JO B 403



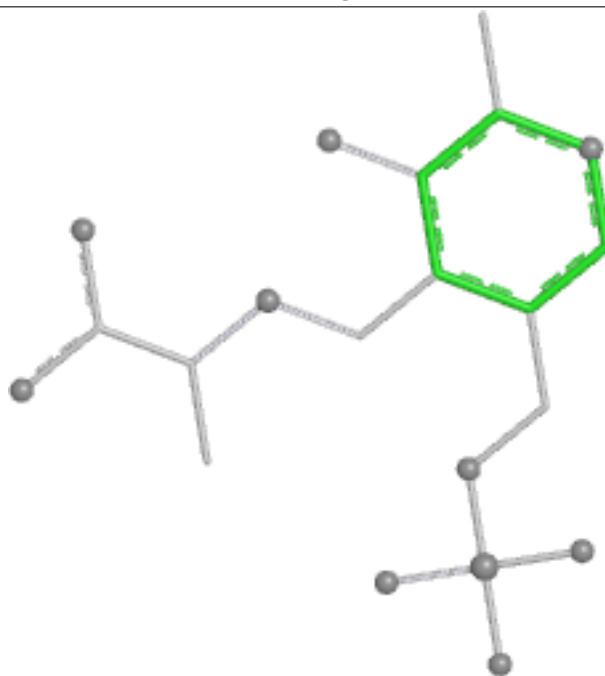
Bond lengths



Bond angles

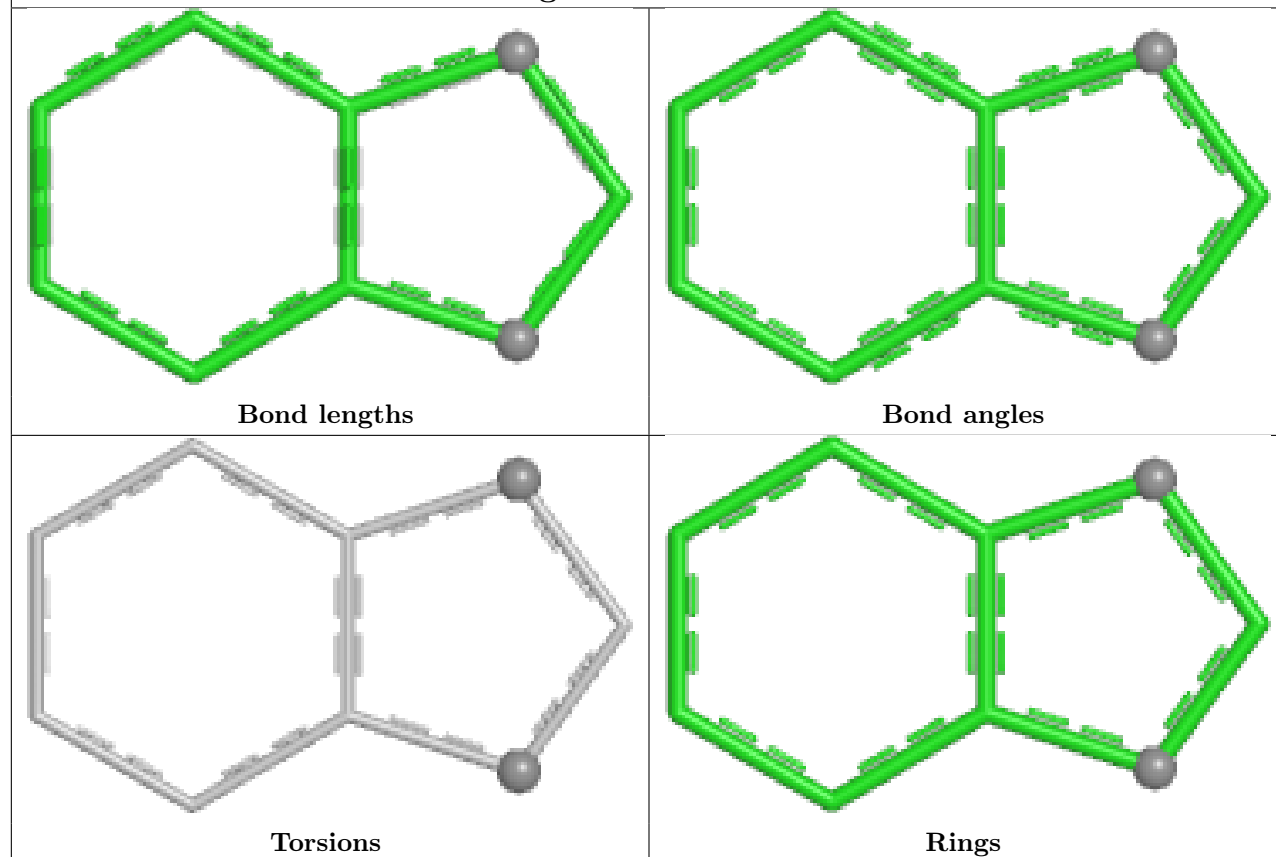


Torsions

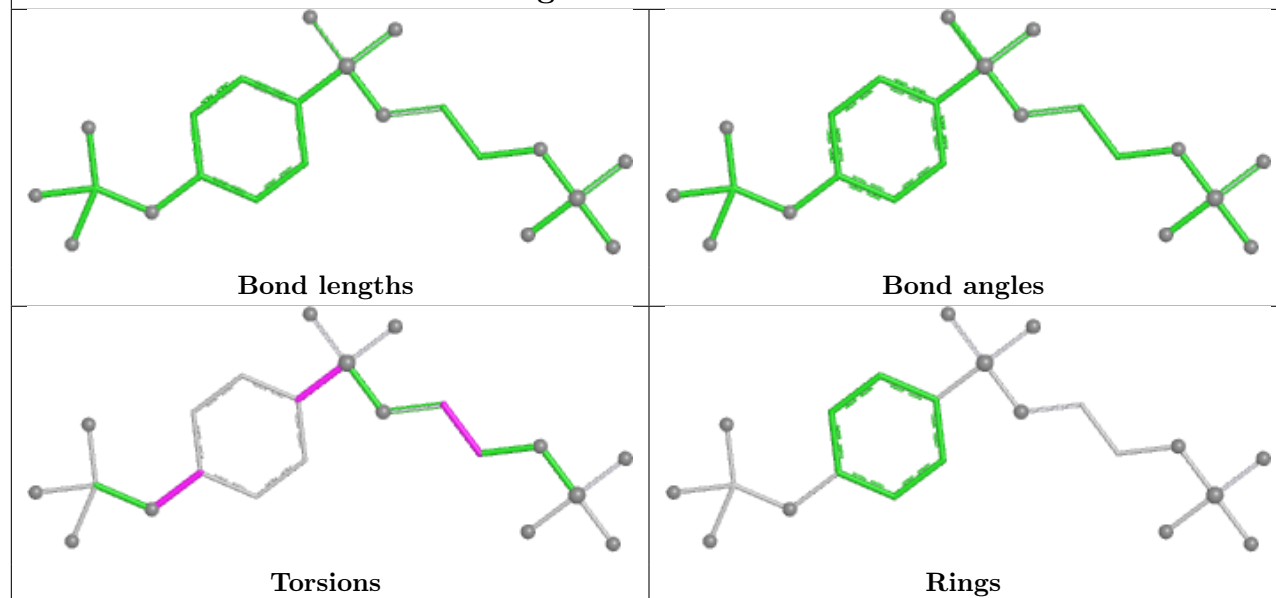


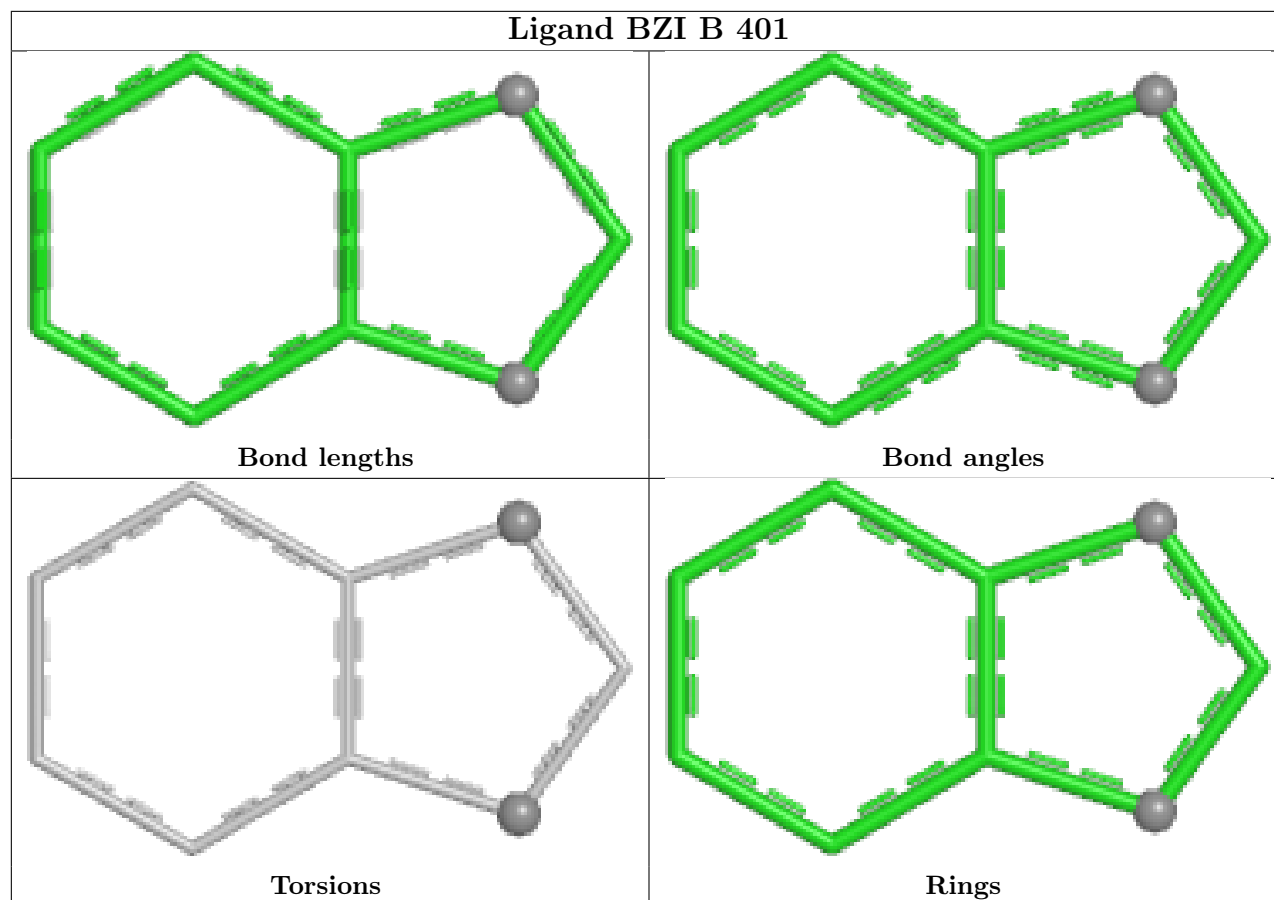
Rings

Ligand BZI B 402



Ligand F9F A 301





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	258/268 (96%)	2.17	128 (49%) 0 0	25, 57, 93, 114	0
2	B	395/397 (99%)	0.95	61 (15%) 5 4	12, 28, 80, 106	5 (1%)
All	All	653/665 (98%)	1.43	189 (28%) 1 1	12, 36, 89, 114	5 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	6.7
1	A	220	VAL	6.6
1	A	214	ILE	5.5
1	A	215	SER	5.5
1	A	58	LEU	5.5
1	A	268	ALA	5.4
1	A	245	LEU	5.2
1	A	193	LEU	5.1
1	A	229	ALA	5.0
2	B	180	SER	5.0
2	B	163	SER	4.7
1	A	237	ILE	4.7
1	A	182	VAL	4.7
1	A	264	ALA	4.7
1	A	265	ALA	4.6
2	B	164	ALA	4.6
2	B	165	THR	4.5
2	B	178	SER	4.5
1	A	224	VAL	4.5
2	B	174	LEU	4.4
1	A	217	PRO	4.4
2	B	160	HIS	4.4
2	B	179	GLY	4.4
1	A	255	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	139	VAL	4.3
1	A	241	ILE	4.3
1	A	235	SER	4.3
1	A	252	LEU	4.3
2	B	159	VAL	4.3
1	A	226	ALA	4.3
1	A	183	THR	4.2
1	A	184	GLY	4.2
1	A	157	ASN	4.2
1	A	211	GLY	4.1
1	A	218	GLU	4.1
1	A	195	HIS	4.0
1	A	233	SER	4.0
1	A	194	HIS	4.0
2	B	156	VAL	4.0
1	A	248	PRO	4.0
2	B	162	GLY	4.0
1	A	196	LEU	4.0
1	A	18	ALA	4.0
2	B	167	THR	3.9
2	B	280	PHE	3.9
1	A	213	GLY	3.9
1	A	225	ARG	3.9
1	A	238	VAL	3.9
1	A	36	ILE	3.8
1	A	240	ILE	3.8
1	A	262	MET	3.8
1	A	95	ILE	3.8
1	A	258	PHE	3.7
1	A	76	VAL	3.7
1	A	181	GLY	3.6
2	B	141	ARG	3.6
2	B	112	ALA	3.6
2	B	136	ALA	3.6
2	B	181	TYR	3.6
1	A	10	GLN	3.6
2	B	279	TYR	3.5
1	A	222	ALA	3.5
2	B	140	GLU	3.5
2	B	142	GLN	3.4
1	A	234	GLY	3.4
2	B	173	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	385	PHE	3.4
1	A	250	GLN	3.3
1	A	221	SER	3.3
2	B	177	TRP	3.3
1	A	257	SER	3.3
2	B	157	ILE	3.3
1	A	156	PRO	3.3
1	A	28	PRO	3.3
1	A	11	LEU	3.2
1	A	177	LEU	3.2
1	A	180	SER	3.2
1	A	228	ALA	3.2
2	B	166	LEU	3.2
2	B	170	CYS	3.2
1	A	232	ILE	3.1
2	B	133	TYR	3.1
1	A	69	LEU	3.1
2	B	375	ASN	3.1
1	A	30	ILE	3.1
2	B	20	ILE	3.1
2	B	384	ILE	3.1
1	A	261	ALA	3.1
1	A	203	TYR	3.0
1	A	236	ALA	3.0
1	A	259	VAL	3.0
1	A	63	THR	3.0
1	A	243	LYS	3.0
2	B	108	ALA	3.0
1	A	227	GLY	3.0
2	B	111	GLY	3.0
2	B	158	PRO	3.0
2	B	172	GLU	3.0
1	A	7	LEU	2.9
2	B	161	SER	2.9
1	A	1	MET	2.9
1	A	216	SER	2.9
1	A	78	PRO	2.9
1	A	67	ALA	2.9
1	A	253	ALA	2.8
1	A	244	ASN	2.8
2	B	107	ILE	2.8
1	A	5	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	64	ILE	2.8
1	A	43	ALA	2.7
2	B	168	ASP	2.7
1	A	8	PHE	2.6
1	A	20	VAL	2.6
1	A	210	GLN	2.6
1	A	2	GLU	2.6
1	A	249	LYS	2.6
1	A	9	ALA	2.6
1	A	158	ALA	2.6
1	A	208	ALA	2.6
1	A	231	ALA	2.6
1	A	66	ASN	2.6
1	A	163	LEU	2.6
1	A	197	ILE	2.6
1	A	12	ASN	2.6
1	A	219	GLN	2.5
2	B	148[A]	ARG	2.5
2	B	138	ASP	2.5
2	B	132	ILE	2.5
2	B	171	ASN	2.5
1	A	22	PHE	2.5
2	B	391	LEU	2.5
1	A	16	GLU	2.5
1	A	223	ALA	2.5
2	B	154	ALA	2.5
1	A	24	THR	2.4
2	B	135	GLY	2.4
1	A	251	MET	2.4
1	A	54	PHE	2.4
1	A	39	THR	2.4
1	A	267	ARG	2.3
1	A	79	ALA	2.3
1	A	263	LYS	2.3
2	B	143	SER	2.3
1	A	40	LEU	2.3
1	A	200	LEU	2.3
2	B	149	MET	2.3
1	A	17	GLY	2.3
1	A	199	LYS	2.3
1	A	239	LYS	2.3
1	A	260	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	394	ARG	2.3
1	A	68	ASN	2.3
2	B	134	MET	2.3
1	A	19	PHE	2.3
2	B	137	LYS	2.3
1	A	44	GLY	2.3
1	A	13	ASP	2.3
2	B	396	GLU	2.3
2	B	175	ARG	2.2
1	A	169	TYR	2.2
2	B	116	GLY	2.2
2	B	169	ALA	2.2
2	B	176	ASP	2.2
2	B	114	GLN	2.2
1	A	179	ARG	2.2
1	A	198	GLU	2.2
1	A	72	PHE	2.2
1	A	175	TYR	2.2
1	A	23	VAL	2.2
1	A	266	SER	2.2
1	A	65	GLN	2.2
1	A	75	GLY	2.2
2	B	106	ILE	2.1
1	A	46	ASP	2.1
2	B	389	ASP	2.1
1	A	178	SER	2.1
1	A	176	LEU	2.1
1	A	35	LYS	2.1
1	A	74	ALA	2.1
1	A	167	ALA	2.1
2	B	381	ASP	2.1
1	A	14	ARG	2.1
1	A	57	PRO	2.1
1	A	93	PRO	2.1
2	B	144	PRO	2.1
1	A	209	LEU	2.1
1	A	33	SER	2.0
2	B	395	GLY	2.0
1	A	155	PRO	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](#)

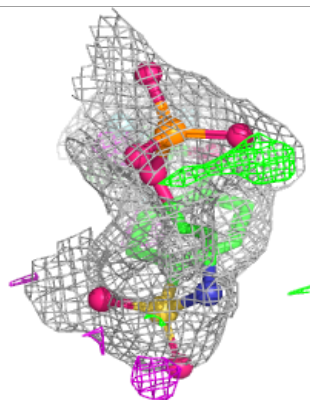
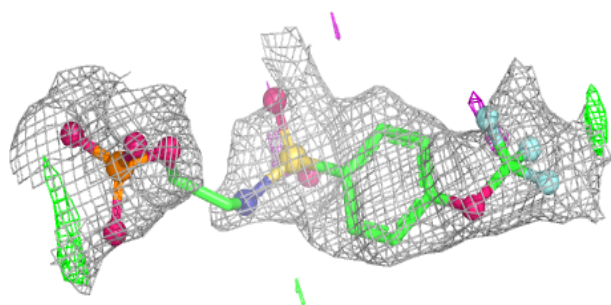
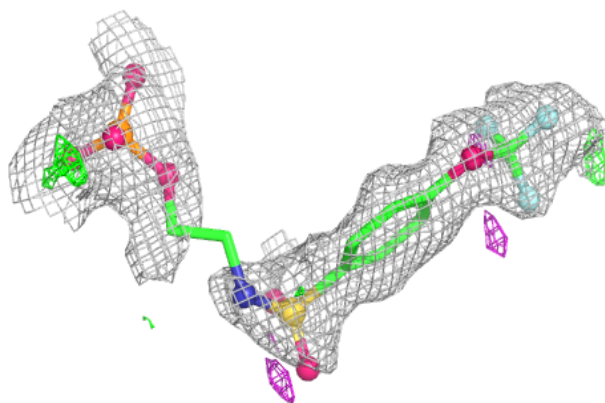
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	404	4/4	0.68	0.16	47,52,55,55	0
4	EDO	B	410	4/4	0.70	0.23	46,49,50,52	0
4	EDO	B	407	4/4	0.72	0.21	39,43,44,49	0
4	EDO	A	302	4/4	0.76	0.16	42,44,46,55	0
5	CL	B	414	1/1	0.76	0.22	81,81,81,81	0
3	F9F	A	301	22/22	0.78	0.21	43,54,83,83	22
9	PEG	B	409	7/7	0.79	0.16	30,37,49,51	0
4	EDO	B	408	4/4	0.80	0.14	40,42,43,46	0
6	BZI	B	401	9/9	0.81	0.16	40,41,49,50	0
6	BZI	B	402	9/9	0.84	0.14	39,41,44,44	0
5	CL	B	415	1/1	0.86	0.12	69,69,69,69	0
5	CL	B	413	1/1	0.86	0.12	56,56,56,56	0
8	DMS	B	406	4/4	0.88	0.15	39,47,51,55	0
8	DMS	B	405	4/4	0.91	0.16	32,46,51,54	0
7	OJO	B	403	21/21	0.94	0.10	19,25,33,38	0
5	CL	A	303	1/1	0.95	0.11	52,52,52,52	0
10	CS	B	411	1/1	0.99	0.02	28,28,28,28	1
10	CS	B	412[A]	1/1	0.99	0.02	23,23,23,23	1
10	CS	B	412[B]	1/1	0.99	0.02	33,33,33,33	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.

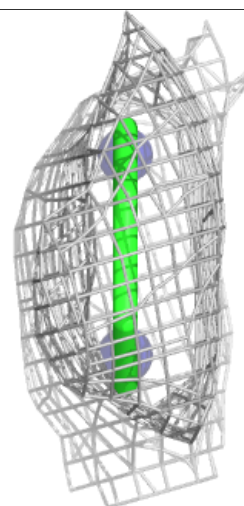
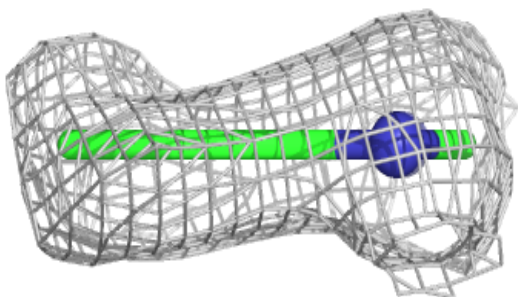
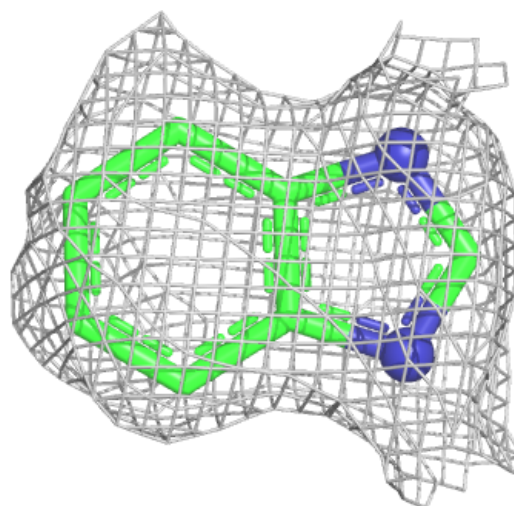
Electron density around F9F A 301:

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



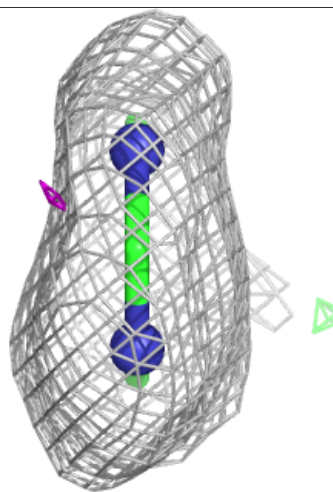
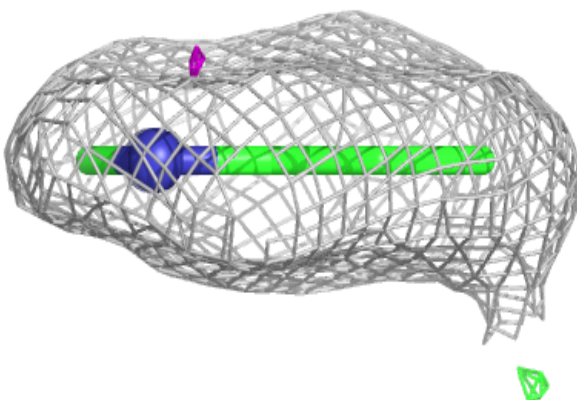
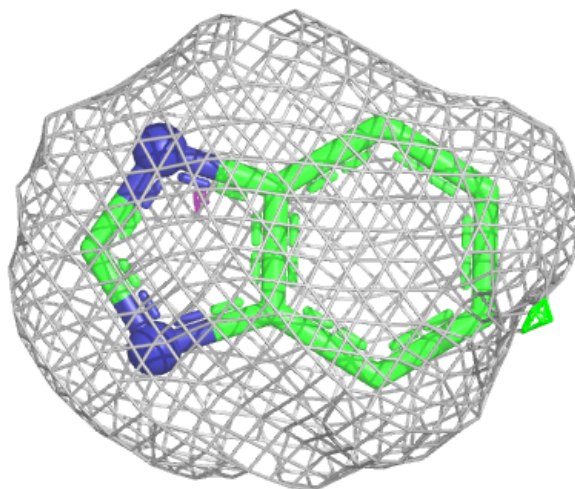
Electron density around BZI B 401:

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



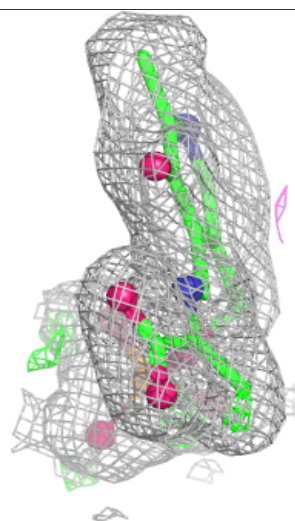
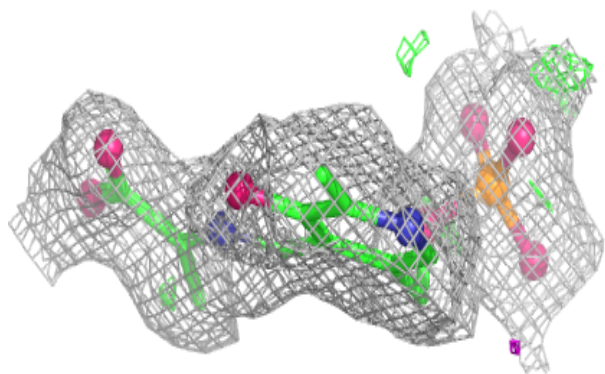
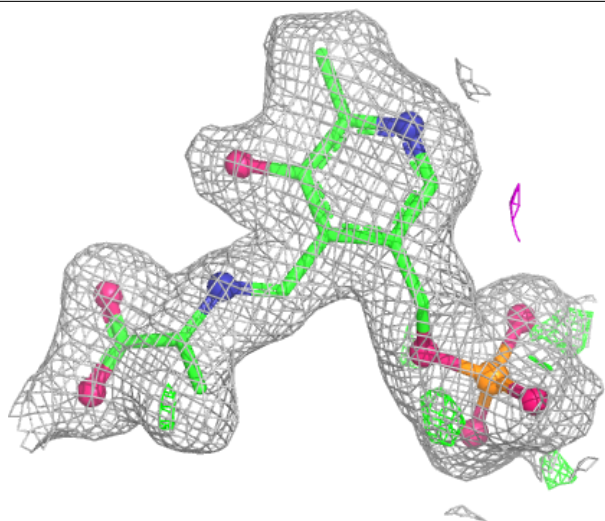
Electron density around BZI B 402:

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



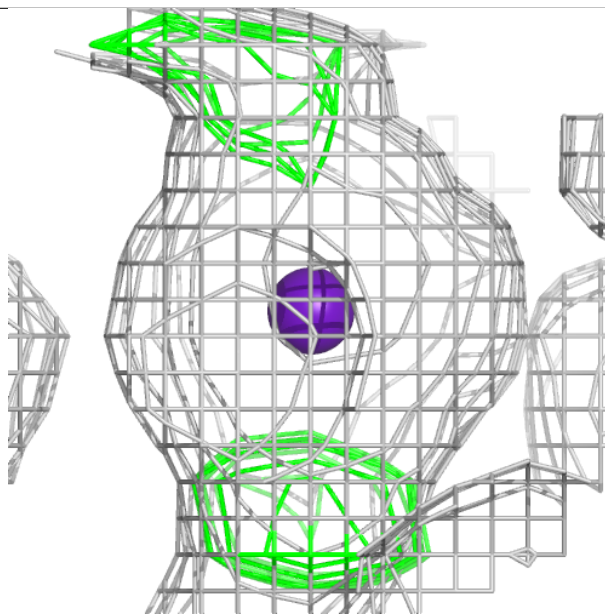
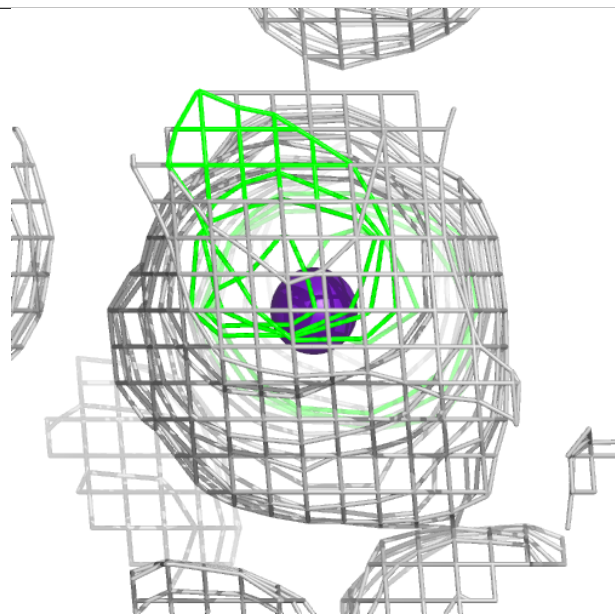
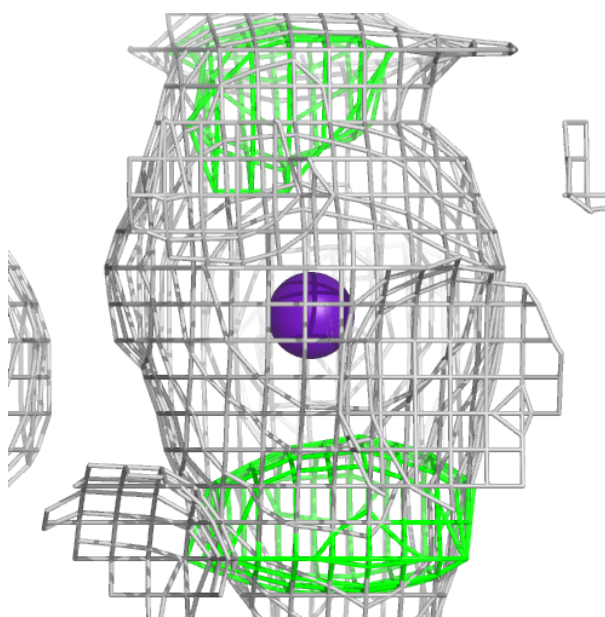
Electron density around 0JO B 403:

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



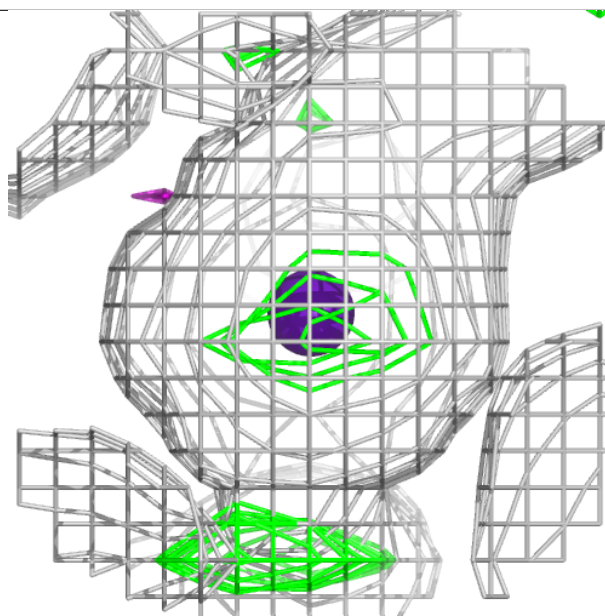
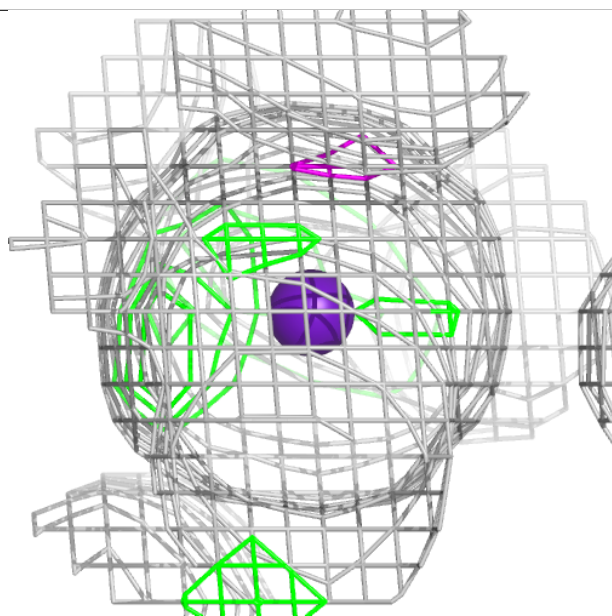
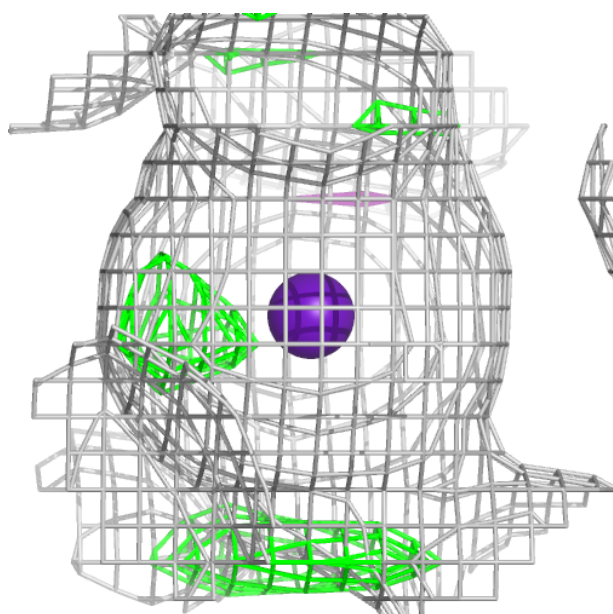
Electron density around CS B 411:

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



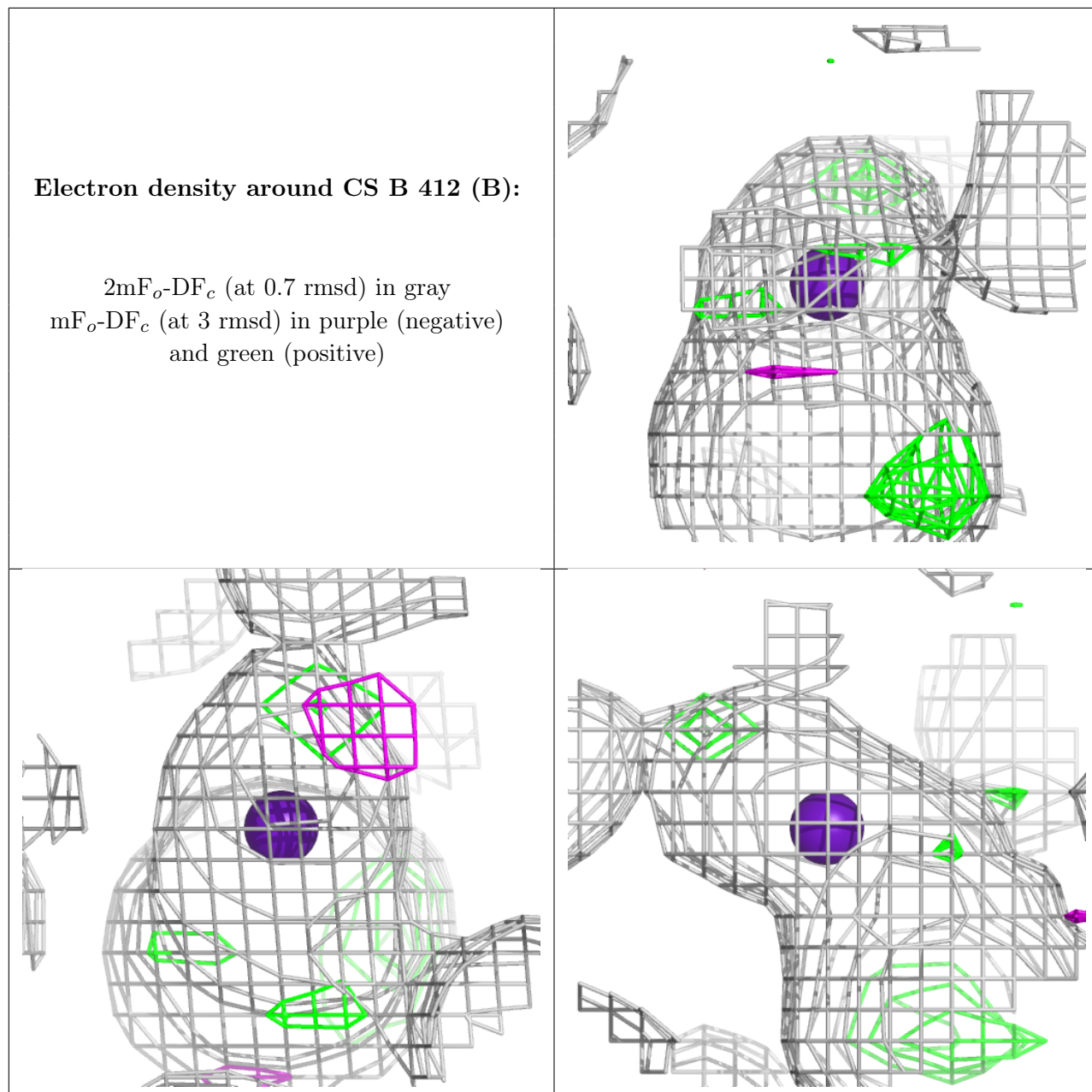
Electron density around CS B 412 (A):

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



Electron density around CS B 412 (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.