



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:10 AM UTC

PDB ID : 9FXI / pdb_00009fxi
Title : Crystal structure of cobalt(II)-substituted double mutant Y115E Y117E human Glutaminyl Cyclase in complex with SEN177
Authors : Tassone, G.; Pozzi, C.; Mangani, S.
Deposited on : 2024-07-01
Resolution : 3.06 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

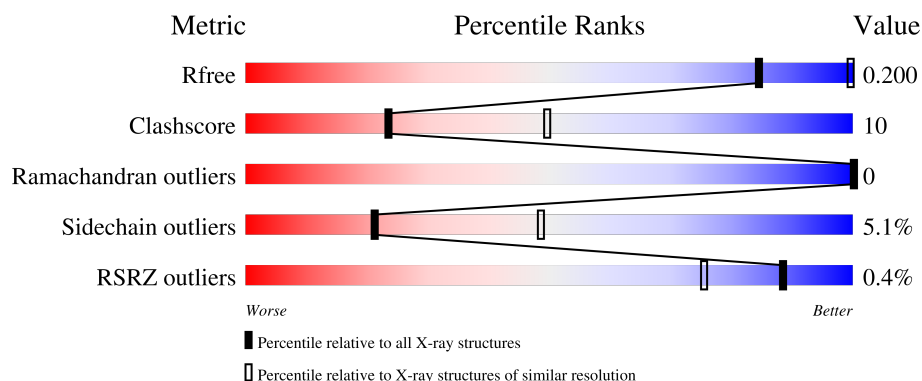
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	341	 72% 24% .
1	B	341	 69% 25% . 5%
1	C	341	 72% 22% . 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8102 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2579	1651	445	474	9			
1	B	325	Total	C	N	O	S	0	0	0
			2586	1655	446	476	9			
1	C	324	Total	C	N	O	S	0	0	0
			2566	1643	442	472	9			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP Q16769
A	22	ARG	-	expression tag	UNP Q16769
A	23	GLY	-	expression tag	UNP Q16769
A	24	SER	-	expression tag	UNP Q16769
A	25	HIS	-	expression tag	UNP Q16769
A	26	HIS	-	expression tag	UNP Q16769
A	27	HIS	-	expression tag	UNP Q16769
A	28	HIS	-	expression tag	UNP Q16769
A	29	HIS	-	expression tag	UNP Q16769
A	30	HIS	-	expression tag	UNP Q16769
A	31	GLY	-	expression tag	UNP Q16769
A	115	GLU	TYR	engineered mutation	UNP Q16769
A	117	GLU	TYR	engineered mutation	UNP Q16769
B	21	MET	-	initiating methionine	UNP Q16769
B	22	ARG	-	expression tag	UNP Q16769
B	23	GLY	-	expression tag	UNP Q16769
B	24	SER	-	expression tag	UNP Q16769
B	25	HIS	-	expression tag	UNP Q16769
B	26	HIS	-	expression tag	UNP Q16769
B	27	HIS	-	expression tag	UNP Q16769
B	28	HIS	-	expression tag	UNP Q16769
B	29	HIS	-	expression tag	UNP Q16769
B	30	HIS	-	expression tag	UNP Q16769

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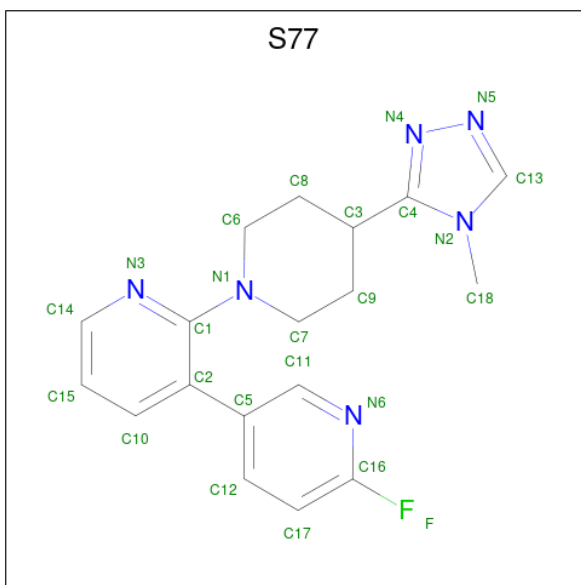
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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	GLY	-	expression tag	UNP Q16769
B	115	GLU	TYR	engineered mutation	UNP Q16769
B	117	GLU	TYR	engineered mutation	UNP Q16769
C	21	MET	-	initiating methionine	UNP Q16769
C	22	ARG	-	expression tag	UNP Q16769
C	23	GLY	-	expression tag	UNP Q16769
C	24	SER	-	expression tag	UNP Q16769
C	25	HIS	-	expression tag	UNP Q16769
C	26	HIS	-	expression tag	UNP Q16769
C	27	HIS	-	expression tag	UNP Q16769
C	28	HIS	-	expression tag	UNP Q16769
C	29	HIS	-	expression tag	UNP Q16769
C	30	HIS	-	expression tag	UNP Q16769
C	31	GLY	-	expression tag	UNP Q16769
C	115	GLU	TYR	engineered mutation	UNP Q16769
C	117	GLU	TYR	engineered mutation	UNP Q16769

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 2-fluoranyl-5-[2-[4-(4-methyl-1,2,4-triazol-3-yl)piperidin-1-yl]pyridin-3-yl]pyridine (CCD ID: S77) (formula: C₁₈H₁₉FN₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			25	18	1	6		
3	B	1	Total	C	F	N	0	0
			25	18	1	6		
3	C	1	Total	C	F	N	0	0
			25	18	1	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

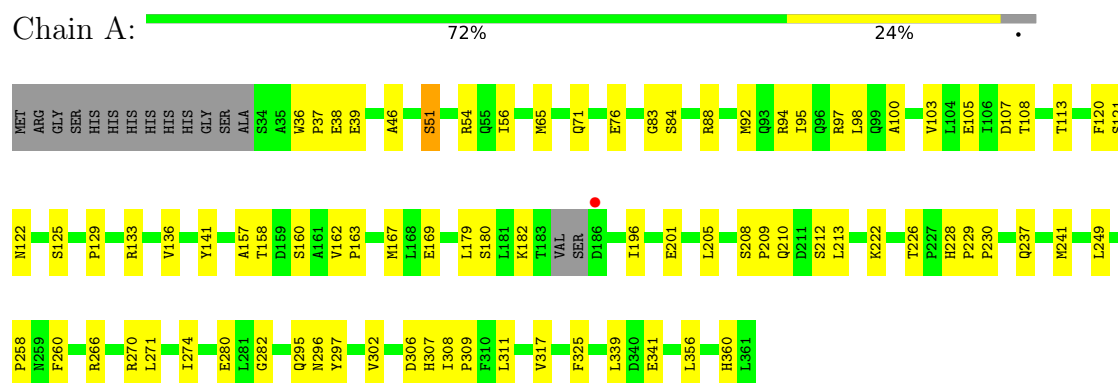
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	95	Total	O	0	0
			95	95		
5	C	91	Total	O	0	0
			91	91		

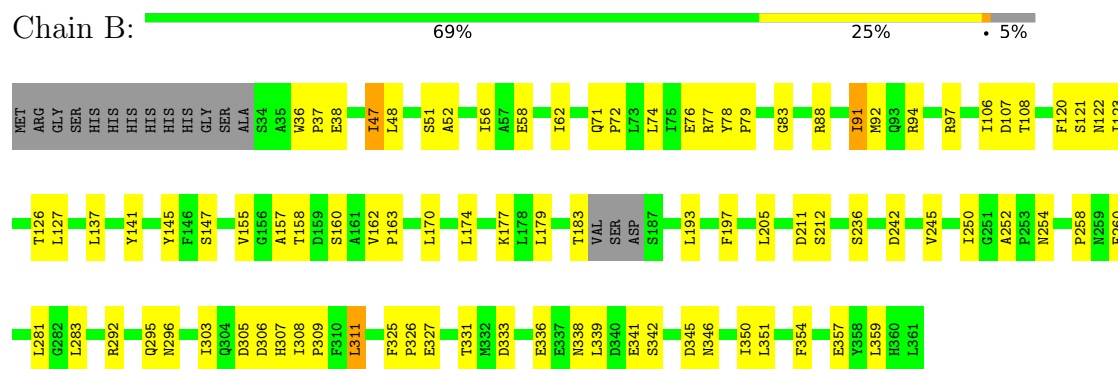
3 Residue-property plots

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.

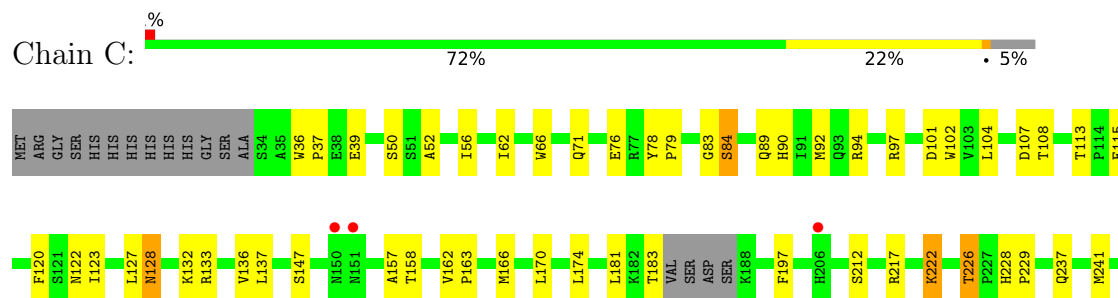
• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 149.74Å 95.65Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	74.87 – 3.06 74.87 – 3.06	Depositor EDS
% Data completeness (in resolution range)	87.0 (74.87-3.06) 87.0 (74.87-3.06)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.228 (Not available) , 0.200	Depositor DCC
R_{free} test set	1015 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8102	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 5.03% 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: CO, S77, SO4

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	0.52	0/2652	1.02	0/3612
1	B	0.51	0/2659	1.05	1/3620 (0.0%)
1	C	0.52	0/2639	1.03	2/3596 (0.1%)
All	All	0.51	0/7950	1.04	3/10828 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	GLU	N-CA-C	-5.73	105.12	111.71
1	B	250	ILE	CB-CA-C	5.71	118.60	110.84
1	C	290	GLU	CB-CA-C	5.21	120.27	110.63

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	2579	0	2467	50	0
1	B	2586	0	2486	52	0
1	C	2566	0	2454	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
4	A	5	0	0	0	0
4	C	10	0	0	0	0
5	A	92	0	0	2	0
5	B	95	0	0	0	0
5	C	91	0	0	2	0
All	All	8102	0	7407	156	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 10.

All (156) 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:C:136:VAL:HG21	1:C:241:MET:HE3	1.58	0.85
1:B:47:ILE:HD12	1:B:47:ILE:H	1.54	0.72
1:B:88:ARG:O	1:B:92:MET:HG3	1.91	0.69
1:B:94:ARG:O	1:B:97:ARG:HG2	1.93	0.69
1:C:163:PRO:HB3	1:C:247:LEU:HB3	1.75	0.68
1:C:123:ILE:HB	1:C:197:PHE:HB2	1.76	0.66
1:B:123:ILE:HB	1:B:197:PHE:HB2	1.76	0.66
1:C:157:ALA:HB1	1:C:339:LEU:HD21	1.77	0.64
1:A:94:ARG:O	1:A:97:ARG:HG2	1.96	0.64
1:B:305:ASP:HB3	1:B:307:HIS:HD2	1.63	0.63
1:C:78:TYR:HB2	1:C:79:PRO:HD3	1.80	0.63
1:B:36:TRP:N	1:B:37:PRO:CD	2.63	0.62
1:B:292:ARG:O	1:B:295:GLN:NE2	2.32	0.62
1:B:108:THR:HA	1:B:120:PHE:O	1.99	0.62
1:C:306:ASP:O	1:C:309:PRO:HD2	2.00	0.61
1:A:136:VAL:HG11	1:A:241:MET:HE3	1.83	0.61
1:A:222:LYS:HE2	5:A:528:HOH:O	2.01	0.60
1:B:305:ASP:HB3	1:B:307:HIS:CD2	2.36	0.60
1:A:36:TRP:N	1:A:37:PRO:CD	2.64	0.60
1:A:108:THR:HA	1:A:120:PHE:O	2.01	0.60
1:B:331:THR:HG22	1:B:333:ASP:H	1.67	0.59
1:B:62:ILE:HG12	1:B:341:GLU:HG2	1.84	0.59
1:B:137:LEU:HD23	1:B:245:VAL:HB	1.84	0.59
1:B:211:ASP:O	1:B:212:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:TYR:HB2	1:C:79:PRO:CD	2.33	0.58
1:A:136:VAL:HG21	1:A:241:MET:HG2	1.86	0.56
1:C:241:MET:HE1	1:C:244:LEU:HD13	1.85	0.56
1:C:157:ALA:CB	1:C:339:LEU:HD21	2.36	0.56
1:B:92:MET:SD	1:B:106:ILE:HD11	2.45	0.56
1:C:128:ASN:HD21	1:C:181:LEU:HB3	1.71	0.56
1:B:183:THR:HG22	1:B:183:THR:O	2.06	0.56
1:C:76:GLU:O	1:C:83:GLY:HA3	2.06	0.56
1:C:181:LEU:HD21	1:C:361:LEU:HD21	1.87	0.55
1:B:107:ASP:HB3	1:B:122:ASN:HB2	1.89	0.55
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.07	0.55
1:B:162:VAL:HB	1:B:163:PRO:HD3	1.87	0.55
1:A:95:ILE:HA	1:A:98:LEU:HD12	1.90	0.54
1:B:311:LEU:C	1:B:311:LEU:HD23	2.32	0.54
1:B:78:TYR:HB2	1:B:79:PRO:CD	2.38	0.54
1:B:336:GLU:C	1:B:338:ASN:H	2.16	0.54
1:C:108:THR:HA	1:C:120:PHE:O	2.08	0.54
1:A:107:ASP:HB3	1:A:122:ASN:HB2	1.90	0.54
1:B:306:ASP:O	1:B:309:PRO:HD2	2.08	0.53
1:C:36:TRP:N	1:C:37:PRO:CD	2.71	0.53
1:B:77:ARG:NH1	1:B:155:VAL:O	2.26	0.53
1:A:51:SER:HB3	1:A:54:ARG:NH1	2.24	0.53
1:A:311:LEU:HB2	1:A:317:VAL:HG21	1.90	0.53
1:C:170:LEU:HD21	1:C:174:LEU:HD12	1.92	0.52
1:C:36:TRP:HA	1:C:39:GLU:HG3	1.90	0.52
1:C:158:THR:HG22	1:C:251:GLY:HA3	1.92	0.52
1:A:208:SER:HB2	1:A:209:PRO:HD2	1.92	0.52
1:C:303:ILE:HG21	1:C:321:ILE:HD13	1.91	0.52
1:C:162:VAL:HB	1:C:163:PRO:HD3	1.91	0.52
1:C:84:SER:HB3	5:C:517:HOH:O	2.10	0.51
1:A:258:PRO:HG2	1:A:260:PHE:CZ	2.46	0.51
1:C:36:TRP:CG	1:C:37:PRO:HD3	2.46	0.51
1:A:100:ALA:HA	1:A:179:LEU:HD13	1.92	0.51
1:A:158:THR:O	1:A:249:LEU:HA	2.11	0.51
1:A:160:SER:HB3	1:A:163:PRO:HG2	1.93	0.50
1:C:212:SER:O	1:C:217:ARG:NH2	2.40	0.50
1:C:260:PHE:CE2	1:C:303:ILE:HD12	2.47	0.50
1:C:36:TRP:O	1:C:39:GLU:HG3	2.12	0.50
1:C:331:THR:HG22	1:C:333:ASP:H	1.77	0.50
1:A:158:THR:HG22	1:A:339:LEU:CD2	2.41	0.50
1:B:158:THR:HG22	1:B:339:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:NH1	1:C:97:ARG:HD3	2.27	0.50
1:C:101:ASP:HB3	5:C:505:HOH:O	2.10	0.50
1:B:260:PHE:HE2	1:B:303:ILE:HD12	1.77	0.49
1:C:259:ASN:HB2	1:C:268:PHE:CD1	2.47	0.49
1:A:228:HIS:HA	1:A:229:PRO:C	2.38	0.49
1:B:258:PRO:HD2	1:B:260:PHE:CE1	2.48	0.49
1:C:39:GLU:HB2	1:C:133:ARG:HD2	1.94	0.49
1:B:52:ALA:O	1:B:56:ILE:HG12	2.12	0.49
1:B:76:GLU:O	1:B:83:GLY:HA3	2.13	0.48
1:B:193:LEU:HB2	1:B:359:LEU:HD11	1.93	0.48
1:B:162:VAL:HB	1:B:163:PRO:CD	2.44	0.48
1:C:228:HIS:HA	1:C:229:PRO:C	2.37	0.48
1:A:266:ARG:HG3	1:A:266:ARG:HH11	1.79	0.48
1:C:92:MET:HG2	1:C:104:LEU:HD13	1.94	0.48
1:C:94:ARG:HH11	1:C:97:ARG:HD3	1.78	0.48
1:C:183:THR:HG22	1:C:183:THR:O	2.15	0.47
1:A:167:MET:HE1	1:A:196:ILE:O	2.15	0.47
1:A:311:LEU:C	1:A:311:LEU:HD23	2.40	0.47
1:A:306:ASP:O	1:A:309:PRO:HD2	2.15	0.47
1:A:280:GLU:C	1:A:282:GLY:H	2.23	0.47
1:A:121:SER:O	1:A:141:TYR:OH	2.21	0.47
1:B:78:TYR:HB2	1:B:79:PRO:HD3	1.96	0.47
1:C:328:VAL:O	1:C:331:THR:HB	2.15	0.47
1:B:91:ILE:HG21	1:B:123:ILE:HG21	1.96	0.46
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.51	0.46
1:B:92:MET:HE2	1:B:92:MET:HB3	1.89	0.46
1:B:157:ALA:O	1:B:162:VAL:HG23	2.15	0.46
1:B:260:PHE:CE2	1:B:303:ILE:HD12	2.50	0.46
1:B:346:ASN:O	1:B:350:ILE:HG13	2.15	0.46
1:A:39:GLU:HB3	1:A:133:ARG:NH1	2.31	0.46
1:B:121:SER:O	1:B:141:TYR:OH	2.26	0.46
1:B:62:ILE:HB	1:B:345:ASP:HB2	1.98	0.46
1:C:241:MET:HE2	1:C:241:MET:HB3	1.88	0.46
1:B:48:LEU:HG	1:B:357:GLU:HG2	1.97	0.45
1:B:252:ALA:HB2	1:B:326:PRO:HB3	1.97	0.45
1:A:201:GLU:HG2	1:A:213:LEU:HD23	1.98	0.45
1:A:228:HIS:HB2	1:A:237:GLN:HG3	1.98	0.45
1:C:162:VAL:O	1:C:166:MET:HG3	2.17	0.45
1:C:359:LEU:O	1:C:360:HIS:HB2	2.15	0.45
1:A:88:ARG:O	1:A:92:MET:HG3	2.16	0.45
1:B:71:GLN:N	1:B:72:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:O	1:A:274:ILE:HG13	2.17	0.44
1:B:308:ILE:N	1:B:309:PRO:CD	2.80	0.44
1:C:279:HIS:HD2	1:C:289:LEU:CD1	2.31	0.44
1:C:333:ASP:O	1:C:335:ASN:N	2.50	0.44
1:B:336:GLU:C	1:B:338:ASN:N	2.76	0.44
1:A:107:ASP:O	1:A:121:SER:HA	2.17	0.44
1:B:281:LEU:HB2	1:B:283:LEU:HD12	2.00	0.44
1:C:90:HIS:O	1:C:94:ARG:HG2	2.18	0.44
1:C:222:LYS:O	1:C:226:THR:OG1	2.36	0.44
1:C:157:ALA:O	1:C:162:VAL:HG23	2.18	0.43
1:B:36:TRP:N	1:B:37:PRO:HD3	2.34	0.43
1:C:113:THR:C	1:C:115:GLU:N	2.76	0.43
1:A:325:PHE:CD1	1:A:325:PHE:N	2.85	0.43
1:A:65:MET:HG3	1:A:169:GLU:HB2	2.00	0.43
1:A:302:VAL:HA	5:A:501:HOH:O	2.19	0.43
1:A:307:HIS:CD2	1:A:317:VAL:HG11	2.53	0.43
1:B:145:TYR:CD1	1:B:145:TYR:C	2.96	0.43
1:C:331:THR:CG2	1:C:333:ASP:H	2.32	0.43
1:C:299:TYR:CE2	1:C:303:ILE:HG13	2.54	0.43
1:C:132:LYS:HG2	1:C:229:PRO:HD3	2.00	0.42
1:C:62:ILE:O	1:C:66:TRP:HB2	2.20	0.42
1:A:270:ARG:HD2	1:A:270:ARG:HA	1.74	0.42
1:A:229:PRO:O	1:A:230:PRO:C	2.62	0.42
1:A:56:ILE:HD13	1:A:56:ILE:HA	1.88	0.42
1:A:103:VAL:HG21	1:A:129:PRO:HG2	2.00	0.42
1:C:113:THR:C	1:C:115:GLU:H	2.26	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.87	0.42
1:A:180:SER:C	1:A:182:LYS:H	2.28	0.42
1:C:107:ASP:HB3	1:C:122:ASN:HB2	2.01	0.41
1:C:228:HIS:HB2	1:C:237:GLN:HG3	2.01	0.41
1:A:308:ILE:HB	1:A:309:PRO:HD3	2.03	0.41
1:A:157:ALA:HB1	1:A:339:LEU:HD21	2.02	0.41
1:B:170:LEU:HG	1:B:174:LEU:HD12	2.01	0.41
1:C:52:ALA:O	1:C:56:ILE:HG12	2.20	0.41
1:A:76:GLU:O	1:A:83:GLY:HA3	2.21	0.41
1:C:308:ILE:HB	1:C:309:PRO:HD3	2.02	0.41
1:B:351:LEU:O	1:B:354:PHE:HB3	2.21	0.41
1:A:295:GLN:HB3	1:A:297:TYR:CE2	2.55	0.41
1:A:162:VAL:HB	1:A:163:PRO:HD3	2.02	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.86	0.41
1:C:102:TRP:HA	1:C:127:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:THR:C	1:C:333:ASP:H	2.28	0.40
1:A:209:PRO:HB2	1:A:210:GLN:NE2	2.36	0.40
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.97	0.40
1:A:36:TRP:HA	1:A:39:GLU:HG3	2.02	0.40
1:A:46:ALA:HB2	1:A:360:HIS:CD2	2.56	0.40
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.96	0.40
1:A:212:SER:O	1:A:213:LEU:C	2.64	0.40
1:B:325:PHE:N	1:B:325:PHE:CD1	2.87	0.40
1:B:170:LEU:O	1:B:174:LEU:HB2	2.21	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	322/341 (94%)	295 (92%)	27 (8%)	0	100	100
1	B	321/341 (94%)	297 (92%)	24 (8%)	0	100	100
1	C	320/341 (94%)	296 (92%)	24 (8%)	0	100	100
All	All	963/1023 (94%)	888 (92%)	75 (8%)	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	274/300 (91%)	263 (96%)	11 (4%)	28	56
1	B	277/300 (92%)	259 (94%)	18 (6%)	15	40
1	C	273/300 (91%)	260 (95%)	13 (5%)	23	50
All	All	824/900 (92%)	782 (95%)	42 (5%)	21	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	51	SER
1	A	71	GLN
1	A	84	SER
1	A	105	GLU
1	A	113	THR
1	A	125	SER
1	A	205	LEU
1	A	226	THR
1	A	296	ASN
1	A	341	GLU
1	B	38	GLU
1	B	47	ILE
1	B	51	SER
1	B	58	GLU
1	B	91	ILE
1	B	126	THR
1	B	147	SER
1	B	160	SER
1	B	177	LYS
1	B	179	LEU
1	B	205	LEU
1	B	236	SER
1	B	242	ASP
1	B	254	ASN
1	B	296	ASN
1	B	311	LEU
1	B	327	GLU
1	B	342	SER
1	C	50	SER
1	C	71	GLN
1	C	84	SER
1	C	89	GLN
1	C	128	ASN

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Mol	Chain	Res	Type
1	C	137	LEU
1	C	147	SER
1	C	222	LYS
1	C	226	THR
1	C	263	ASN
1	C	298	SER
1	C	302	VAL
1	C	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	210	GLN
1	A	335	ASN
1	B	134	HIS
1	B	319	HIS
1	B	338	ASN
1	C	68	ASN
1	C	128	ASN
1	C	194	GLN
1	C	254	ASN
1	C	263	ASN
1	C	279	HIS
1	C	296	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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
3	S77	B	401	2	28,28,28	0.59	1 (3%)	37,39,39	1.89	3 (8%)
4	SO4	C	404	-	4,4,4	0.31	0	6,6,6	0.11	0
3	S77	A	402	2	28,28,28	0.78	1 (3%)	37,39,39	1.93	3 (8%)
3	S77	C	402	2	28,28,28	0.97	2 (7%)	37,39,39	2.01	2 (5%)
4	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.11	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
3	S77	B	401	2	-	2/12/22/22	0/4/4/4
3	S77	C	402	2	-	2/12/22/22	0/4/4/4
3	S77	A	402	2	-	2/12/22/22	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	S77	C4-N2	3.78	1.39	1.36
3	A	402	S77	C4-N2	3.10	1.38	1.36
3	C	402	S77	C2-C1	2.91	1.46	1.42
3	B	401	S77	C4-N2	2.43	1.38	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	S77	N2-C4-N4	-9.39	107.27	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	S77	N2-C4-N4	-9.35	107.28	110.99
3	B	401	S77	N2-C4-N4	-8.84	107.48	110.99
3	C	402	S77	C3-C4-N2	5.64	128.22	123.24
3	B	401	S77	C3-C4-N2	4.86	127.53	123.24
3	A	402	S77	C3-C4-N2	4.54	127.25	123.24
3	B	401	S77	C8-C3-C4	2.79	114.85	111.29
3	A	402	S77	C9-C3-C4	2.49	114.47	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

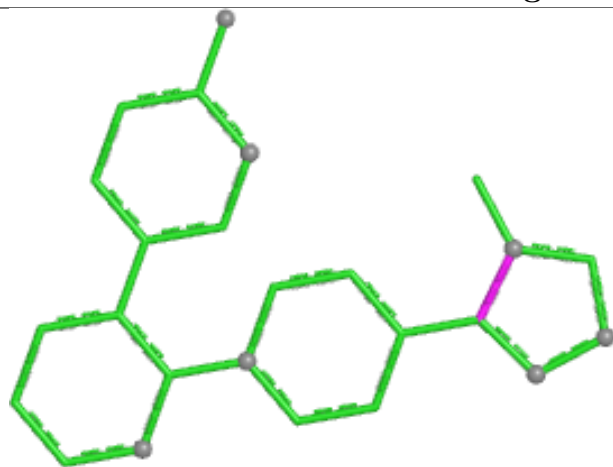
Mol	Chain	Res	Type	Atoms
3	A	402	S77	N3-C1-N1-C7
3	A	402	S77	C2-C1-N1-C7
3	B	401	S77	N3-C1-N1-C7
3	B	401	S77	C2-C1-N1-C7
3	C	402	S77	N3-C1-N1-C7
3	C	402	S77	C2-C1-N1-C7

There are no ring outliers.

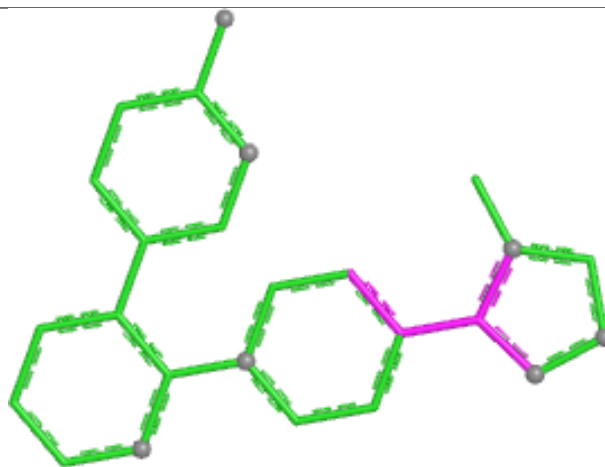
No monomer is involved in short contacts.

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.

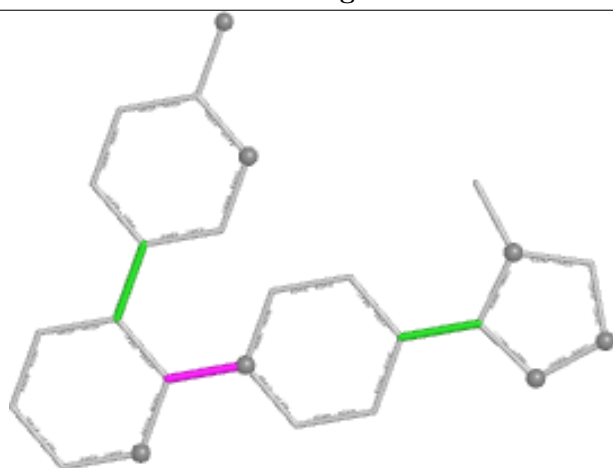
Ligand S77 B 401



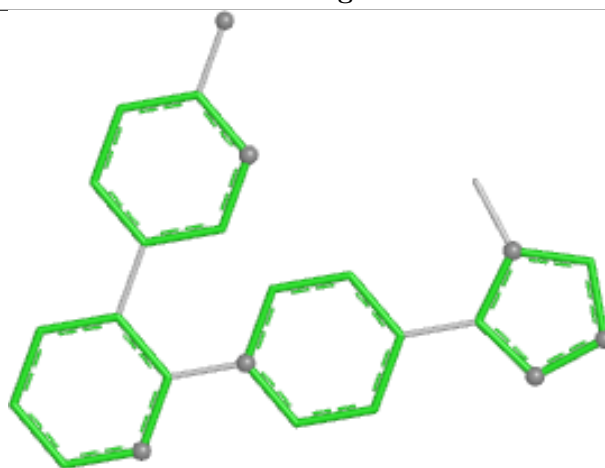
Bond lengths



Bond angles

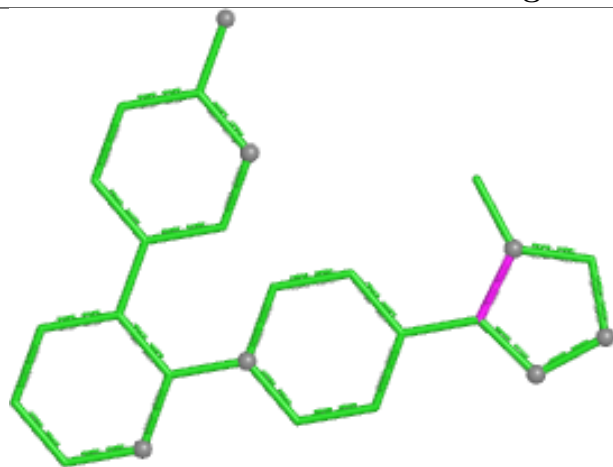


Torsions

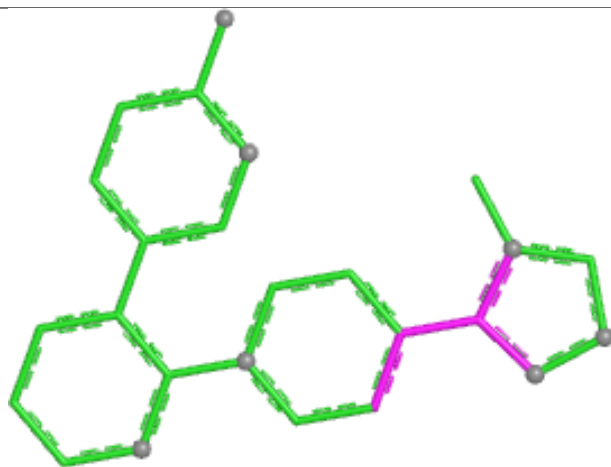


Rings

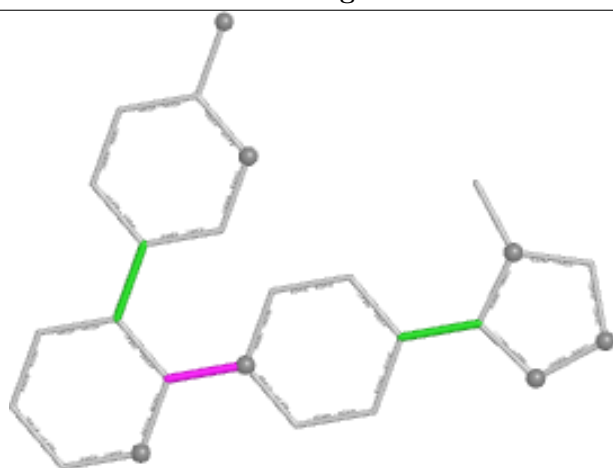
Ligand S77 A 402



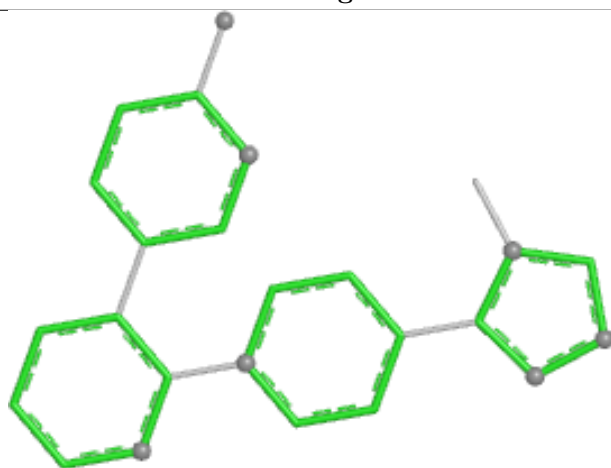
Bond lengths



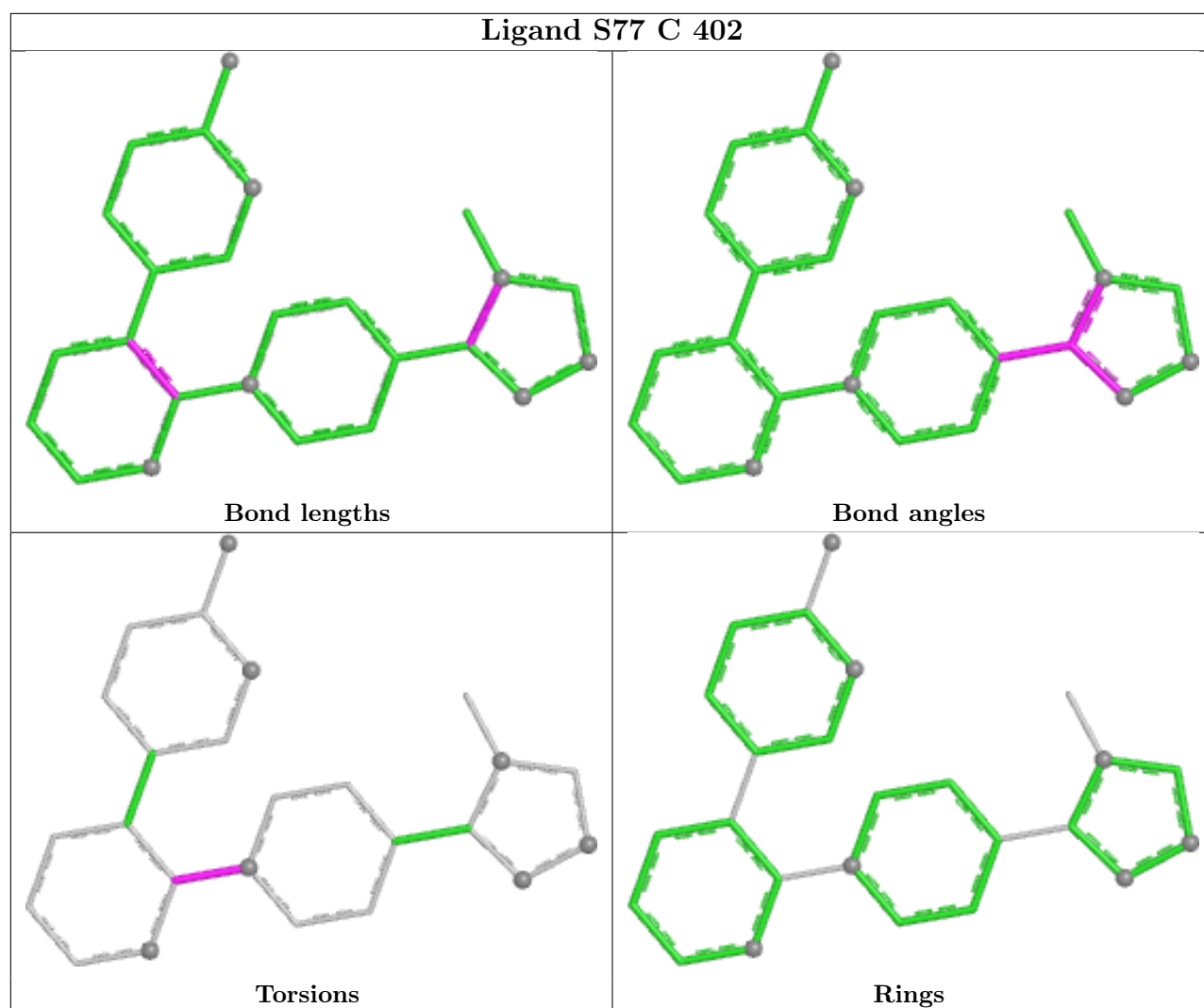
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	326/341 (95%)	-0.50	1 (0%) 90 80	16, 31, 54, 88	0
1	B	325/341 (95%)	-0.61	0 100 100	15, 28, 49, 75	0
1	C	324/341 (95%)	-0.57	3 (0%) 81 61	14, 29, 49, 100	0
All	All	975/1023 (95%)	-0.56	4 (0%) 88 75	14, 29, 51, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	HIS	2.4
1	C	151	ASN	2.3
1	C	150	ASN	2.3
1	A	186	ASP	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](#)

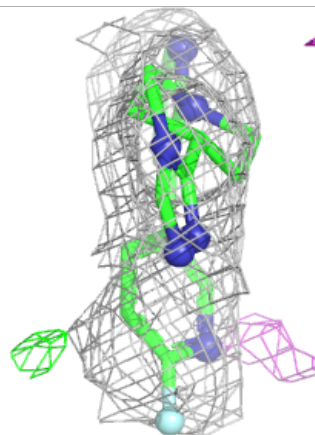
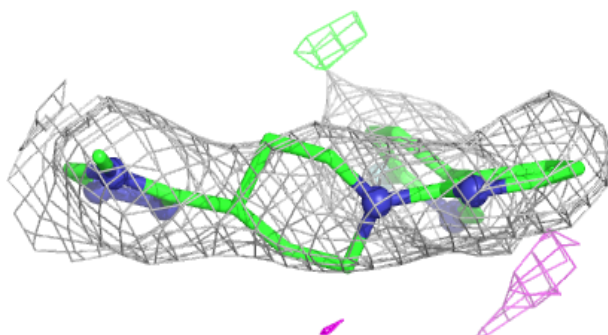
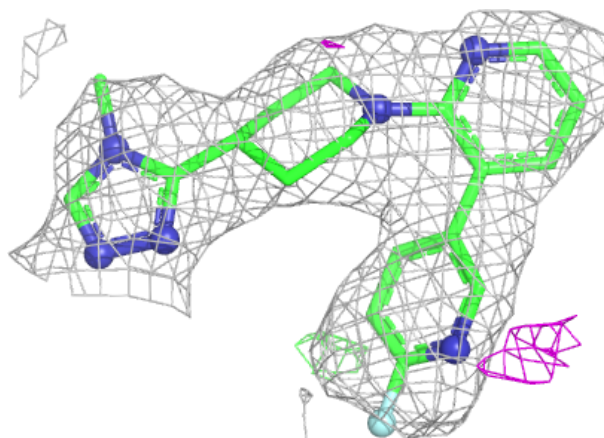
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	S77	A	402	25/25	0.95	0.09	35,40,52,52	0
3	S77	C	402	25/25	0.96	0.07	30,33,45,51	0
4	SO4	A	403	5/5	0.96	0.07	36,36,38,38	0
3	S77	B	401	25/25	0.97	0.07	28,32,37,39	0
4	SO4	C	403	5/5	0.98	0.05	25,25,26,28	0
4	SO4	C	404	5/5	0.98	0.05	31,31,33,35	0
2	CO	A	401	1/1	1.00	0.02	24,24,24,24	0
2	CO	B	402	1/1	1.00	0.01	22,22,22,22	0
2	CO	C	401	1/1	1.00	0.01	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

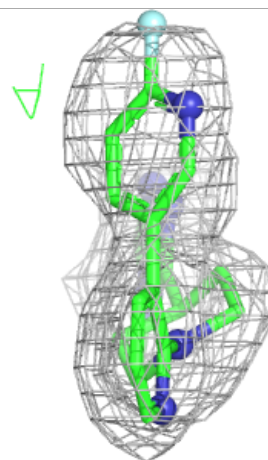
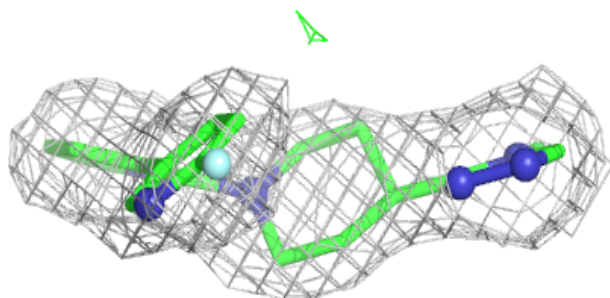
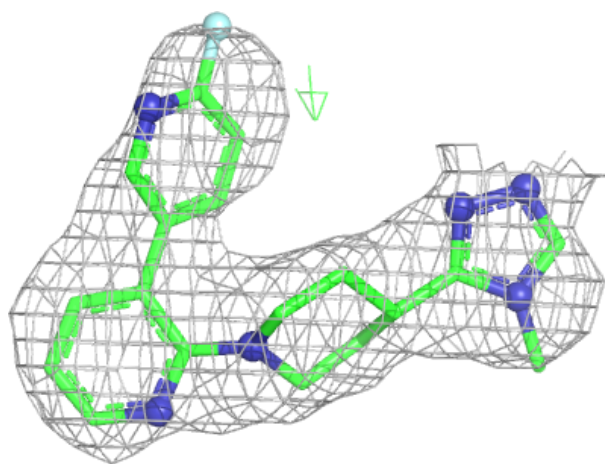
Electron density around S77 A 402:

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



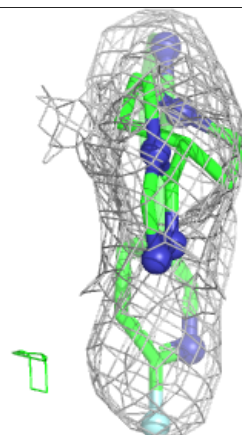
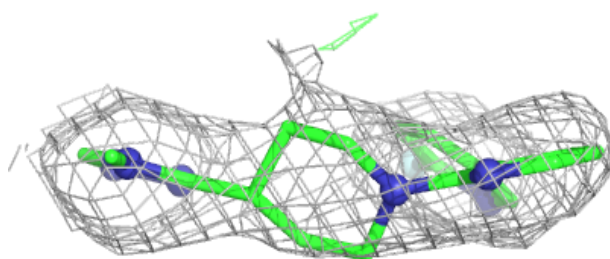
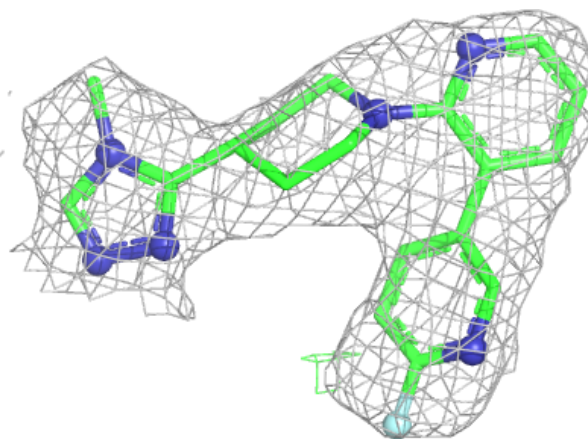
Electron density around S77 C 402:

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



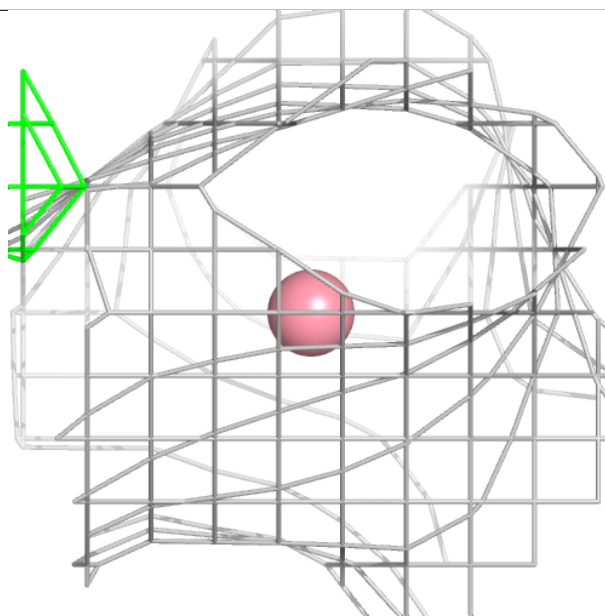
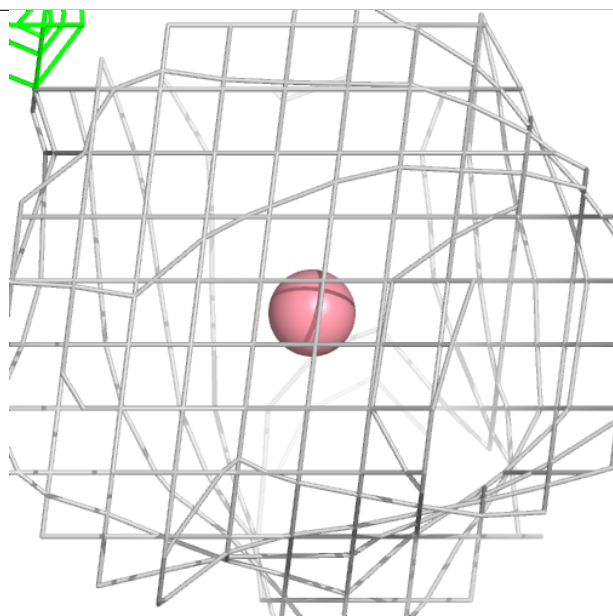
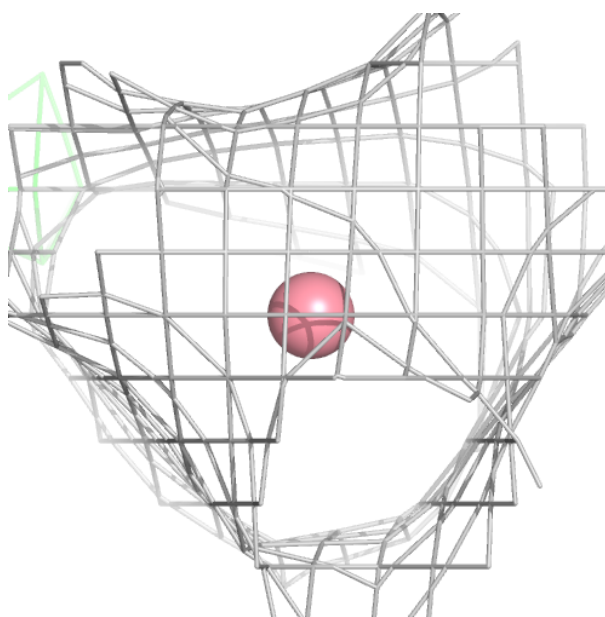
Electron density around S77 B 401:

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



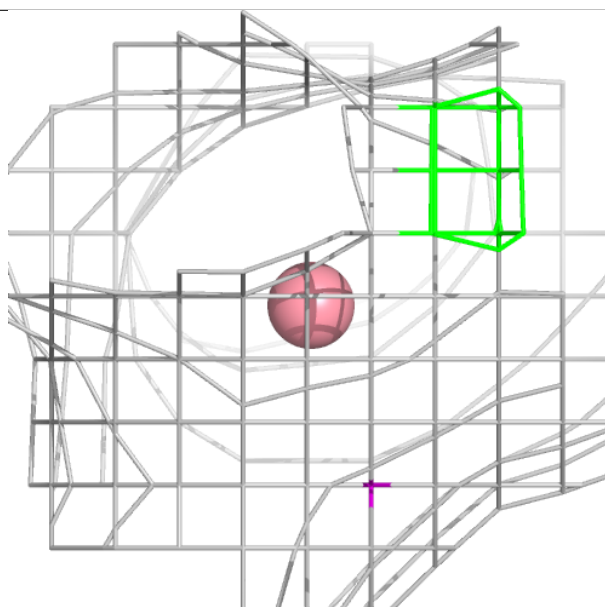
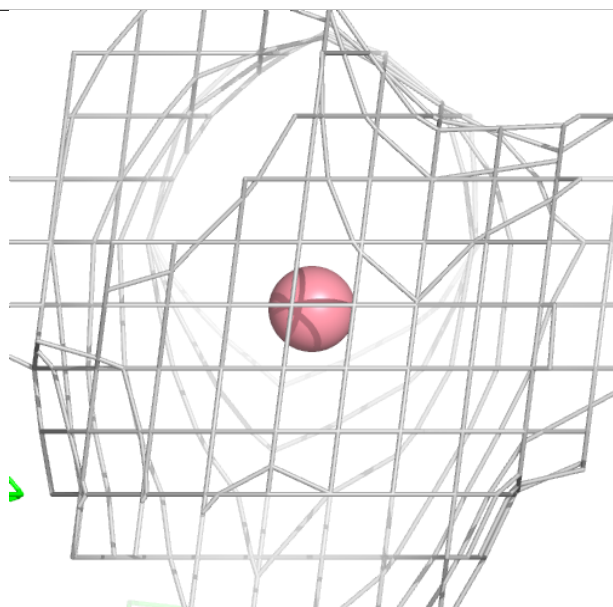
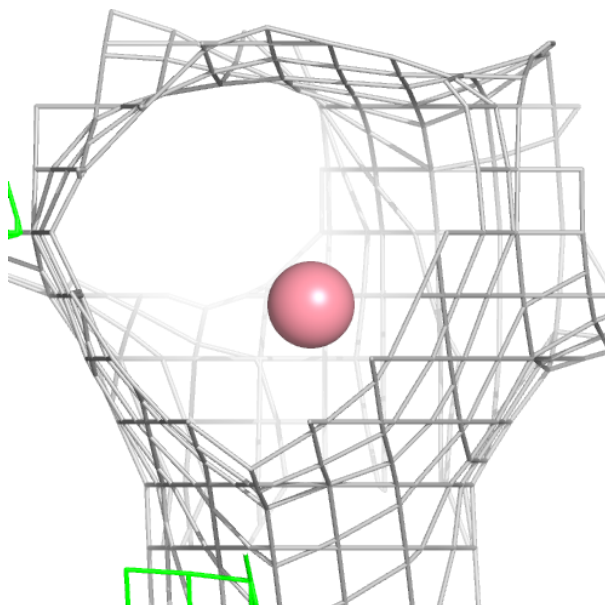
Electron density around CO A 401:

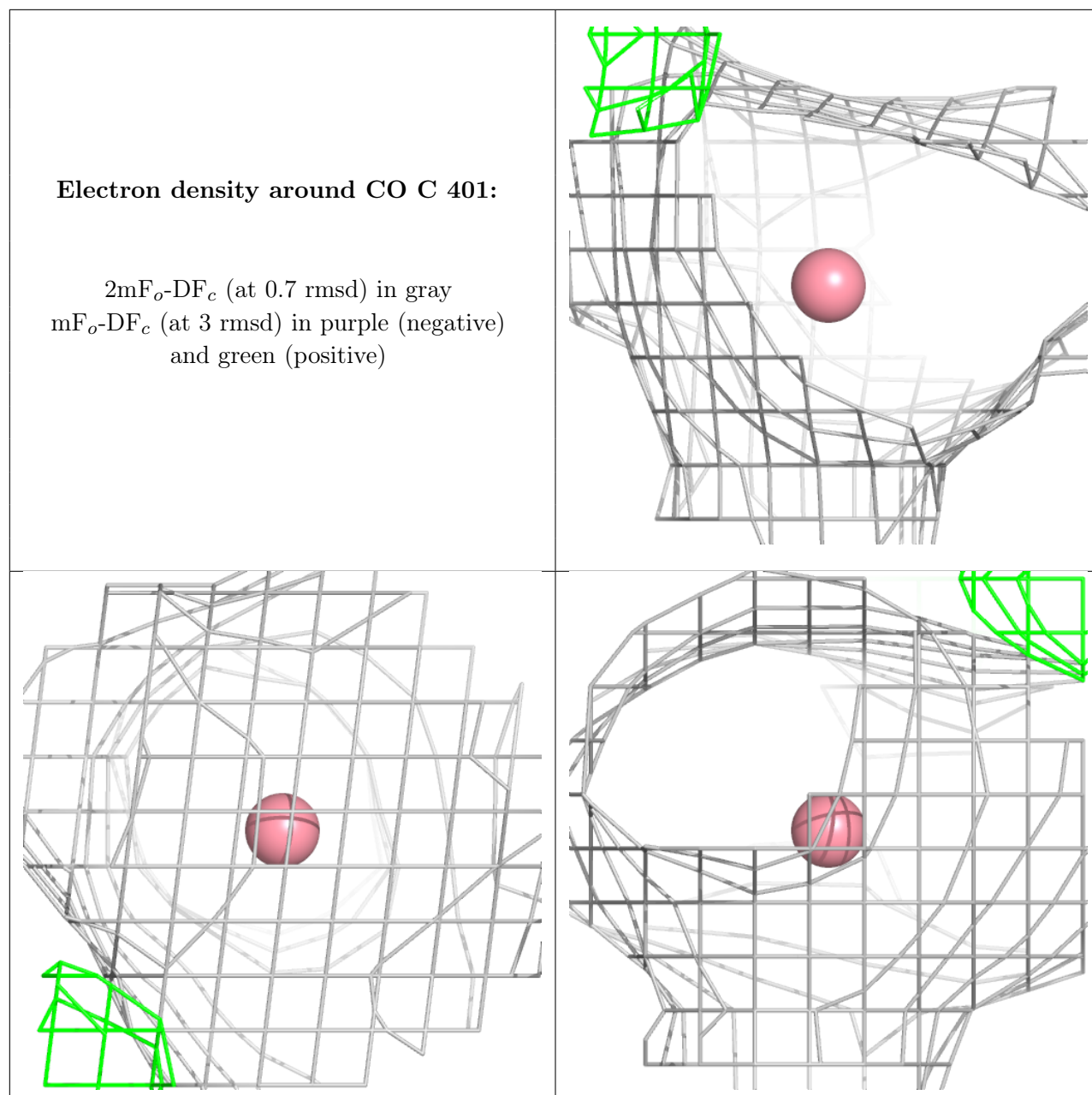
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CO 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.