



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:02 PM UTC

PDB ID : 9FXJ / pdb_00009fxj
Title : Crystal structure of cobalt(II)-substituted double mutant Y115E Y117E human Glutaminyl Cyclase in complex with PBD-150
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

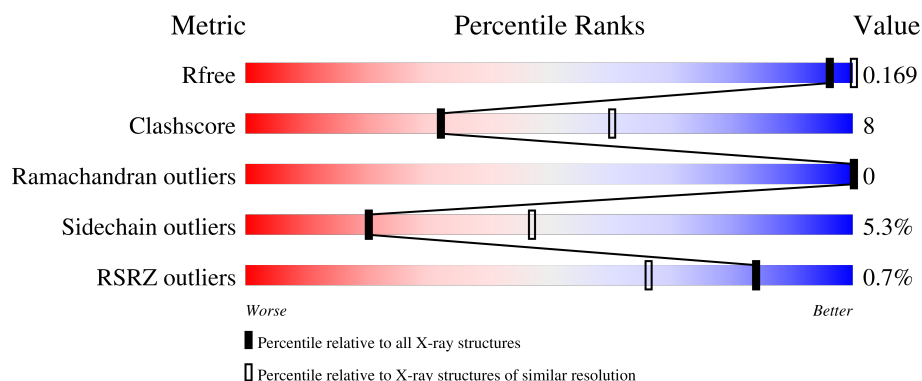
1 Overall quality at a glance

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	% 75% 21% .
1	B	341	% 74% 21% ..
1	C	341	72% 22% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8154 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
			2586	1654	446	477	9			
1	B	326	Total	C	N	O	S	0	0	0
			2585	1654	446	476	9			
1	C	326	Total	C	N	O	S	0	0	0
			2594	1659	448	478	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

Continued on next page...

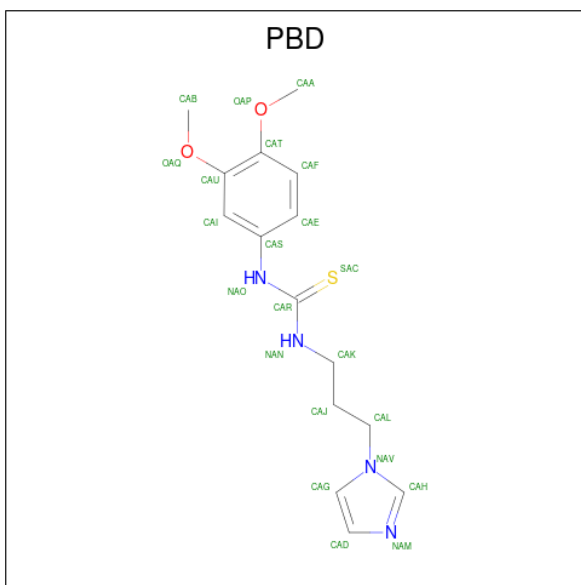
Continued from previous page...

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 1-(3,4-dimethoxyphenyl)-3-[3-(1H-imidazol-1-yl)propyl]thiourea (CCD ID: PBD) (formula: C₁₅H₂₀N₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
3	B	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
3	C	1	Total	C	N	O	S	0	0
			22	15	4	2	1		

- 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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	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	102	Total	O	0	0
			102	102		
5	B	104	Total	O	0	0
			104	104		
5	C	99	Total	O	0	0
			99	99		

S298
Y299
D305
D306
H307
T308
P309
F310
L311
P322
P326
T331
H332
D333
D334
N335
N338
L339
V353
F354
V355
L356
E357
Y358
L361

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.39Å 149.63Å 96.16Å 90.00° 96.82° 90.00°	Depositor
Resolution (Å)	74.81 – 3.06 74.81 – 3.06	Depositor EDS
% Data completeness (in resolution range)	87.5 (74.81-3.06) 87.4 (74.81-3.06)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.171 , 0.202 (Not available) , 0.169	Depositor DCC
R_{free} test set	1043 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8154	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, SO4, PBD

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	0.53	0/2659	1.07	2/3622 (0.1%)
1	B	0.54	0/2657	1.09	2/3618 (0.1%)
1	C	0.53	0/2667	1.07	3/3631 (0.1%)
All	All	0.53	0/7983	1.08	7/10871 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	THR	CB-CA-C	5.72	120.30	109.37
1	B	82	PRO	N-CA-C	-5.50	106.22	113.65
1	C	72	PRO	CB-CA-C	-5.32	103.85	111.62
1	C	299	TYR	CA-C-N	5.24	125.80	119.98
1	C	299	TYR	C-N-CA	5.24	125.80	119.98
1	A	159	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	199	ASP	CA-CB-CG	5.04	117.64	112.60

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	2586	0	2475	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2585	0	2483	40	0
1	C	2594	0	2492	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	20	0	0
3	B	22	0	20	1	0
3	C	22	0	20	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	102	0	0	1	0
5	B	104	0	0	0	0
5	C	99	0	0	0	0
All	All	8154	0	7510	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (123) 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:207:TRP:CH2	3:C:402:PBD:HAL	2.14	0.82
1:B:92:MET:HG2	1:B:104:LEU:HD13	1.68	0.75
1:C:158:THR:HG22	1:C:251:GLY:HA3	1.71	0.71
1:A:141:TYR:CE2	1:A:199:ASP:HB2	2.28	0.69
1:A:161:ALA:O	1:A:164:CYS:HB2	1.93	0.68
1:B:123:ILE:HB	1:B:197:PHE:HB2	1.77	0.67
1:C:335:ASN:OD1	1:C:338:ASN:ND2	2.28	0.66
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.31	0.66
1:C:36:TRP:N	1:C:37:PRO:CD	2.59	0.65
1:C:306:ASP:O	1:C:309:PRO:HD2	1.99	0.62
1:B:267:TRP:O	1:B:270:ARG:HB2	1.99	0.62
1:A:105:GLU:HB3	5:A:524:HOH:O	1.99	0.62
1:A:123:ILE:HB	1:A:197:PHE:HB2	1.82	0.60
1:B:92:MET:SD	1:B:106:ILE:HD11	2.42	0.60
1:A:141:TYR:CZ	1:A:199:ASP:HB2	2.39	0.58
1:C:108:THR:HA	1:C:120:PHE:O	2.04	0.57
1:C:311:LEU:C	1:C:311:LEU:HD23	2.30	0.57
1:C:252:ALA:HB2	1:C:326:PRO:HB3	1.86	0.57
1:C:157:ALA:CB	1:C:339:LEU:HD21	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:MET:HE2	1:C:197:PHE:CE2	2.39	0.56
1:A:359:LEU:O	1:A:360:HIS:HB2	2.04	0.56
1:B:228:HIS:HB2	1:B:237:GLN:HG3	1.88	0.56
1:A:125:SER:HB3	1:A:195:LEU:HB2	1.88	0.55
1:C:274:ILE:HD13	1:C:353:VAL:HG12	1.87	0.55
1:A:92:MET:SD	1:A:106:ILE:HD11	2.48	0.54
1:C:170:LEU:HD11	1:C:355:VAL:HG21	1.91	0.54
1:B:36:TRP:CD1	1:B:37:PRO:HD3	2.43	0.53
1:B:114:PRO:HG2	1:B:211:ASP:OD2	2.08	0.53
1:A:268:PHE:CZ	1:A:294:PHE:HB3	2.43	0.53
1:A:36:TRP:N	1:A:37:PRO:CD	2.72	0.53
1:A:228:HIS:HB2	1:A:237:GLN:HG2	1.91	0.53
1:C:78:TYR:HB2	1:C:79:PRO:CD	2.39	0.53
1:A:258:PRO:HG2	1:A:260:PHE:CZ	2.44	0.52
1:A:209:PRO:HB2	1:A:210:GLN:OE1	2.10	0.52
1:B:39:GLU:HB3	1:B:133:ARG:NH1	2.24	0.52
1:B:331:THR:C	1:B:333:ASP:H	2.18	0.52
1:B:331:THR:HG22	1:B:333:ASP:H	1.74	0.52
1:B:94:ARG:O	1:B:97:ARG:HG3	2.11	0.51
1:C:106:ILE:HG22	1:C:108:THR:OG1	2.10	0.51
1:A:107:ASP:HB3	1:A:122:ASN:HB2	1.92	0.51
1:A:88:ARG:HG3	1:A:123:ILE:HD11	1.94	0.50
1:C:228:HIS:HA	1:C:229:PRO:C	2.35	0.50
1:C:211:ASP:O	1:C:212:SER:HB3	2.11	0.50
1:C:137:LEU:HD23	1:C:245:VAL:HB	1.93	0.49
1:C:157:ALA:HB3	1:C:339:LEU:HD21	1.94	0.49
1:B:108:THR:HA	1:B:120:PHE:O	2.13	0.49
1:C:207:TRP:CZ3	3:C:402:PBD:HAL	2.48	0.49
1:C:247:LEU:HG	1:C:250:ILE:HD12	1.95	0.49
1:C:305:ASP:HB3	1:C:307:HIS:ND1	2.27	0.49
1:C:138:ALA:HA	1:C:196:ILE:O	2.13	0.48
1:C:333:ASP:O	1:C:338:ASN:ND2	2.46	0.48
1:B:162:VAL:O	1:B:166:MET:HG3	2.14	0.47
1:B:205:LEU:HB3	1:B:206:HIS:H	1.54	0.47
1:B:319:HIS:CE1	1:B:321:ILE:HG21	2.49	0.47
1:C:295:GLN:HB3	1:C:297:TYR:CE2	2.48	0.47
1:A:309:PRO:HA	1:A:312:ARG:HG2	1.96	0.47
1:C:249:LEU:HB2	1:C:322:PRO:HD2	1.96	0.47
1:B:157:ALA:O	1:B:162:VAL:HG23	2.15	0.46
1:A:76:GLU:O	1:A:83:GLY:HA3	2.15	0.46
1:C:158:THR:HG22	1:C:251:GLY:CA	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:HD22	1:C:356:LEU:HD21	1.96	0.46
1:C:331:THR:HG22	1:C:333:ASP:H	1.79	0.46
1:B:76:GLU:O	1:B:83:GLY:HA3	2.15	0.46
1:A:136:VAL:HG22	1:A:194:GLN:HB3	1.97	0.46
1:B:96:GLN:C	1:B:98:LEU:H	2.23	0.46
1:B:107:ASP:HB3	1:B:122:ASN:HB2	1.97	0.46
1:C:242:ASP:HB3	1:C:358:TYR:OH	2.15	0.46
1:C:205:LEU:HB3	1:C:206:HIS:H	1.35	0.45
1:C:213:LEU:O	1:C:217:ARG:HB2	2.17	0.45
1:C:157:ALA:HB1	1:C:339:LEU:HD21	1.98	0.45
1:A:108:THR:HA	1:A:120:PHE:O	2.16	0.44
1:A:272:GLN:HG2	1:A:294:PHE:HB2	1.99	0.44
1:C:255:PRO:HD2	1:C:293:TYR:CE1	2.53	0.44
1:B:145:TYR:CD1	1:B:145:TYR:C	2.95	0.44
1:B:203:ALA:CB	1:B:207:TRP:HA	2.48	0.44
1:C:55:GLN:NE2	1:C:177:LYS:HE2	2.33	0.44
1:C:181:LEU:C	1:C:183:THR:N	2.75	0.44
1:A:88:ARG:HD2	1:A:121:SER:HB3	2.00	0.43
1:B:241:MET:HE1	1:B:244:LEU:HD13	2.00	0.43
1:C:36:TRP:CG	1:C:37:PRO:HD3	2.53	0.43
1:B:69:ASP:O	1:B:90:HIS:HE1	2.01	0.43
1:B:170:LEU:HD11	1:B:355:VAL:HG21	2.00	0.43
1:B:193:LEU:HD12	1:B:194:GLN:H	1.82	0.43
1:C:40:LYS:HD2	1:C:242:ASP:HA	2.01	0.43
1:C:94:ARG:HA	1:C:94:ARG:HD2	1.70	0.43
1:A:109:PHE:CE1	1:A:120:PHE:HB2	2.53	0.43
1:B:65:MET:HG3	1:B:169:GLU:HB2	1.99	0.43
1:C:308:ILE:HB	1:C:309:PRO:HD3	2.00	0.43
1:C:71:GLN:HB3	1:C:72:PRO:HD3	2.00	0.43
1:A:204:PHE:HE1	1:A:214:TYR:CE2	2.37	0.42
1:A:213:LEU:O	1:A:217:ARG:HB2	2.19	0.42
1:B:118:ARG:HD3	1:B:118:ARG:HA	1.76	0.42
1:B:228:HIS:HA	1:B:229:PRO:C	2.42	0.42
1:C:92:MET:SD	1:C:106:ILE:HD11	2.59	0.42
1:B:207:TRP:CH2	3:B:402:PBD:HAL	2.55	0.42
1:B:311:LEU:O	1:B:314:GLY:N	2.46	0.42
1:C:36:TRP:C	1:C:38:GLU:H	2.26	0.42
1:B:246:LEU:HD22	1:B:307:HIS:HB3	2.01	0.42
1:C:94:ARG:O	1:C:97:ARG:HG2	2.19	0.42
1:A:120:PHE:CD2	1:A:200:GLY:HA3	2.55	0.42
1:C:157:ALA:HB1	1:C:339:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:HG2	1:A:104:LEU:HD13	2.02	0.41
1:C:335:ASN:OD1	1:C:335:ASN:C	2.64	0.41
1:A:181:LEU:HD21	1:A:361:LEU:HD21	2.02	0.41
1:B:265:ALA:O	1:B:269:GLU:HG3	2.20	0.41
1:C:107:ASP:HB3	1:C:122:ASN:HB2	2.02	0.41
1:A:65:MET:HG3	1:A:169:GLU:HB2	2.02	0.41
1:A:54:ARG:HG2	1:A:283:LEU:HD11	2.03	0.41
1:C:39:GLU:HB3	1:C:133:ARG:NH1	2.36	0.41
1:A:174:LEU:O	1:A:178:LEU:HG	2.21	0.41
1:A:211:ASP:O	1:A:212:SER:HB3	2.20	0.41
1:B:211:ASP:O	1:B:212:SER:HB3	2.20	0.41
1:B:331:THR:C	1:B:333:ASP:N	2.79	0.41
1:A:311:LEU:C	1:A:311:LEU:HD23	2.46	0.41
1:B:36:TRP:N	1:B:37:PRO:CD	2.84	0.41
1:C:55:GLN:HE22	1:C:177:LYS:HE2	1.86	0.41
1:A:120:PHE:CE2	1:A:200:GLY:HA3	2.56	0.40
1:A:356:LEU:O	1:A:360:HIS:N	2.55	0.40
1:B:359:LEU:O	1:B:360:HIS:HB2	2.22	0.40
1:B:136:VAL:HG11	1:B:241:MET:HE3	2.03	0.40
1:B:138:ALA:HA	1:B:196:ILE:O	2.21	0.40
1:B:328:VAL:O	1:B:331:THR:HB	2.22	0.40
1:A:226:THR:HB	1:A:237:GLN:HG3	2.04	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	145/341 (42%)	140 (97%)	5 (3%)	0	100	100
1	B	322/341 (94%)	303 (94%)	19 (6%)	0	100	100
1	C	322/341 (94%)	294 (91%)	28 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	789/1023 (77%)	737 (93%)	52 (7%)	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	276/300 (92%)	262 (95%)	14 (5%)	21	48
1	B	276/300 (92%)	261 (95%)	15 (5%)	20	46
1	C	278/300 (93%)	263 (95%)	15 (5%)	20	46
All	All	830/900 (92%)	786 (95%)	44 (5%)	20	47

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	49	ASN
1	A	63	SER
1	A	64	GLU
1	A	71	GLN
1	A	84	SER
1	A	91	ILE
1	A	113	THR
1	A	126	THR
1	A	130	THR
1	A	142	ASP
1	A	160	SER
1	A	205	LEU
1	A	254	ASN
1	B	38	GLU
1	B	71	GLN
1	B	84	SER
1	B	92	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	97	ARG
1	B	105	GLU
1	B	152	ARG
1	B	155	VAL
1	B	205	LEU
1	B	208	SER
1	B	298	SER
1	B	312	ARG
1	B	327	GLU
1	B	328	VAL
1	B	332	MET
1	C	38	GLU
1	C	75	ILE
1	C	91	ILE
1	C	96	GLN
1	C	113	THR
1	C	128	ASN
1	C	135	LEU
1	C	147	SER
1	C	153	VAL
1	C	160	SER
1	C	177	LYS
1	C	181	LEU
1	C	205	LEU
1	C	254	ASN
1	C	298	SER

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	55	GLN
1	A	68	ASN
1	A	140	HIS
1	A	272	GLN
1	A	307	HIS
1	A	348	ASN
1	B	90	HIS
1	B	259	ASN
1	B	276	HIS
1	B	335	ASN
1	B	338	ASN
1	C	55	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	296	ASN

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 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	$\# Z > 2$
4	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.12	0
3	PBD	B	402	2	23,23,23	0.30	0	29,29,29	0.59	0
3	PBD	A	402	2	23,23,23	0.30	0	29,29,29	0.61	1 (3%)
3	PBD	C	402	2	23,23,23	0.31	0	29,29,29	0.39	0
4	SO4	C	403	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.14	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	PBD	A	402	2	-	2/15/15/15	0/2/2/2
3	PBD	C	402	2	-	6/15/15/15	0/2/2/2
3	PBD	B	402	2	-	4/15/15/15	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	PBD	SAC-CAR-NAN	-2.67	118.83	123.26

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	PBD	NAO-CAR-NAN-CAK
3	B	402	PBD	CAU-CAT-OAP-CAA
3	C	402	PBD	CAK-CAJ-CAL-NAV
3	B	402	PBD	CAK-CAJ-CAL-NAV
3	C	402	PBD	SAC-CAR-NAN-CAK
3	B	402	PBD	CAF-CAT-OAP-CAA
3	A	402	PBD	CAU-CAT-OAP-CAA
3	A	402	PBD	CAF-CAT-OAP-CAA
3	C	402	PBD	CAU-CAT-OAP-CAA
3	C	402	PBD	CAJ-CAK-NAN-CAR
3	C	402	PBD	CAI-CAS-NAO-CAR
3	B	402	PBD	CAI-CAS-NAO-CAR

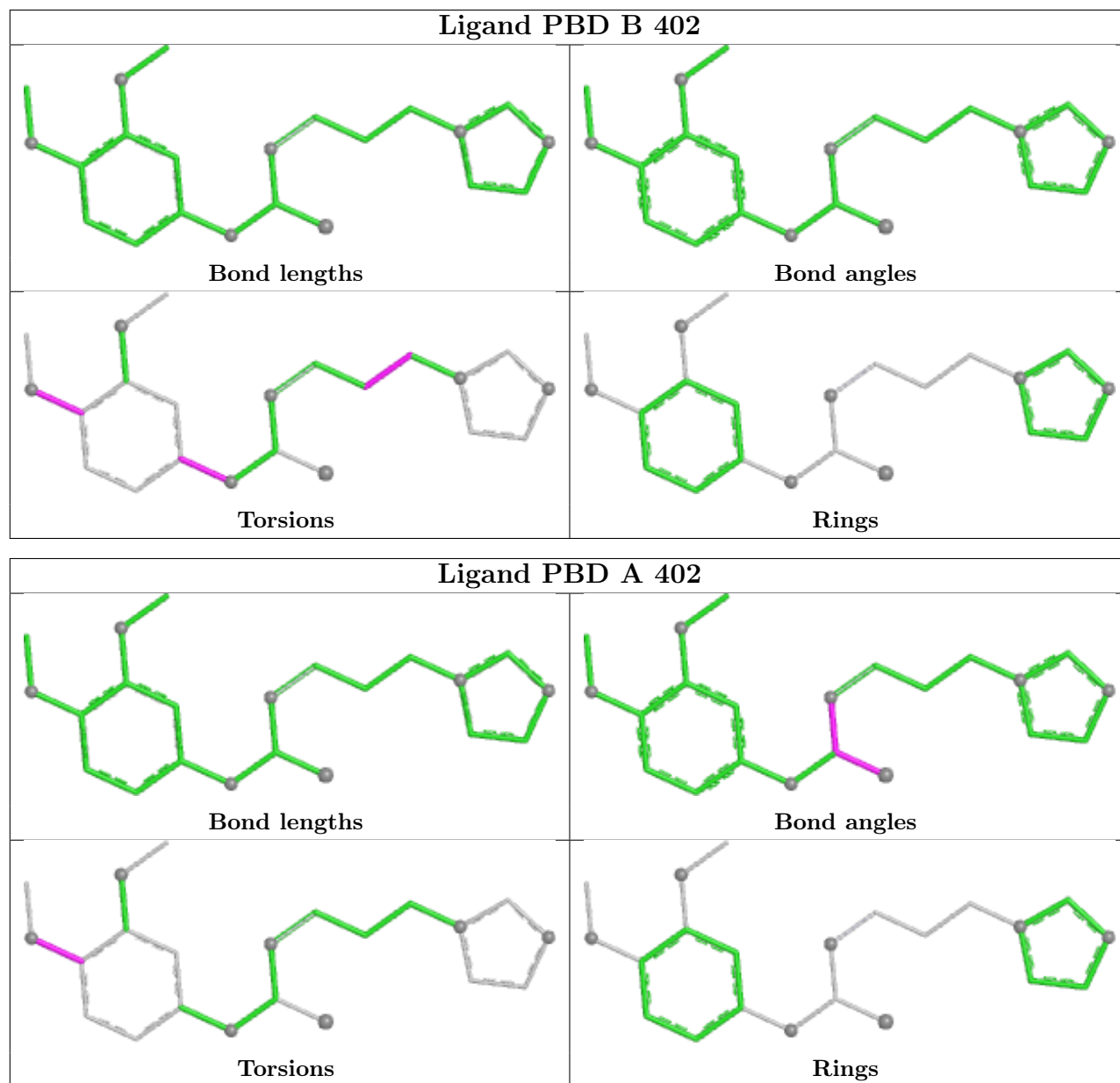
There are no ring outliers.

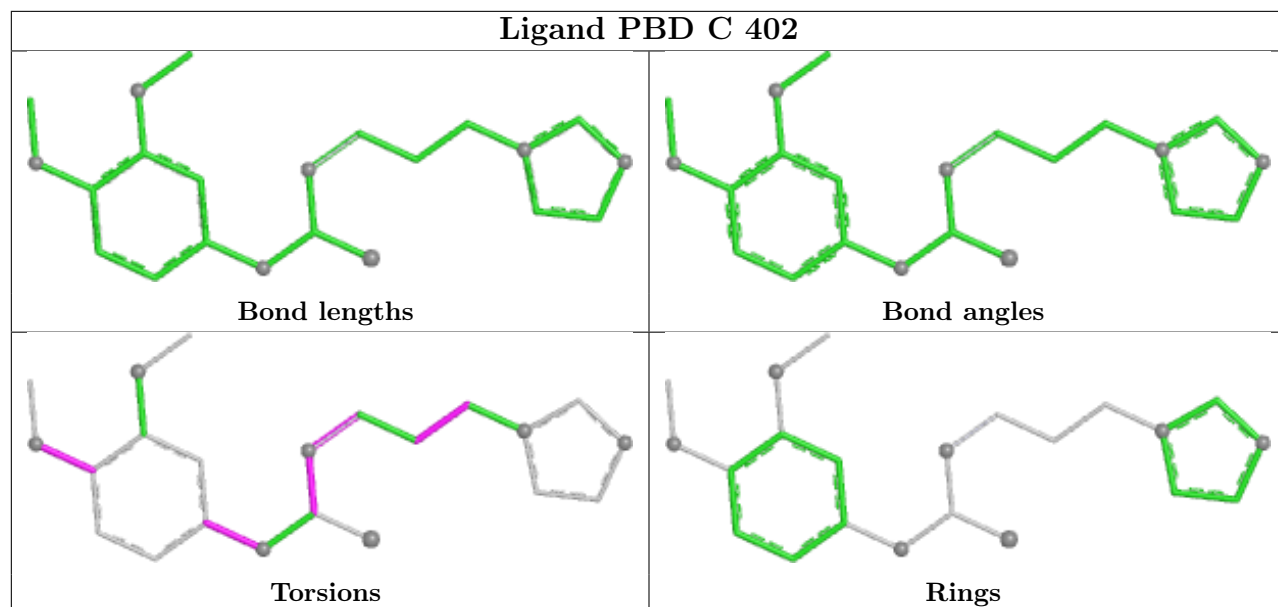
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	PBD	1	0
3	C	402	PBD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	-0.64	2 (0%) 85 69	14, 26, 45, 73	0
1	B	326/341 (95%)	-0.61	4 (1%) 76 55	13, 25, 41, 93	0
1	C	326/341 (95%)	-0.67	1 (0%) 90 80	14, 25, 43, 76	0
All	All	978/1023 (95%)	-0.64	7 (0%) 84 66	13, 25, 44, 93	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	SER	3.3
1	A	151	ASN	3.0
1	B	150	ASN	2.7
1	B	151	ASN	2.6
1	C	206	HIS	2.2
1	A	187	SER	2.2
1	B	184	VAL	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.

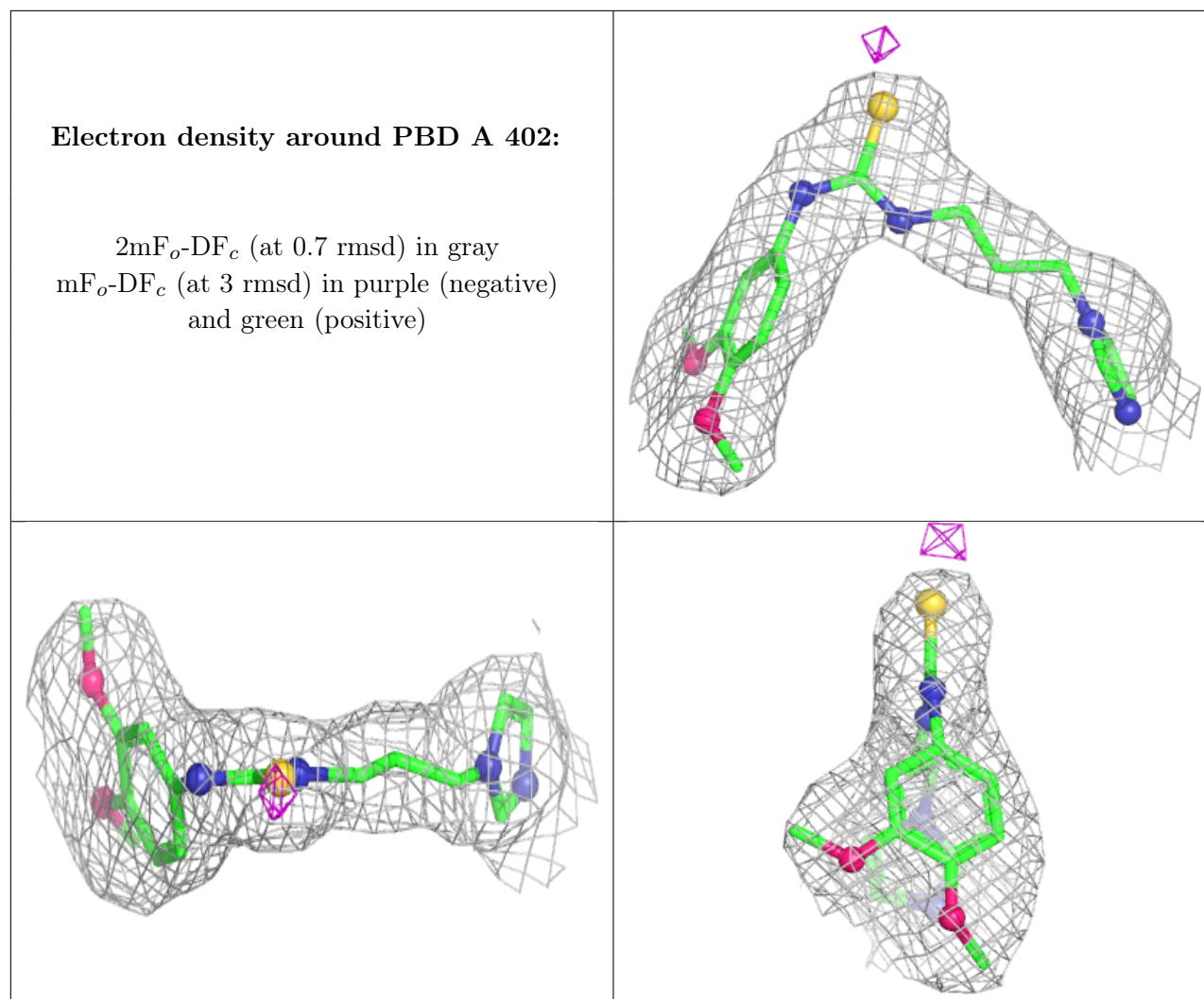
6.4 Ligands [i](#)

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.

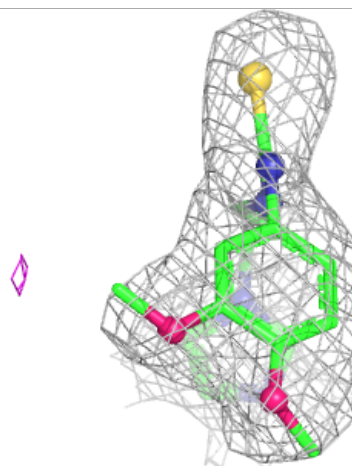
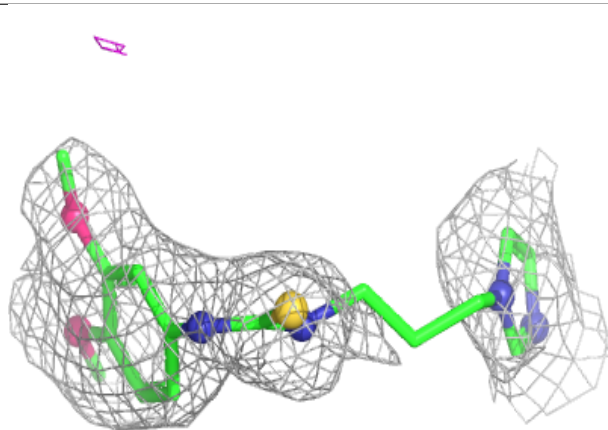
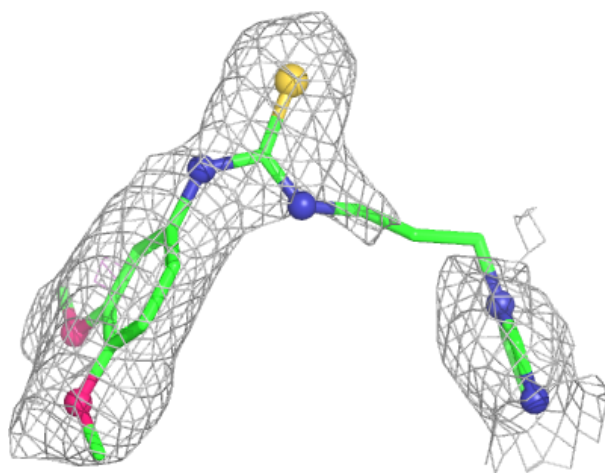
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PBD	A	402	22/22	0.96	0.07	24,27,29,30	0
4	SO4	A	403	5/5	0.96	0.07	36,37,40,43	0
3	PBD	C	402	22/22	0.97	0.08	24,29,30,34	0
3	PBD	B	402	22/22	0.97	0.07	21,26,28,29	0
4	SO4	B	403	5/5	0.98	0.05	37,39,41,41	0
4	SO4	C	403	5/5	0.98	0.05	30,33,35,35	0
2	CO	C	401	1/1	0.99	0.02	21,21,21,21	0
2	CO	B	401	1/1	1.00	0.02	20,20,20,20	0
2	CO	A	401	1/1	1.00	0.02	23,23,23,23	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.



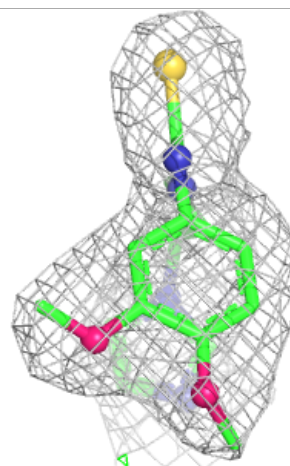
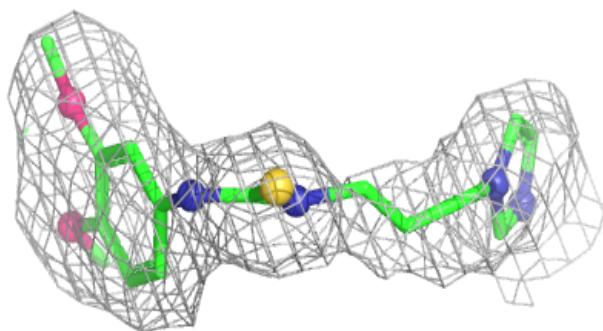
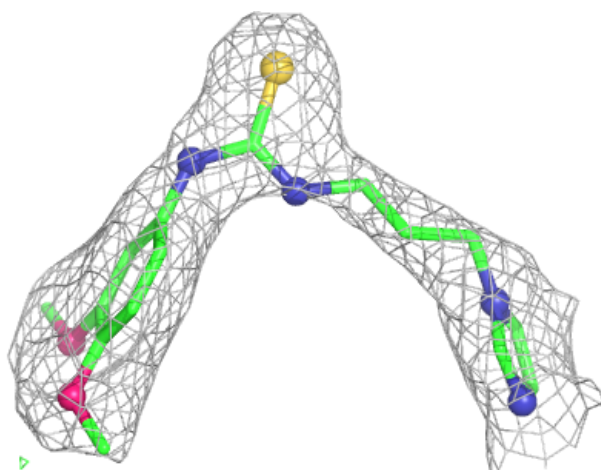
Electron density around PBD C 402:

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



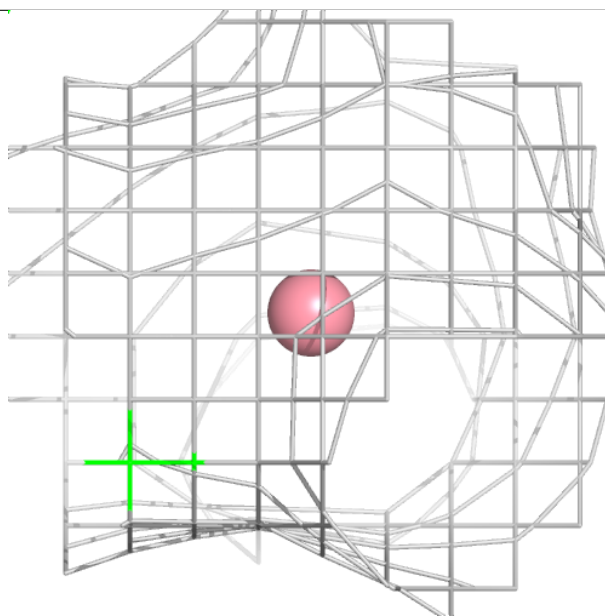
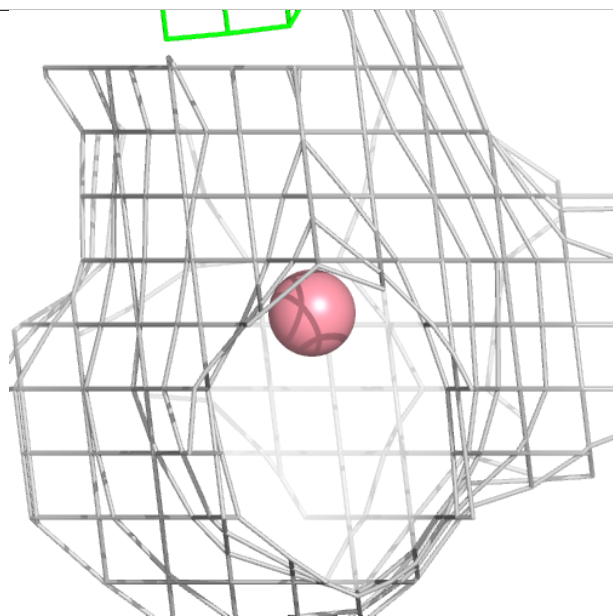
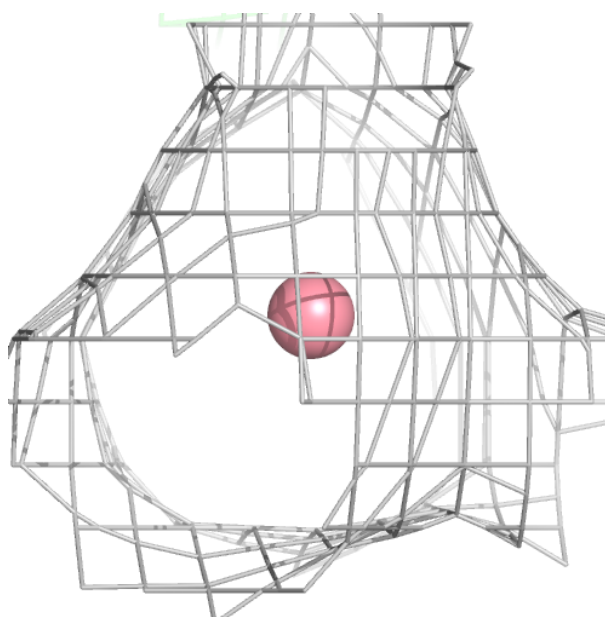
Electron density around PBD B 402:

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



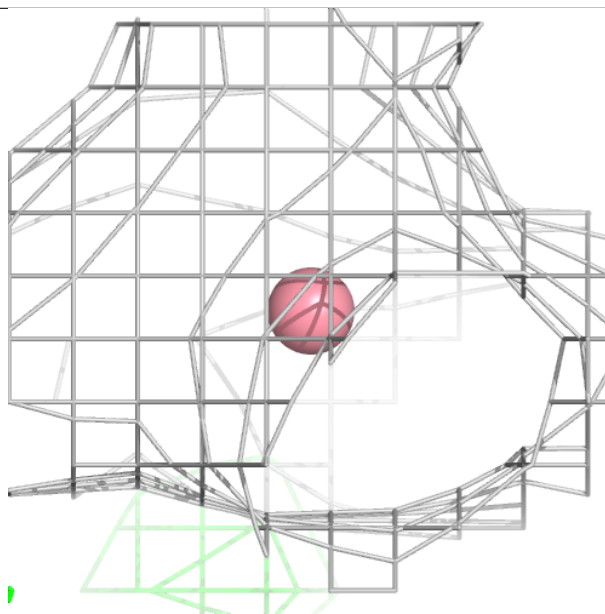
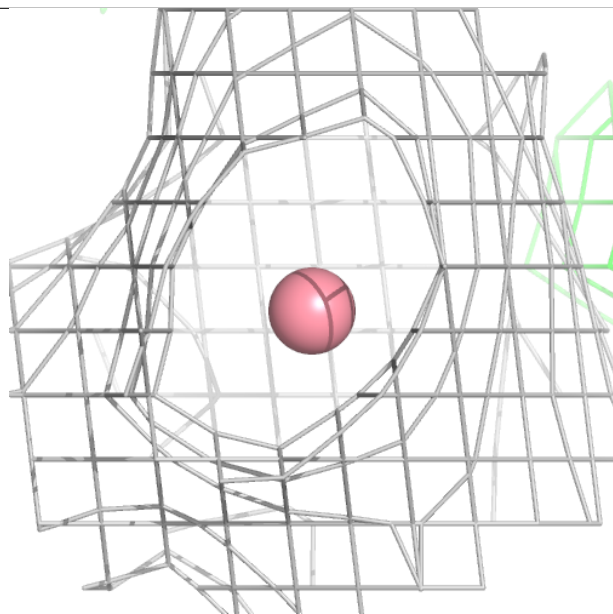
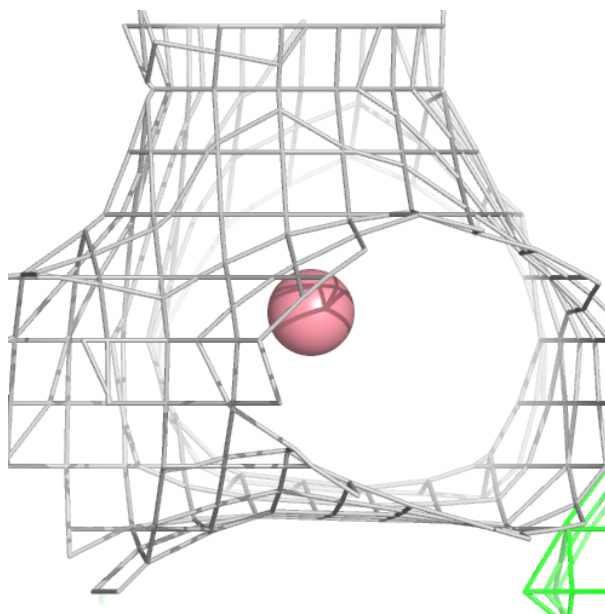
Electron density around CO C 401:

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



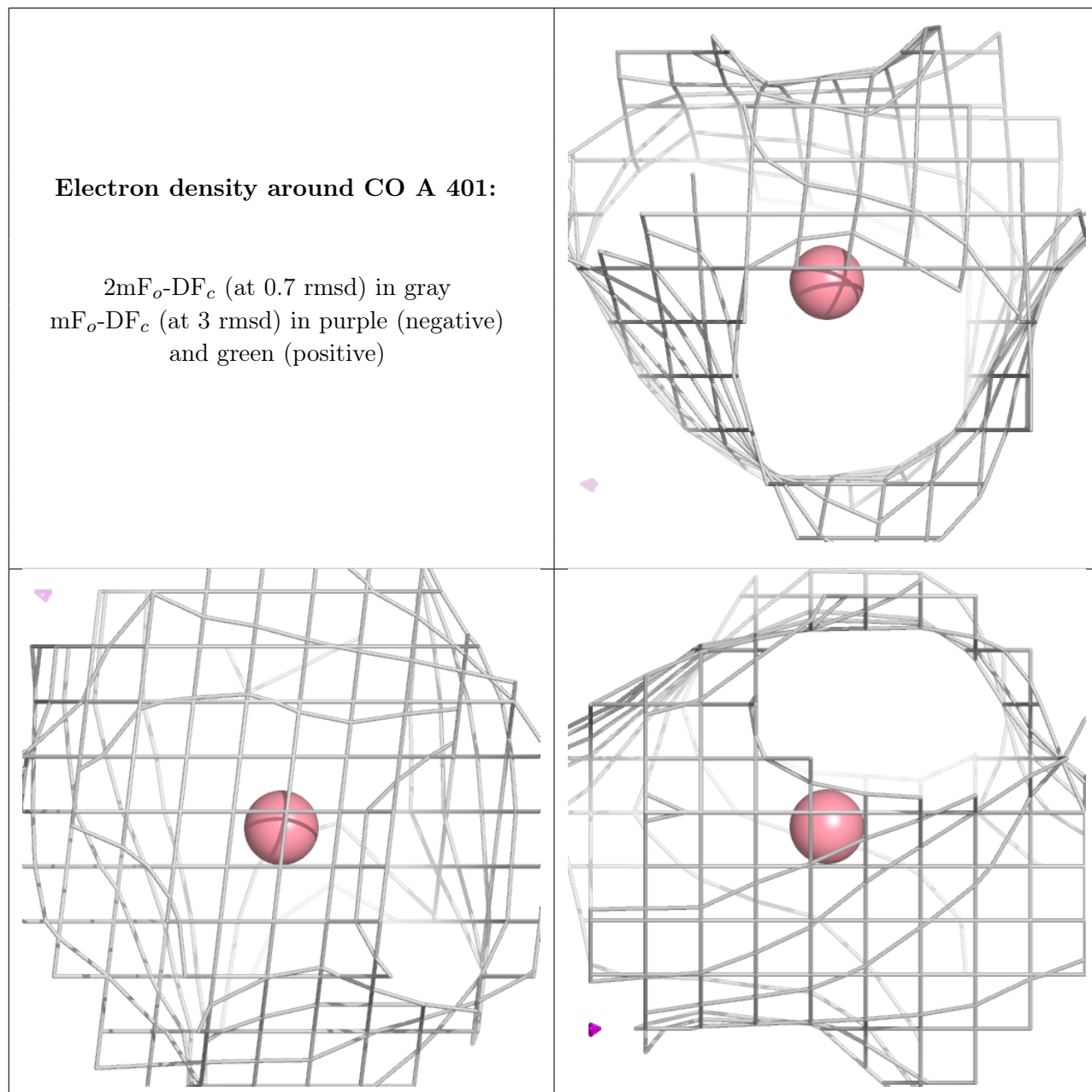
Electron density around CO B 401:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.