



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:00 PM UTC

PDB ID : 7Q2A / pdb_00007q2a
Title : Crystal structure of AphC in complex with 4-ethylcatechol
Authors : Zahn, M.; Grigg, J.C.; Eltis, L.D.; McGeehan, J.E.
Deposited on : 2021-10-25
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

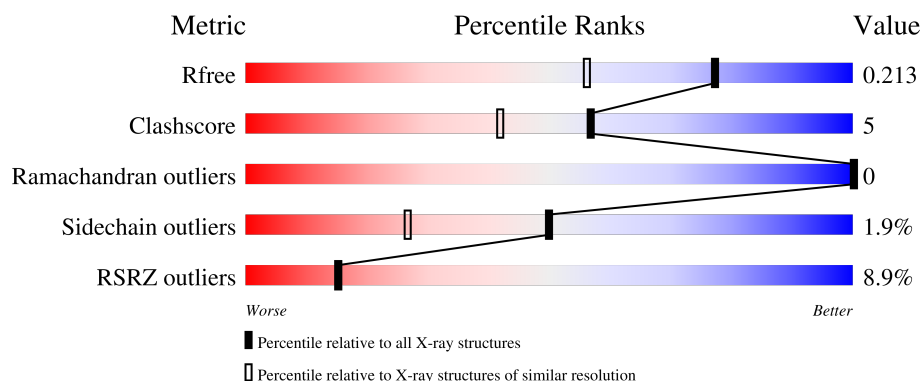
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	381	10% 83% 8% 8%
1	B	381	9% 83% 9% 8%
1	C	381	7% 83% 7% 9%
1	D	381	7% 83% 8% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11975 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 Catechol 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	1	0
			2775	1757	474	534	10			
1	B	352	Total	C	N	O	S	0	1	0
			2793	1770	476	537	10			
1	C	347	Total	C	N	O	S	0	2	0
			2757	1747	471	529	10			
1	D	350	Total	C	N	O	S	0	2	0
			2785	1767	476	532	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q0S9X1
A	-19	GLY	-	expression tag	UNP Q0S9X1
A	-18	SER	-	expression tag	UNP Q0S9X1
A	-17	SER	-	expression tag	UNP Q0S9X1
A	-16	HIS	-	expression tag	UNP Q0S9X1
A	-15	HIS	-	expression tag	UNP Q0S9X1
A	-14	HIS	-	expression tag	UNP Q0S9X1
A	-13	HIS	-	expression tag	UNP Q0S9X1
A	-12	HIS	-	expression tag	UNP Q0S9X1
A	-11	SER	-	expression tag	UNP Q0S9X1
A	-10	SER	-	expression tag	UNP Q0S9X1
A	-9	GLY	-	expression tag	UNP Q0S9X1
A	-8	GLU	-	expression tag	UNP Q0S9X1
A	-7	ASN	-	expression tag	UNP Q0S9X1
A	-6	LEU	-	expression tag	UNP Q0S9X1
A	-5	TYR	-	expression tag	UNP Q0S9X1
A	-4	PHE	-	expression tag	UNP Q0S9X1
A	-3	GLN	-	expression tag	UNP Q0S9X1
A	-2	GLY	-	expression tag	UNP Q0S9X1
A	-1	HIS	-	expression tag	UNP Q0S9X1
A	0	MET	-	expression tag	UNP Q0S9X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q0S9X1
B	-19	GLY	-	expression tag	UNP Q0S9X1
B	-18	SER	-	expression tag	UNP Q0S9X1
B	-17	SER	-	expression tag	UNP Q0S9X1
B	-16	HIS	-	expression tag	UNP Q0S9X1
B	-15	HIS	-	expression tag	UNP Q0S9X1
B	-14	HIS	-	expression tag	UNP Q0S9X1
B	-13	HIS	-	expression tag	UNP Q0S9X1
B	-12	HIS	-	expression tag	UNP Q0S9X1
B	-11	SER	-	expression tag	UNP Q0S9X1
B	-10	SER	-	expression tag	UNP Q0S9X1
B	-9	GLY	-	expression tag	UNP Q0S9X1
B	-8	GLU	-	expression tag	UNP Q0S9X1
B	-7	ASN	-	expression tag	UNP Q0S9X1
B	-6	LEU	-	expression tag	UNP Q0S9X1
B	-5	TYR	-	expression tag	UNP Q0S9X1
B	-4	PHE	-	expression tag	UNP Q0S9X1
B	-3	GLN	-	expression tag	UNP Q0S9X1
B	-2	GLY	-	expression tag	UNP Q0S9X1
B	-1	HIS	-	expression tag	UNP Q0S9X1
B	0	MET	-	expression tag	UNP Q0S9X1
C	-20	MET	-	initiating methionine	UNP Q0S9X1
C	-19	GLY	-	expression tag	UNP Q0S9X1
C	-18	SER	-	expression tag	UNP Q0S9X1
C	-17	SER	-	expression tag	UNP Q0S9X1
C	-16	HIS	-	expression tag	UNP Q0S9X1
C	-15	HIS	-	expression tag	UNP Q0S9X1
C	-14	HIS	-	expression tag	UNP Q0S9X1
C	-13	HIS	-	expression tag	UNP Q0S9X1
C	-12	HIS	-	expression tag	UNP Q0S9X1
C	-11	SER	-	expression tag	UNP Q0S9X1
C	-10	SER	-	expression tag	UNP Q0S9X1
C	-9	GLY	-	expression tag	UNP Q0S9X1
C	-8	GLU	-	expression tag	UNP Q0S9X1
C	-7	ASN	-	expression tag	UNP Q0S9X1
C	-6	LEU	-	expression tag	UNP Q0S9X1
C	-5	TYR	-	expression tag	UNP Q0S9X1
C	-4	PHE	-	expression tag	UNP Q0S9X1
C	-3	GLN	-	expression tag	UNP Q0S9X1
C	-2	GLY	-	expression tag	UNP Q0S9X1
C	-1	HIS	-	expression tag	UNP Q0S9X1
C	0	MET	-	expression tag	UNP Q0S9X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP Q0S9X1
D	-19	GLY	-	expression tag	UNP Q0S9X1
D	-18	SER	-	expression tag	UNP Q0S9X1
D	-17	SER	-	expression tag	UNP Q0S9X1
D	-16	HIS	-	expression tag	UNP Q0S9X1
D	-15	HIS	-	expression tag	UNP Q0S9X1
D	-14	HIS	-	expression tag	UNP Q0S9X1
D	-13	HIS	-	expression tag	UNP Q0S9X1
D	-12	HIS	-	expression tag	UNP Q0S9X1
D	-11	SER	-	expression tag	UNP Q0S9X1
D	-10	SER	-	expression tag	UNP Q0S9X1
D	-9	GLY	-	expression tag	UNP Q0S9X1
D	-8	GLU	-	expression tag	UNP Q0S9X1
D	-7	ASN	-	expression tag	UNP Q0S9X1
D	-6	LEU	-	expression tag	UNP Q0S9X1
D	-5	TYR	-	expression tag	UNP Q0S9X1
D	-4	PHE	-	expression tag	UNP Q0S9X1
D	-3	GLN	-	expression tag	UNP Q0S9X1
D	-2	GLY	-	expression tag	UNP Q0S9X1
D	-1	HIS	-	expression tag	UNP Q0S9X1
D	0	MET	-	expression tag	UNP Q0S9X1

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

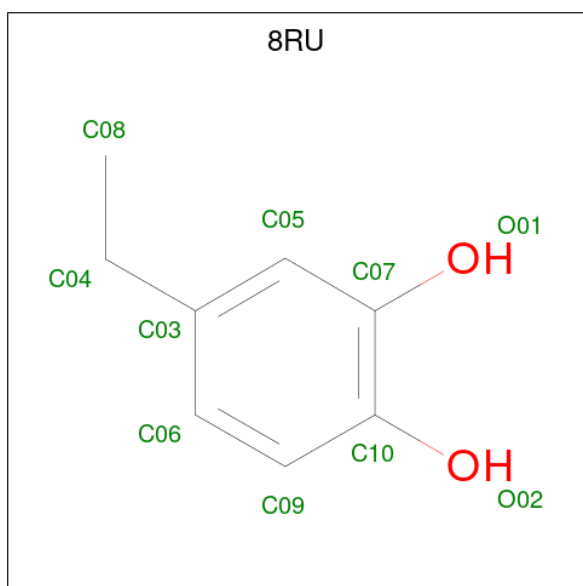
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 4-ethylbenzene-1,2-diol (CCD ID: 8RU) (formula: $C_8H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	8	2		
4	B	1	Total	C	O	0	0
			10	8	2		
4	C	1	Total	C	O	0	0
			10	8	2		
4	D	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	0
			186	186		
5	B	236	Total	O	0	0
			236	236		

Continued on next page...

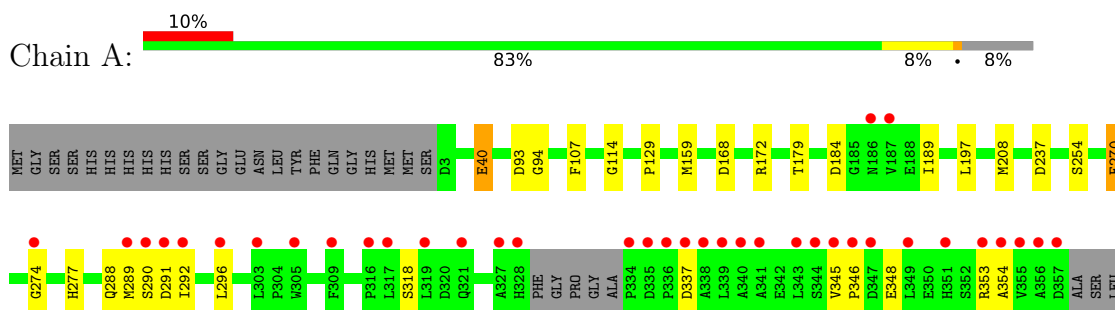
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	202	Total 202	O 202	0	0
5	D	191	Total 191	O 191	0	0

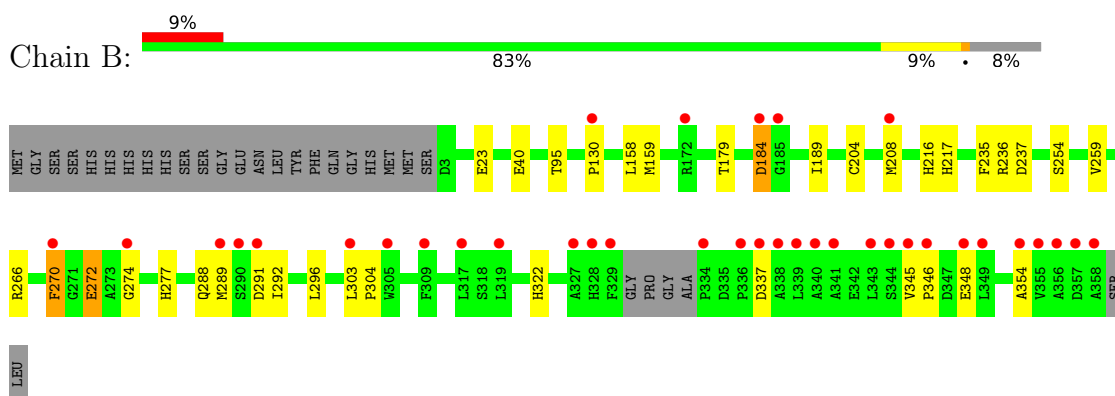
3 Residue-property plots [i](#)

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.

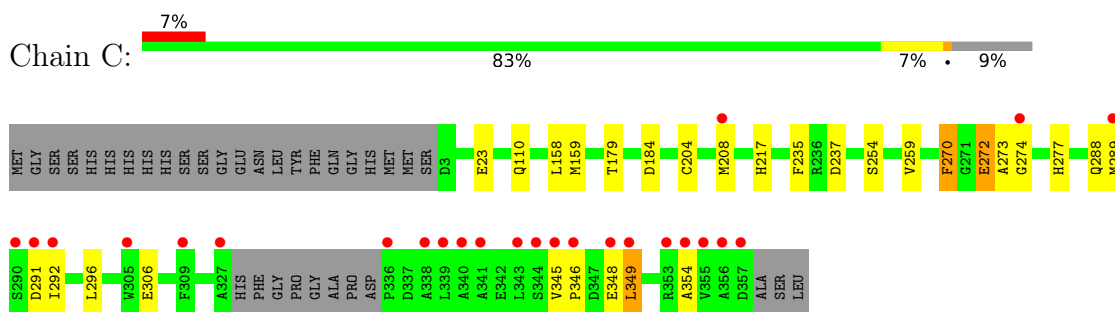
- Molecule 1: Catechol 2,3-dioxygenase



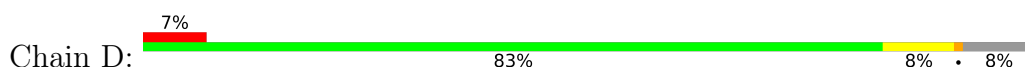
- Molecule 1: Catechol 2,3-dioxygenase

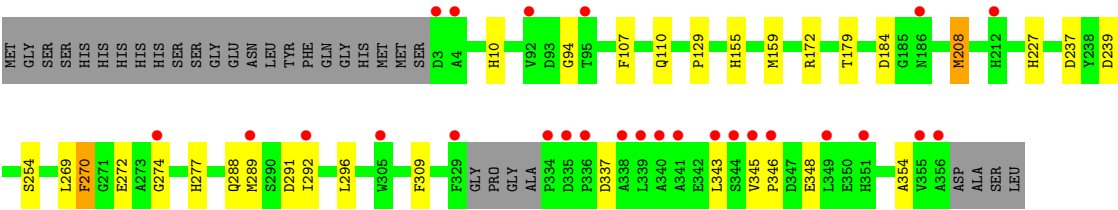


- Molecule 1: Catechol 2,3-dioxygenase



- Molecule 1: Catechol 2,3-dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 119.35Å 84.53Å 90.00° 114.56° 90.00°	Depositor
Resolution (Å)	47.19 – 1.60 47.19 – 1.60	Depositor EDS
% Data completeness (in resolution range)	70.7 (47.19-1.60) 71.1 (47.19-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.179 , 0.209 0.187 , 0.213	Depositor DCC
R_{free} test set	6888 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: 8RU, FE, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	1/2855 (0.0%)	1.20	1/3871 (0.0%)
1	B	1.12	3/2874 (0.1%)	1.23	3/3897 (0.1%)
1	C	1.10	2/2839 (0.1%)	1.21	1/3848 (0.0%)
1	D	1.11	4/2870 (0.1%)	1.21	2/3891 (0.1%)
All	All	1.11	10/11438 (0.1%)	1.21	7/15507 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	GLU	CD-OE2	8.55	1.41	1.25
1	B	272	GLU	CD-OE2	8.16	1.40	1.25
1	A	274	GLY	C-O	7.88	1.34	1.23
1	D	272	GLU	CD-OE1	7.56	1.39	1.25
1	D	227	HIS	CE1-NE2	5.81	1.38	1.32
1	D	10	HIS	CE1-NE2	5.62	1.38	1.32
1	C	274	GLY	C-O	5.49	1.37	1.23
1	D	274	GLY	C-O	5.11	1.36	1.23
1	B	274	GLY	C-O	5.03	1.34	1.23
1	B	130	PRO	C-O	-5.01	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	PHE	CA-CB-CG	7.94	121.74	113.80
1	B	272	GLU	CB-CG-CD	7.87	125.98	112.60
1	B	95	THR	CA-CB-OG1	-7.19	98.81	109.60
1	D	272	GLU	CB-CG-CD	6.79	124.14	112.60
1	C	272	GLU	CB-CG-CD	6.60	123.82	112.60
1	A	129	PRO	N-CA-CB	5.65	106.35	103.19
1	D	129	PRO	N-CA-CB	5.52	106.28	103.19

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	ASP	Peptide
1	B	291	ASP	Peptide
1	C	291	ASP	Peptide
1	D	291	ASP	Peptide

5.2 Too-close contacts ⓘ

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	2775	0	2637	23	0
1	B	2793	0	2650	32	0
1	C	2757	0	2626	23	0
1	D	2785	0	2649	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	0	0	0
5	A	186	0	0	5	0
5	B	236	0	0	6	0
5	C	202	0	0	4	0
5	D	191	0	0	3	0
All	All	11975	0	10562	99	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 5.

All (99) 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:110:GLN:NE2	5:C:501:HOH:O	2.09	0.84
1:D:110:GLN:NE2	5:D:501:HOH:O	2.11	0.84
1:B:337:ASP:OD2	5:B:501:HOH:O	2.03	0.77
1:B:184:ASP:OD2	1:B:346:PRO:HB3	1.85	0.74
1:C:289:MET:HB3	1:C:348:GLU:HB2	1.72	0.70
1:B:289:MET:HA	1:B:289:MET:HE2	1.76	0.68
1:A:289:MET:HB3	1:A:348:GLU:HB2	1.77	0.67
1:A:114:GLY:O	5:A:501:HOH:O	2.12	0.67
1:B:289:MET:HB3	1:B:348:GLU:HB2	1.77	0.67
1:D:239:ASP:OD1	5:D:502:HOH:O	2.13	0.66
1:B:272:GLU:O	5:B:503:HOH:O	2.14	0.66
1:B:272:GLU:OE1	5:B:502:HOH:O	2.13	0.64
1:D:289:MET:HB3	1:D:348:GLU:HB2	1.78	0.64
1:C:23:GLU:OE1	5:C:502:HOH:O	2.15	0.63
1:A:289:MET:HE2	1:A:289:MET:HA	1.79	0.62
1:A:296:LEU:HD12	1:A:354:ALA:HB3	1.81	0.62
1:C:292:ILE:HG12	1:C:349:LEU:HD13	1.83	0.61
1:C:272:GLU:OE1	5:C:503:HOH:O	2.15	0.61
1:D:289:MET:HA	1:D:289:MET:HE2	1.83	0.60
1:C:296:LEU:HD12	1:C:354:ALA:HB3	1.82	0.60
1:D:309:PHE:O	5:D:503:HOH:O	2.15	0.60
1:A:93:ASP:OD1	5:A:502:HOH:O	2.16	0.60
1:B:208:MET:HE3	1:B:345:VAL:HG22	1.83	0.60
1:C:289:MET:HA	1:C:289:MET:HE2	1.84	0.60
1:C:273:ALA:O	5:C:504:HOH:O	2.17	0.60
1:B:184:ASP:OD2	1:B:346:PRO:CB	2.50	0.59
1:B:184:ASP:OD2	1:B:346:PRO:HG3	2.02	0.58
1:A:208:MET:HE3	1:A:345:VAL:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:LEU:HD12	1:D:354:ALA:HB3	1.86	0.57
1:D:343:LEU:O	1:D:343:LEU:HD23	2.04	0.57
1:D:208:MET:HG2	1:D:345:VAL:CG2	2.36	0.56
1:B:296:LEU:HD12	1:B:354:ALA:HB3	1.88	0.55
1:C:288:GLN:C	1:C:289:MET:HE2	2.31	0.55
1:B:184:ASP:OD2	1:B:346:PRO:CG	2.56	0.54
1:D:288:GLN:C	1:D:289:MET:HE2	2.32	0.53
1:D:208:MET:CG	1:D:345:VAL:CG2	2.86	0.53
1:B:289:MET:HE2	1:B:289:MET:CA	2.39	0.52
1:B:254:SER:HB2	1:B:270:PHE:CZ	2.45	0.51
1:D:208:MET:HG3	1:D:345:VAL:HG23	1.92	0.51
1:B:184:ASP:HB2	1:B:346:PRO:HG3	1.93	0.51
1:B:40:GLU:HG2	5:B:609:HOH:O	2.10	0.51
1:D:289:MET:HE2	1:D:289:MET:CA	2.41	0.51
1:A:288:GLN:C	1:A:289:MET:HE2	2.36	0.50
1:B:288:GLN:C	1:B:289:MET:HE2	2.36	0.50
1:A:289:MET:HE2	1:A:289:MET:CA	2.40	0.50
1:A:184:ASP:CG	1:A:346:PRO:HG3	2.37	0.49
1:A:353:ARG:NH2	1:B:236:ARG:CZ	2.75	0.49
1:A:254[A]:SER:HB2	1:A:270:PHE:CZ	2.47	0.49
1:D:94:GLY:HA3	1:D:107:PHE:CZ	2.47	0.49
1:C:184:ASP:CG	1:C:346:PRO:HG3	2.37	0.49
1:D:254[A]:SER:HB2	1:D:270:PHE:CZ	2.48	0.49
1:A:168:ASP:O	1:A:172:ARG:HG3	2.12	0.48
1:C:254[A]:SER:HB2	1:C:270:PHE:CZ	2.48	0.48
1:C:289:MET:HE2	1:C:289:MET:CA	2.43	0.48
1:D:254[B]:SER:HB3	1:D:270:PHE:CZ	2.48	0.48
1:B:23:GLU:HG3	5:B:682:HOH:O	2.13	0.48
1:C:288:GLN:O	1:C:289:MET:HE2	2.14	0.47
1:A:254[A]:SER:CB	1:A:270:PHE:CZ	2.98	0.47
1:A:254[B]:SER:CB	1:A:270:PHE:CZ	2.98	0.46
1:D:184:ASP:CG	1:D:346:PRO:HG3	2.40	0.46
1:D:254[B]:SER:CB	1:D:270:PHE:CZ	2.98	0.46
1:A:40:GLU:HG3	5:A:620:HOH:O	2.15	0.46
1:C:254[A]:SER:CB	1:C:270:PHE:CZ	2.98	0.46
1:A:290:SER:O	5:A:503:HOH:O	2.21	0.46
1:D:254[A]:SER:CB	1:D:270:PHE:CZ	2.99	0.46
1:A:289:MET:O	1:A:292:ILE:HG22	2.15	0.46
1:C:289:MET:O	1:C:292:ILE:HG22	2.15	0.46
1:A:254[B]:SER:HB3	1:A:270:PHE:CZ	2.50	0.45
1:D:289:MET:O	1:D:292:ILE:HG22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:HB	1:B:277:HIS:CE1	2.52	0.45
1:C:179:THR:HB	1:C:277:HIS:CE1	2.52	0.45
1:A:197:LEU:HG	5:A:658:HOH:O	2.17	0.44
1:B:304:PRO:HG3	5:B:580:HOH:O	2.18	0.44
1:B:217:HIS:CE1	4:B:403:8RU:O01	2.70	0.44
1:A:353:ARG:CZ	1:B:236:ARG:CZ	2.96	0.44
1:C:254[B]:SER:CB	1:C:270:PHE:CZ	3.01	0.43
1:A:179:THR:HB	1:A:277:HIS:CE1	2.54	0.43
1:A:94:GLY:HA3	1:A:107:PHE:CZ	2.54	0.43
1:C:254[B]:SER:HB3	1:C:270:PHE:CZ	2.54	0.43
1:C:217:HIS:CE1	4:C:404:8RU:O01	2.72	0.42
1:B:288:GLN:O	1:B:289:MET:HE2	2.19	0.42
1:D:179:THR:HB	1:D:277:HIS:CE1	2.54	0.42
1:D:208:MET:HG2	1:D:345:VAL:HG22	2.01	0.42
1:B:254:SER:CB	1:B:270:PHE:CZ	3.02	0.42
1:B:254:SER:HB2	1:B:270:PHE:CE1	2.55	0.42
1:B:289:MET:O	1:B:292:ILE:HG22	2.20	0.42
1:C:208:MET:HE3	1:C:345:VAL:HG22	2.01	0.42
1:D:288:GLN:O	1:D:289:MET:HE2	2.20	0.42
1:B:303:LEU:HA	1:B:304:PRO:HD3	1.96	0.42
1:D:155:HIS:CE1	1:D:270:PHE:CZ	3.08	0.42
1:C:306:GLU:H	1:C:306:GLU:CD	2.28	0.41
1:A:288:GLN:O	1:A:289:MET:HE2	2.21	0.41
1:B:216:HIS:O	1:B:266:ARG:HB3	2.21	0.41
1:B:235:PHE:CD2	1:B:259:VAL:HG11	2.56	0.41
1:B:184:ASP:CG	1:B:346:PRO:HG3	2.46	0.40
1:C:158:LEU:O	1:C:204:CYS:HA	2.21	0.40
1:C:235:PHE:CD2	1:C:259:VAL:HG11	2.56	0.40
1:B:158:LEU:O	1:B:204:CYS:HA	2.21	0.40
1:B:322:HIS:CD2	1:B:322:HIS:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	347/381 (91%)	338 (97%)	9 (3%)	0	100	100
1	B	349/381 (92%)	340 (97%)	9 (3%)	0	100	100
1	C	345/381 (91%)	336 (97%)	9 (3%)	0	100	100
1	D	348/381 (91%)	340 (98%)	8 (2%)	0	100	100
All	All	1389/1524 (91%)	1354 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/316 (93%)	286 (98%)	7 (2%)	43	19
1	B	294/316 (93%)	290 (99%)	4 (1%)	59	38
1	C	291/316 (92%)	287 (99%)	4 (1%)	59	38
1	D	294/316 (93%)	287 (98%)	7 (2%)	43	19
All	All	1172/1264 (93%)	1150 (98%)	22 (2%)	50	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	159	MET
1	A	189	ILE
1	A	237	ASP
1	A	270	PHE
1	A	318	SER
1	A	337	ASP
1	B	159	MET
1	B	184	ASP
1	B	189	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	237	ASP
1	C	159	MET
1	C	237	ASP
1	C	270	PHE
1	C	349	LEU
1	D	159	MET
1	D	172	ARG
1	D	208	MET
1	D	237	ASP
1	D	269	LEU
1	D	270	PHE
1	D	337	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	186	ASN
1	D	186	ASN
1	D	277	HIS

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 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	8RU	A	403	2	10,10,10	1.25	1 (10%)	13,13,13	1.10	0
4	8RU	B	403	2	10,10,10	1.12	1 (10%)	13,13,13	0.81	0
4	8RU	D	404	2	10,10,10	1.00	0	13,13,13	1.05	0
4	8RU	C	404	2	10,10,10	1.35	1 (10%)	13,13,13	1.21	1 (7%)

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	8RU	A	403	2	-	0/2/2/2	0/1/1/1
4	8RU	B	403	2	-	0/2/2/2	0/1/1/1
4	8RU	D	404	2	-	1/2/2/2	0/1/1/1
4	8RU	C	404	2	-	0/2/2/2	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	8RU	C10-C07	-3.08	1.34	1.40
4	C	404	8RU	O01-C07	2.60	1.41	1.36
4	B	403	8RU	O01-C07	2.18	1.40	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	8RU	O01-C07-C05	2.07	125.03	119.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

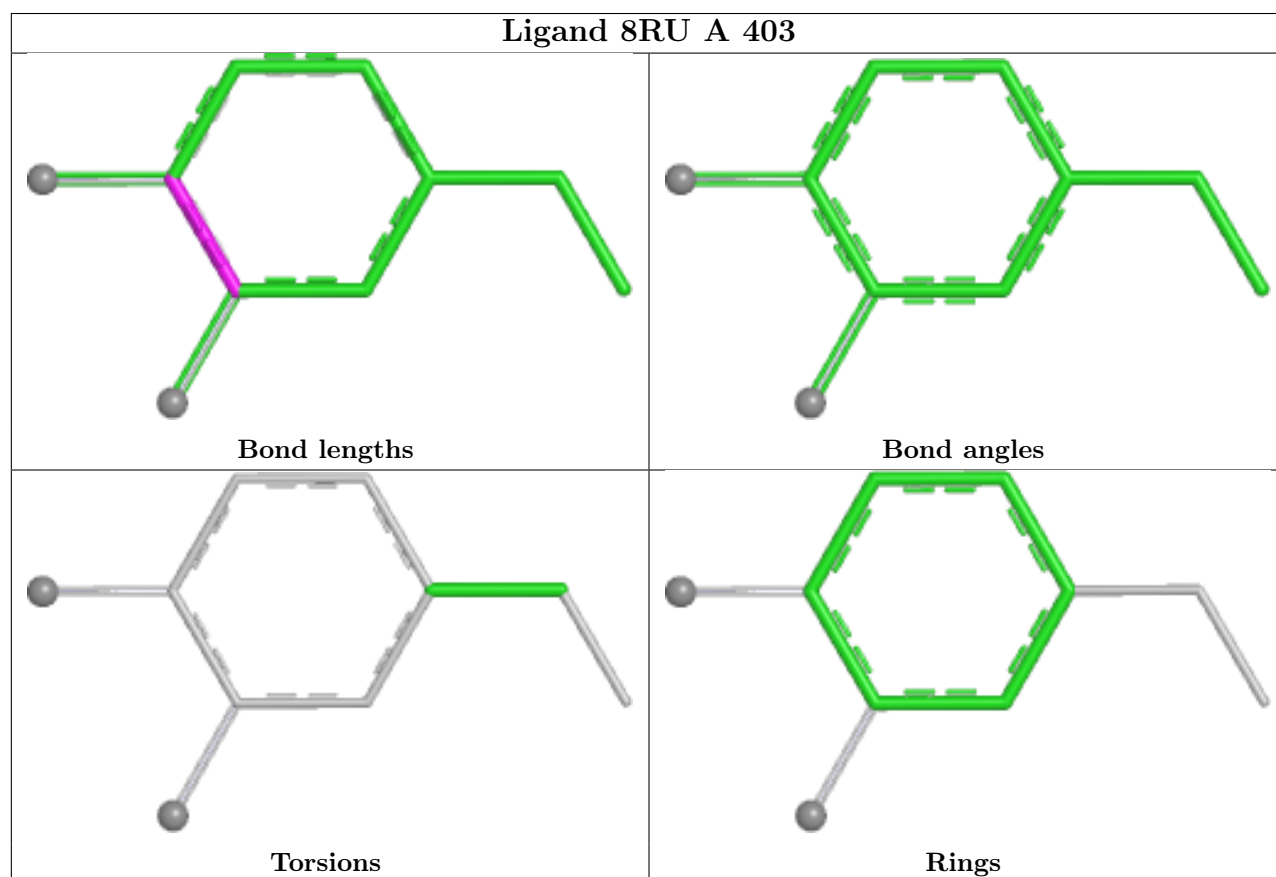
Mol	Chain	Res	Type	Atoms
4	D	404	8RU	C05-C03-C04-C08

There are no ring outliers.

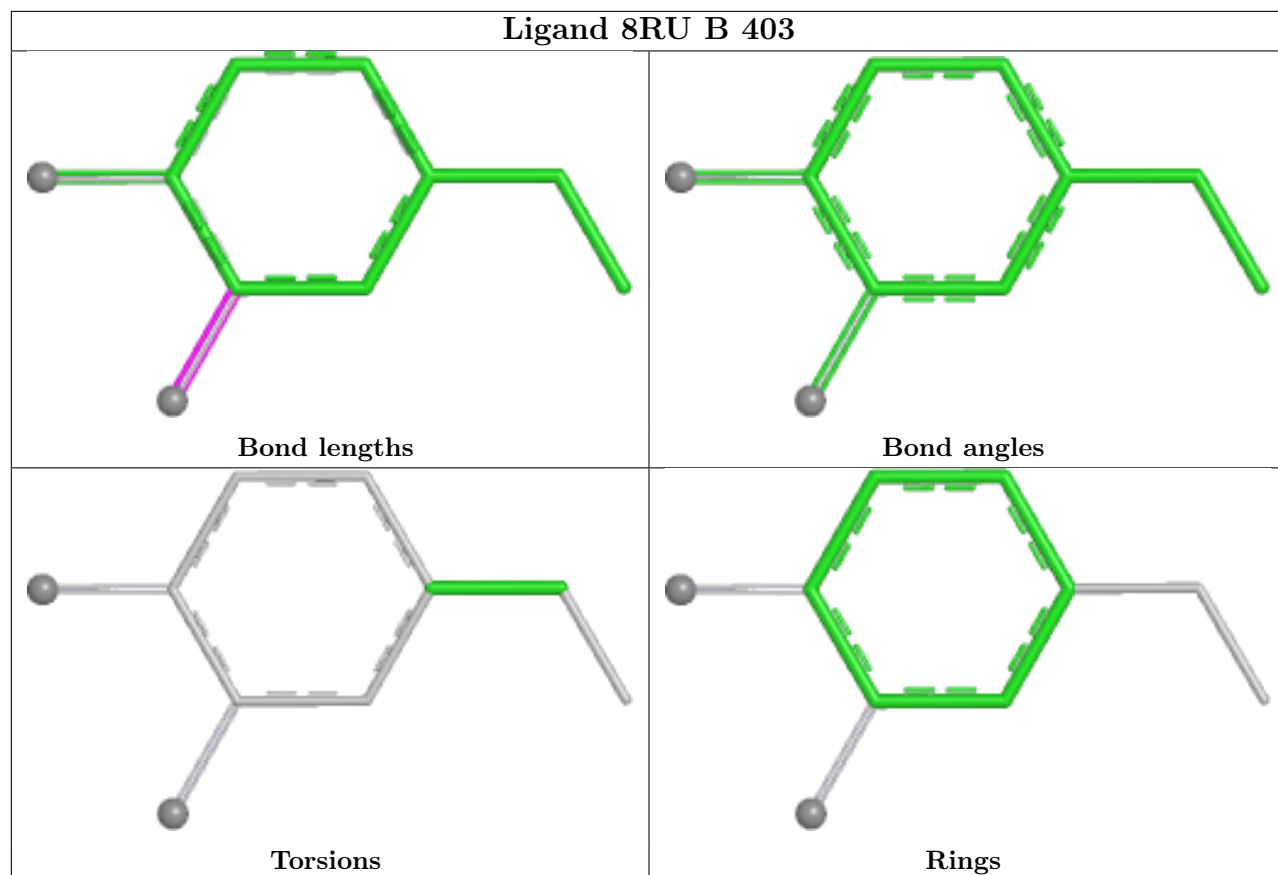
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	8RU	1	0
4	C	404	8RU	1	0

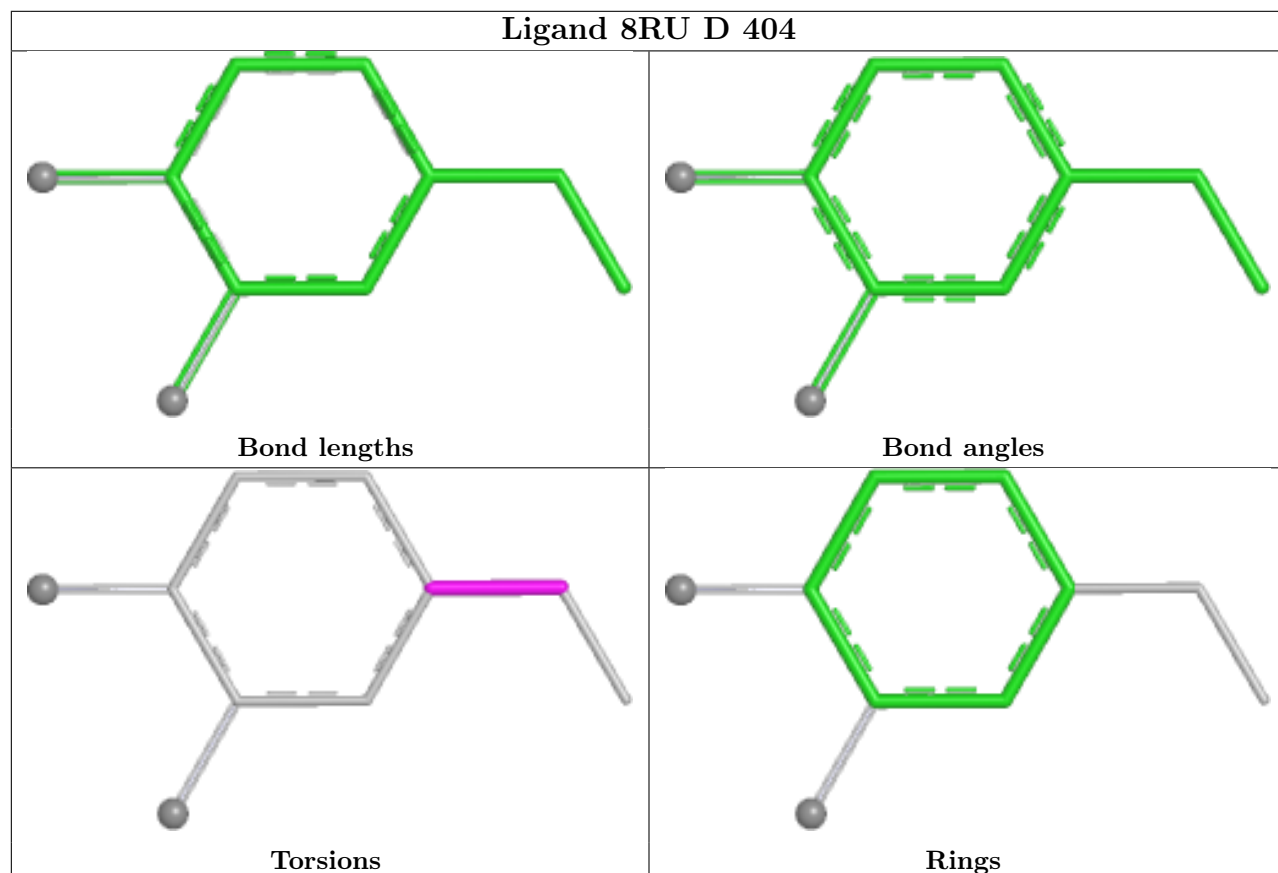
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

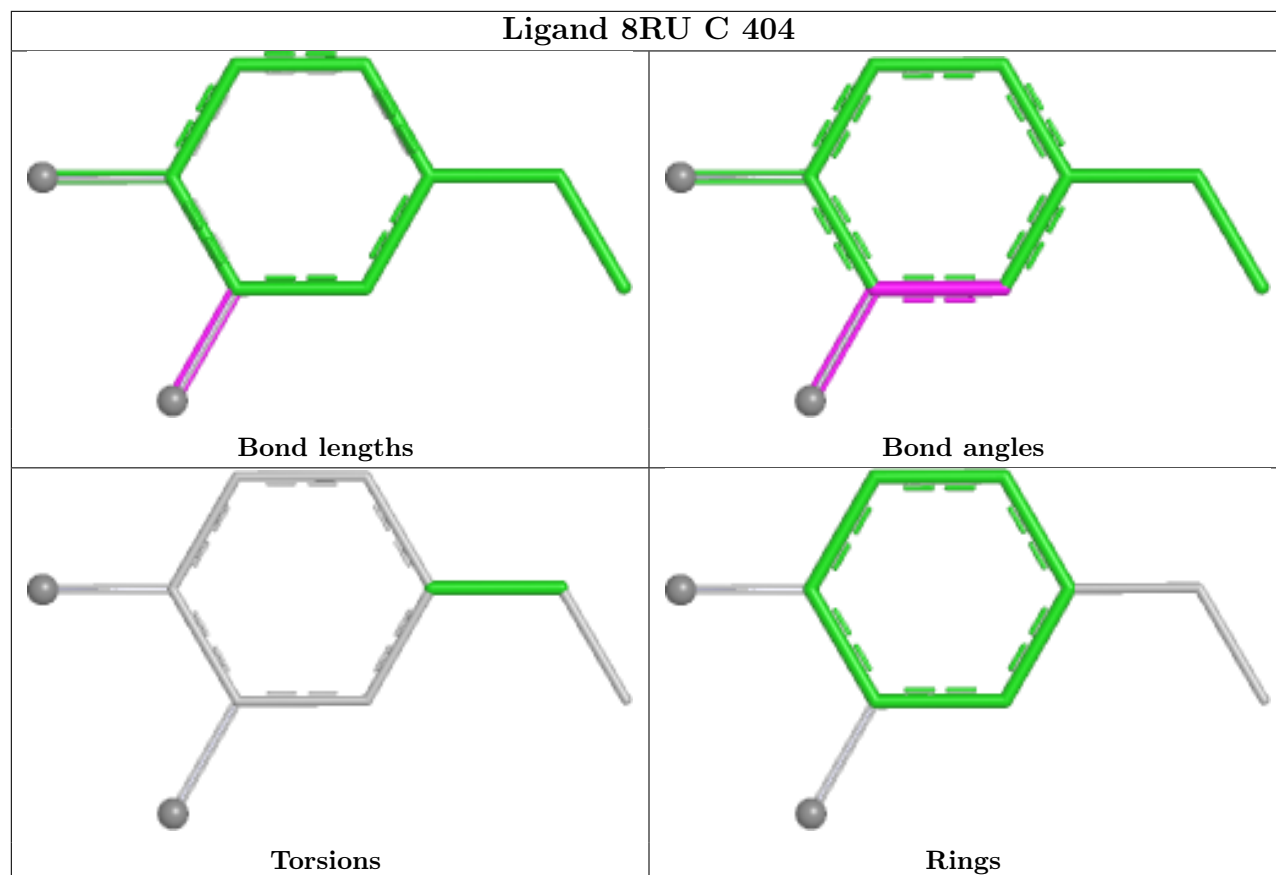


Ligand 8RU B 403



Ligand 8RU D 404





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	350/381 (91%)	0.51	37 (10%)	11 11	18, 30, 76, 104	1 (0%)
1	B	352/381 (92%)	0.31	36 (10%)	12 12	17, 27, 59, 97	1 (0%)
1	C	347/381 (91%)	0.39	25 (7%)	21 22	18, 29, 64, 105	2 (0%)
1	D	350/381 (91%)	0.31	26 (7%)	20 21	17, 28, 64, 96	2 (0%)
All	All	1399/1524 (91%)	0.38	124 (8%)	15 15	17, 29, 65, 105	6 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	LEU	7.0
1	C	355	VAL	6.7
1	C	349	LEU	6.6
1	B	329	PHE	6.3
1	D	329	PHE	6.1
1	D	349	LEU	5.8
1	C	341	ALA	5.6
1	A	343	LEU	5.3
1	A	339	LEU	5.2
1	C	343	LEU	5.2
1	A	346	PRO	5.2
1	A	345	VAL	5.1
1	C	345	VAL	5.1
1	A	338	ALA	5.0
1	C	338	ALA	5.0
1	D	339	LEU	4.9
1	C	305	TRP	4.8
1	A	341	ALA	4.7
1	B	349	LEU	4.6
1	A	356	ALA	4.6
1	A	340	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	4.5
1	B	345	VAL	4.5
1	B	355	VAL	4.5
1	B	341	ALA	4.5
1	C	339	LEU	4.5
1	B	336	PRO	4.3
1	D	355	VAL	4.3
1	D	336	PRO	4.2
1	D	343	LEU	4.1
1	C	340	ALA	4.0
1	A	305	TRP	4.0
1	C	346	PRO	3.9
1	B	334	PRO	3.9
1	C	291	ASP	3.9
1	D	338	ALA	3.9
1	C	336	PRO	3.9
1	A	351	HIS	3.8
1	B	339	LEU	3.7
1	B	340	ALA	3.7
1	A	334	PRO	3.7
1	A	354	ALA	3.7
1	B	358	ALA	3.7
1	C	274	GLY	3.7
1	A	292	ILE	3.6
1	A	309	PHE	3.6
1	A	336	PRO	3.6
1	C	292	ILE	3.6
1	D	345	VAL	3.5
1	B	290	SER	3.5
1	A	344	SER	3.5
1	B	327	ALA	3.4
1	A	289	MET	3.4
1	C	327	ALA	3.3
1	D	305	TRP	3.3
1	B	343	LEU	3.2
1	C	356	ALA	3.2
1	B	346	PRO	3.2
1	B	305	TRP	3.1
1	D	274	GLY	3.1
1	C	354	ALA	3.1
1	A	187	VAL	3.0
1	D	356	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	334	PRO	3.0
1	A	353	ARG	3.0
1	C	344	SER	3.0
1	D	212[A]	HIS	3.0
1	D	341	ALA	3.0
1	B	274	GLY	3.0
1	A	274	GLY	2.9
1	C	290	SER	2.9
1	B	354	ALA	2.9
1	D	344	SER	2.8
1	B	356	ALA	2.8
1	B	317	LEU	2.8
1	C	348	GLU	2.8
1	C	309	PHE	2.8
1	D	340	ALA	2.8
1	D	292	ILE	2.8
1	B	338	ALA	2.7
1	B	348	GLU	2.6
1	D	346	PRO	2.6
1	D	4	ALA	2.6
1	B	185	GLY	2.6
1	A	291	ASP	2.6
1	A	303	LEU	2.6
1	A	328	HIS	2.6
1	B	344	SER	2.6
1	B	270	PHE	2.6
1	D	289	MET	2.6
1	A	317	LEU	2.5
1	C	357	ASP	2.5
1	A	335	ASP	2.5
1	A	296	LEU	2.4
1	B	309	PHE	2.4
1	A	327	ALA	2.4
1	B	289	MET	2.4
1	B	328	HIS	2.4
1	A	321	GLN	2.4
1	A	316	PRO	2.4
1	B	208	MET	2.4
1	C	208	MET	2.4
1	B	184	ASP	2.3
1	A	347	ASP	2.3
1	B	291	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	337	ASP	2.3
1	D	351	HIS	2.3
1	A	337	ASP	2.3
1	B	130	PRO	2.3
1	A	290	SER	2.3
1	D	335	ASP	2.3
1	A	186	ASN	2.2
1	D	186	ASN	2.2
1	B	357	ASP	2.2
1	D	95	THR	2.2
1	D	92	VAL	2.2
1	A	357	ASP	2.2
1	B	319	LEU	2.2
1	C	353	ARG	2.1
1	D	3	ASP	2.1
1	A	319	LEU	2.1
1	C	289	MET	2.1
1	B	172	ARG	2.1
1	B	303	LEU	2.1

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	CA	C	402	1/1	0.84	0.13	85,85,85,85	0
3	CA	A	402	1/1	0.86	0.14	84,84,84,84	0
4	8RU	A	403	10/10	0.89	0.11	34,37,40,40	0
4	8RU	B	403	10/10	0.90	0.11	29,33,35,35	0

Continued on next page...

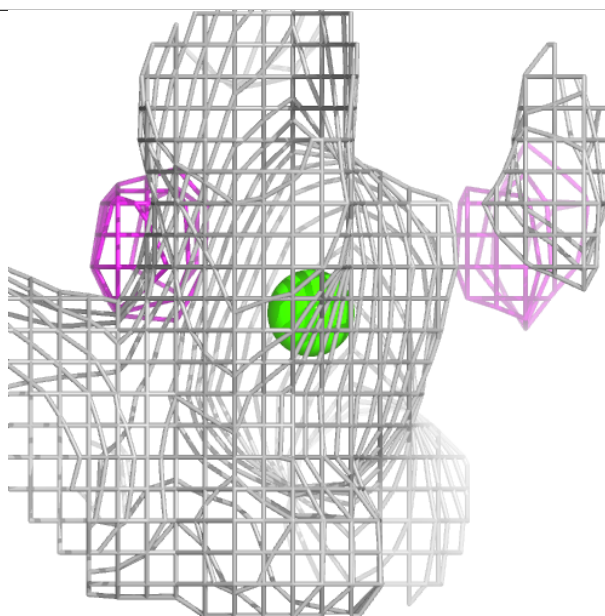
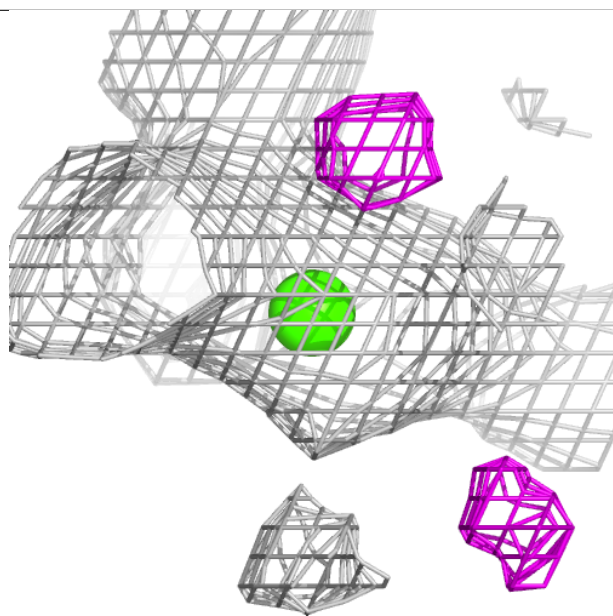
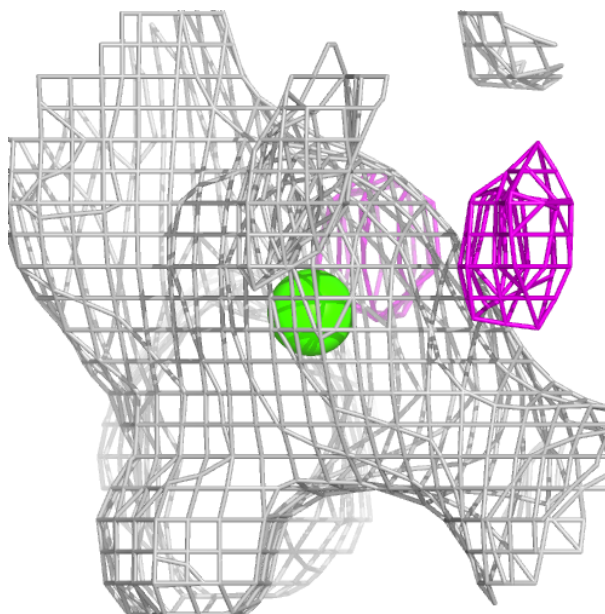
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	8RU	C	404	10/10	0.90	0.09	29,31,33,34	0
4	8RU	D	404	10/10	0.90	0.10	33,35,37,39	0
3	CA	D	402	1/1	0.94	0.14	62,62,62,62	0
3	CA	B	402	1/1	0.95	0.14	51,51,51,51	0
3	CA	C	403	1/1	0.96	0.12	35,35,35,35	0
3	CA	D	403	1/1	0.96	0.10	57,57,57,57	0
2	FE	A	401	1/1	0.99	0.07	30,30,30,30	0
2	FE	C	401	1/1	0.99	0.06	28,28,28,28	0
2	FE	B	401	1/1	1.00	0.07	25,25,25,25	0
2	FE	D	401	1/1	1.00	0.07	30,30,30,30	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.

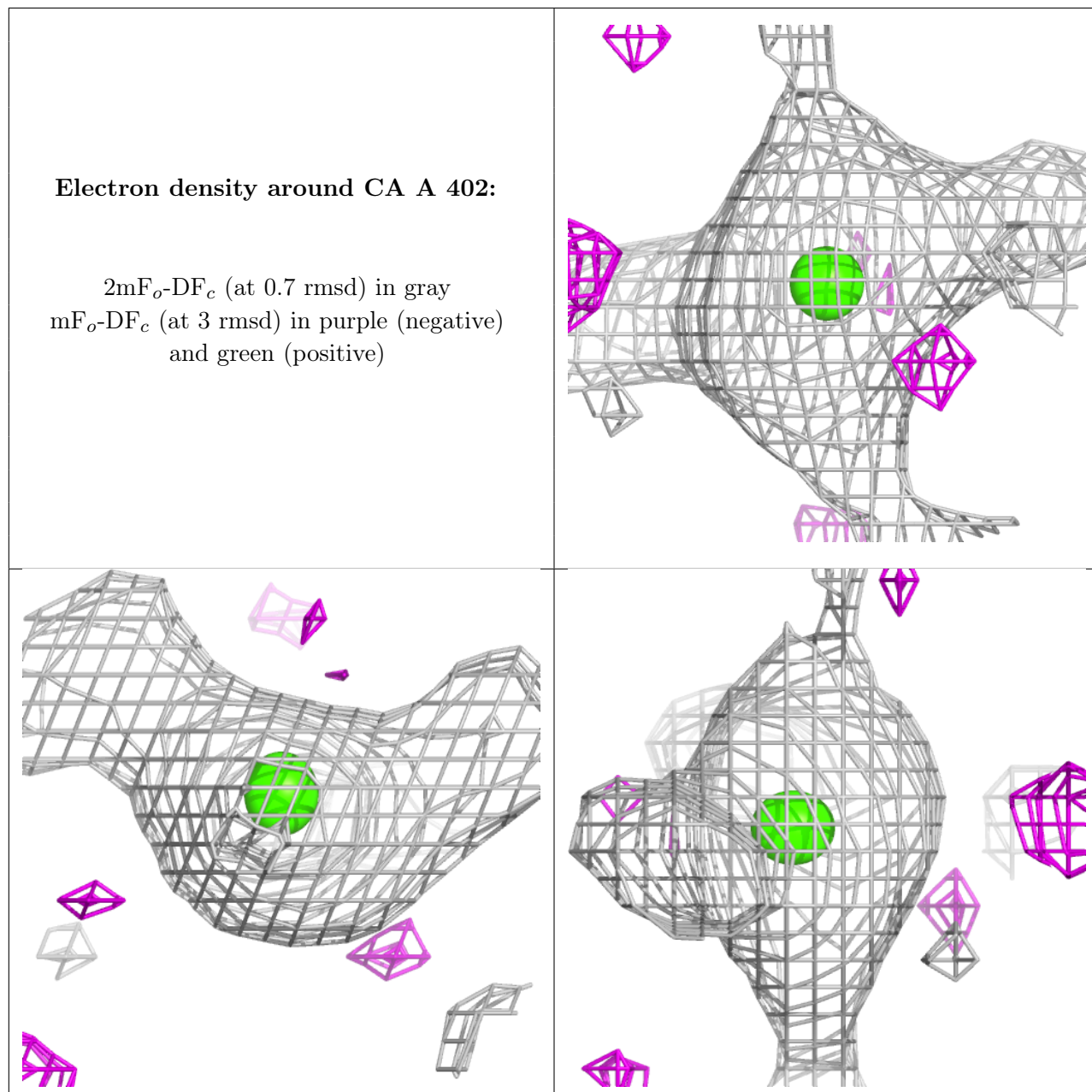
Electron density around CA C 402:

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



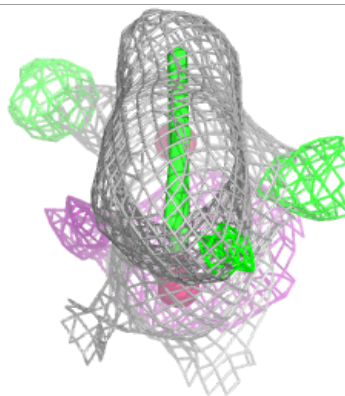
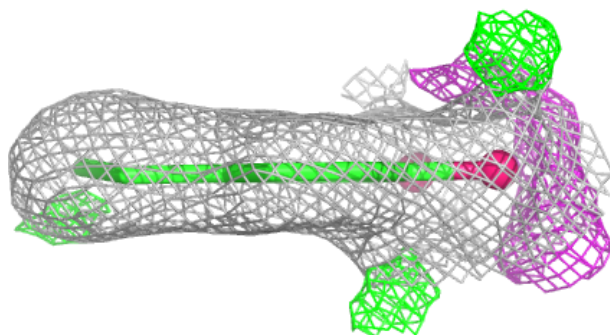
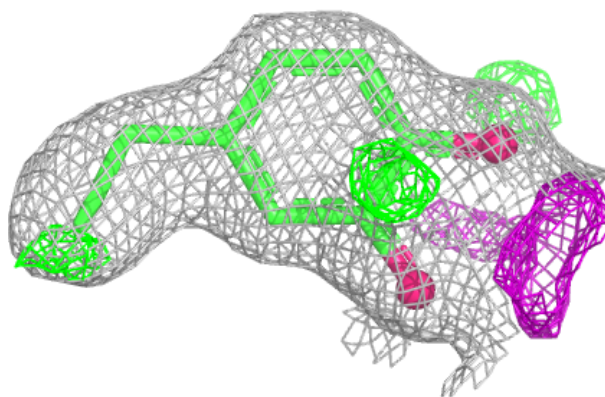
Electron density around CA A 402:

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

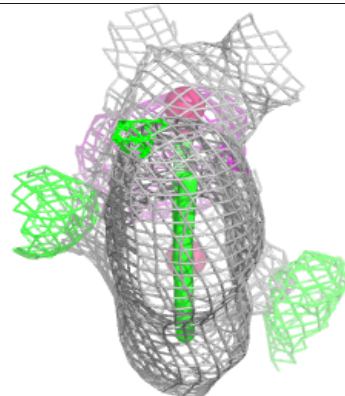
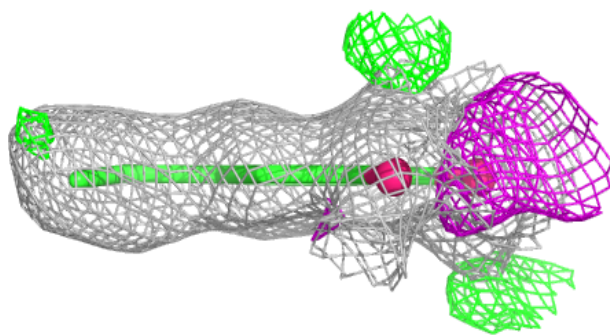
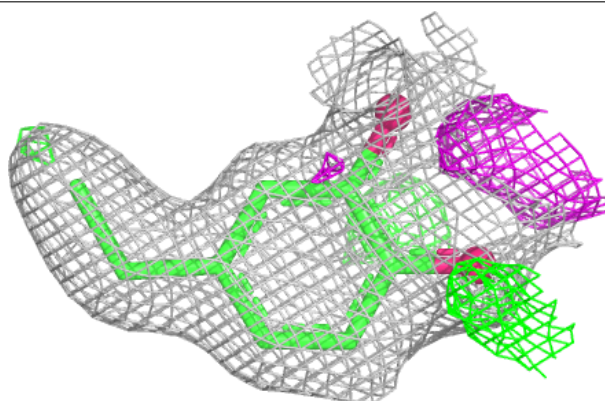


Electron density around 8RU A 403:

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

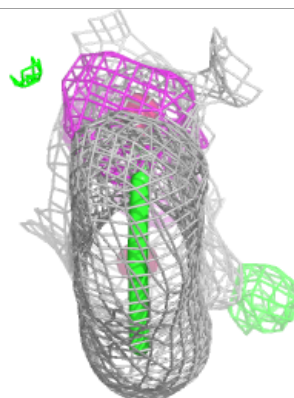
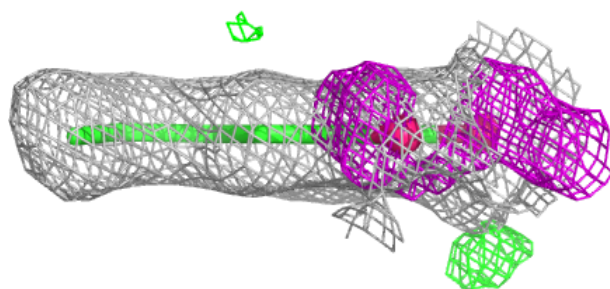
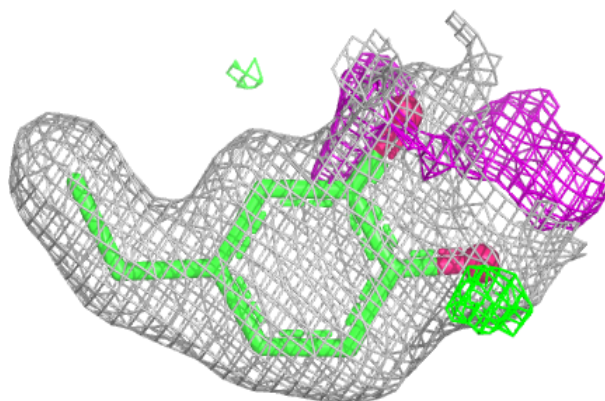
**Electron density around 8RU B 403:**

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

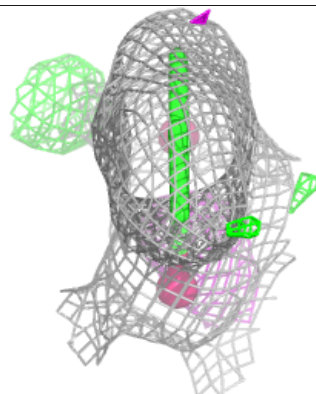
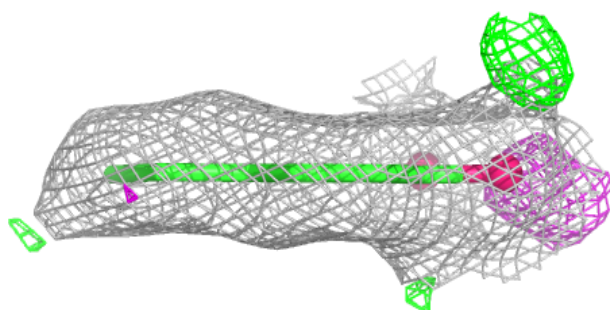
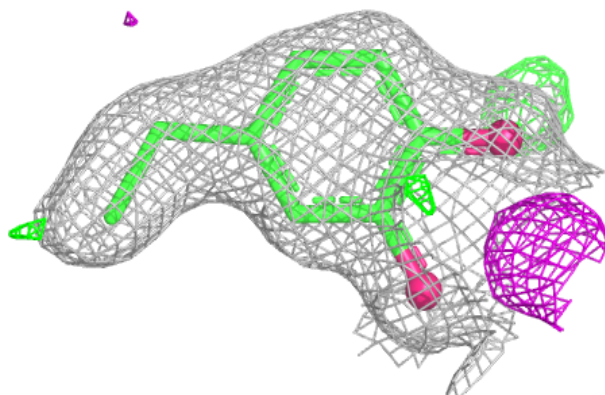


Electron density around 8RU C 404:

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

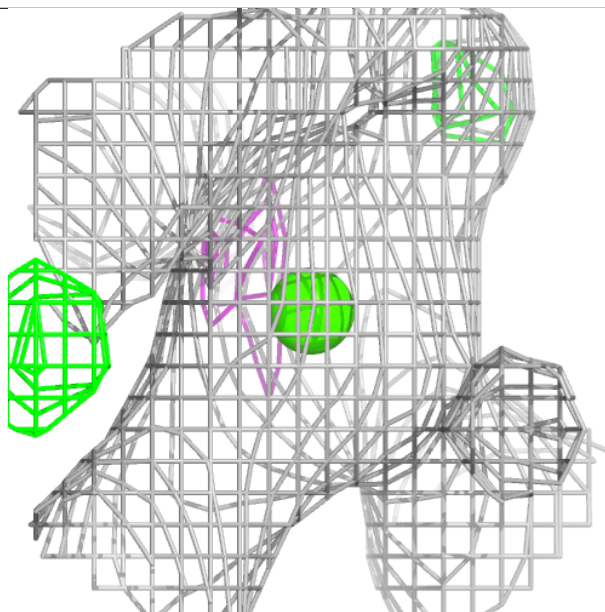
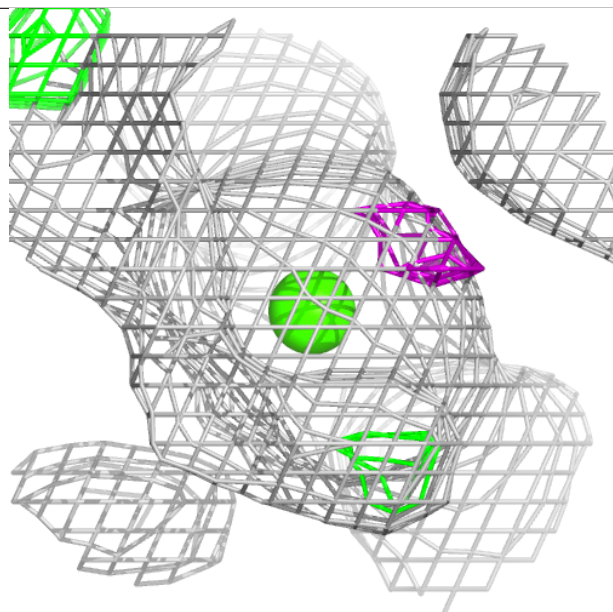
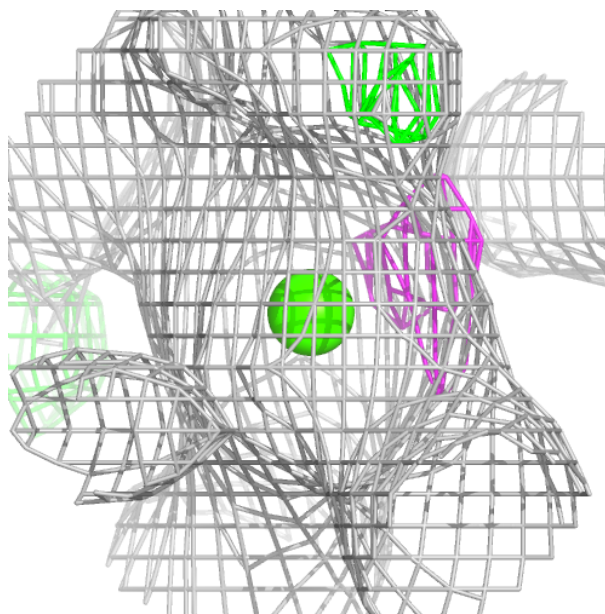
**Electron density around 8RU D 404:**

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



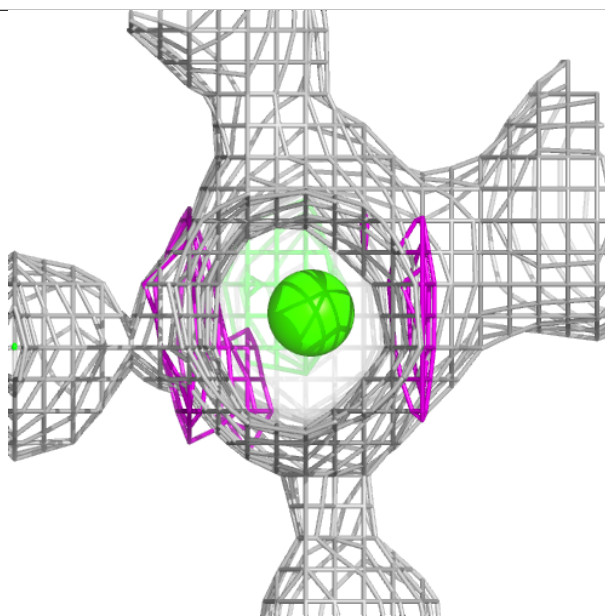
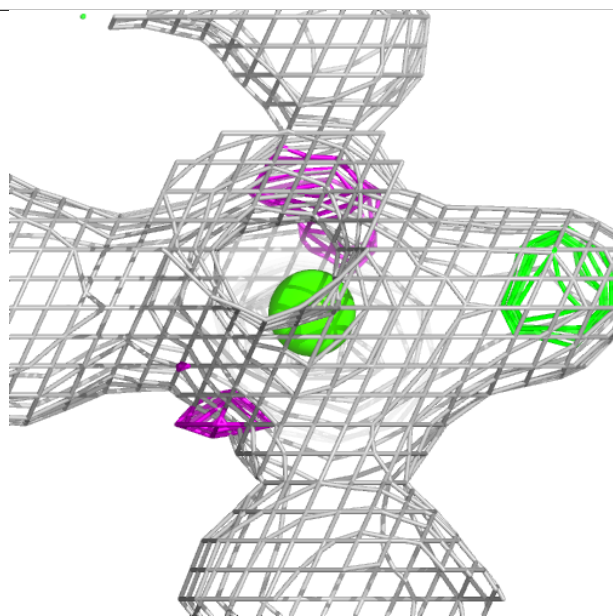
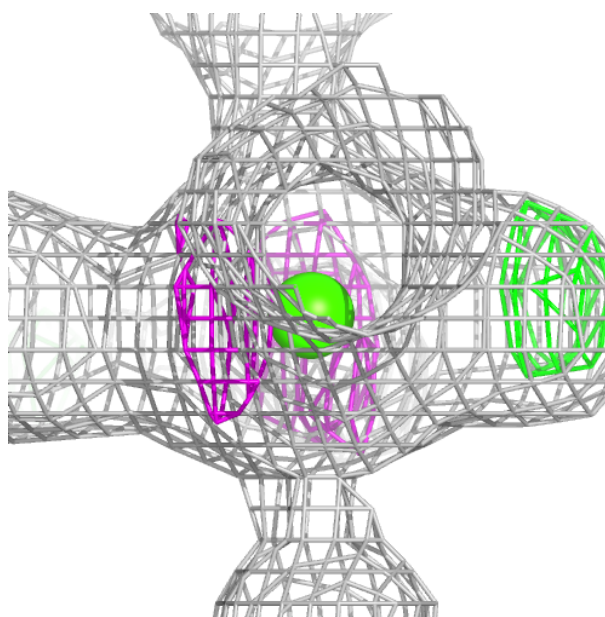
Electron density around CA D 402:

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



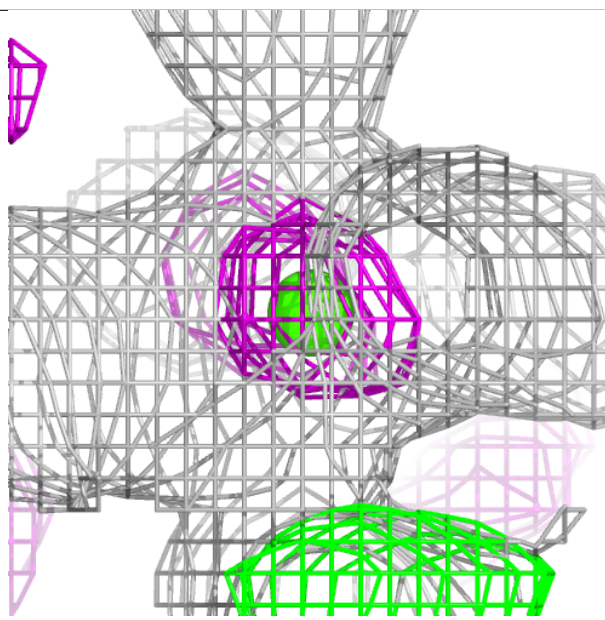
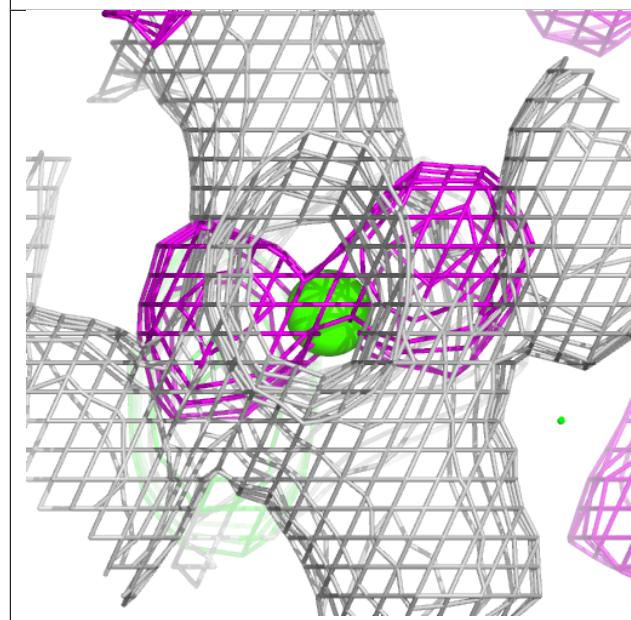
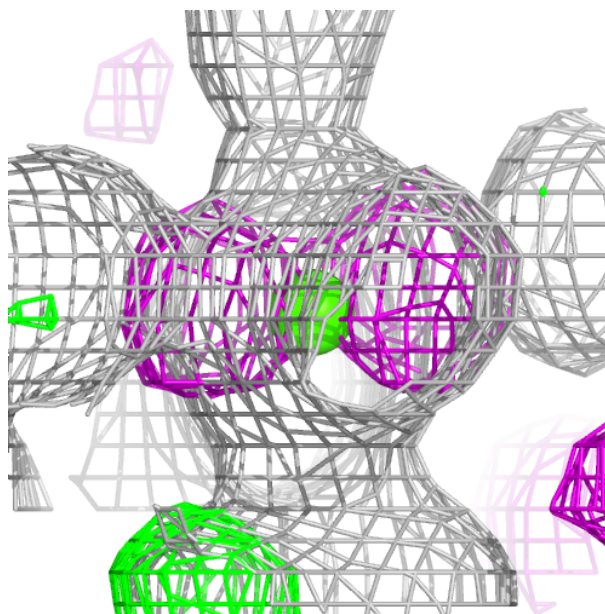
Electron density around CA B 402:

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



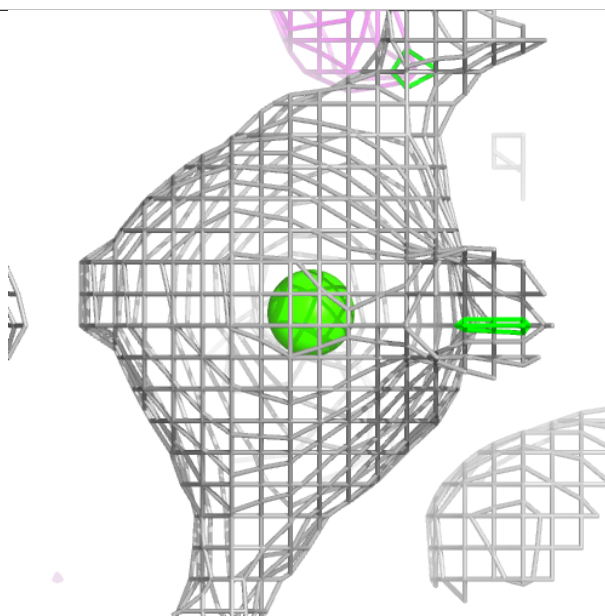
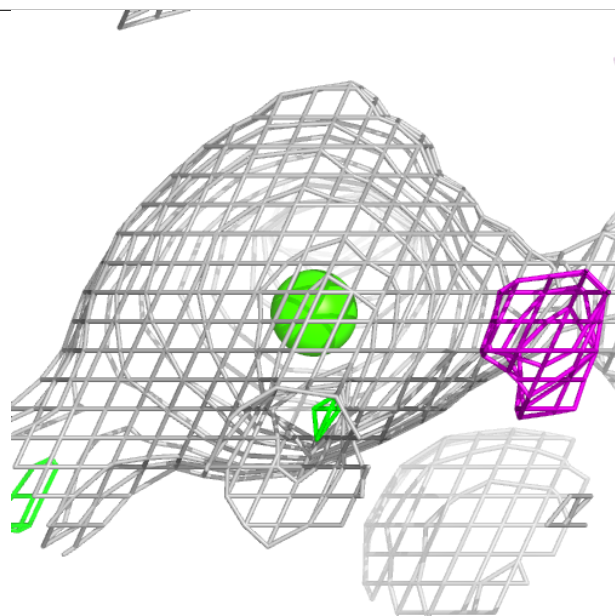
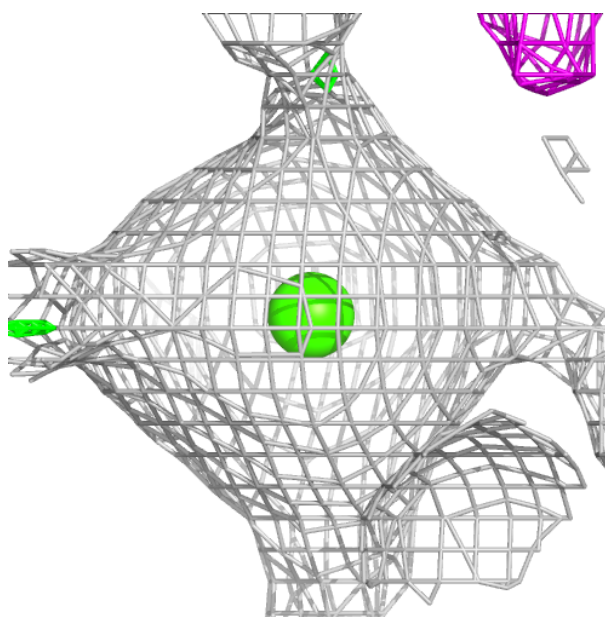
Electron density around CA C 403:

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



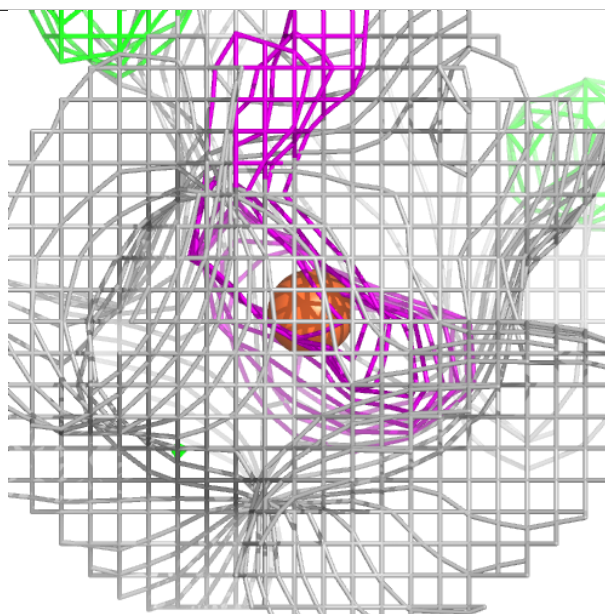
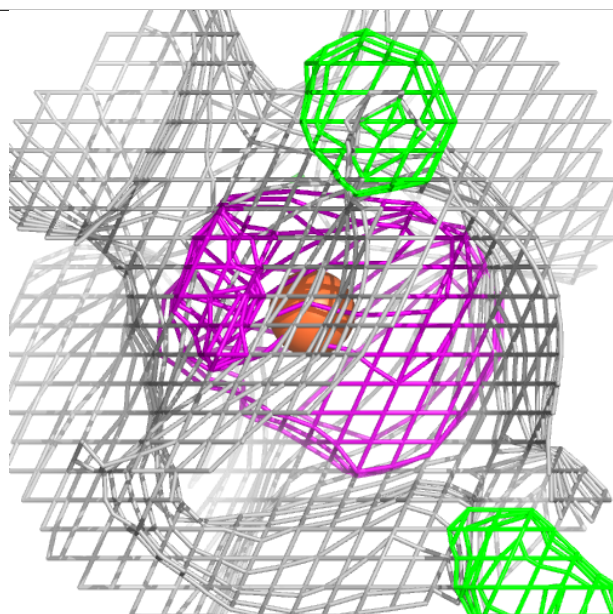
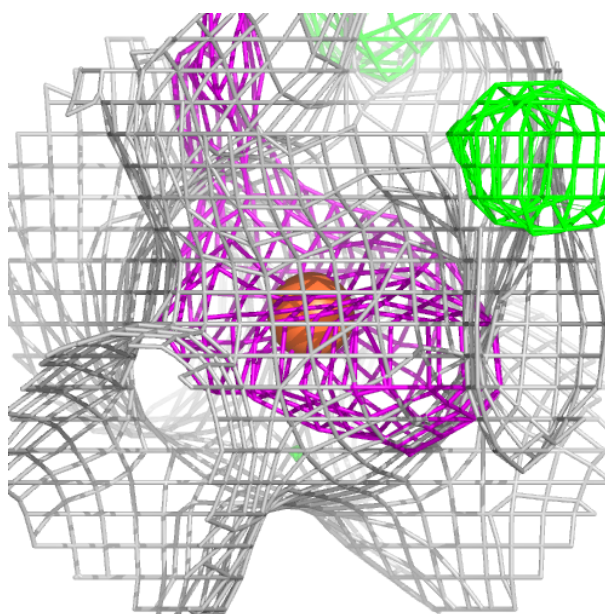
Electron density around CA D 403:

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



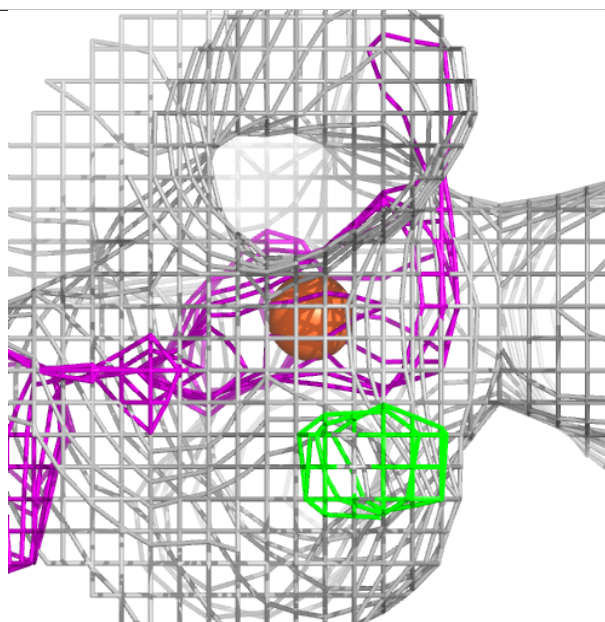
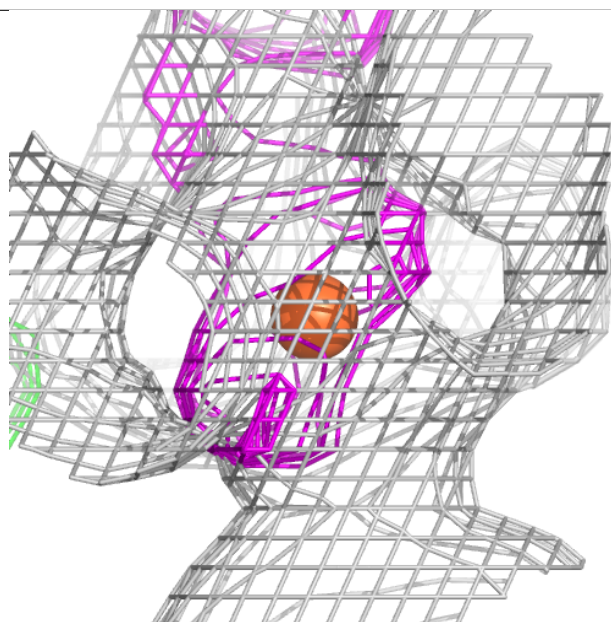
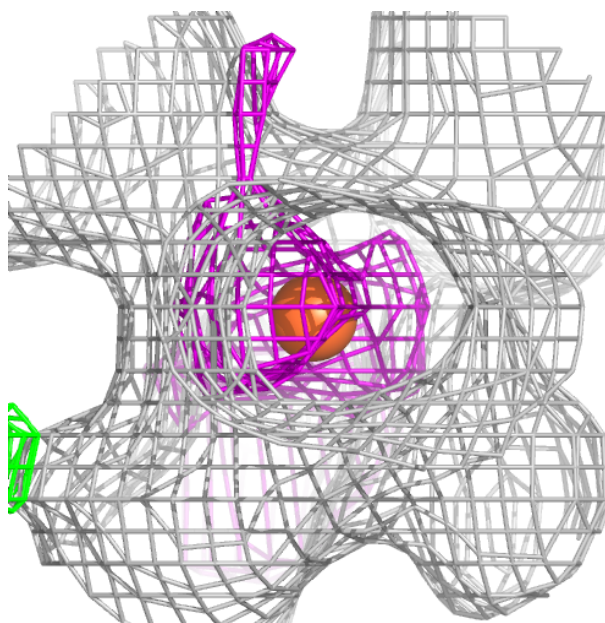
Electron density around FE A 401:

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



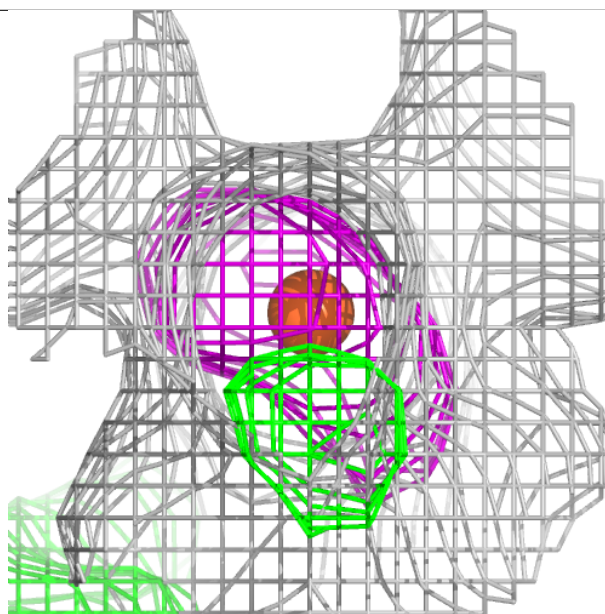
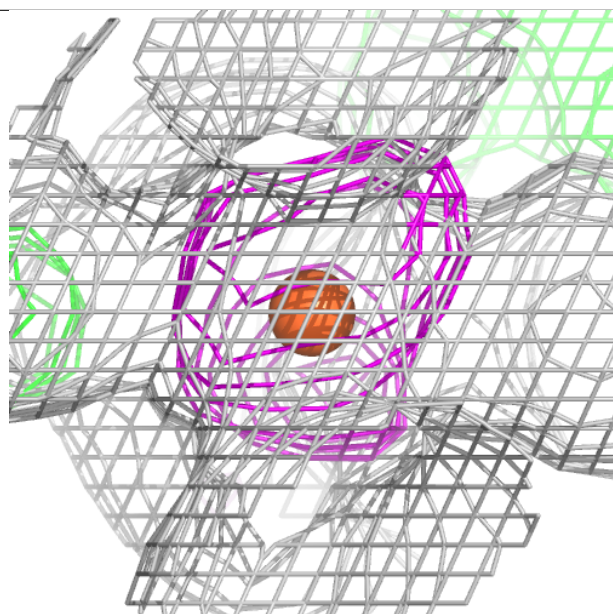
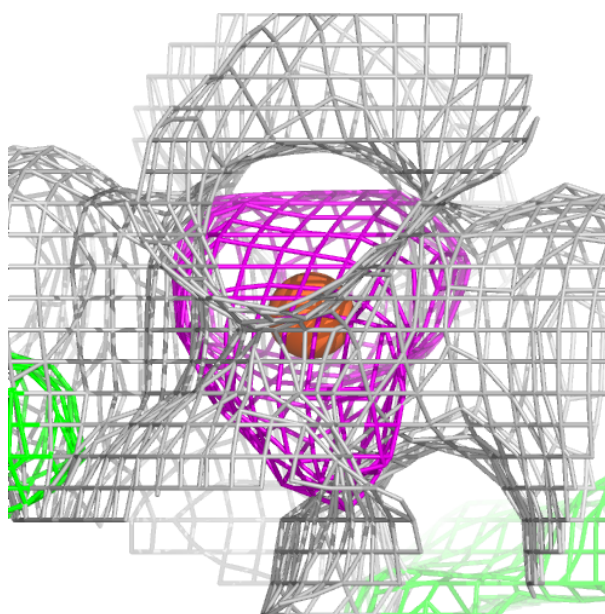
Electron density around FE C 401:

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



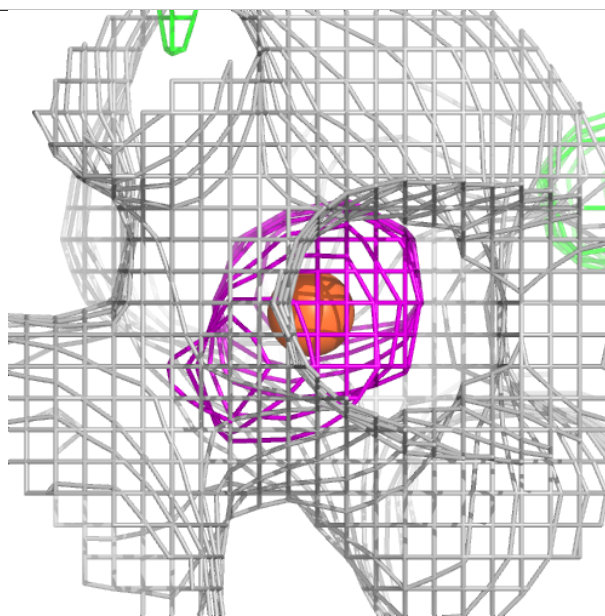
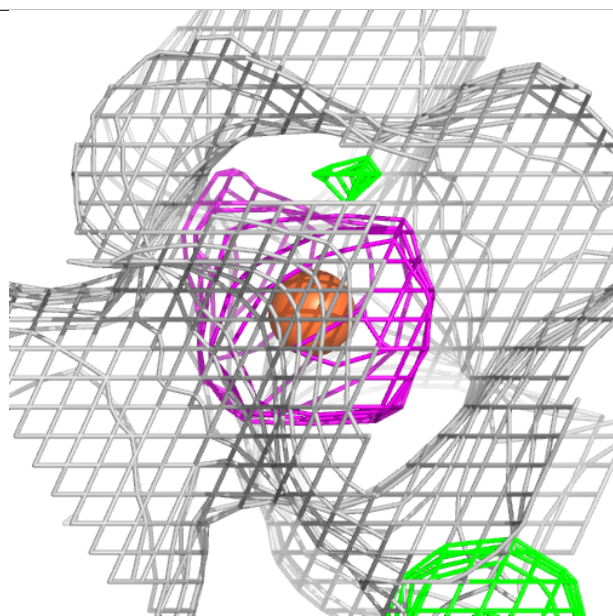
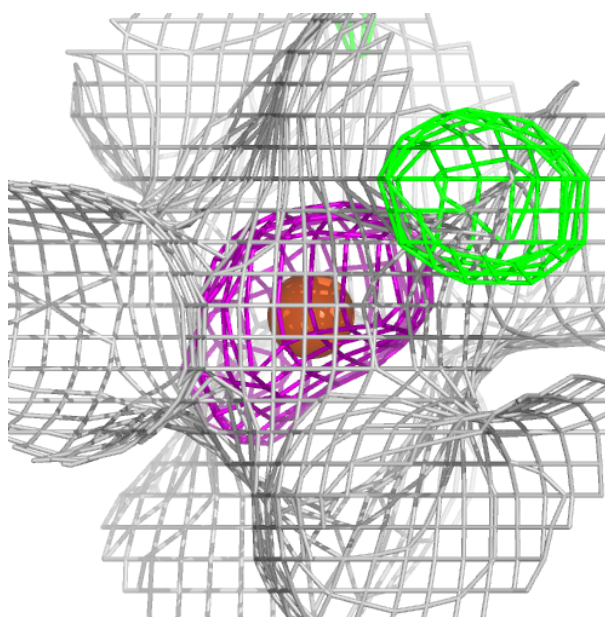
Electron density around FE B 401:

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



Electron density around FE D 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.