



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8P7K / pdb_00008p7k
Title : The impact of molecular variants, crystallization conditions and space group on structure-ligand complexes: A case study on Bacterial Phosphotriesterase Variants and complexes
Authors : Dym, O.; Aggawal, N.; Ashani, Y.; Albeck, S.; Unger, T.; Hamer Rogotner, S.; Silman, I.; Sussman, J.L.
Deposited on : 2023-05-30
Resolution : 1.93 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](#) ①) 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

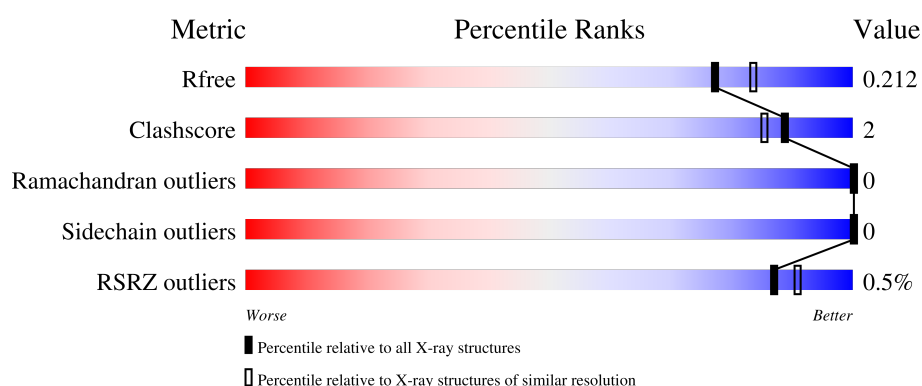
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	340	
1	B	340	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5508 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	3	0
			2498	1578	441	472	7			
1	B	334	Total	C	N	O	S	0	1	0
			2517	1589	442	479	7			

There are 36 discrepancies between the modelled and reference sequences:

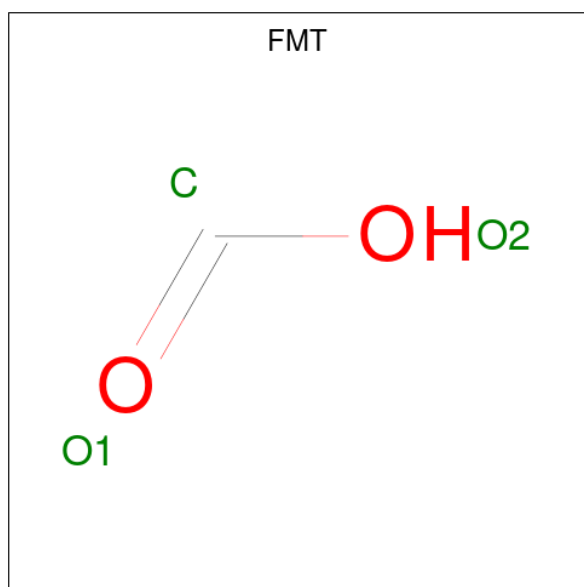
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ILE	-	expression tag	UNP P0A434
A	27	SER	-	expression tag	UNP P0A434
A	28	GLU	-	expression tag	UNP P0A434
A	29	PHE	-	expression tag	UNP P0A434
A	30	ILE	-	expression tag	UNP P0A434
A	31	THR	-	expression tag	UNP P0A434
A	32	ASN	-	expression tag	UNP P0A434
A	33	SER	-	expression tag	UNP P0A434
A	77	ALA	LYS	conflict	UNP P0A434
A	80	VAL	ALA	conflict	UNP P0A434
A	106	ALA	ILE	conflict	UNP P0A434
A	132	GLU	PHE	conflict	UNP P0A434
A	173	GLN	THR	conflict	UNP P0A434
A	185	ARG	LYS	conflict	UNP P0A434
A	203	PHE	ALA	conflict	UNP P0A434
A	254	GLY	HIS	conflict	UNP P0A434
A	274	ASN	ILE	conflict	UNP P0A434
A	319	SER	ARG	conflict	UNP P0A434
B	26	ILE	-	expression tag	UNP P0A434
B	27	SER	-	expression tag	UNP P0A434
B	28	GLU	-	expression tag	UNP P0A434
B	29	PHE	-	expression tag	UNP P0A434
B	30	ILE	-	expression tag	UNP P0A434
B	31	THR	-	expression tag	UNP P0A434
B	32	ASN	-	expression tag	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
B	33	SER	-	expression tag	UNP P0A434
B	77	ALA	LYS	conflict	UNP P0A434
B	80	VAL	ALA	conflict	UNP P0A434
B	106	ALA	ILE	conflict	UNP P0A434
B	132	GLU	PHE	conflict	UNP P0A434
B	173	GLN	THR	conflict	UNP P0A434
B	185	ARG	LYS	conflict	UNP P0A434
B	203	PHE	ALA	conflict	UNP P0A434
B	254	GLY	HIS	conflict	UNP P0A434
B	274	ASN	ILE	conflict	UNP P0A434
B	319	SER	ARG	conflict	UNP P0A434

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).

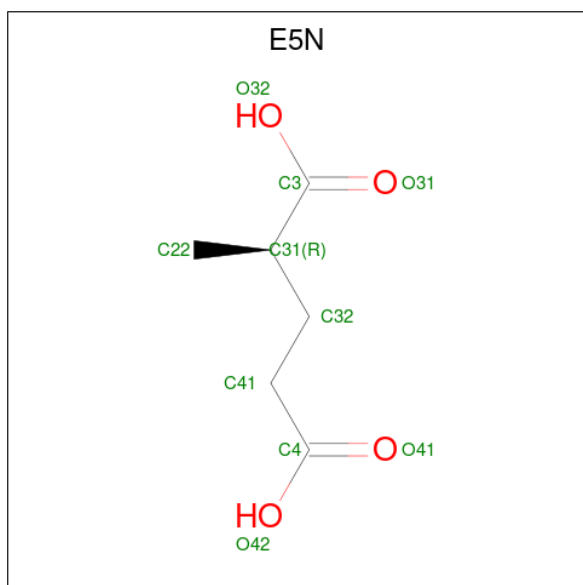


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (2 {R})-2-methylpentanedioic acid (CCD ID: E5N) (formula: C₆H₁₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	211	Total	O	0	0
			211	211		

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: Parathion hydrolase

Chain A:  91% 5% .



- Molecule 1: Parathion hydrolase

Chain B:  % 95% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.03Å 81.49Å 70.81Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	32.70 – 1.93 32.70 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.7 (32.70-1.93) 98.7 (32.70-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.160 , 0.212 0.160 , 0.212	Depositor DCC
R_{free} test set	2356 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, E5N, ZN

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	0.31	0/2545	0.49	0/3459
1	B	0.29	0/2567	0.49	0/3488
All	All	0.30	0/5112	0.49	0/6947

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2498	0	2488	11	0
1	B	2517	0	2509	8	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	252	0	0	1	0
5	B	211	0	0	0	0
All	All	5508	0	4997	19	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 2.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD12	1:A:116:VAL:HG12	1.70	0.72
1:B:131:TRP:CG	1:B:132:GLU:H	2.18	0.61
1:A:91:ARG:NH2	1:A:121:ASP:OD2	2.37	0.57
1:A:57:HIS:O	1:A:303:LEU:HA	2.07	0.55
1:B:57:HIS:O	1:B:303:LEU:HA	2.06	0.55
1:A:131:TRP:CG	1:A:132:GLU:H	2.25	0.54
1:B:57:HIS:HB2	1:B:303:LEU:HB3	1.91	0.53
1:B:293:MET:HE2	1:B:349:ILE:HG13	1.95	0.48
1:A:356:ARG:HD2	5:A:670:HOH:O	2.12	0.48
1:B:314:MET:HA	1:B:314:MET:HE3	1.96	0.46
1:B:131:TRP:CG	1:B:132:GLU:N	2.85	0.45
1:A:344:GLU:CD	1:A:344:GLU:H	2.25	0.45
1:A:202:THR:HB	1:A:208:ASP:HB2	1.99	0.45
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.98	0.44
1:A:314:MET:HA	1:A:314:MET:HE3	2.00	0.43
1:B:40:VAL:HA	1:B:163:ILE:HG23	2.00	0.42
1:B:197:PRO:HB2	1:B:357:PHE:CE1	2.55	0.41
1:A:35:ASP:HA	1:A:46:ILE:HD11	2.03	0.40
1:A:57:HIS:HB2	1:A:303:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/340 (96%)	320 (98%)	8 (2%)	0	100	100
1	B	331/340 (97%)	321 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	659/680 (97%)	641 (97%)	18 (3%)	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	260/273 (95%)	260 (100%)	0	100	100
1	B	262/273 (96%)	262 (100%)	0	100	100
All	All	522/546 (96%)	522 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	ASN
1	B	343	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\# Z > 2$
2	FMT	B	401	1,3	2,2,2	0.68	0	1,1,1	0.22	0
4	E5N	B	404	3	9,9,9	1.01	0	10,11,11	1.51	2 (20%)
4	E5N	A	404	3	9,9,9	1.04	0	10,11,11	1.16	1 (10%)
2	FMT	A	401	1,3	2,2,2	0.69	0	1,1,1	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	E5N	B	404	3	-	1/9/9/9	-
4	E5N	A	404	3	-	2/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	E5N	O41-C4-C41	-2.98	113.64	123.09
4	A	404	E5N	O31-C3-C31	-2.30	115.26	122.27
4	B	404	E5N	O42-C4-C41	2.05	120.49	114.00

There are no chirality outliers.

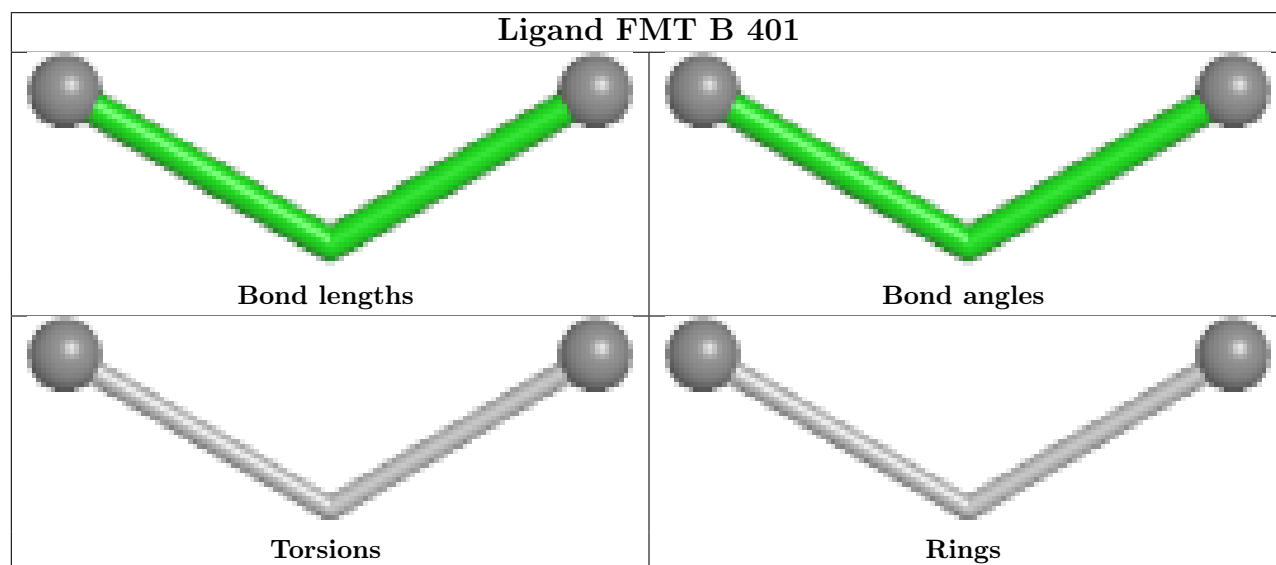
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	E5N	O31-C3-C31-C32
4	A	404	E5N	O32-C3-C31-C32
4	B	404	E5N	O41-C4-C41-C32

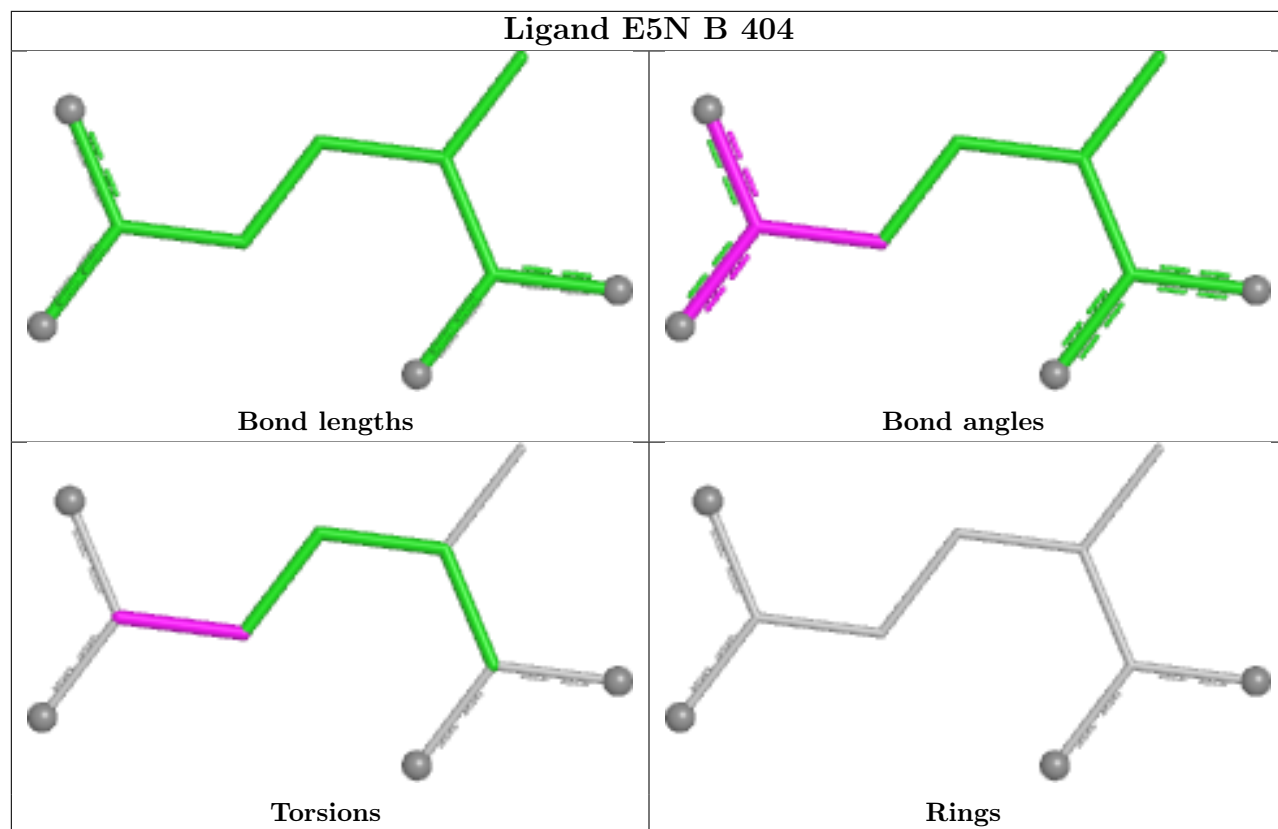
There are no ring outliers.

No monomer is involved in short contacts.

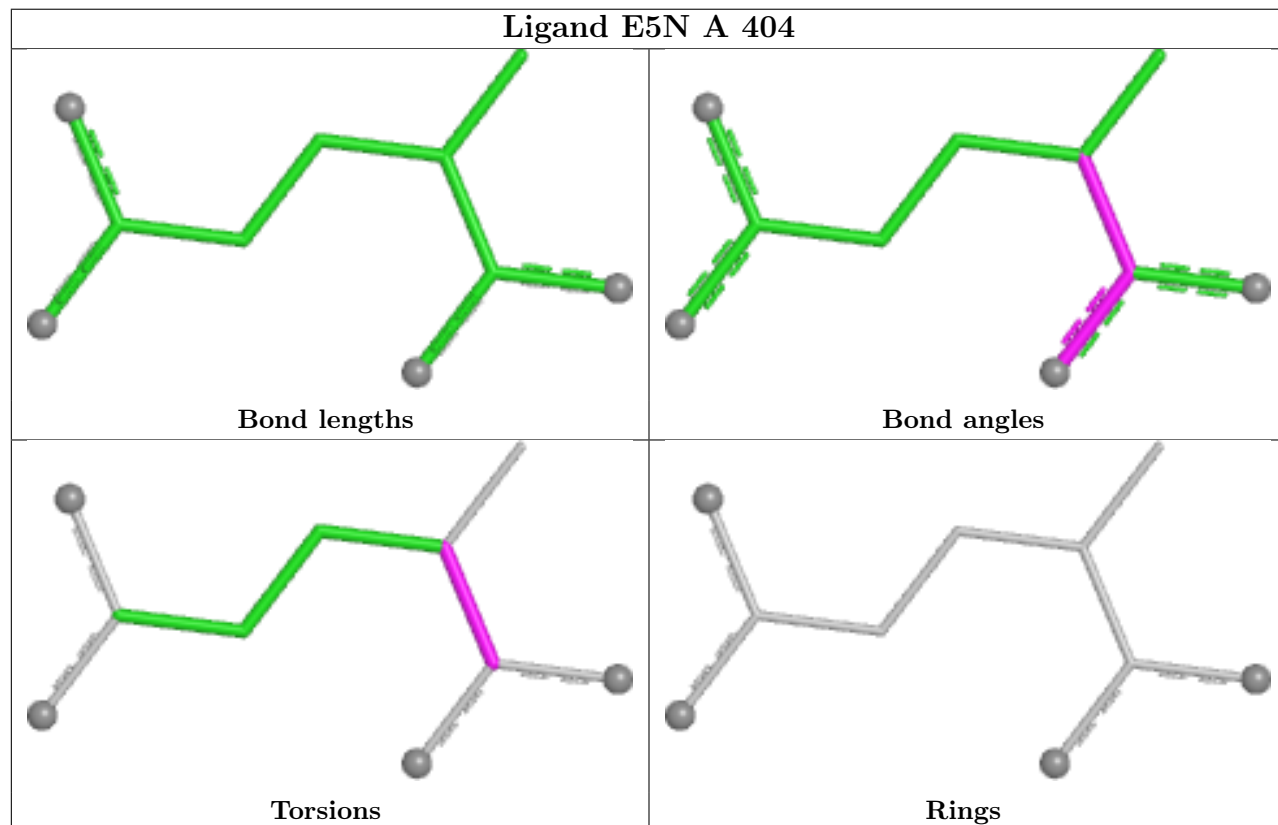
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

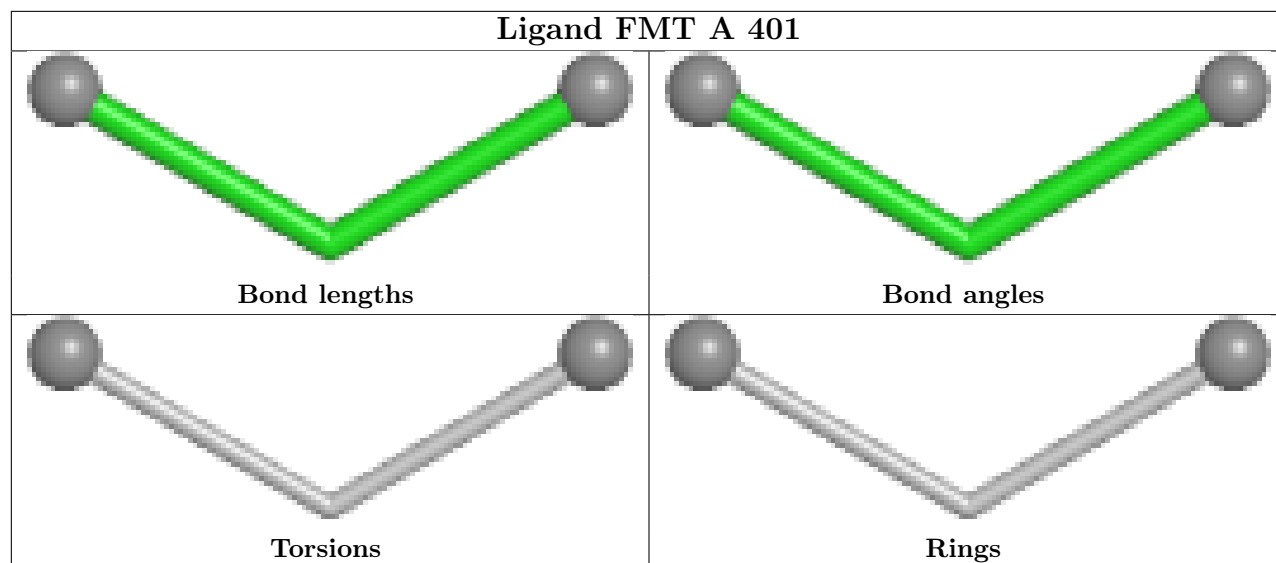


Ligand E5N B 404



Ligand E5N A 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 [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	327/340 (96%)	-0.44	0	100 100	12, 24, 33, 64	3 (0%)
1	B	334/340 (98%)	-0.26	3 (0%)	81 86	20, 27, 38, 76	1 (0%)
All	All	661/680 (97%)	-0.35	3 (0%)	87 91	12, 25, 36, 76	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	GLU	3.1
1	B	35	ASP	3.0
1	B	27	SER	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
4	E5N	A	404	10/10	0.92	0.11	20,25,42,58	0
4	E5N	B	404	10/10	0.92	0.12	21,28,44,56	0

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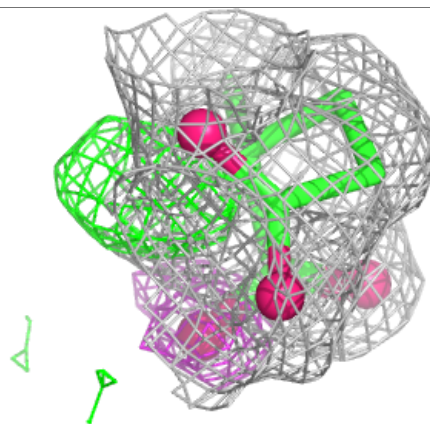
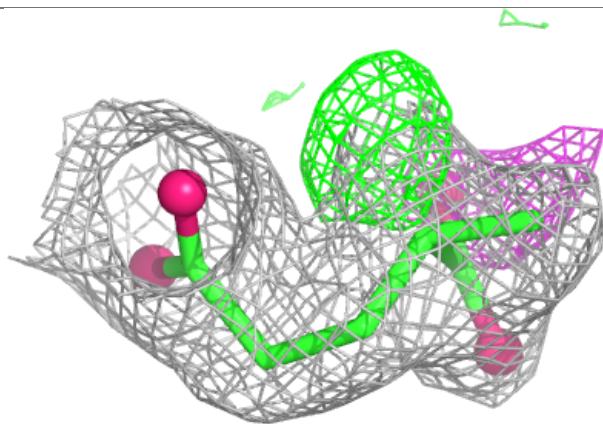
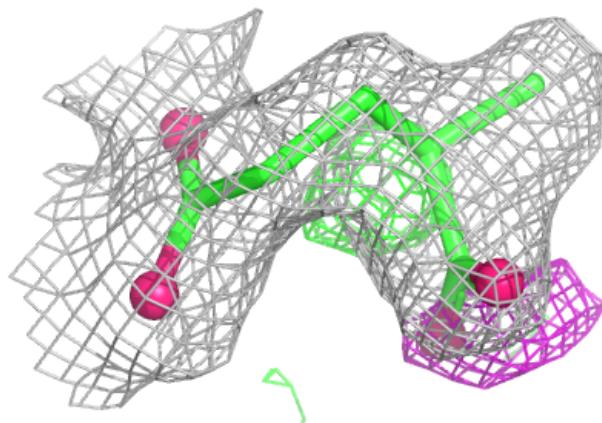
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMT	A	401	3/3	0.97	0.06	18,18,23,23	0
2	FMT	B	401	3/3	0.97	0.06	25,25,26,27	0
3	ZN	B	402	1/1	1.00	0.02	26,26,26,26	0
3	ZN	B	403	1/1	1.00	0.02	30,30,30,30	0
3	ZN	A	402	1/1	1.00	0.01	23,23,23,23	0
3	ZN	A	403	1/1	1.00	0.03	24,24,24,24	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.

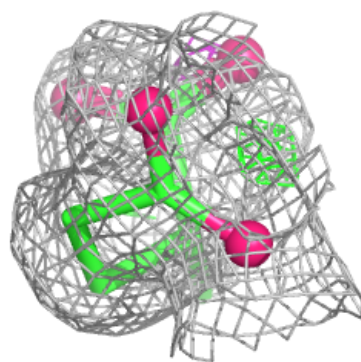
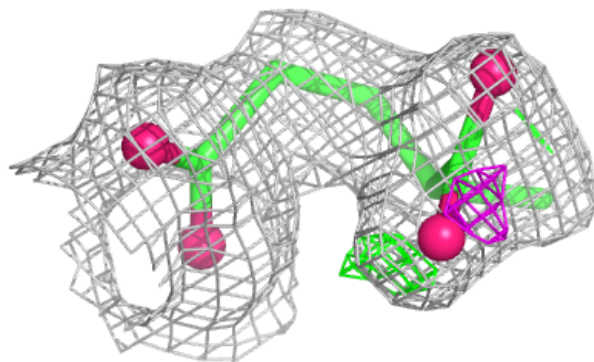
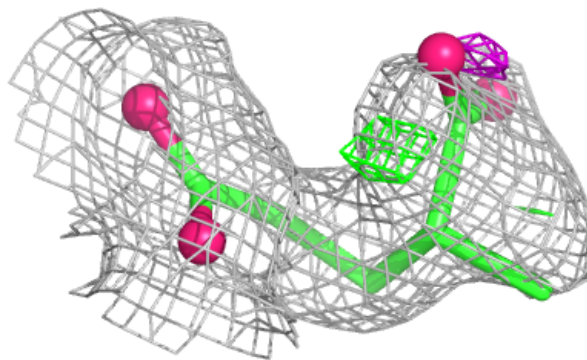
Electron density around E5N A 404:

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



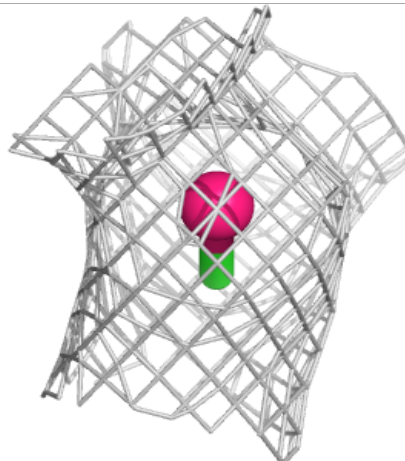
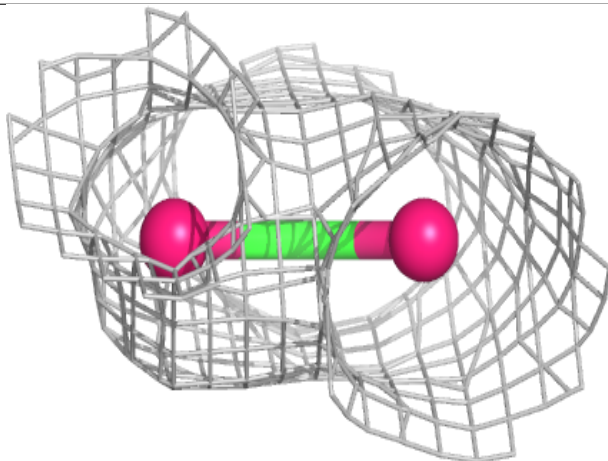
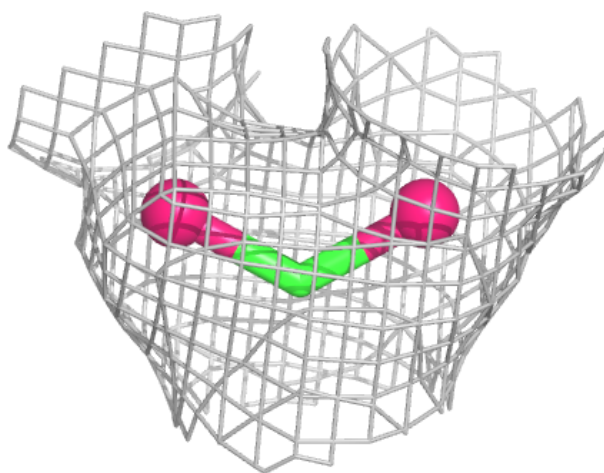
Electron density around E5N B 404:

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



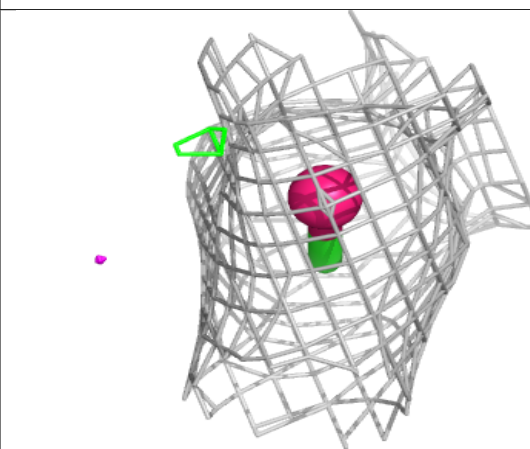
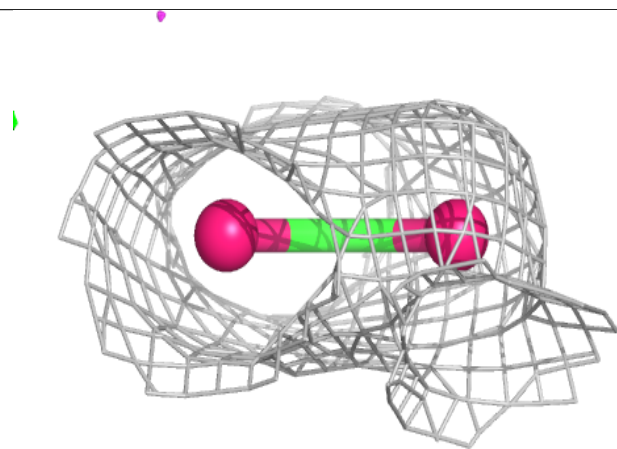
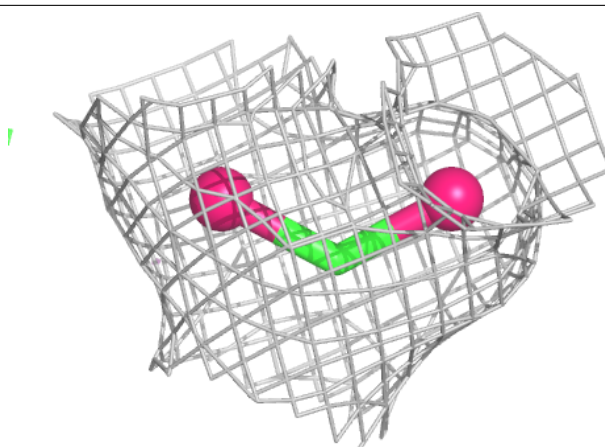
Electron density around FMT A 401:

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



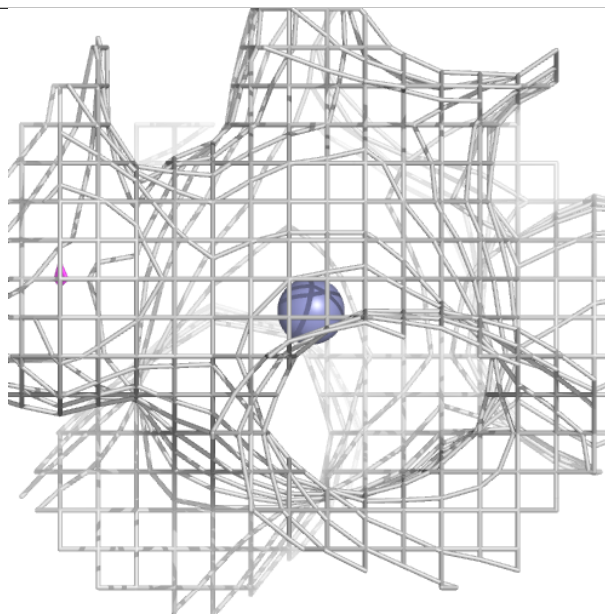
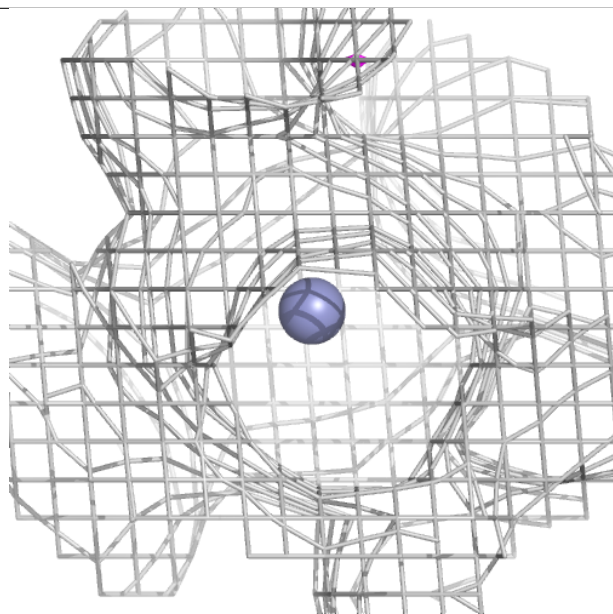
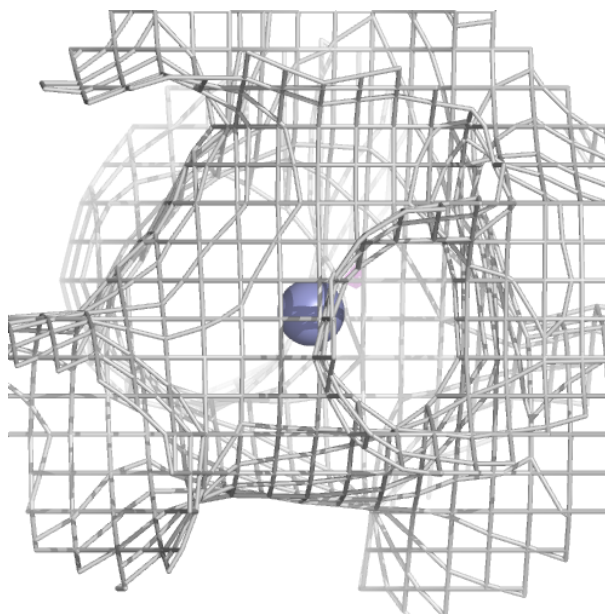
Electron density around FMT B 401:

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



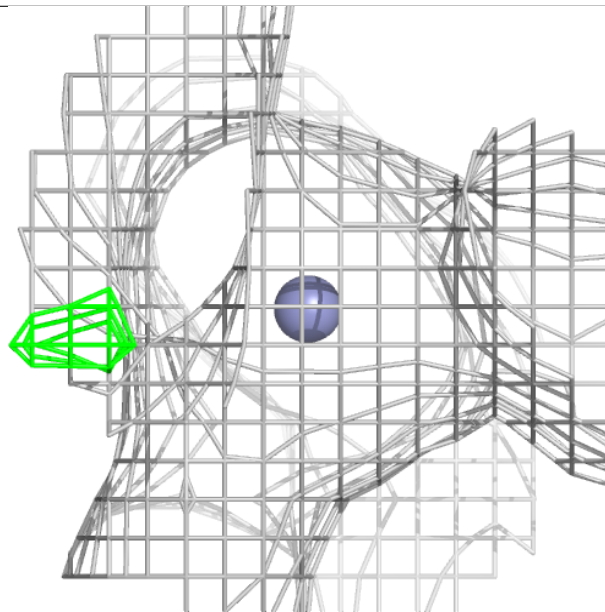
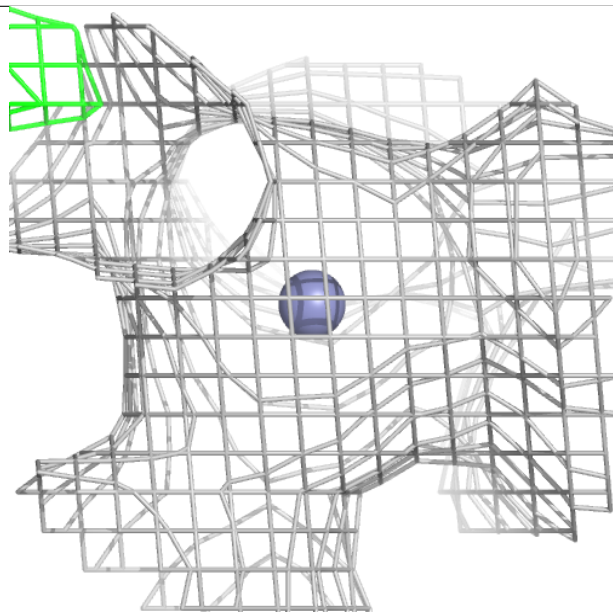
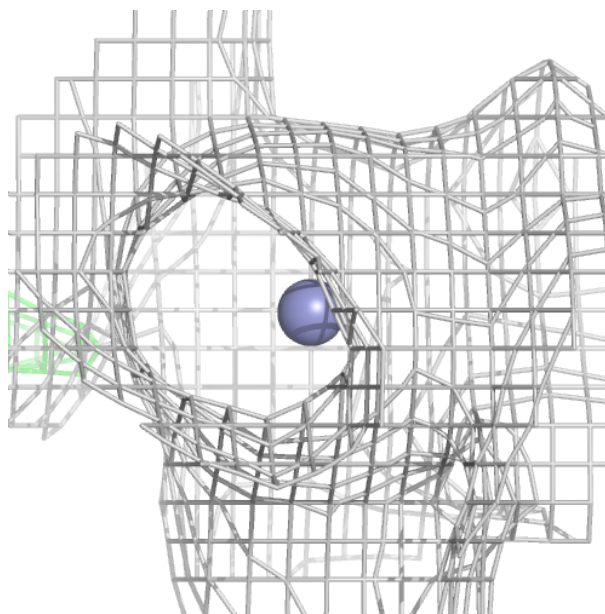
Electron density around ZN B 402:

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



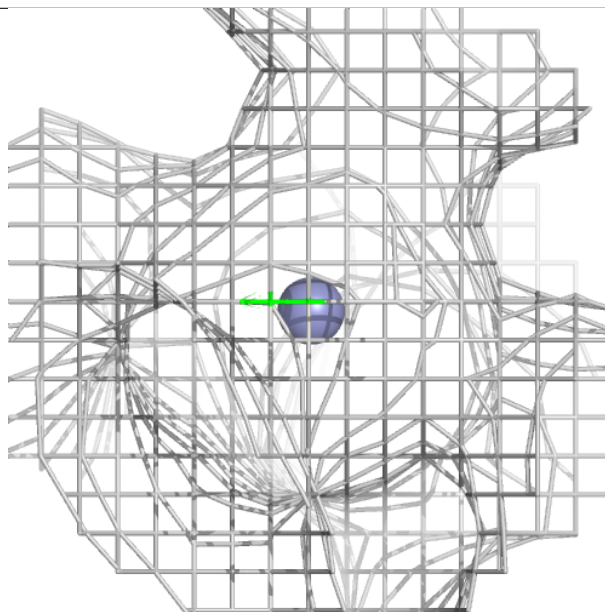
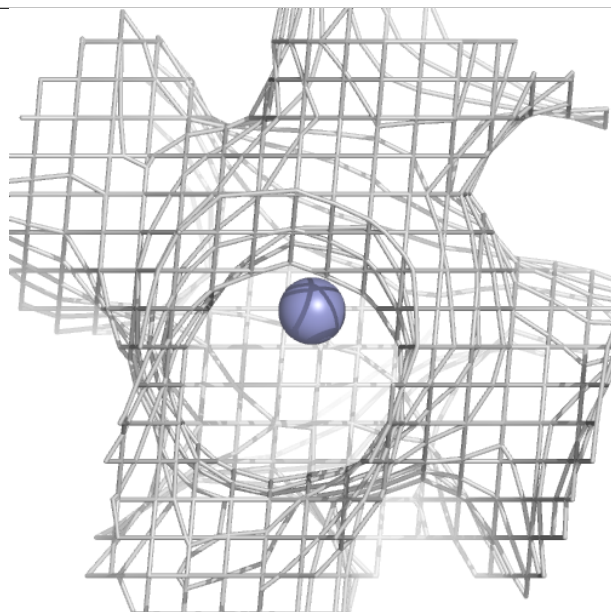
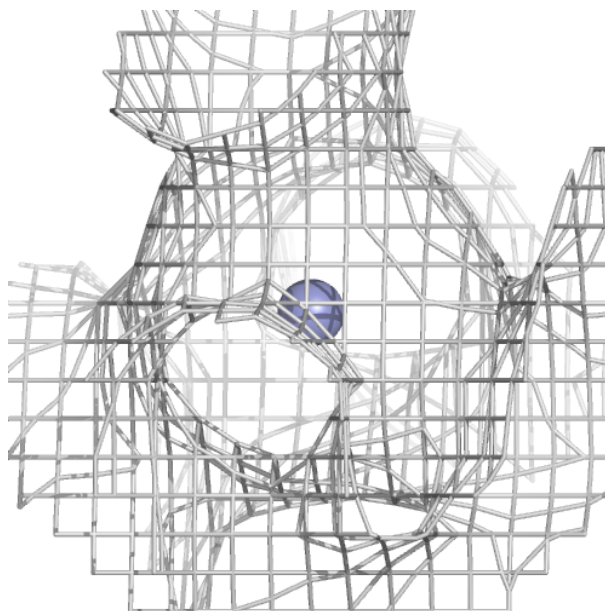
Electron density around ZN B 403:

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



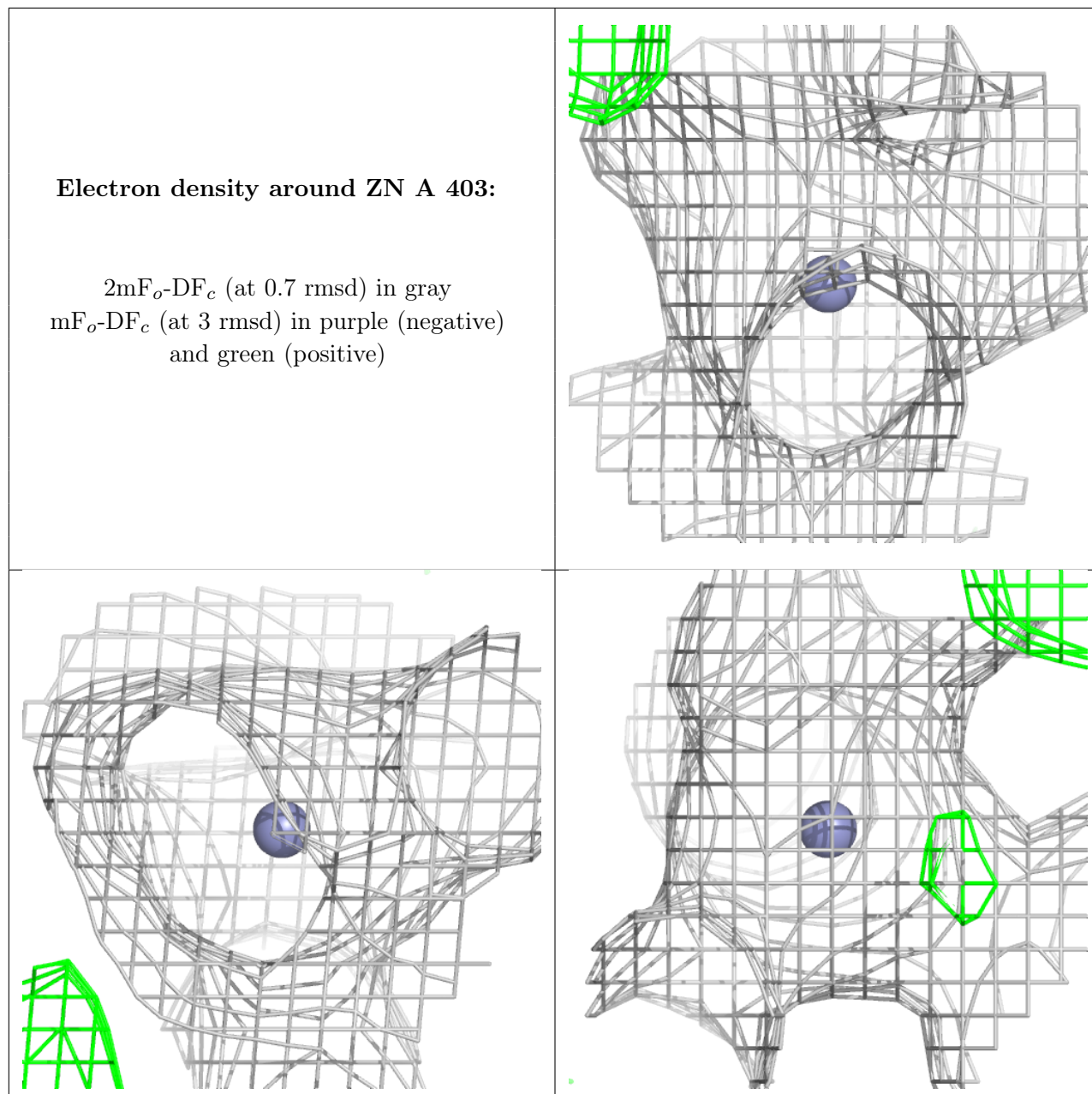
Electron density around ZN A 402:

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



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.