



wwPDB X-ray Structure Validation Summary Report

Jan 30, 2025 – 09:13 am GMT

PDB ID : 8AW0
Title : Crystal structure of PksD, the trans-acting acyl hydrolase domain from the bacillaene trans-AT PKS (native)
Authors : Fage, C.D.; Challis, G.L.; Lewandowski, J.; Jenner, M.
Deposited on : 2022-08-28
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

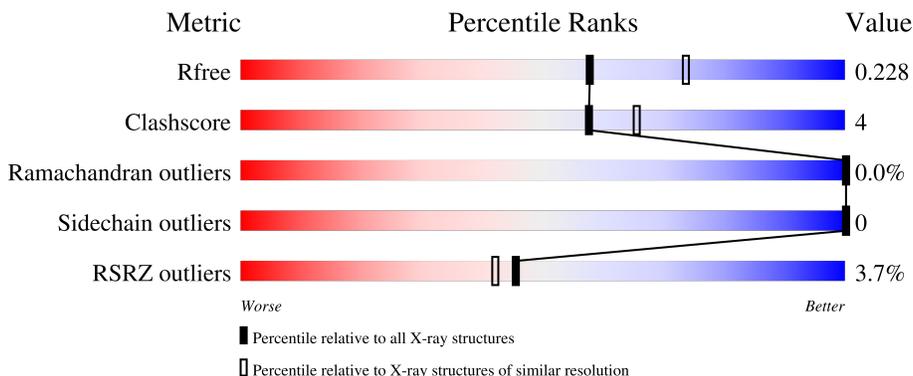
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

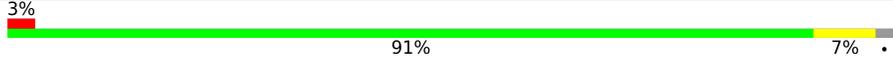
The reported resolution of this entry is 2.20 Å.

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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	327	 3% 91% 7%
1	B	327	 3% 86% 11%
1	C	327	 2% 87% 9%
1	D	327	 2% 88% 9%
1	E	327	 2% 86% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	327	 2% 87% 10% .
1	G	327	 2% 87% 9% .
1	H	327	 12% 74% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20885 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 Polyketide biosynthesis acyltransferase homolog PksD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2578	1646	428	485	19	0	3	0
1	B	317	2554	1632	421	483	18	0	4	0
1	C	317	2555	1634	420	482	19	0	4	0
1	D	316	2519	1612	413	475	19	0	1	0
1	E	317	2553	1631	425	478	19	0	3	0
1	F	316	2528	1617	414	478	19	0	2	0
1	G	315	2525	1615	416	476	18	0	2	0
1	H	316	2512	1608	412	474	18	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O34877
A	-1	SER	-	expression tag	UNP O34877
A	0	HIS	-	expression tag	UNP O34877
B	-2	GLY	-	expression tag	UNP O34877
B	-1	SER	-	expression tag	UNP O34877
B	0	HIS	-	expression tag	UNP O34877
C	-2	GLY	-	expression tag	UNP O34877
C	-1	SER	-	expression tag	UNP O34877
C	0	HIS	-	expression tag	UNP O34877
D	-2	GLY	-	expression tag	UNP O34877
D	-1	SER	-	expression tag	UNP O34877
D	0	HIS	-	expression tag	UNP O34877
E	-2	GLY	-	expression tag	UNP O34877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP O34877
E	0	HIS	-	expression tag	UNP O34877
F	-2	GLY	-	expression tag	UNP O34877
F	-1	SER	-	expression tag	UNP O34877
F	0	HIS	-	expression tag	UNP O34877
G	-2	GLY	-	expression tag	UNP O34877
G	-1	SER	-	expression tag	UNP O34877
G	0	HIS	-	expression tag	UNP O34877
H	-2	GLY	-	expression tag	UNP O34877
H	-1	SER	-	expression tag	UNP O34877
H	0	HIS	-	expression tag	UNP O34877

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	77	Total O 77 77	0	0
3	C	76	Total O 76 76	0	0
3	D	77	Total O 77 77	0	0
3	E	63	Total O 63 63	0	0
3	F	58	Total O 58 58	0	0
3	G	73	Total O 73 73	0	0

Continued on next page...

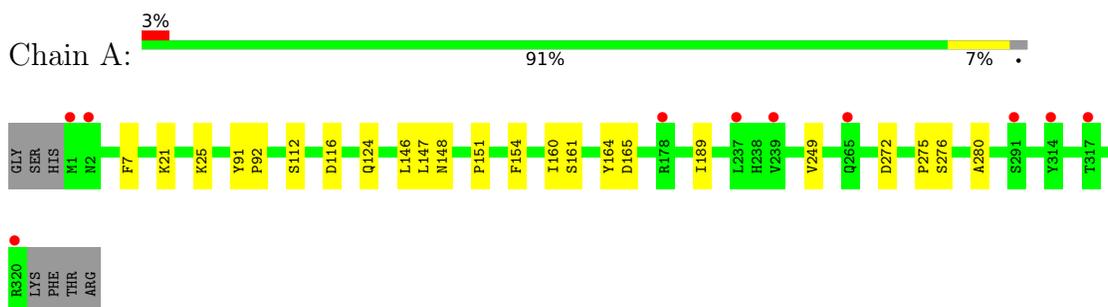
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	34	Total	O	0	0
			34	34		

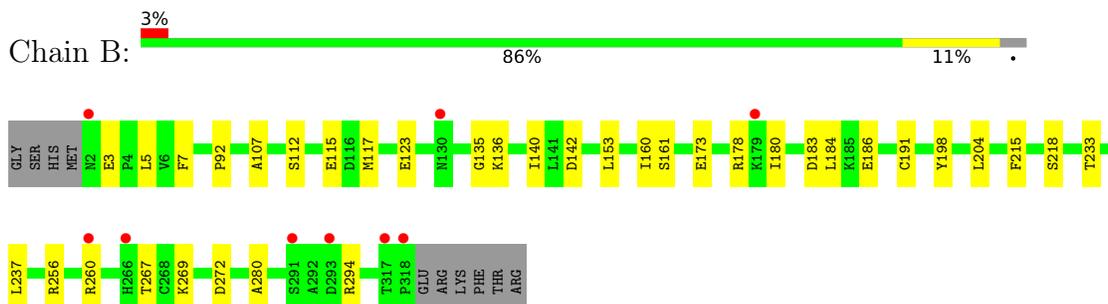
3 Residue-property plots [i](#)

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.

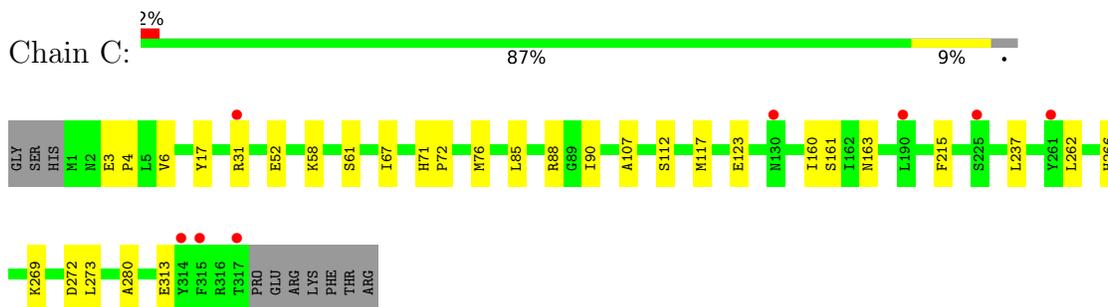
- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD



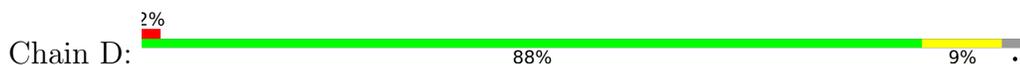
- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD

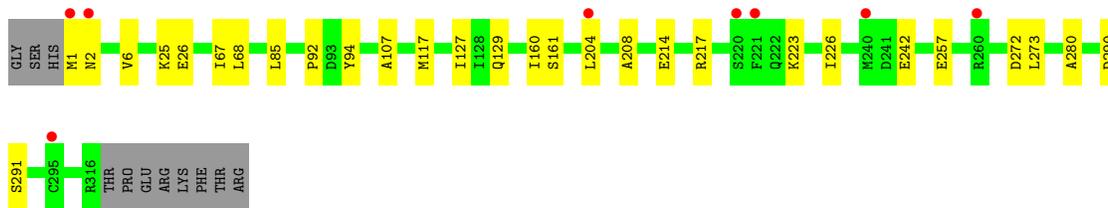


- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD

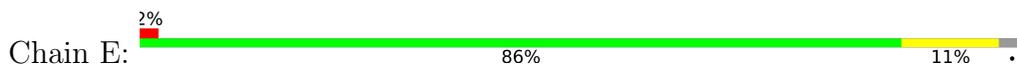


- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD

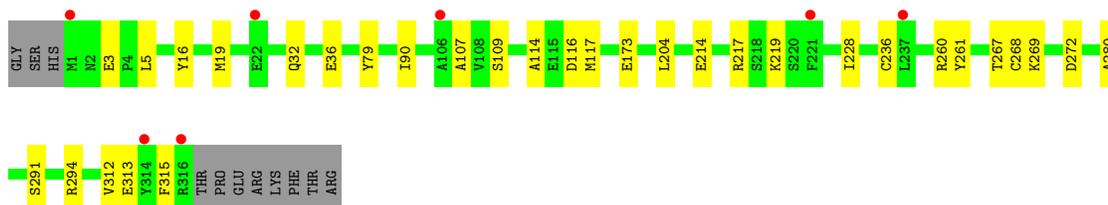
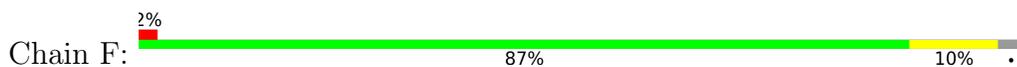




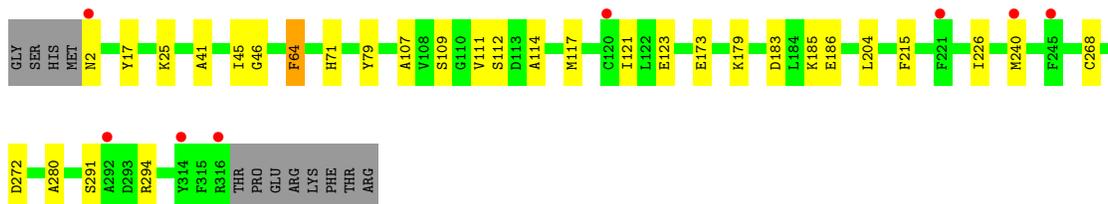
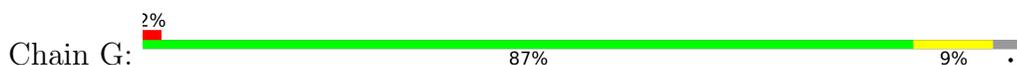
- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD



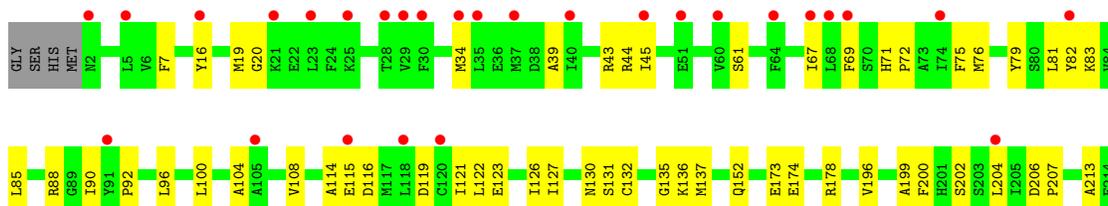
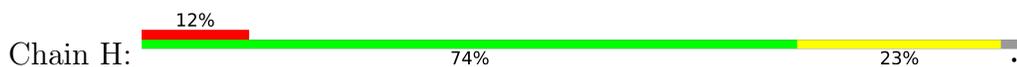
- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD

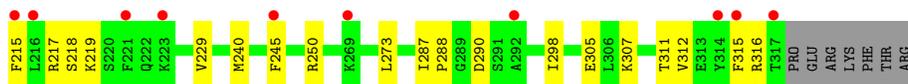


- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD



- Molecule 1: Polyketide biosynthesis acyltransferase homolog PksD





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.20Å 163.33Å 186.87Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	51.08 – 2.20 51.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (51.08-2.20) 99.5 (51.08-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.198 , 0.227 0.199 , 0.228	Depositor DCC
R_{free} test set	11316 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtrriage
Anisotropy	0.440	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20885	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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:
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	0.33	0/2637	0.49	0/3560
1	B	0.35	0/2613	0.52	2/3530 (0.1%)
1	C	0.34	0/2614	0.52	0/3530
1	D	0.32	0/2577	0.53	1/3480 (0.0%)
1	E	0.32	0/2611	0.51	1/3524 (0.0%)
1	F	0.34	0/2586	0.50	0/3492
1	G	0.32	0/2583	0.54	2/3488 (0.1%)
1	H	0.31	0/2570	0.53	0/3472
All	All	0.33	0/20791	0.52	6/28076 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	E	293	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	178	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	G	64	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	B	142	ASP	C-N-CA	-6.19	106.23	121.70

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	2578	0	2535	12	0
1	B	2554	0	2503	20	0
1	C	2555	0	2508	20	1
1	D	2519	0	2477	17	0
1	E	2553	0	2516	20	0
1	F	2528	0	2482	23	0
1	G	2525	0	2479	20	1
1	H	2512	0	2468	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	99	0	0	0	0
3	B	77	0	0	2	0
3	C	76	0	0	2	0
3	D	77	0	0	1	0
3	E	63	0	0	0	0
3	F	58	0	0	1	0
3	G	73	0	0	1	0
3	H	34	0	0	0	0
All	All	20885	0	19968	176	1

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 4.

The worst 5 of 176 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:3:GLU:OE2	1:C:269:LYS:HE3	1.79	0.83
1:E:90:ILE:HD11	1:E:313:GLU:HG2	1.64	0.80
1:F:16:TYR:O	1:F:19:MET:HG3	1.87	0.74
1:H:126:ILE:O	1:H:130:ASN:ND2	2.20	0.74
1:F:32:GLN:O	1:F:36:GLU:HG3	1.92	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:SER:OG	1:G:186:GLU:OE2[3_455]	2.16	0.04

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	321/327 (98%)	315 (98%)	6 (2%)	0	100	100
1	B	319/327 (98%)	313 (98%)	6 (2%)	0	100	100
1	C	319/327 (98%)	311 (98%)	8 (2%)	0	100	100
1	D	315/327 (96%)	307 (98%)	8 (2%)	0	100	100
1	E	318/327 (97%)	313 (98%)	5 (2%)	0	100	100
1	F	316/327 (97%)	304 (96%)	12 (4%)	0	100	100
1	G	315/327 (96%)	306 (97%)	9 (3%)	0	100	100
1	H	314/327 (96%)	300 (96%)	13 (4%)	1 (0%)	37	42
All	All	2537/2616 (97%)	2469 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	218	SER

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	287/290 (99%)	287 (100%)	0	100	100
1	B	285/290 (98%)	285 (100%)	0	100	100
1	C	285/290 (98%)	285 (100%)	0	100	100
1	D	281/290 (97%)	281 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	284/290 (98%)	284 (100%)	0	100	100
1	F	282/290 (97%)	282 (100%)	0	100	100
1	G	281/290 (97%)	281 (100%)	0	100	100
1	H	280/290 (97%)	280 (100%)	0	100	100
All	All	2265/2320 (98%)	2265 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	129	GLN
1	D	130	ASN
1	D	150	HIS
1	E	148	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	320/327 (97%)	0.13	10 (3%) 51 48	30, 65, 93, 116	3 (0%)
1	B	317/327 (96%)	0.35	9 (2%) 55 52	29, 71, 95, 109	4 (1%)
1	C	317/327 (96%)	0.22	8 (2%) 58 55	28, 67, 91, 133	4 (1%)
1	D	316/327 (96%)	0.27	8 (2%) 58 55	30, 73, 98, 136	1 (0%)
1	E	317/327 (96%)	0.23	7 (2%) 62 58	34, 71, 95, 131	3 (0%)
1	F	316/327 (96%)	0.24	7 (2%) 62 58	29, 71, 96, 144	2 (0%)
1	G	315/327 (96%)	0.25	8 (2%) 58 55	37, 72, 98, 120	2 (0%)
1	H	316/327 (96%)	0.96	38 (12%) 10 8	62, 92, 117, 141	0
All	All	2534/2616 (96%)	0.33	95 (3%) 45 42	28, 72, 105, 144	19 (0%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314[A]	TYR	5.0
1	B	317	THR	4.1
1	A	237	LEU	4.1
1	D	1	MET	4.0
1	E	178[A]	ARG	3.8

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 monosaccharides in this entry.

6.4 Ligands

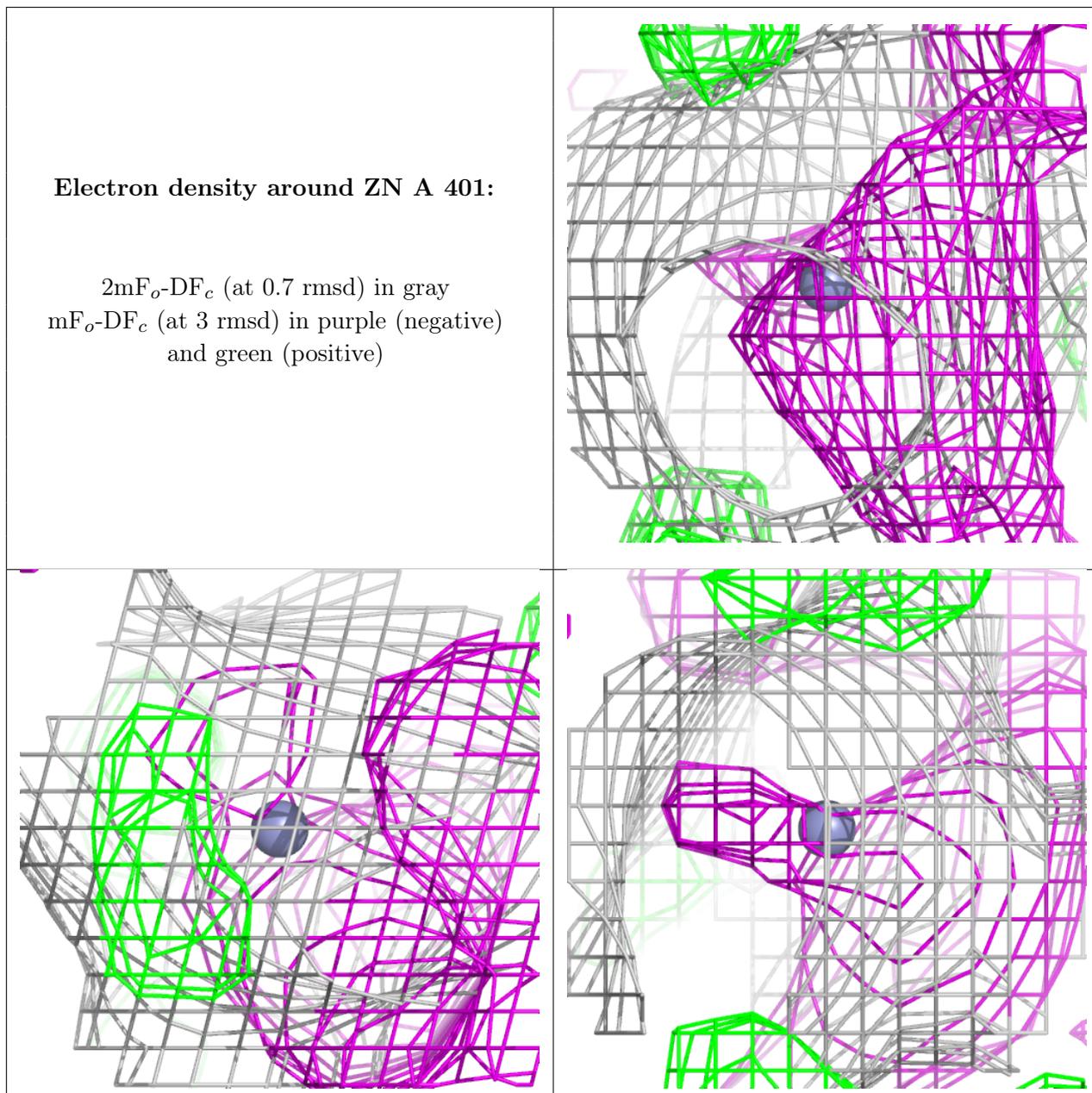
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	401	1/1	0.98	0.07	80,80,80,80	0
2	ZN	C	401	1/1	0.99	0.03	76,76,76,76	0
2	ZN	E	401	1/1	0.99	0.03	76,76,76,76	0
2	ZN	B	401	1/1	1.00	0.02	68,68,68,68	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.

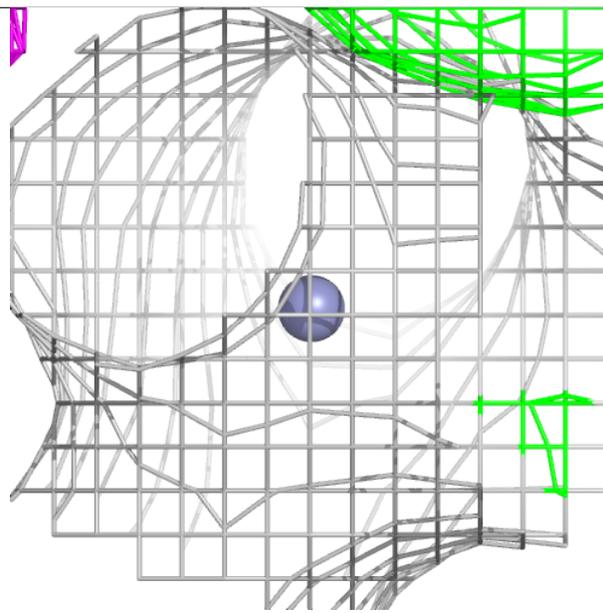
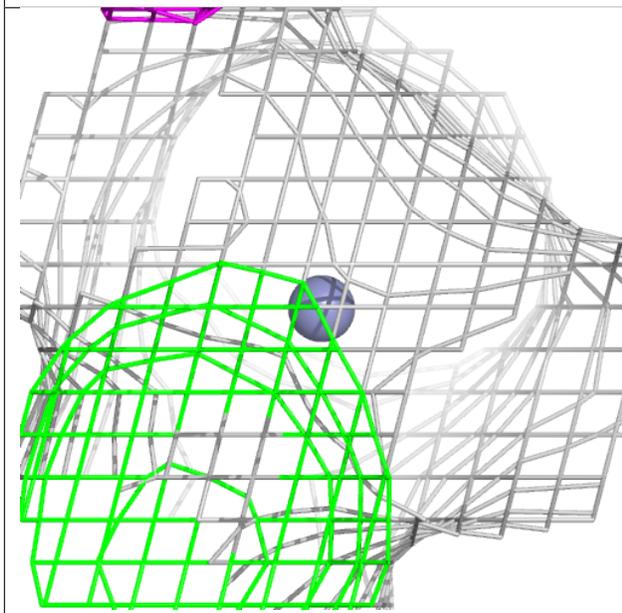
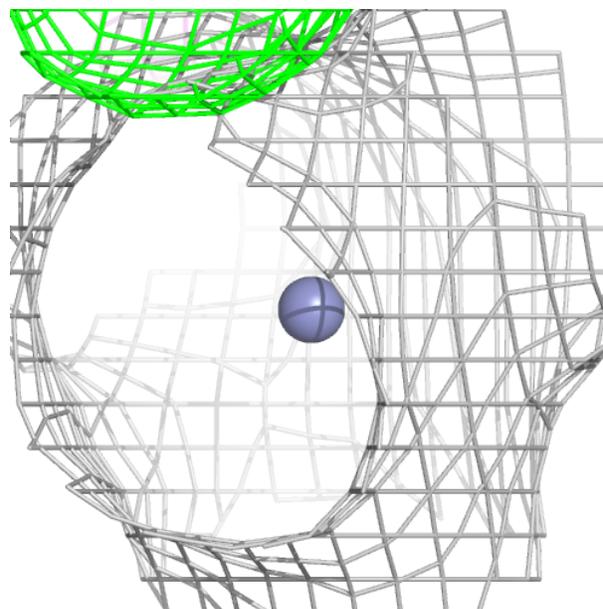
Electron density around ZN A 401:

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



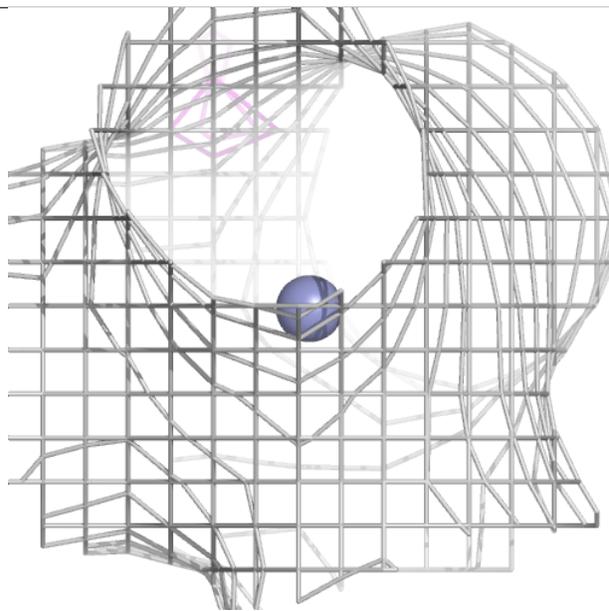
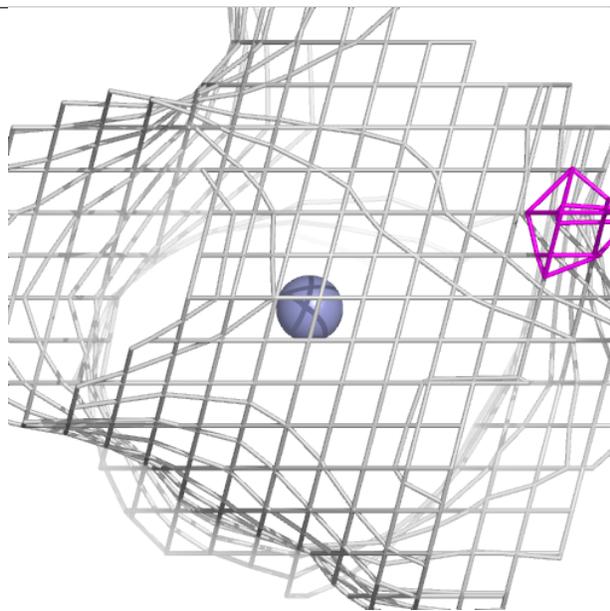
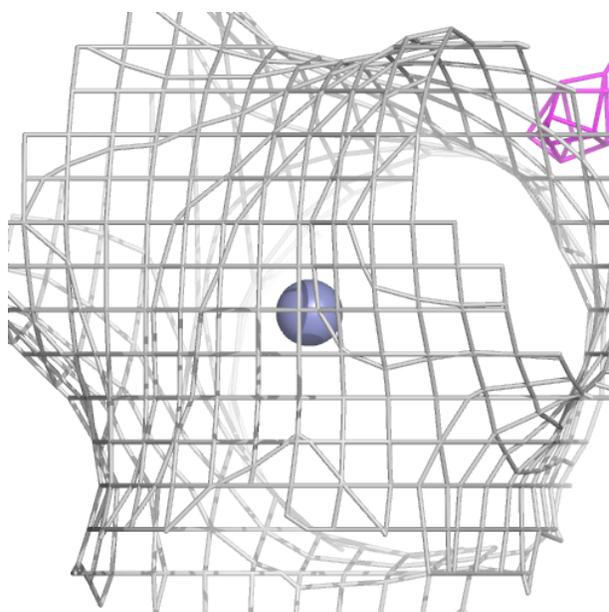
Electron density around ZN C 401:

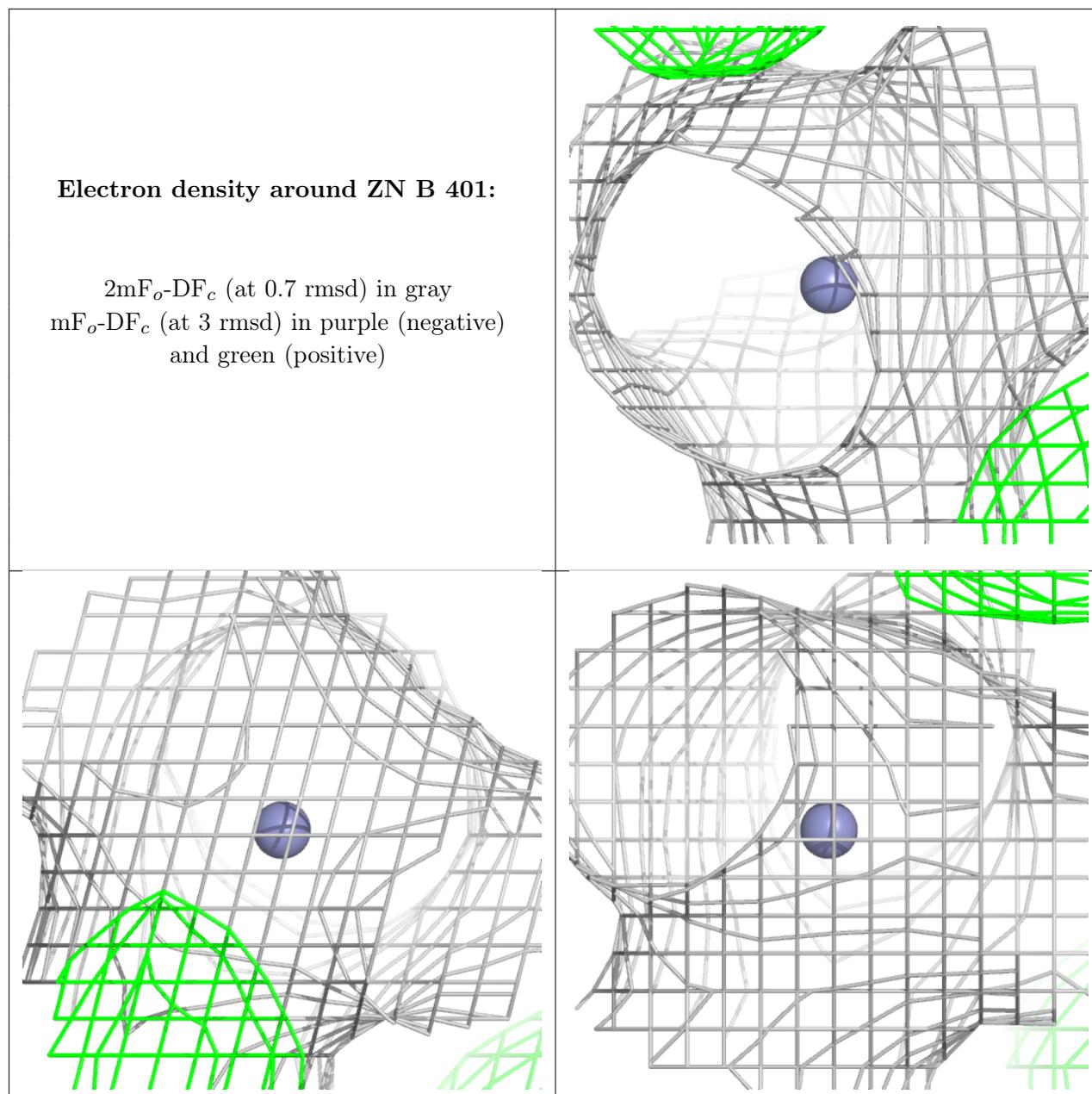
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 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 [i](#)

There are no such residues in this entry.