



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:33 PM EDT

PDB ID : 7KWD
Title : Crystal structure of Thermus thermophilus alkaline phosphatase
Authors : Gallo, G.; Coelho, C.; Borges, B.; Negri, N.; Maiello, F.; Hardy, L.; Wurtele, M.
Deposited on : 2020-11-30
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

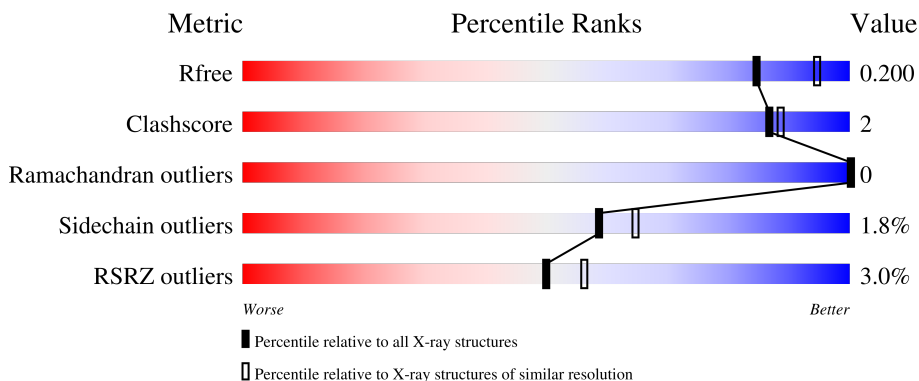
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	501	 88% 6% 6%
1	B	501	 88% 6% 6% 4%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	A	601	-	X	-	-
2	TLA	B	601	-	X	-	-

2 Entry composition [i](#)

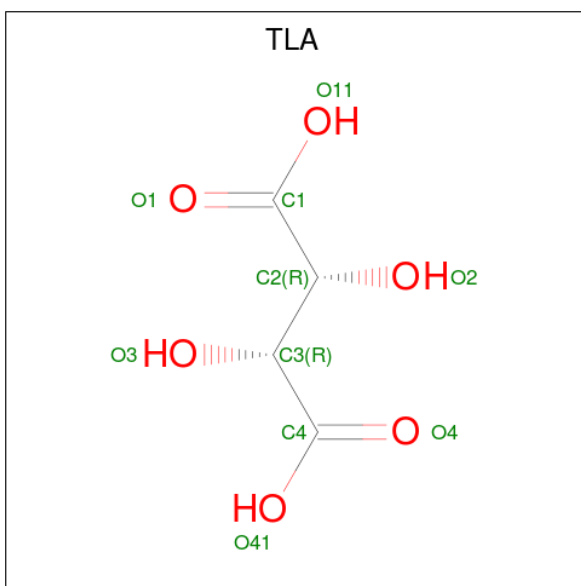
There are 5 unique types of molecules in this entry. The entry contains 15084 atoms, of which 7249 are hydrogens and 0 are deuteriums.

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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	473	Total 7279	C 2306	H 3621	N 666	O 677	S 9	0	1	0
1	B	473	Total 7278	C 2306	H 3620	N 666	O 677	S 9	0	1	0

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
2	A	1	Total 14	C 4	H 4	O 6	0	0
2	B	1	Total 14	C 4	H 4	O 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

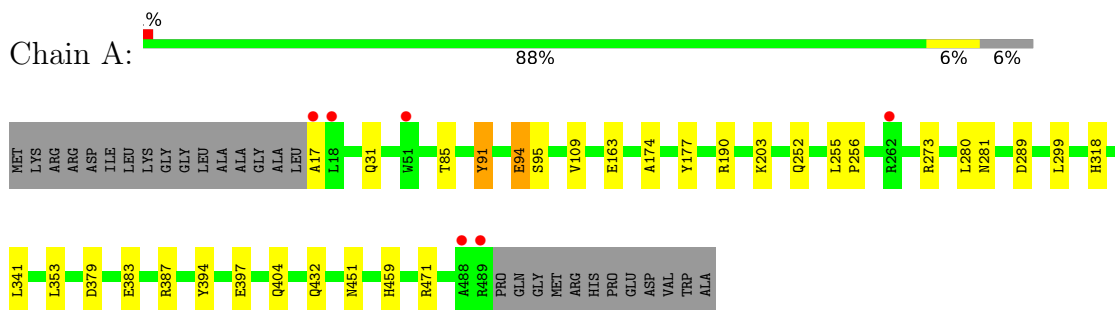
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	272	Total O 272 272	0	0
5	B	221	Total O 221 221	0	0

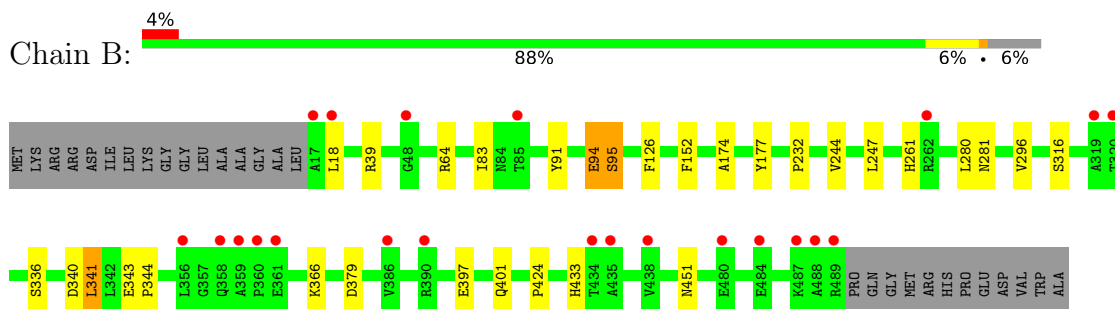
3 Residue-property plots [i](#)

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: Alkaline phosphatase



- Molecule 1: Alkaline phosphatase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	163.18Å 163.18Å 163.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.26 – 2.10 47.10 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.26-2.10) 97.9 (47.10-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.163 , 0.201 0.164 , 0.200	Depositor DCC
R_{free} test set	4710 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.028 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15084	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: MG, ZN, TLA

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	0.56	1/3737 (0.0%)	0.73	1/5069 (0.0%)
1	B	0.55	1/3737 (0.0%)	0.70	0/5069
All	All	0.55	2/7474 (0.0%)	0.71	1/10138 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TYR	CD1-CE1	-6.25	1.29	1.39
1	B	91	TYR	CD1-CE1	-5.88	1.30	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ARG	NE-CZ-NH2	-5.94	117.33	120.30

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	3658	3621	3621	16	0
1	B	3658	3620	3620	16	0
2	A	10	4	4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	4	4	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	272	0	0	2	0
5	B	221	0	0	2	0
All	All	7835	7249	7249	30	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 (30) 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:B:261:HIS:ND1	5:B:701:HOH:O	2.18	0.76
1:A:451:ASN:OD1	1:B:451:ASN:ND2	2.21	0.73
1:A:17:ALA:O	5:A:701:HOH:O	2.08	0.71
1:A:91:TYR:HD2	1:B:336:SER:HG	1.38	0.69
1:B:95:SER:OG	2:B:601:TLA:O4	2.15	0.65
1:B:39:ARG:NH2	5:B:703:HOH:O	2.33	0.60
1:A:387:ARG:HH11	1:A:387:ARG:HG2	1.70	0.57
1:A:94:GLU:HB2	2:A:601:TLA:O3	2.10	0.52
1:A:379:ASP:O	1:A:383:GLU:HG2	2.13	0.48
1:B:247:LEU:HG	1:B:296:VAL:HG21	1.95	0.48
1:A:174:ALA:HB3	1:A:177:TYR:CZ	2.49	0.48
1:B:341:LEU:HB3	1:B:424:PRO:HG3	1.96	0.47
1:B:174:ALA:HB3	1:B:177:TYR:CZ	2.50	0.47
1:B:83:ILE:HD11	1:B:316:SER:O	2.16	0.45
1:A:109:VAL:O	5:A:703:HOH:O	2.21	0.44
1:B:343:GLU:N	1:B:344:PRO:CD	2.80	0.43
1:B:232:PRO:HD2	1:B:244:VAL:HG21	2.00	0.43
1:A:31:GLN:HA	1:A:459:HIS:CE1	2.53	0.43
1:B:126:PHE:HB2	1:B:152:PHE:O	2.19	0.43
1:A:273:ARG:HB2	1:A:289:ASP:OD2	2.18	0.43
1:A:252:GLN:HG2	1:A:299:LEU:HD21	2.01	0.42
1:A:394:TYR:CE1	1:A:404:GLN:HB3	2.55	0.42
1:B:64:ARG:HD3	1:B:340:ASP:HA	2.02	0.42
1:A:255:LEU:N	1:A:256:PRO:HD2	2.36	0.41
1:B:280:LEU:O	1:B:281:ASN:HB2	2.20	0.41
1:B:366:LYS:NZ	1:B:379:ASP:OD1	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG2	1:A:190:ARG:CZ	2.51	0.41
1:A:280:LEU:O	1:A:281:ASN:HB2	2.20	0.41
1:B:94:GLU:HA	1:B:433:HIS:CE1	2.56	0.40
1:A:85:THR:HG21	1:A:318:HIS:HA	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	472/501 (94%)	461 (98%)	11 (2%)	0	100	100
1	B	472/501 (94%)	459 (97%)	13 (3%)	0	100	100
All	All	944/1002 (94%)	920 (98%)	24 (2%)	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	370/389 (95%)	363 (98%)	7 (2%)	57	63
1	B	370/389 (95%)	364 (98%)	6 (2%)	62	69
All	All	740/778 (95%)	727 (98%)	13 (2%)	59	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	95	SER
1	A	203	LYS
1	A	341	LEU
1	A	353	LEU
1	A	397	GLU
1	A	432	GLN
1	B	18	LEU
1	B	94	GLU
1	B	95	SER
1	B	341	LEU
1	B	397	GLU
1	B	401	GLN

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

Mol	Chain	Res	Type
1	A	218	ASN
1	B	451	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	TLA	B	601	-	9,9,9	1.33	1 (11%)	12,12,12	2.71	5 (41%)
2	TLA	A	601	4	9,9,9	1.16	0	12,12,12	2.07	7 (58%)

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
2	TLA	B	601	-	-	8/12/12/12	-
2	TLA	A	601	4	-	8/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TLA	C2-C1	2.73	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TLA	O3-C3-C4	-5.74	98.63	110.66
2	B	601	TLA	O41-C4-C3	4.07	124.28	113.27
2	B	601	TLA	O4-C4-C3	-3.50	112.43	121.63
2	B	601	TLA	O3-C3-C2	3.37	116.93	110.23
2	A	601	TLA	O3-C3-C4	-3.15	104.06	110.66
2	A	601	TLA	O11-C1-C2	2.88	121.06	113.27
2	A	601	TLA	C3-C2-C1	-2.70	103.85	109.87
2	A	601	TLA	O41-C4-C3	2.63	120.38	113.27
2	B	601	TLA	O11-C1-C2	2.49	120.02	113.27
2	A	601	TLA	C2-C3-C4	2.19	114.77	109.87
2	A	601	TLA	O11-C1-O1	-2.15	119.20	124.09
2	A	601	TLA	O3-C3-C2	2.15	114.50	110.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	TLA	C1-C2-C3-C4
2	B	601	TLA	O2-C2-C3-C4
2	A	601	TLA	O3-C3-C4-O4
2	A	601	TLA	O3-C3-C4-O41
2	A	601	TLA	C1-C2-C3-O3
2	B	601	TLA	C1-C2-C3-O3
2	A	601	TLA	O1-C1-C2-O2
2	A	601	TLA	O11-C1-C2-O2
2	A	601	TLA	O2-C2-C3-C4
2	A	601	TLA	C1-C2-C3-C4
2	B	601	TLA	O11-C1-C2-O2
2	B	601	TLA	O1-C1-C2-O2
2	A	601	TLA	O2-C2-C3-O3
2	B	601	TLA	O2-C2-C3-O3
2	B	601	TLA	O1-C1-C2-C3
2	B	601	TLA	O11-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	TLA	1	0
2	A	601	TLA	1	0

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	473/501 (94%)	-0.41	6 (1%) 77 80	19, 28, 49, 75	0
1	B	473/501 (94%)	-0.05	22 (4%) 31 37	19, 30, 52, 94	0
All	All	946/1002 (94%)	-0.23	28 (2%) 50 56	19, 29, 51, 94	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	8.5
1	B	18	LEU	4.6
1	B	359	ALA	4.4
1	A	488	ALA	3.9
1	B	488	ALA	3.8
1	A	17	ALA	3.8
1	B	487	LYS	3.5
1	A	489	ARG	3.4
1	B	361	GLU	3.3
1	B	489	ARG	3.1
1	A	18	LEU	3.0
1	B	390	ARG	2.9
1	B	358	GLN	2.8
1	B	386	VAL	2.8
1	B	484	GLU	2.7
1	B	262	ARG	2.7
1	A	51	TRP	2.6
1	B	434	THR	2.6
1	A	262	ARG	2.5
1	B	319	ALA	2.5
1	B	435	ALA	2.5
1	B	48	GLY	2.4
1	B	438	VAL	2.2
1	B	356	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	360	PRO	2.2
1	B	320	THR	2.2
1	B	480	GLU	2.2
1	B	85	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

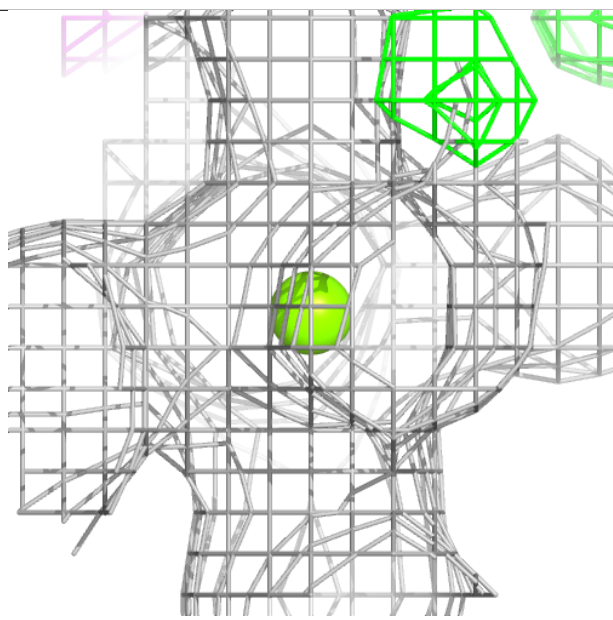
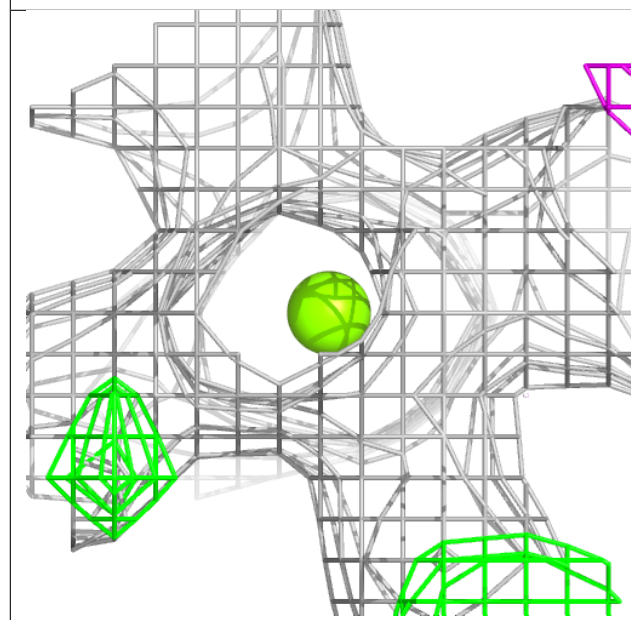
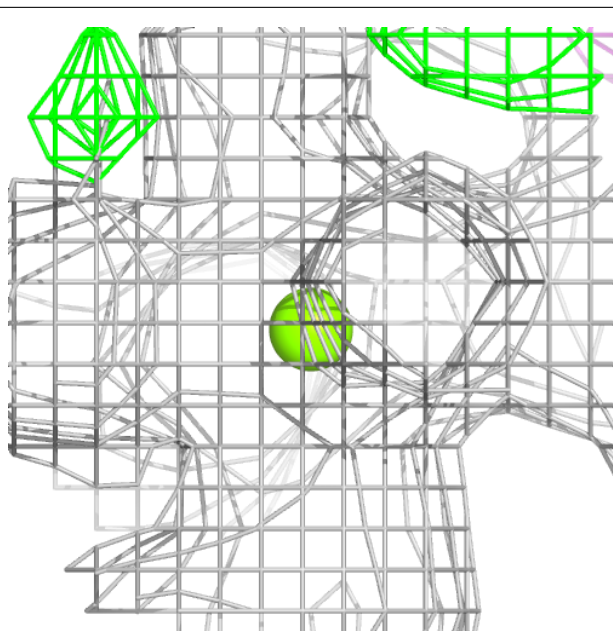
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TLA	B	601	10/10	0.80	0.22	41,57,70,71	0
2	TLA	A	601	10/10	0.83	0.16	40,54,65,65	0
3	MG	B	602	1/1	0.96	0.13	34,34,34,34	0
3	MG	A	602	1/1	0.99	0.09	33,33,33,33	0
4	ZN	A	603	1/1	1.00	0.09	37,37,37,37	0
4	ZN	A	604	1/1	1.00	0.10	30,30,30,30	0
4	ZN	B	603	1/1	1.00	0.10	38,38,38,38	0
4	ZN	B	604	1/1	1.00	0.13	33,33,33,33	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.

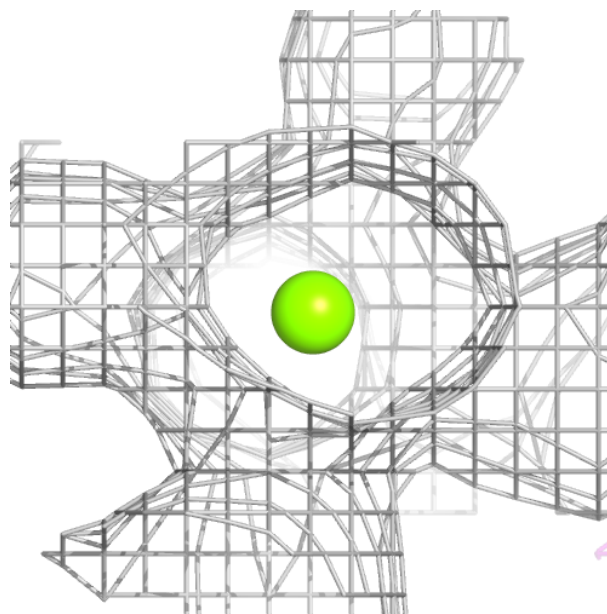
Electron density around MG B 602:

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



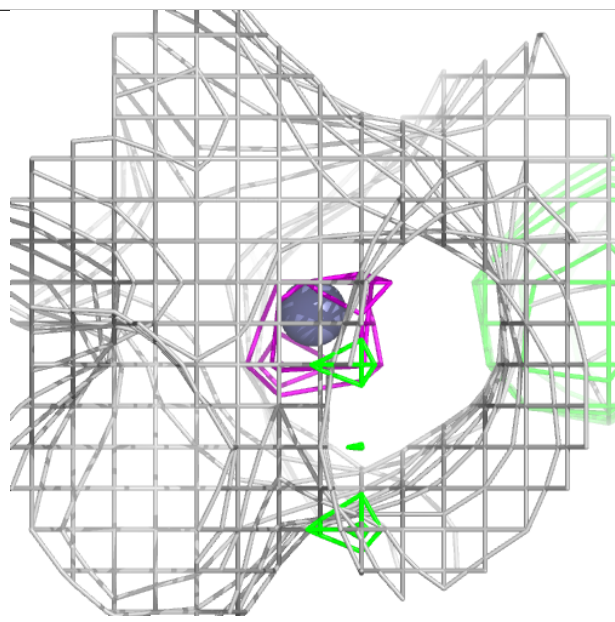
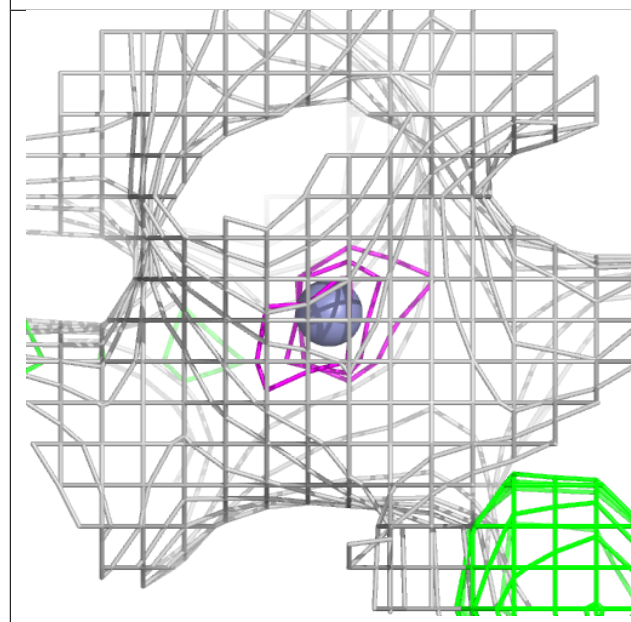
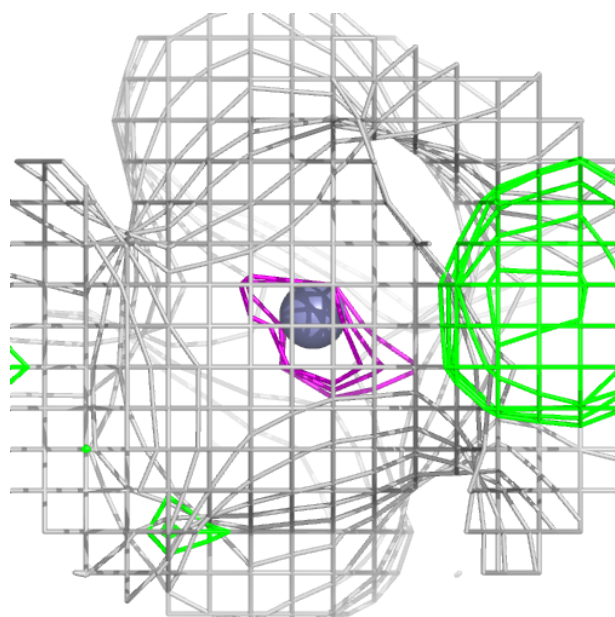
Electron density around MG A 602:

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



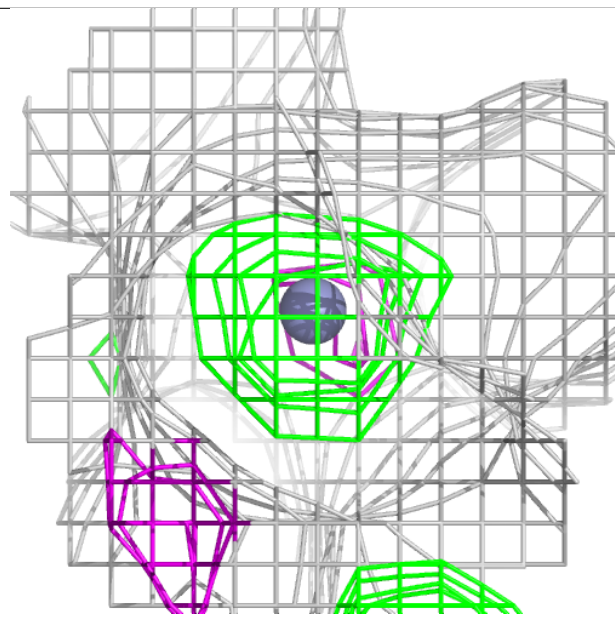
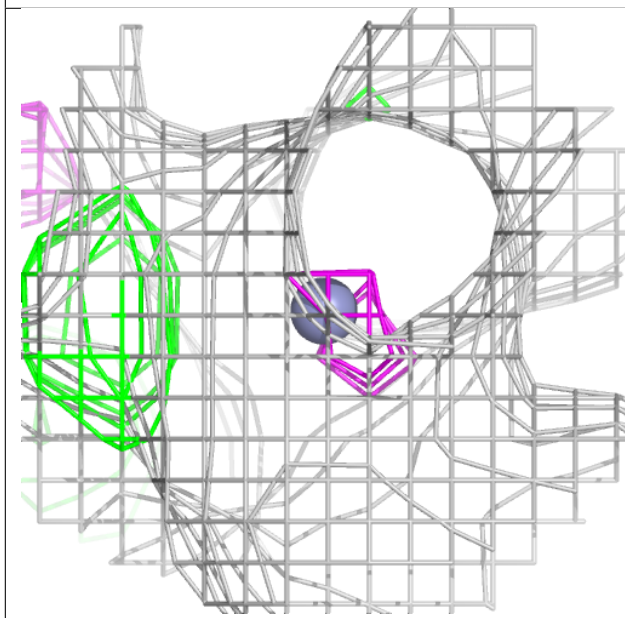
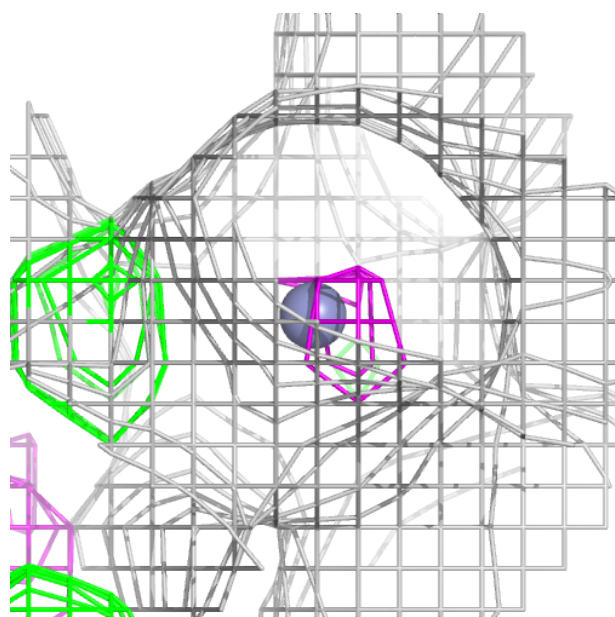
Electron density around ZN A 603:

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



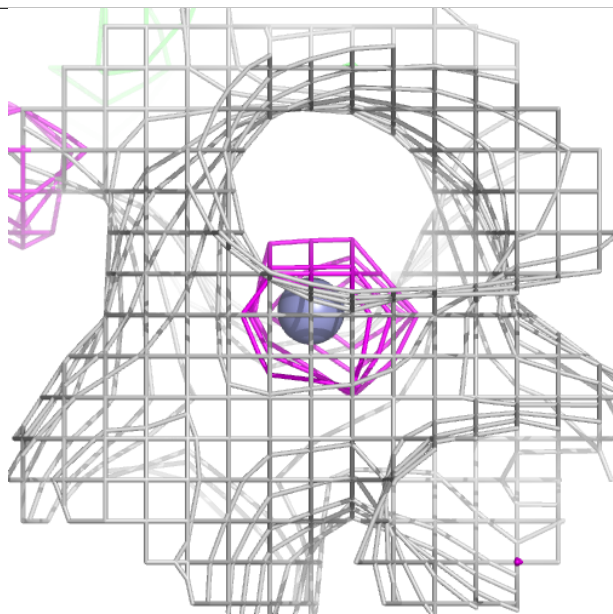
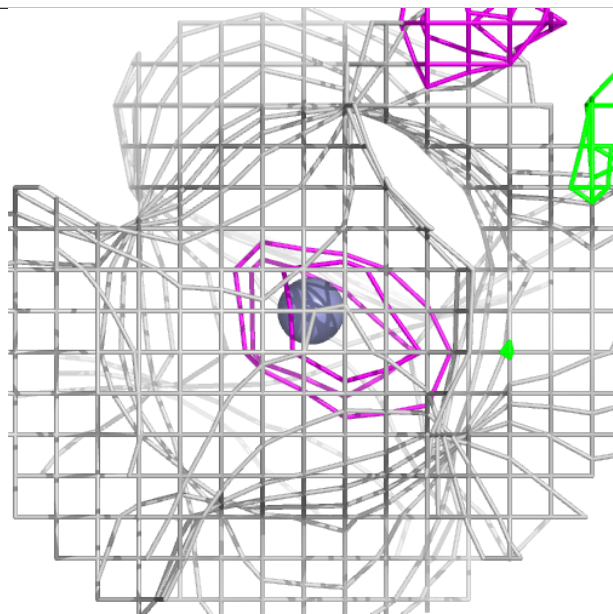
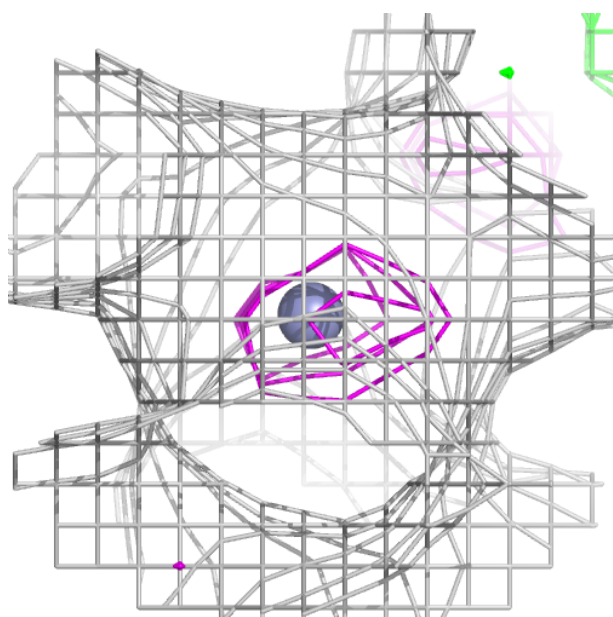
Electron density around ZN A 604:

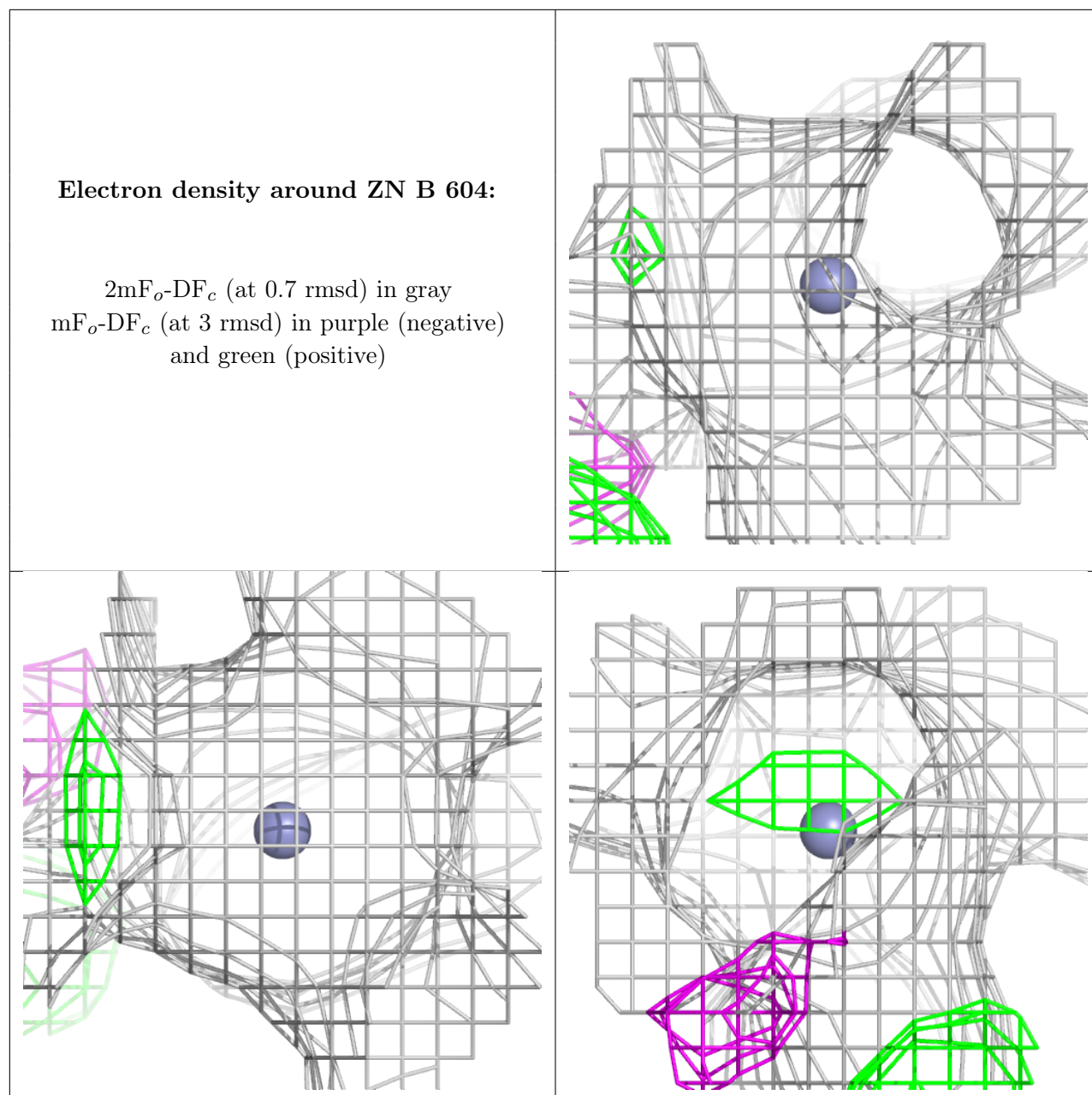
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 603:

$2mF_o-DF_c$ (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.