



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:32 AM UTC

PDB ID : 8P6F / pdb_00008p6f
Title : Crystal structure of PorX-Fj
Authors : Leone, P.
Deposited on : 2023-05-26
Resolution : 2.00 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
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

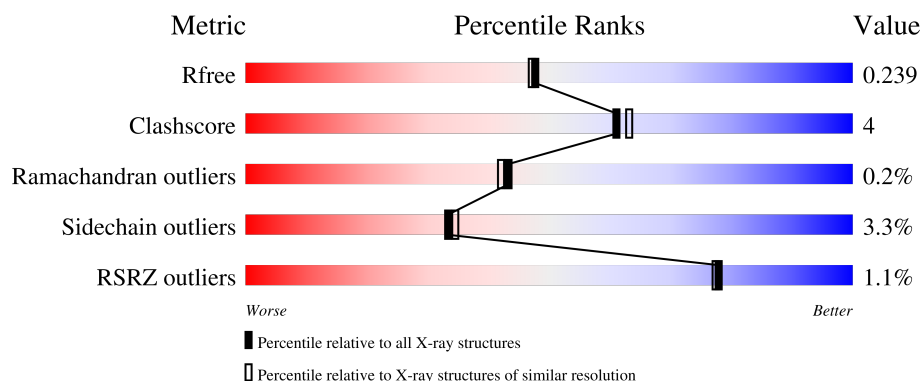
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	540	82% 12% • 5%
1	B	540	81% 13% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8988 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 Response regulator receiver domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4207	2731	665	796	15			
1	B	510	Total	C	N	O	S	0	0	0
			4191	2721	663	792	15			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0A1M5SPD1
A	-21	GLY	-	expression tag	UNP A0A1M5SPD1
A	-20	HIS	-	expression tag	UNP A0A1M5SPD1
A	-19	HIS	-	expression tag	UNP A0A1M5SPD1
A	-18	HIS	-	expression tag	UNP A0A1M5SPD1
A	-17	HIS	-	expression tag	UNP A0A1M5SPD1
A	-16	HIS	-	expression tag	UNP A0A1M5SPD1
A	-15	HIS	-	expression tag	UNP A0A1M5SPD1
A	-14	SER	-	expression tag	UNP A0A1M5SPD1
A	-13	SER	-	expression tag	UNP A0A1M5SPD1
A	-12	GLY	-	expression tag	UNP A0A1M5SPD1
A	-11	VAL	-	expression tag	UNP A0A1M5SPD1
A	-10	ASP	-	expression tag	UNP A0A1M5SPD1
A	-9	LEU	-	expression tag	UNP A0A1M5SPD1
A	-8	GLY	-	expression tag	UNP A0A1M5SPD1
A	-7	THR	-	expression tag	UNP A0A1M5SPD1
A	-6	GLU	-	expression tag	UNP A0A1M5SPD1
A	-5	ASN	-	expression tag	UNP A0A1M5SPD1
A	-4	LEU	-	expression tag	UNP A0A1M5SPD1
A	-3	TYR	-	expression tag	UNP A0A1M5SPD1
A	-2	PHE	-	expression tag	UNP A0A1M5SPD1
A	-1	GLN	-	expression tag	UNP A0A1M5SPD1
A	0	SER	-	expression tag	UNP A0A1M5SPD1
B	-22	MET	-	initiating methionine	UNP A0A1M5SPD1
B	-21	GLY	-	expression tag	UNP A0A1M5SPD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP A0A1M5SPD1
B	-19	HIS	-	expression tag	UNP A0A1M5SPD1
B	-18	HIS	-	expression tag	UNP A0A1M5SPD1
B	-17	HIS	-	expression tag	UNP A0A1M5SPD1
B	-16	HIS	-	expression tag	UNP A0A1M5SPD1
B	-15	HIS	-	expression tag	UNP A0A1M5SPD1
B	-14	SER	-	expression tag	UNP A0A1M5SPD1
B	-13	SER	-	expression tag	UNP A0A1M5SPD1
B	-12	GLY	-	expression tag	UNP A0A1M5SPD1
B	-11	VAL	-	expression tag	UNP A0A1M5SPD1
B	-10	ASP	-	expression tag	UNP A0A1M5SPD1
B	-9	LEU	-	expression tag	UNP A0A1M5SPD1
B	-8	GLY	-	expression tag	UNP A0A1M5SPD1
B	-7	THR	-	expression tag	UNP A0A1M5SPD1
B	-6	GLU	-	expression tag	UNP A0A1M5SPD1
B	-5	ASN	-	expression tag	UNP A0A1M5SPD1
B	-4	LEU	-	expression tag	UNP A0A1M5SPD1
B	-3	TYR	-	expression tag	UNP A0A1M5SPD1
B	-2	PHE	-	expression tag	UNP A0A1M5SPD1
B	-1	GLN	-	expression tag	UNP A0A1M5SPD1
B	0	SER	-	expression tag	UNP A0A1M5SPD1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- 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 2 2	0	0
3	B	2	Total Zn 2 2	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

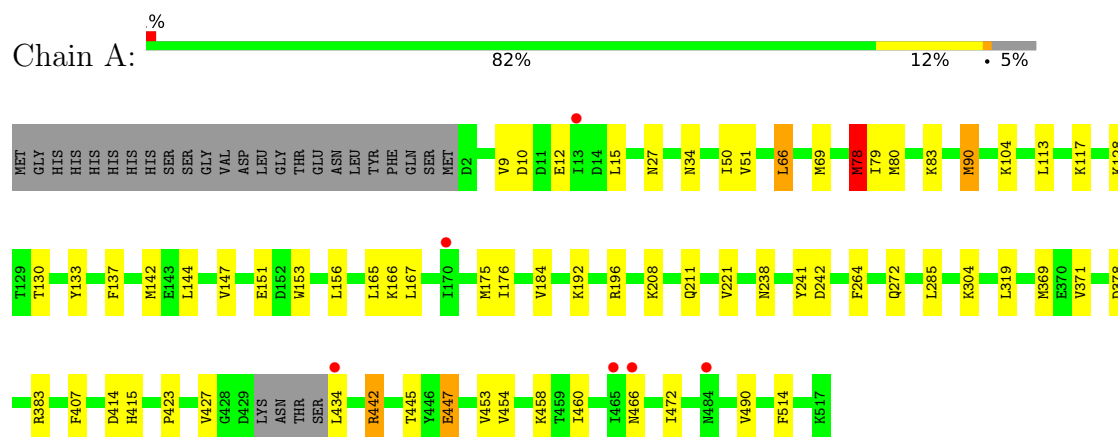
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	284	Total	O	0	0
			284	284		
5	B	276	Total	O	0	0
			276	276		

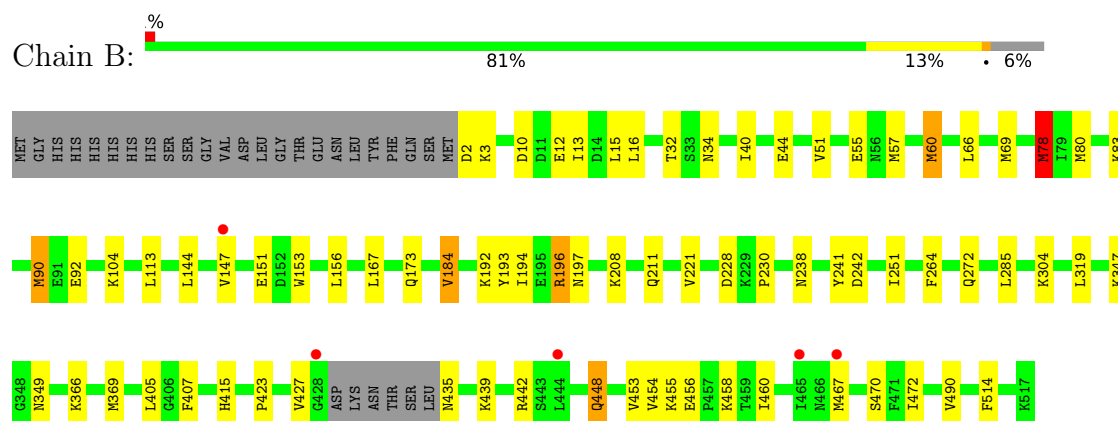
3 Residue-property plots [i](#)

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: Response regulator receiver domain-containing protein



- Molecule 1: Response regulator receiver domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.61Å 97.48Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.16 – 2.00 29.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.16-2.00) 99.9 (29.16-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.98Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.216 , 0.255 0.205 , 0.239	Depositor DCC
R_{free} test set	3710 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8988	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: ACT, ZN, MG

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	0.76	3/4298 (0.1%)	1.07	7/5802 (0.1%)
1	B	0.75	4/4282 (0.1%)	1.08	8/5780 (0.1%)
All	All	0.75	7/8580 (0.1%)	1.08	15/11582 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	MET	SD-CE	-8.23	1.58	1.79
1	A	78	MET	SD-CE	-8.22	1.59	1.79
1	B	60	MET	SD-CE	-7.92	1.59	1.79
1	B	78	MET	SD-CE	-7.50	1.60	1.79
1	B	57	MET	SD-CE	-7.41	1.61	1.79
1	B	90	MET	SD-CE	-6.82	1.62	1.79
1	A	142	MET	SD-CE	-6.15	1.64	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ASP	CA-C-N	6.50	133.95	121.54
1	B	2	ASP	C-N-CA	6.50	133.95	121.54
1	B	184	VAL	N-CA-CB	6.33	120.08	110.58
1	B	196	ARG	N-CA-C	-6.16	101.40	110.52
1	B	514	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	137	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	407	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	407	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	442	ARG	N-CA-C	5.38	116.95	111.14
1	B	242	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	514	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	55	GLU	CB-CG-CD	5.05	121.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	GLU	CA-C-N	5.02	127.32	120.54
1	A	447	GLU	C-N-CA	5.02	127.32	120.54
1	A	378	ASP	CA-CB-CG	5.02	117.62	112.60

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	4207	0	4223	37	0
1	B	4191	0	4208	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	3	0	0
4	B	20	0	15	1	0
5	A	284	0	0	4	0
5	B	276	0	0	0	0
All	All	8988	0	8449	70	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 4.

All (70) 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:427:VAL:HB	1:A:445:THR:HB	1.42	1.01
1:B:448:GLN:HE21	1:B:448:GLN:H	1.25	0.84
1:B:66:LEU:HD12	1:B:78:MET:HE2	1.71	0.71
1:A:113:LEU:HD23	1:B:90:MET:HG2	1.75	0.69
1:A:90:MET:HG2	1:B:113:LEU:HD23	1.77	0.67
1:A:130:THR:HA	1:A:175:MET:HE1	1.76	0.66
1:A:369:MET:HE3	1:B:369:MET:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HG12	1:B:32:THR:HB	1.77	0.64
1:A:133:TYR:HB3	1:A:175:MET:HE3	1.79	0.63
1:A:66:LEU:HD12	1:A:78:MET:HE2	1.79	0.63
1:A:69:MET:HB2	1:A:78:MET:HE1	1.79	0.62
1:B:69:MET:HB2	1:B:78:MET:HE1	1.81	0.61
1:A:50:ILE:HD11	1:A:79:ILE:HD12	1.83	0.61
1:B:193:TYR:O	1:B:196:ARG:O	2.19	0.61
1:B:51:VAL:HB	1:B:78:MET:CG	2.35	0.57
1:B:51:VAL:HB	1:B:78:MET:HG2	1.87	0.56
1:A:51:VAL:HB	1:A:78:MET:CG	2.35	0.55
1:A:51:VAL:HB	1:A:78:MET:HG2	1.89	0.55
1:A:128:LYS:HE3	1:B:92:GLU:HG3	1.88	0.54
1:B:456:GLU:HG2	1:B:467:MET:HE1	1.89	0.54
1:B:12:GLU:HB3	1:B:15:LEU:HD13	1.90	0.53
1:B:40:ILE:HD12	1:B:60:MET:HE1	1.91	0.53
1:B:44:GLU:OE1	4:B:608:ACT:O	2.30	0.50
1:A:221:VAL:HG21	1:A:319:LEU:HD13	1.94	0.50
1:B:144:LEU:HG	1:B:156:LEU:HD21	1.94	0.49
1:A:12:GLU:HB3	1:A:15:LEU:HD13	1.95	0.49
1:A:453:VAL:HG22	1:A:472:ILE:HG22	1.94	0.49
1:B:453:VAL:HG22	1:B:472:ILE:HG22	1.96	0.48
1:B:147:VAL:HG11	1:B:153:TRP:CD2	2.49	0.47
1:B:83:LYS:HG3	1:B:104:LYS:HD2	1.96	0.47
1:B:221:VAL:HG21	1:B:319:LEU:HD13	1.97	0.47
1:A:147:VAL:HG11	1:A:153:TRP:CD2	2.49	0.47
1:A:423:PRO:HB3	1:A:490:VAL:HG22	1.96	0.47
1:B:238:ASN:HA	1:B:415:HIS:O	2.15	0.46
1:A:10:ASP:O	1:A:34:ASN:HA	2.16	0.46
1:B:423:PRO:HB3	1:B:490:VAL:HG22	1.98	0.46
1:A:66:LEU:HA	1:A:78:MET:CE	2.46	0.46
1:A:238:ASN:HA	1:A:415:HIS:O	2.16	0.45
1:B:347:LYS:HE2	1:B:405:LEU:HD22	1.98	0.45
1:A:272:GLN:HG3	1:A:304:LYS:HB3	1.99	0.45
1:B:455:LYS:HA	1:B:470:SER:HB2	1.99	0.45
1:A:113:LEU:HA	1:B:90:MET:HE3	1.98	0.45
1:A:458:LYS:NZ	5:A:712:HOH:O	2.50	0.44
1:B:272:GLN:HG3	1:B:304:LYS:HB3	1.99	0.44
1:A:211:GLN:HA	1:A:264:PHE:O	2.18	0.44
1:B:211:GLN:HA	1:B:264:PHE:O	2.18	0.44
1:B:194:ILE:O	1:B:196:ARG:O	2.35	0.44
1:A:83:LYS:HG3	1:A:104:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HG	1:A:156:LEU:HD21	2.00	0.44
1:B:285:LEU:HD21	1:B:458:LYS:HE2	2.00	0.44
1:B:435:ASN:O	1:B:439:LYS:HE3	2.18	0.43
1:A:117:LYS:HD3	5:A:792:HOH:O	2.18	0.43
1:A:117:LYS:NZ	5:A:714:HOH:O	2.51	0.43
1:B:10:ASP:O	1:B:34:ASN:HA	2.18	0.43
1:A:369:MET:CE	1:B:369:MET:HG3	2.47	0.43
1:B:13:ILE:HD12	1:B:16:LEU:HD12	2.01	0.42
1:B:147:VAL:HG21	1:B:156:LEU:HD22	2.02	0.42
1:B:230:PRO:HB3	1:B:349:ASN:O	2.19	0.41
1:B:51:VAL:HB	1:B:78:MET:HG3	2.01	0.41
1:A:454:VAL:HG21	1:A:460:ILE:HD13	2.02	0.41
1:B:196:ARG:O	1:B:197:ASN:HB2	2.21	0.41
1:A:51:VAL:HB	1:A:78:MET:HG3	2.01	0.41
1:A:285:LEU:HD21	1:A:458:LYS:HE2	2.02	0.41
1:B:454:VAL:HG21	1:B:460:ILE:HD13	2.02	0.41
1:A:133:TYR:HD2	1:A:175:MET:HE3	1.86	0.41
1:A:242:ASP:HB2	1:A:383:ARG:HD3	2.03	0.40
1:A:166:LYS:NZ	5:A:703:HOH:O	2.55	0.40
1:A:192:LYS:O	1:A:196:ARG:HB2	2.22	0.40
1:A:414:ASP:CG	1:A:415:HIS:CD2	3.00	0.40
1:B:454:VAL:HG11	1:B:460:ILE:HG12	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	508/540 (94%)	495 (97%)	12 (2%)	1 (0%)	43	42
1	B	506/540 (94%)	490 (97%)	15 (3%)	1 (0%)	43	42
All	All	1014/1080 (94%)	985 (97%)	27 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	A	466	ASN

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	468/493 (95%)	452 (97%)	16 (3%)	32	33
1	B	466/493 (94%)	451 (97%)	15 (3%)	34	35
All	All	934/986 (95%)	903 (97%)	31 (3%)	33	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	27	ASN
1	A	66	LEU
1	A	78	MET
1	A	80	MET
1	A	151	GLU
1	A	165	LEU
1	A	167	LEU
1	A	176	ILE
1	A	184	VAL
1	A	208	LYS
1	A	241	TYR
1	A	371	VAL
1	A	434	LEU
1	A	442	ARG
1	A	447	GLU
1	B	78	MET
1	B	80	MET
1	B	151	GLU
1	B	167	LEU
1	B	173	GLN

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Mol	Chain	Res	Type
1	B	184	VAL
1	B	192	LYS
1	B	208	LYS
1	B	228	ASP
1	B	241	TYR
1	B	251	ILE
1	B	366	LYS
1	B	427	VAL
1	B	442	ARG
1	B	448	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	253	ASN
1	A	349	ASN
1	A	419	ASN
1	A	495	ASN
1	B	19	HIS
1	B	197	ASN
1	B	211	GLN
1	B	253	ASN
1	B	419	ASN
1	B	448	GLN
1	B	495	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	B	604	-	3,3,3	0.94	0	3,3,3	1.60	1 (33%)
4	ACT	A	604	-	3,3,3	0.90	0	3,3,3	1.60	1 (33%)
4	ACT	B	605	-	3,3,3	0.90	0	3,3,3	1.51	1 (33%)
4	ACT	B	606	-	3,3,3	0.77	0	3,3,3	1.61	1 (33%)
4	ACT	B	607	-	3,3,3	0.98	0	3,3,3	1.62	1 (33%)
4	ACT	B	608	-	3,3,3	0.70	0	3,3,3	1.90	1 (33%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	ACT	O-C-CH3	-2.51	112.25	122.53
4	B	607	ACT	OXT-C-O	2.21	130.22	122.03
4	A	604	ACT	OXT-C-O	2.15	130.01	122.03
4	B	604	ACT	OXT-C-O	2.06	129.66	122.03
4	B	605	ACT	OXT-C-O	2.02	129.51	122.03
4	B	606	ACT	OXT-C-O	2.01	129.47	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	608	ACT	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 [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	512/540 (94%)	0.06	6 (1%) 76 76	35, 49, 73, 97	0
1	B	510/540 (94%)	0.13	5 (0%) 79 79	35, 53, 77, 111	0
All	All	1022/1080 (94%)	0.09	11 (1%) 78 77	35, 51, 76, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	ASN	3.1
1	A	465	ILE	2.8
1	B	428	GLY	2.7
1	A	484	ASN	2.6
1	B	467	MET	2.5
1	B	465	ILE	2.2
1	A	170	ILE	2.2
1	A	434	LEU	2.2
1	A	13	ILE	2.1
1	B	444	LEU	2.1
1	B	147	VAL	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

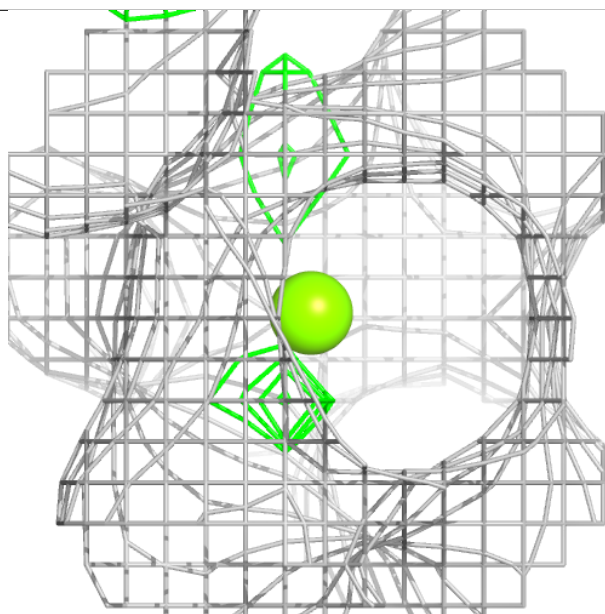
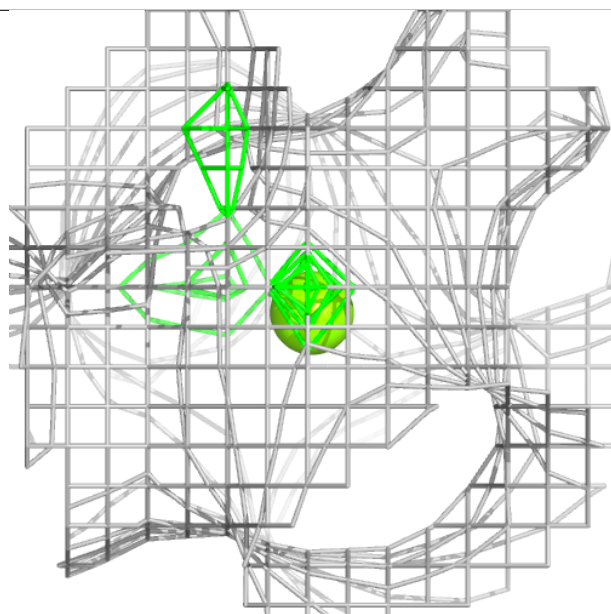
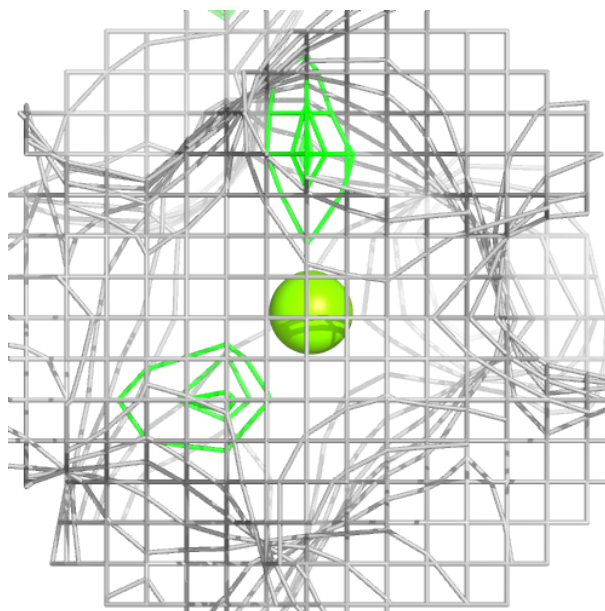
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	B	608	4/4	0.65	0.17	65,65,65,65	0
4	ACT	B	604	4/4	0.68	0.14	85,85,85,85	0
4	ACT	B	607	4/4	0.70	0.16	81,81,81,81	0
4	ACT	B	606	4/4	0.72	0.17	84,85,85,85	0
4	ACT	A	604	4/4	0.76	0.14	89,89,89,89	0
4	ACT	B	605	4/4	0.79	0.13	82,82,82,82	0
2	MG	B	601	1/1	0.97	0.10	40,40,40,40	0
2	MG	A	601	1/1	0.98	0.10	37,37,37,37	0
3	ZN	B	603	1/1	0.98	0.04	45,45,45,45	0
3	ZN	A	603	1/1	0.99	0.04	41,41,41,41	0
3	ZN	B	602	1/1	0.99	0.04	44,44,44,44	0
3	ZN	A	602	1/1	0.99	0.04	41,41,41,41	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.

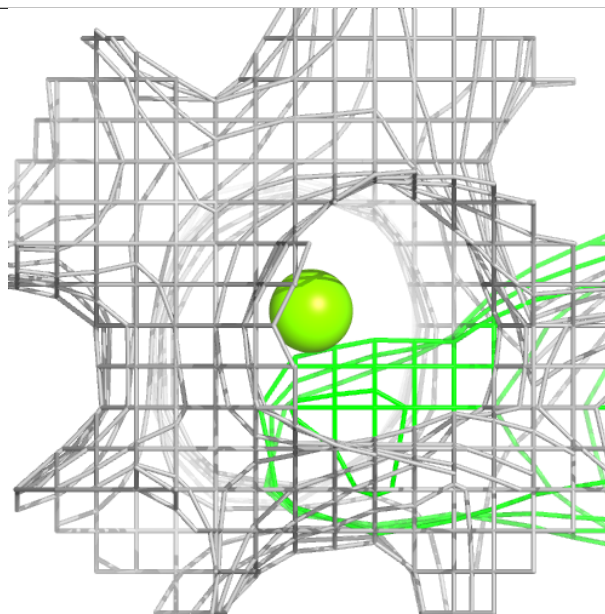
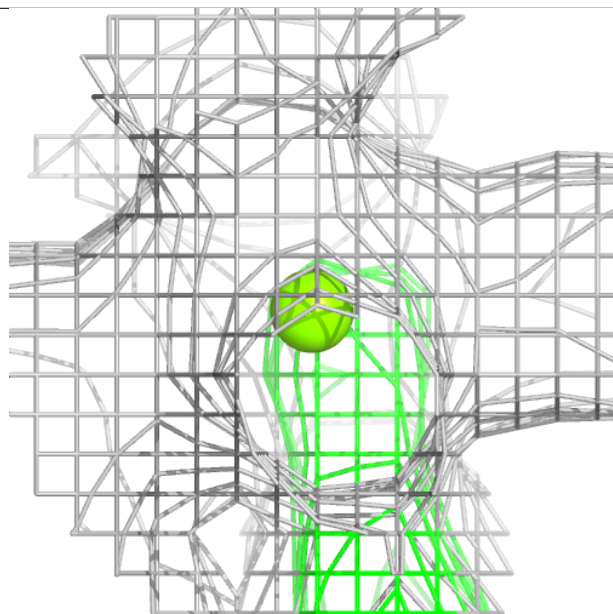
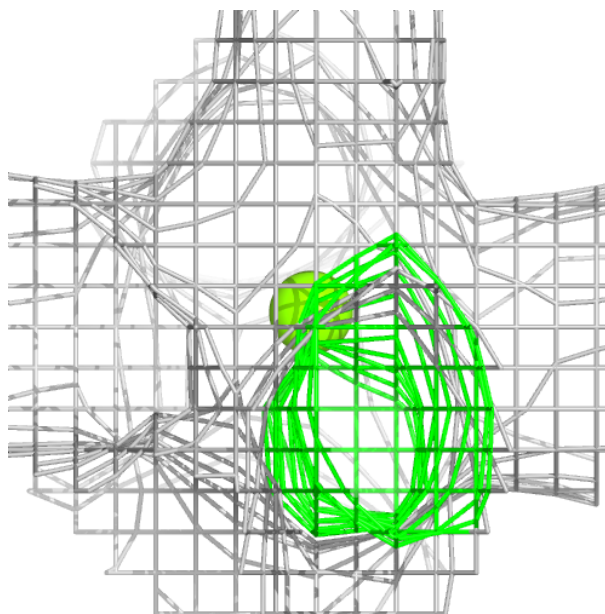
Electron density around MG B 601:

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



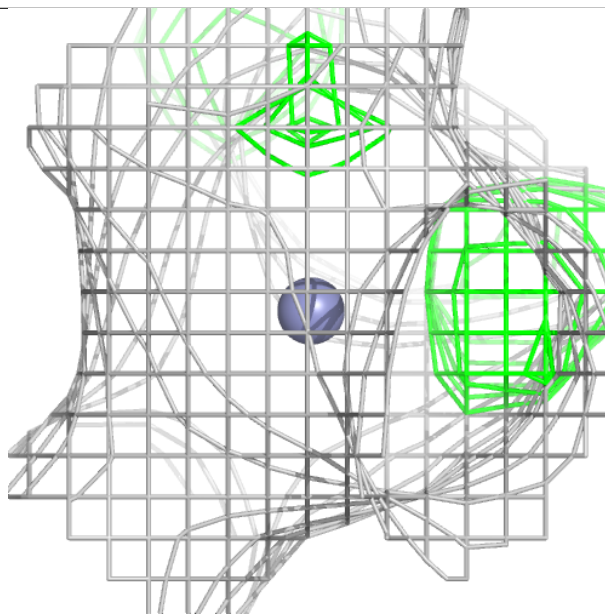
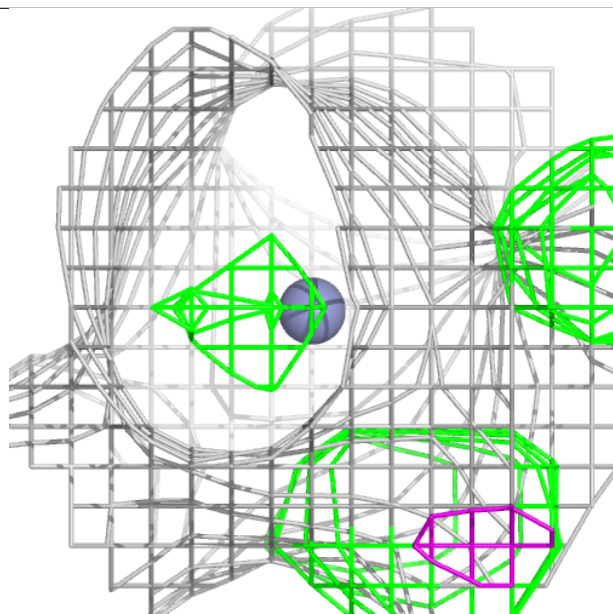
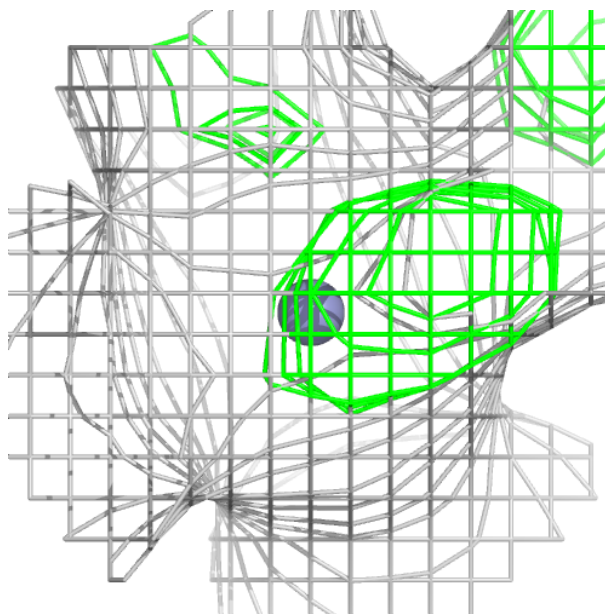
Electron density around MG A 601:

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and green (positive)



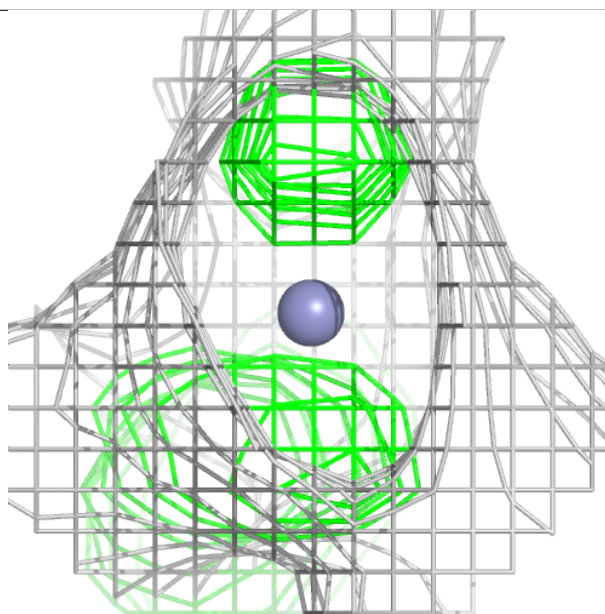
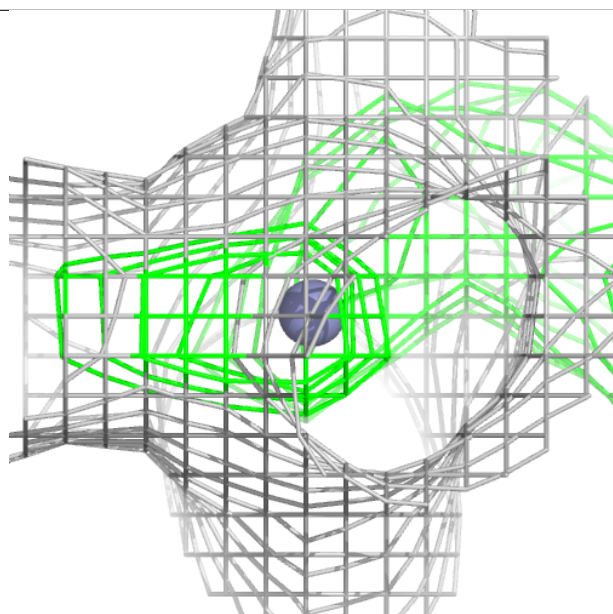
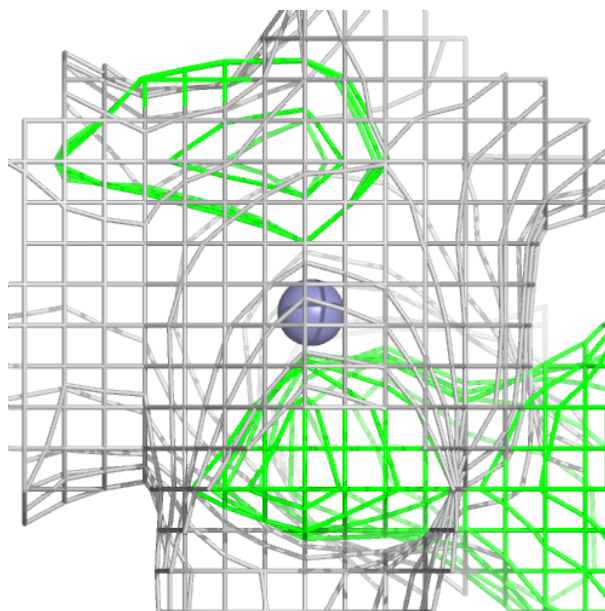
Electron density around ZN B 603:

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



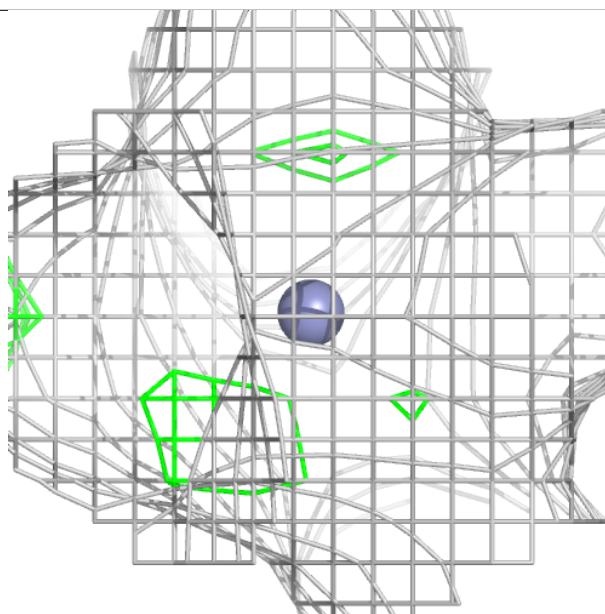
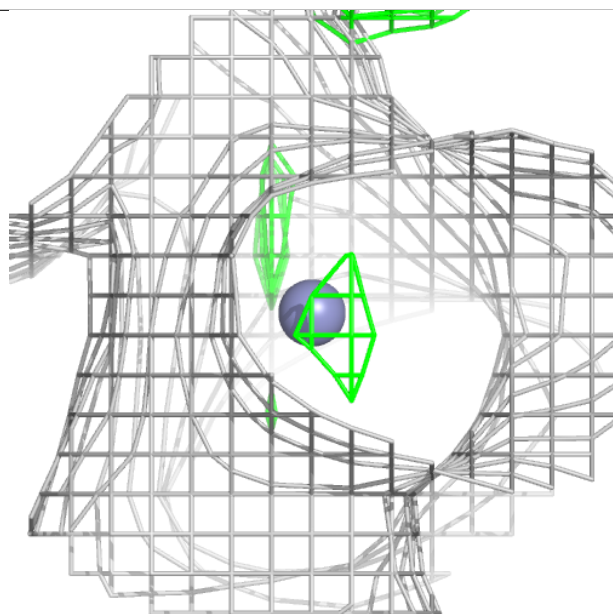
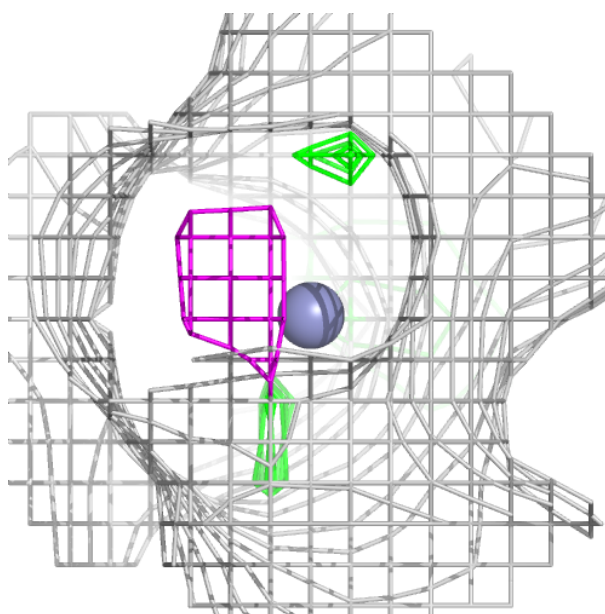
Electron density around ZN A 603:

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and green (positive)



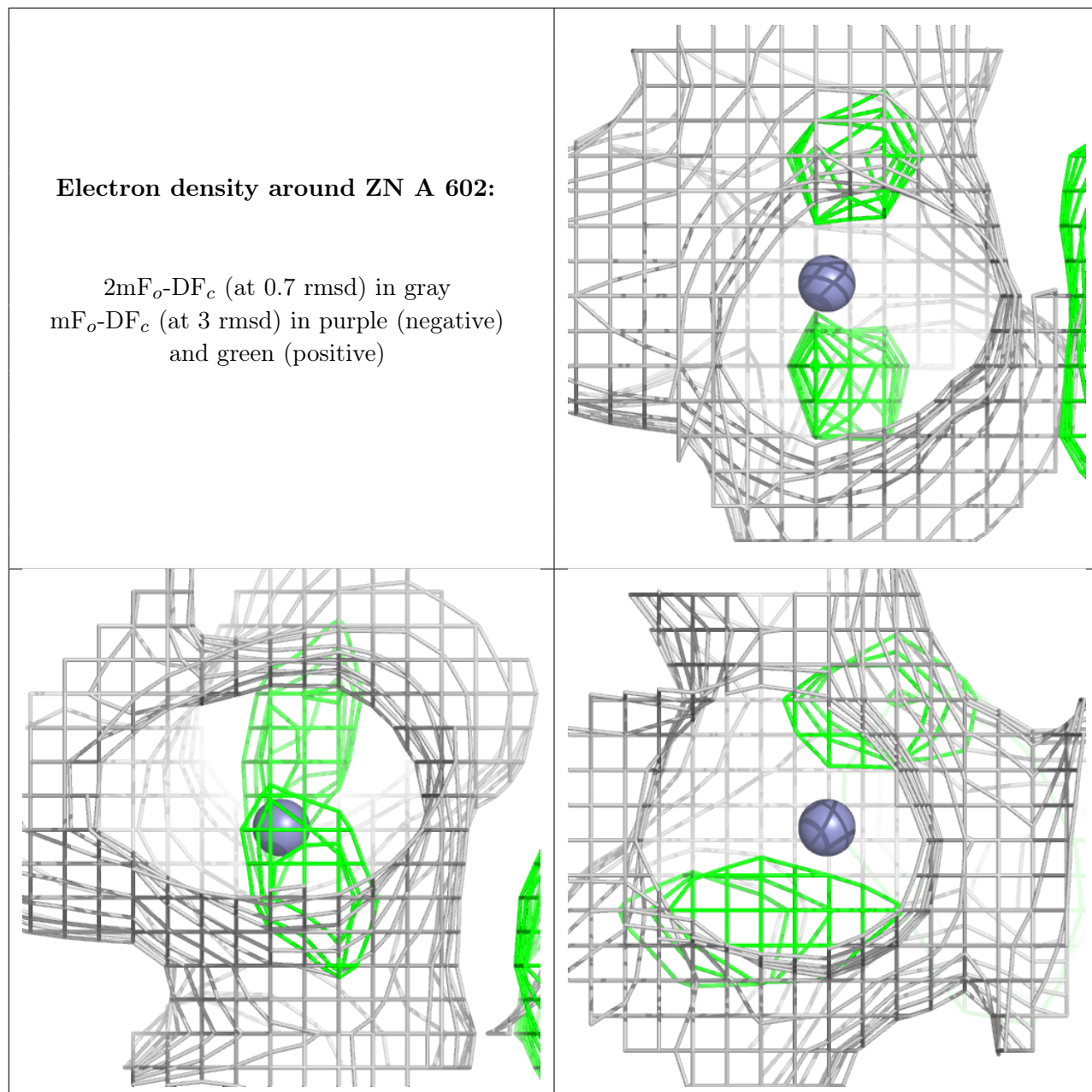
Electron density around ZN B 602:

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



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.