Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2022 – 01:22 am BST

PDB ID	:	7BBJ
Title	:	CD73 in complex with the humanized antagonistic antibody mAb19
Authors	:	Boettcher, J.; Han, F.
Deposited on	:	2020-12-17
Resolution	:	2.72 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 (i) 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:

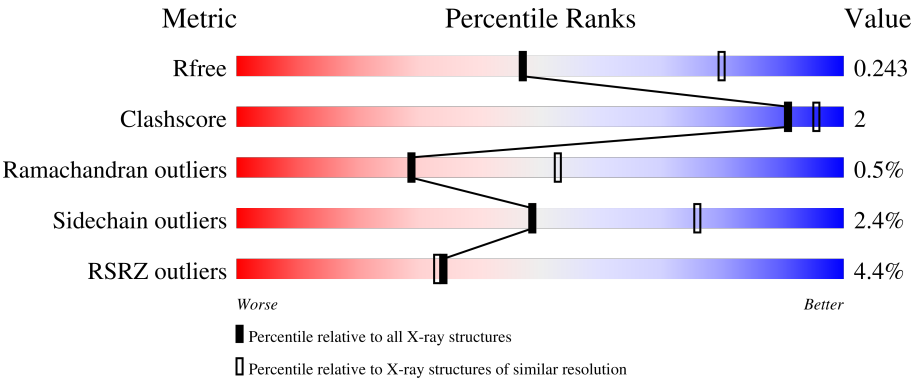
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 <=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	546	89% 7% .
1	B	546	89% 7% .
2	H	222	10% 92% 5% ..
2	M	222	13% 86% 6% 8%
3	L	214	4% 92% 7% .

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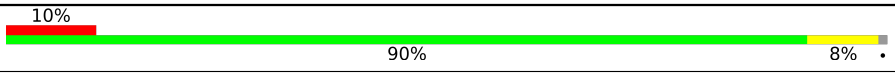
Mol	Chain	Length	Quality of chain
3	N	214	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14874 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4079	2591	693	776	19			
1	B	524	Total	C	N	O	S	0	0	0
			4079	2591	693	776	19			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P21589
A	5	ALA	-	expression tag	UNP P21589
A	6	HIS	-	expression tag	UNP P21589
A	7	HIS	-	expression tag	UNP P21589
A	8	HIS	-	expression tag	UNP P21589
A	9	HIS	-	expression tag	UNP P21589
A	10	HIS	-	expression tag	UNP P21589
A	11	HIS	-	expression tag	UNP P21589
A	12	VAL	-	expression tag	UNP P21589
A	13	GLY	-	expression tag	UNP P21589
A	14	THR	-	expression tag	UNP P21589
A	15	GLY	-	expression tag	UNP P21589
A	16	SER	-	expression tag	UNP P21589
A	17	ASN	-	expression tag	UNP P21589
A	18	ASP	-	expression tag	UNP P21589
A	19	ASP	-	expression tag	UNP P21589
A	20	ASP	-	expression tag	UNP P21589
A	21	ASP	-	expression tag	UNP P21589
A	22	LYS	-	expression tag	UNP P21589
A	23	SER	-	expression tag	UNP P21589
A	24	PRO	-	expression tag	UNP P21589
A	25	ASP	-	expression tag	UNP P21589
A	26	PRO	-	expression tag	UNP P21589
A	53	ASP	ASN	engineered mutation	UNP P21589
A	145	SER	LYS	engineered mutation	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
A	147	SER	LYS	engineered mutation	UNP P21589
A	311	ASP	ASN	engineered mutation	UNP P21589
A	333	ASP	ASN	engineered mutation	UNP P21589
A	376	ALA	THR	conflict	UNP P21589
A	403	ASP	ASN	engineered mutation	UNP P21589
A	478	SER	LYS	engineered mutation	UNP P21589
B	4	MET	-	initiating methionine	UNP P21589
B	5	ALA	-	expression tag	UNP P21589
B	6	HIS	-	expression tag	UNP P21589
B	7	HIS	-	expression tag	UNP P21589
B	8	HIS	-	expression tag	UNP P21589
B	9	HIS	-	expression tag	UNP P21589
B	10	HIS	-	expression tag	UNP P21589
B	11	HIS	-	expression tag	UNP P21589
B	12	VAL	-	expression tag	UNP P21589
B	13	GLY	-	expression tag	UNP P21589
B	14	THR	-	expression tag	UNP P21589
B	15	GLY	-	expression tag	UNP P21589
B	16	SER	-	expression tag	UNP P21589
B	17	ASN	-	expression tag	UNP P21589
B	18	ASP	-	expression tag	UNP P21589
B	19	ASP	-	expression tag	UNP P21589
B	20	ASP	-	expression tag	UNP P21589
B	21	ASP	-	expression tag	UNP P21589
B	22	LYS	-	expression tag	UNP P21589
B	23	SER	-	expression tag	UNP P21589
B	24	PRO	-	expression tag	UNP P21589
B	25	ASP	-	expression tag	UNP P21589
B	26	PRO	-	expression tag	UNP P21589
B	53	ASP	ASN	engineered mutation	UNP P21589
B	145	SER	LYS	engineered mutation	UNP P21589
B	147	SER	LYS	engineered mutation	UNP P21589
B	311	ASP	ASN	engineered mutation	UNP P21589
B	333	ASP	ASN	engineered mutation	UNP P21589
B	376	ALA	THR	conflict	UNP P21589
B	403	ASP	ASN	engineered mutation	UNP P21589
B	478	SER	LYS	engineered mutation	UNP P21589

- Molecule 2 is a protein called heavy chain mAb19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1641	1039	271	322	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	205	Total	C	N	O	S	0	0	0
			1565	996	257	303	9			

- Molecule 3 is a protein called light chain mAB19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1643	1029	281	328	5			
3	N	211	Total	C	N	O	S	0	0	0
			1643	1029	281	328	5			

- 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	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	88	Total	O	0	0
			88	88		
6	H	5	Total	O	0	0
			5	5		
6	L	6	Total	O	0	0
			6	6		
6	M	9	Total	O	0	0
			9	9		

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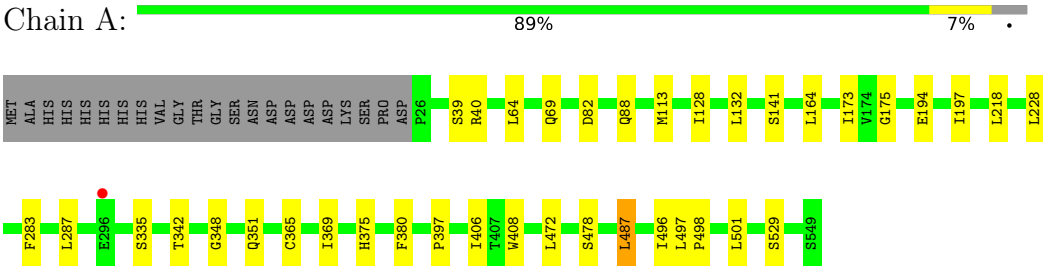
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	4	Total O 4 4	0	0

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.

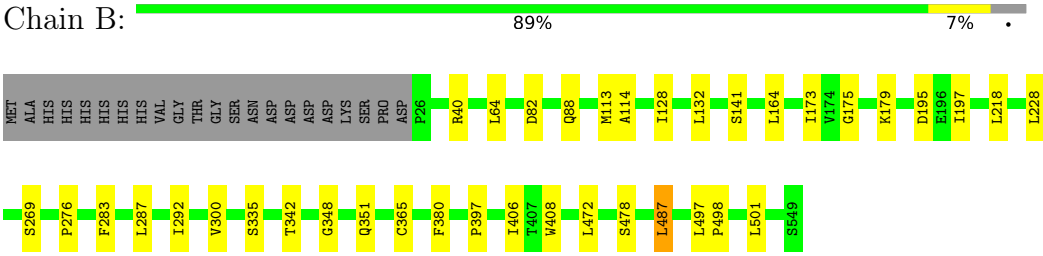
• Molecule 1: 5'-nucleotidase

Chain A:



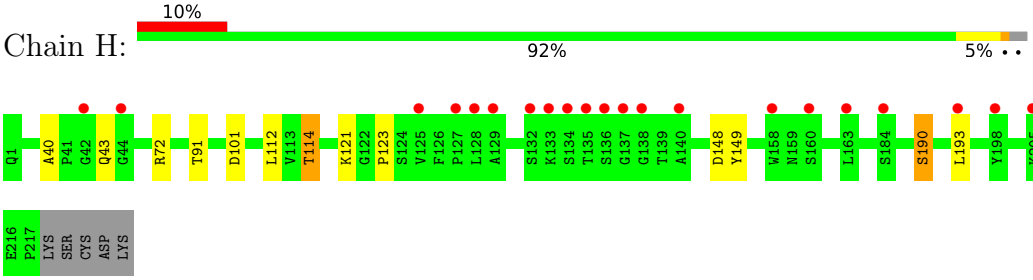
• Molecule 1: 5'-nucleotidase

Chain B:



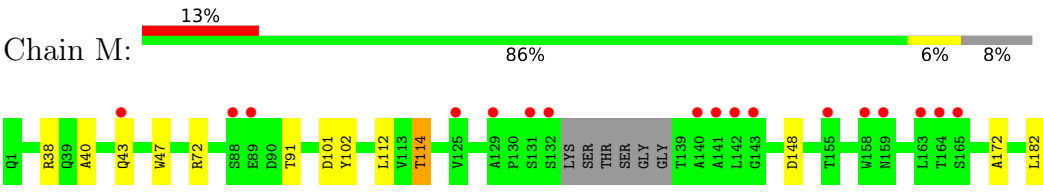
• Molecule 2: heavy chain mAb19

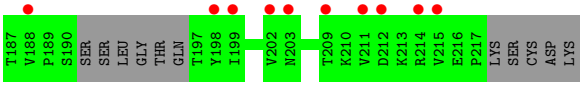
Chain H:



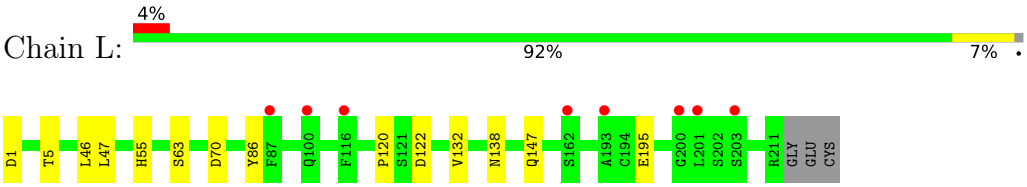
• Molecule 2: heavy chain mAb19

Chain M:

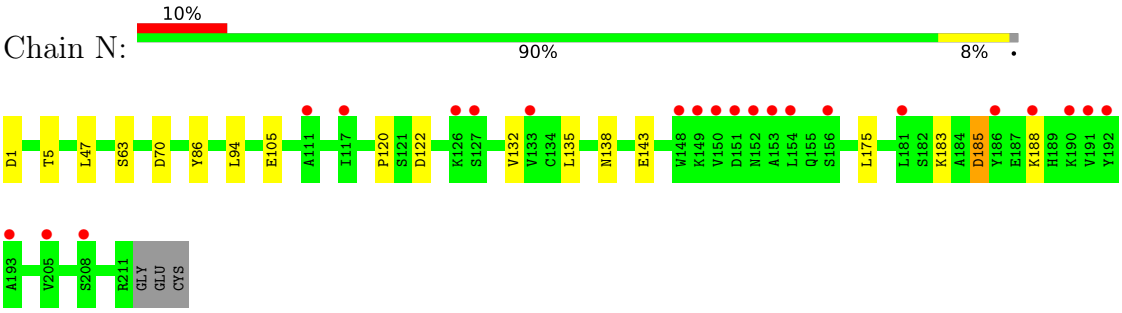




• Molecule 3: light chain mAB19



• Molecule 3: light chain mAB19



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.35Å 67.74Å 150.05Å 90.00° 100.13° 90.00°	Depositor
Resolution (Å)	39.83 – 2.72 39.83 – 2.72	Depositor EDS
% Data completeness (in resolution range)	83.5 (39.83-2.72) 83.6 (39.83-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.208 , 0.234 0.216 , 0.243	Depositor DCC
R_{free} test set	2990 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14874	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 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	0.40	0/4166	0.64	0/5645
1	B	0.39	0/4166	0.64	0/5645
2	H	0.37	0/1682	0.58	0/2293
2	M	0.38	0/1604	0.58	0/2186
3	L	0.38	0/1681	0.56	0/2283
3	N	0.37	0/1681	0.56	0/2283
All	All	0.39	0/14980	0.61	0/20335

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	4079	0	4041	14	0
1	B	4079	0	4041	17	0
2	H	1641	0	1617	4	0
2	M	1565	0	1540	6	0
3	L	1643	0	1599	4	0
3	N	1643	0	1599	5	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	106	0	0	0	0
6	B	88	0	0	0	0
6	H	5	0	0	0	0
6	L	6	0	0	0	0
6	M	9	0	0	0	0
6	N	4	0	0	0	0
All	All	14874	0	14437	48	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 (48) 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:335:SER:HA	1:B:408:TRP:HB3	1.75	0.67
1:A:335:SER:HA	1:A:408:TRP:HB3	1.76	0.65
2:H:190:SER:HA	2:H:193:LEU:HD23	1.86	0.57
1:A:164:LEU:HD13	1:A:173:ILE:HD12	1.87	0.56
1:B:164:LEU:HD13	1:B:173:ILE:HD12	1.87	0.56
1:A:197:ILE:HD11	1:A:228:LEU:HB3	1.89	0.53
1:B:197:ILE:HD11	1:B:228:LEU:HB3	1.91	0.53
1:A:348:GLY:H	1:A:397:PRO:HB3	1.74	0.53
1:B:40:ARG:HG3	1:B:283:PHE:HB3	1.91	0.52
1:B:348:GLY:H	1:B:397:PRO:HB3	1.73	0.52
1:B:179:LYS:HD3	1:B:195:ASP:HA	1.93	0.51
2:M:91:THR:HG23	2:M:114:THR:HA	1.94	0.50
1:A:40:ARG:HG3	1:A:283:PHE:HB3	1.94	0.50
1:A:82:ASP:HB3	1:A:113:MET:HG3	1.95	0.48
2:H:91:THR:HG23	2:H:114:THR:HA	1.95	0.48
1:B:342:THR:HB	1:B:406:ILE:HD11	1.96	0.47
1:A:175:GLY:HA2	1:A:218:LEU:O	2.15	0.47
1:B:82:ASP:HB3	1:B:113:MET:HG3	1.96	0.47
2:M:40:ALA:HB3	2:M:43:GLN:HB2	1.97	0.47
1:B:114:ALA:HB2	1:B:218:LEU:HG	1.97	0.47
1:B:175:GLY:HA2	1:B:218:LEU:O	2.15	0.47
1:B:64:LEU:HD11	1:B:287:LEU:HD13	1.97	0.47
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.96	0.46
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:VAL:HG22	1:B:276:PRO:HG2	1.97	0.46
1:A:342:THR:HB	1:A:406:ILE:HD11	1.98	0.46
1:A:369:ILE:HD13	1:A:496:ILE:HD12	1.97	0.45
1:A:64:LEU:HD11	1:A:287:LEU:HD13	1.98	0.45
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.98	0.45
2:M:185:VAL:HG21	3:N:135:LEU:HD11	2.00	0.44
3:L:46:LEU:HD23	3:L:55:HIS:HD2	1.83	0.44
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.99	0.44
2:M:101:ASP:HB3	2:M:102:TYR:CD2	2.53	0.44
1:A:472:LEU:HD23	1:A:487:LEU:HD22	1.99	0.43
2:H:123:PRO:HB3	2:H:149:TYR:HB3	2.00	0.43
2:M:47:TRP:CH2	3:N:94:LEU:HD22	2.54	0.43
1:A:231:GLN:HA	1:A:269:SER:HA	2.00	0.43
1:B:231:GLN:HA	1:B:269:SER:HA	2.00	0.42
1:B:472:LEU:HD23	1:B:487:LEU:HD22	2.00	0.42
3:N:185:ASP:HA	3:N:188:LYS:HD2	2.01	0.42
1:B:498:PRO:HG2	1:B:501:LEU:HG	2.03	0.41
2:M:172:ALA:HA	2:M:182:LEU:HB3	2.03	0.41
1:A:128:ILE:HA	1:A:132:LEU:HB2	2.02	0.41
1:B:128:ILE:HA	1:B:132:LEU:HB2	2.03	0.41
1:A:498:PRO:HG2	1:A:501:LEU:HG	2.02	0.40
1:B:292:ILE:HG23	1:B:300:VAL:HG13	2.02	0.40
3:N:47:LEU:HD11	3:N:86:TYR:HE2	1.86	0.40
3:L:47:LEU:HD11	3:L:86:TYR:HE2	1.86	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	522/546 (96%)	497 (95%)	22 (4%)	3 (1%)	25 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/546 (96%)	496 (95%)	24 (5%)	2 (0%)	34	58
2	H	215/222 (97%)	205 (95%)	9 (4%)	1 (0%)	29	53
2	M	199/222 (90%)	190 (96%)	8 (4%)	1 (0%)	29	53
3	L	209/214 (98%)	196 (94%)	12 (6%)	1 (0%)	29	53
3	N	209/214 (98%)	191 (91%)	16 (8%)	2 (1%)	15	35
All	All	1876/1964 (96%)	1775 (95%)	91 (5%)	10 (0%)	29	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	138	ASN
3	N	138	ASN
1	A	141	SER
1	B	141	SER
2	H	148	ASP
2	M	148	ASP
1	A	88	GLN
1	B	88	GLN
3	N	143	GLU
1	A	375	HIS

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	451/470 (96%)	441 (98%)	10 (2%)	52	78
1	B	451/470 (96%)	445 (99%)	6 (1%)	69	86
2	H	186/191 (97%)	180 (97%)	6 (3%)	39	67
2	M	177/191 (93%)	173 (98%)	4 (2%)	50	77
3	L	188/190 (99%)	183 (97%)	5 (3%)	44	72
3	N	188/190 (99%)	179 (95%)	9 (5%)	25	51
All	All	1641/1702 (96%)	1601 (98%)	40 (2%)	49	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	69	GLN
1	A	194	GLU
1	A	351	GLN
1	A	365	CYS
1	A	380	PHE
1	A	478	SER
1	A	487	LEU
1	A	497	LEU
1	A	529	SER
1	B	351	GLN
1	B	365	CYS
1	B	380	PHE
1	B	478	SER
1	B	487	LEU
1	B	497	LEU
2	H	72	ARG
2	H	101	ASP
2	H	112	LEU
2	H	114	THR
2	H	121	LYS
2	H	190	SER
3	L	1	ASP
3	L	5	THR
3	L	63	SER
3	L	70	ASP
3	L	122	ASP
2	M	38	ARG
2	M	72	ARG
2	M	112	LEU
2	M	114	THR
3	N	1	ASP
3	N	5	THR
3	N	63	SER
3	N	70	ASP
3	N	105	GLU
3	N	122	ASP
3	N	175	LEU
3	N	183	LYS
3	N	185	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
3	L	55	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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, 95^{th} 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	524/546 (95%)	-0.31	1 (0%) 95 96	31, 48, 72, 96	0
1	B	524/546 (95%)	-0.29	0 100 100	33, 48, 73, 97	0
2	H	217/222 (97%)	0.48	23 (10%) 6 4	66, 100, 136, 152	0
2	M	205/222 (92%)	0.77	29 (14%) 2 2	68, 111, 153, 164	0
3	L	211/214 (98%)	0.27	8 (3%) 40 40	61, 97, 122, 138	0
3	N	211/214 (98%)	0.62	22 (10%) 6 5	57, 106, 164, 192	0
All	All	1892/1964 (96%)	0.07	83 (4%) 34 33	31, 65, 139, 192	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	150	VAL	9.4
3	N	127	SER	6.7
2	H	134	SER	6.7
2	M	186	VAL	6.2
2	M	199	ILE	5.2
3	N	192	TYR	5.1
2	H	136	SER	4.9
3	N	193	ALA	4.9
2	H	133	LYS	4.8
2	H	137	GLY	4.6
2	M	125	VAL	4.6
2	M	214	ARG	4.5
3	L	87	PHE	4.4
2	M	165	SER	4.1
2	H	135	THR	4.0
2	H	44	GLY	4.0
3	L	100	GLN	3.9
3	N	153	ALA	3.8
3	N	188	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	138	GLY	3.8
3	N	149	LYS	3.7
3	N	152	ASN	3.7
3	N	205	VAL	3.5
2	M	158	TRP	3.4
3	N	190	LYS	3.3
2	M	211	VAL	3.2
3	N	181	LEU	3.2
2	M	198	TYR	3.2
2	H	205	LYS	3.1
2	M	142	LEU	3.0
3	L	203	SER	3.0
2	H	132	SER	3.0
2	H	193	LEU	2.9
2	M	203	ASN	2.8
2	M	184	SER	2.8
3	N	111	ALA	2.8
3	L	201	LEU	2.8
3	L	116	PHE	2.7
2	M	155	THR	2.7
2	H	140	ALA	2.6
2	M	143	GLY	2.6
3	N	133	VAL	2.6
2	M	188	VAL	2.6
2	M	140	ALA	2.5
3	N	117	ILE	2.5
2	H	215	VAL	2.5
3	N	154	LEU	2.5
3	N	208	SER	2.5
2	M	159	ASN	2.5
2	M	89	GLU	2.4
3	L	200	GLY	2.4
3	N	126	LYS	2.4
3	N	156	SER	2.4
2	H	127	PRO	2.3
3	L	193	ALA	2.3
2	H	160	SER	2.3
2	M	215	VAL	2.3
2	M	129	ALA	2.3
2	M	43	GLN	2.3
2	H	158	TRP	2.2
1	A	296	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	125	VAL	2.2
2	H	163	LEU	2.2
2	M	88	SER	2.2
2	H	42	GLY	2.2
2	H	184	SER	2.1
2	M	131	SER	2.1
2	M	163	LEU	2.1
2	H	198	TYR	2.1
2	M	202	VAL	2.1
2	H	129	ALA	2.1
2	M	141	ALA	2.1
2	M	209	THR	2.1
2	H	212	ASP	2.1
3	N	151	ASP	2.1
3	N	191	VAL	2.1
3	N	148	TRP	2.1
3	N	186	TYR	2.1
2	M	212	ASP	2.1
3	L	162	SER	2.1
2	H	128	LEU	2.0
2	M	132	SER	2.0
2	M	164	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, 95^{th} 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
5	MG	A	803	1/1	0.93	0.06	59,59,59,59	0

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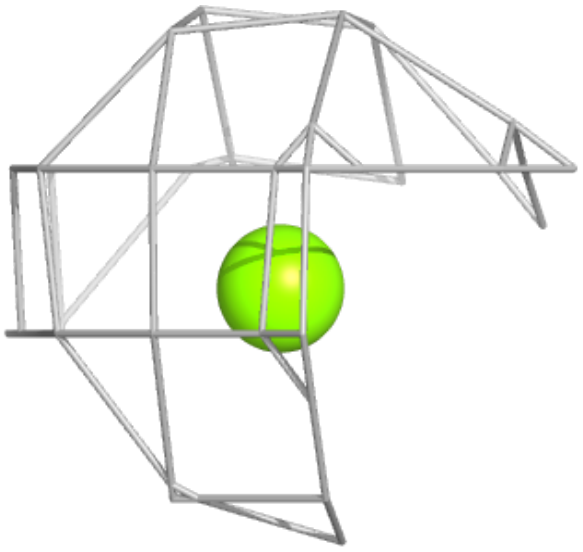
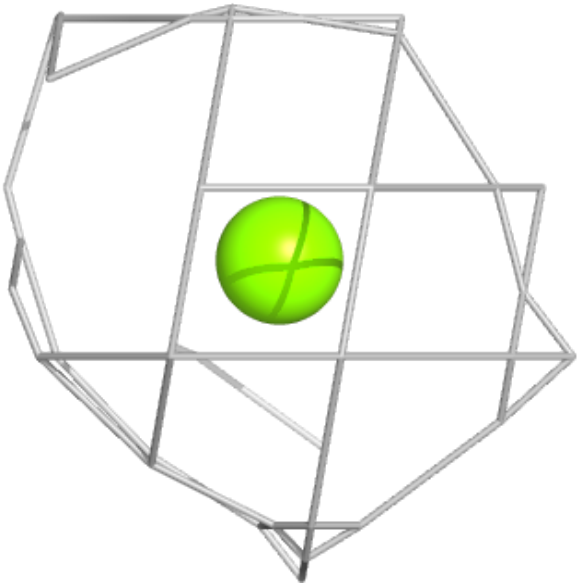
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	803	1/1	0.94	0.06	53,53,53,53	0
4	ZN	B	802	1/1	0.99	0.19	41,41,41,41	0
4	ZN	A	801	1/1	0.99	0.16	57,57,57,57	0
4	ZN	B	801	1/1	0.99	0.20	53,53,53,53	0
4	ZN	A	802	1/1	1.00	0.15	42,42,42,42	0

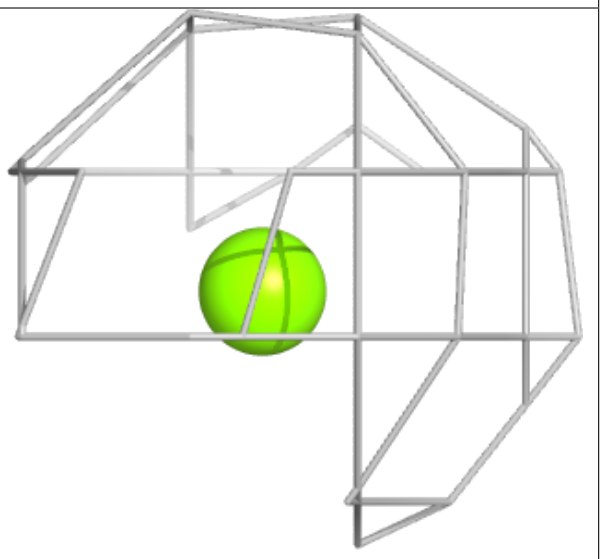
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MG A 803:

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

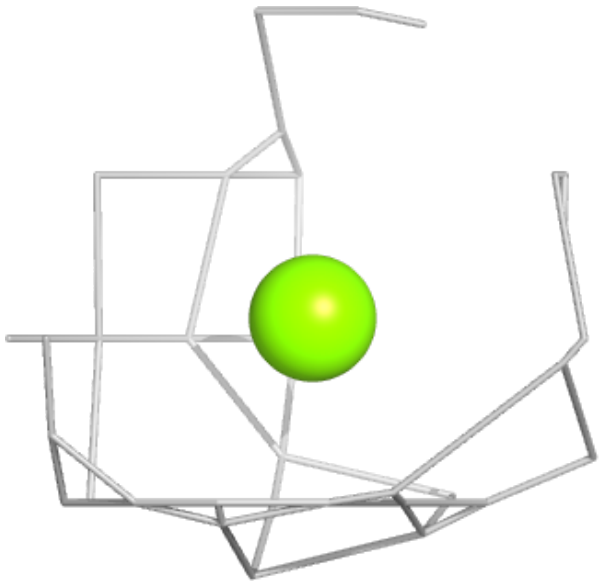


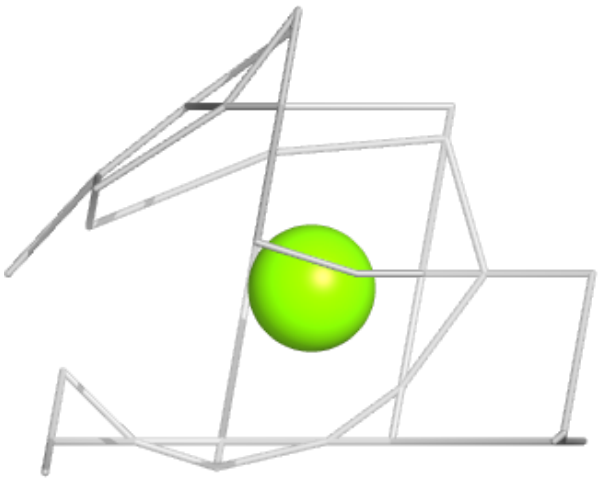


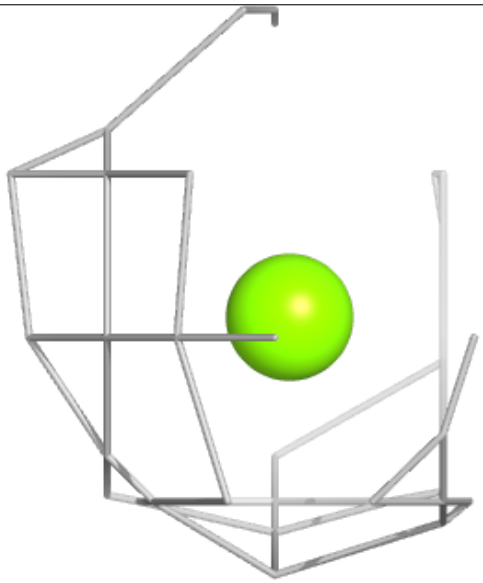


Electron density around MG B 803:

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

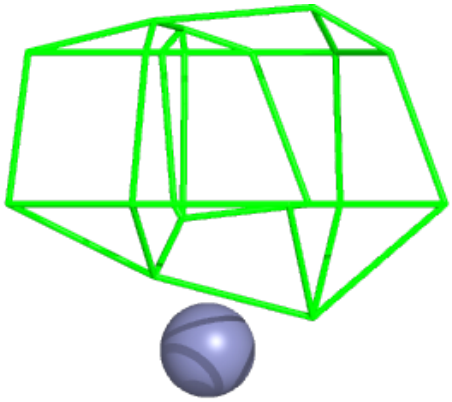


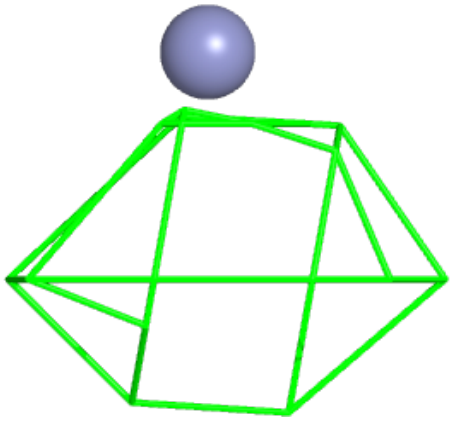


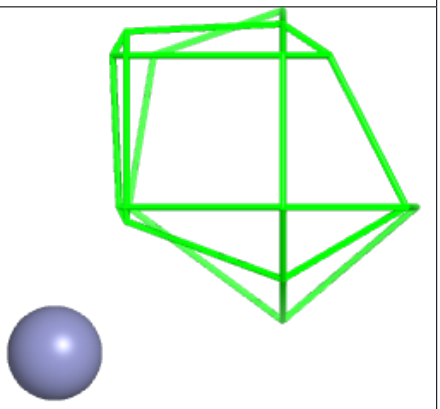


Electron density around ZN B 802:

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

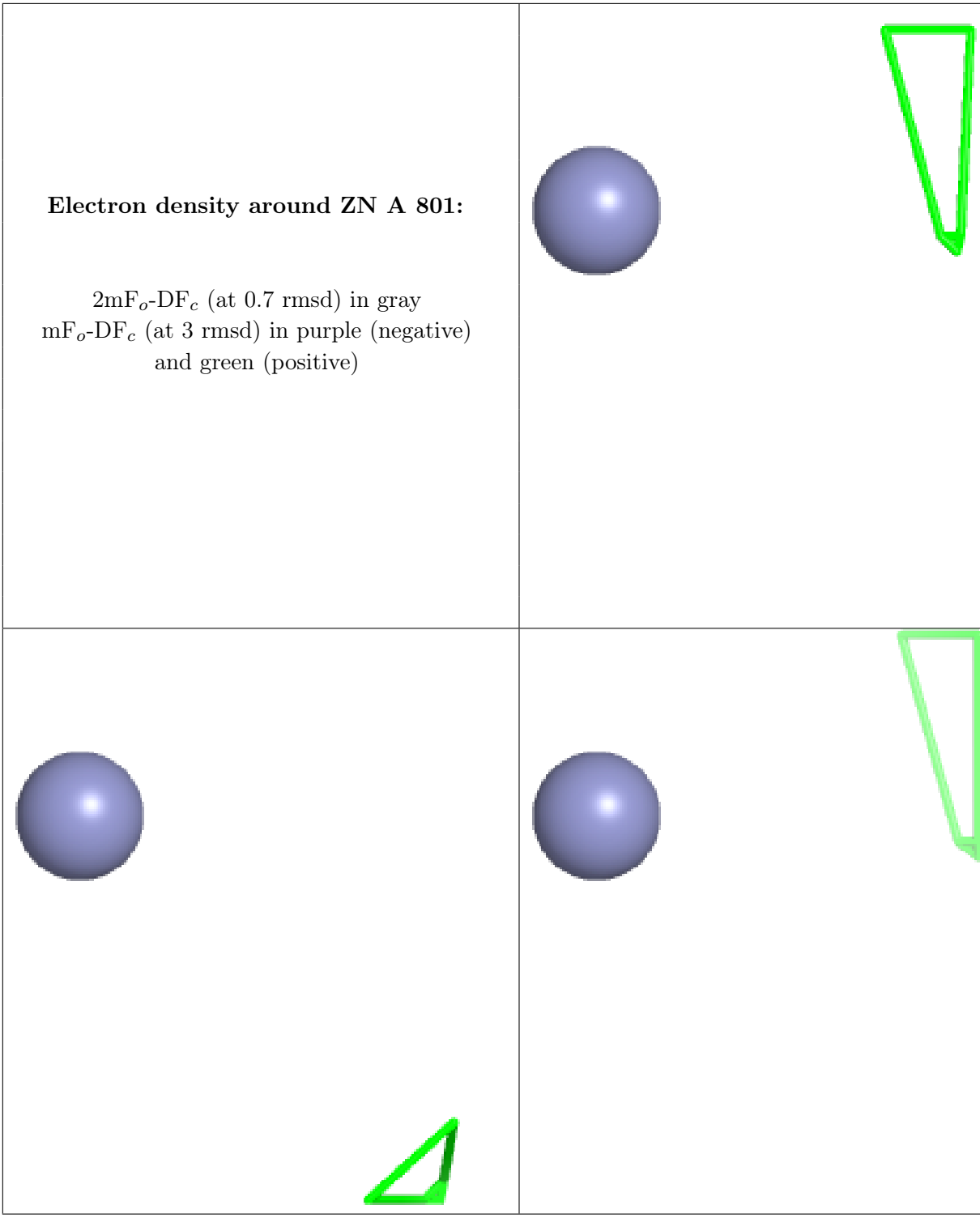






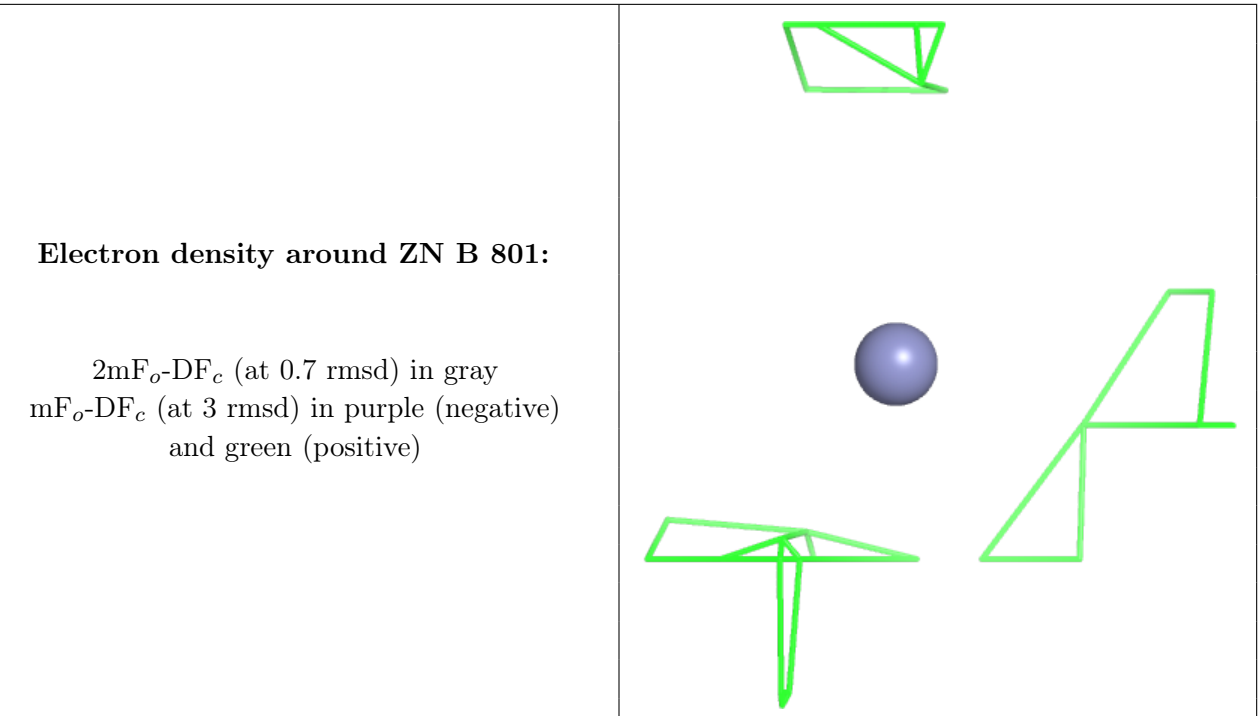
Electron density around ZN A 801:

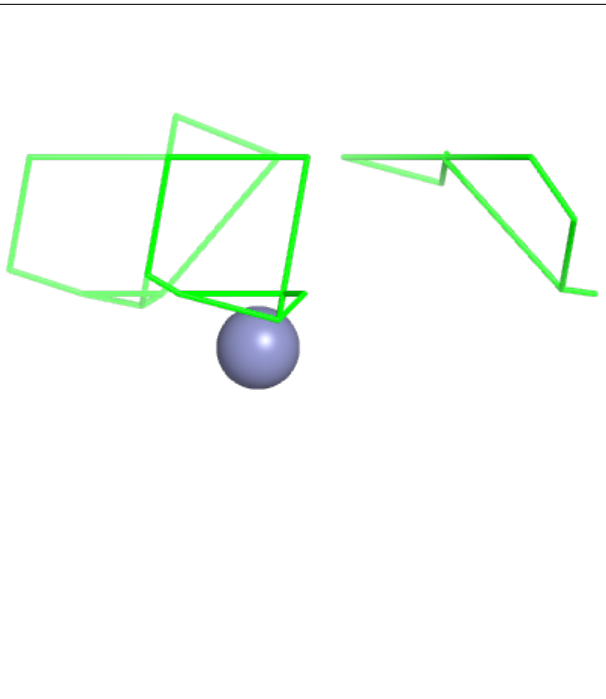
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

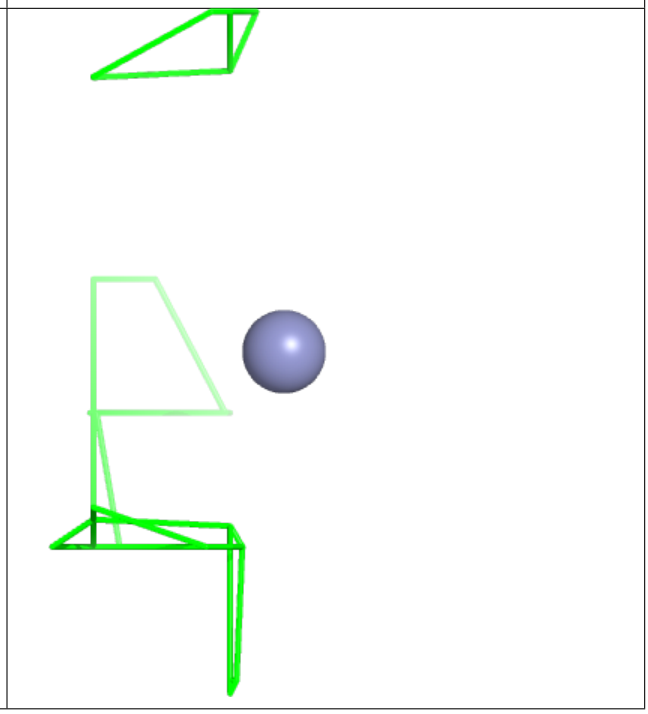


Electron density around ZN B 801:

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

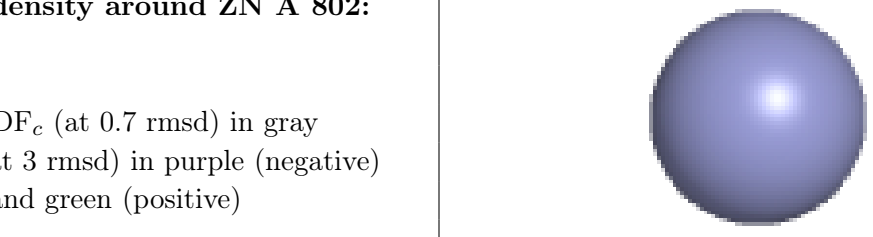


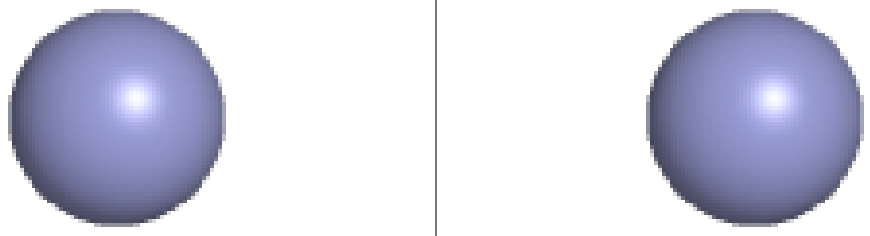




Electron density around ZN A 802:

$2mF_o$-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.