



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:58 AM UTC

PDB ID : 8GDW / pdb_00008gdw
Title : Crystal structure of Domain Related to Iron (DRI) from cyanobacteria
Authors : Kumaran, D.; Grosjean, N.; Blaby, E.C.
Deposited on : 2023-03-06
Resolution : 2.35 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
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

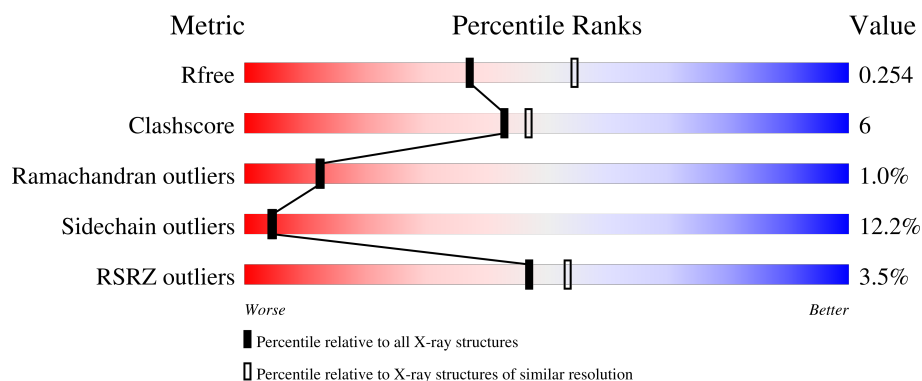
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	AAA	103	5% 76% 17% 6% .
1	BBB	103	% 80% 15% . .
1	CCC	103	4% 71% 24% . .
1	DDD	103	4% 73% 24% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3134 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 Ssr1698 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	101	Total	C	N	O	S	0	0	0
			774	478	133	157	6			
1	BBB	101	Total	C	N	O	S	0	0	0
			774	478	133	157	6			
1	CCC	101	Total	C	N	O	S	0	0	0
			774	478	133	157	6			
1	DDD	101	Total	C	N	O	S	0	0	0
			774	478	133	157	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	97	ALA	-	expression tag	UNP P73129
AAA	98	GLU	-	expression tag	UNP P73129
AAA	99	ASN	-	expression tag	UNP P73129
AAA	100	LEU	-	expression tag	UNP P73129
AAA	101	TYR	-	expression tag	UNP P73129
AAA	102	PHE	-	expression tag	UNP P73129
AAA	103	GLN	-	expression tag	UNP P73129
BBB	97	ALA	-	expression tag	UNP P73129
BBB	98	GLU	-	expression tag	UNP P73129
BBB	99	ASN	-	expression tag	UNP P73129
BBB	100	LEU	-	expression tag	UNP P73129
BBB	101	TYR	-	expression tag	UNP P73129
BBB	102	PHE	-	expression tag	UNP P73129
BBB	103	GLN	-	expression tag	UNP P73129
CCC	97	ALA	-	expression tag	UNP P73129
CCC	98	GLU	-	expression tag	UNP P73129
CCC	99	ASN	-	expression tag	UNP P73129
CCC	100	LEU	-	expression tag	UNP P73129
CCC	101	TYR	-	expression tag	UNP P73129
CCC	102	PHE	-	expression tag	UNP P73129
CCC	103	GLN	-	expression tag	UNP P73129

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	97	ALA	-	expression tag	UNP P73129
DDD	98	GLU	-	expression tag	UNP P73129
DDD	99	ASN	-	expression tag	UNP P73129
DDD	100	LEU	-	expression tag	UNP P73129
DDD	101	TYR	-	expression tag	UNP P73129
DDD	102	PHE	-	expression tag	UNP P73129
DDD	103	GLN	-	expression tag	UNP P73129

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Zn 1 1	0	0
2	BBB	1	Total Zn 1 1	0	0
2	CCC	1	Total Zn 1 1	0	0
2	DDD	1	Total Zn 1 1	0	0

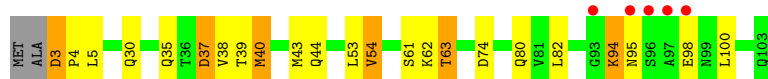
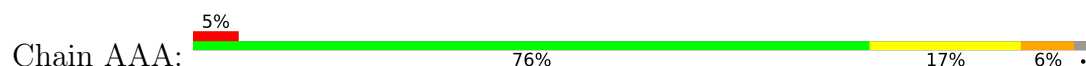
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	13	Total O 13 13	0	0
3	BBB	5	Total O 5 5	0	0
3	CCC	3	Total O 3 3	0	0
3	DDD	13	Total O 13 13	0	0

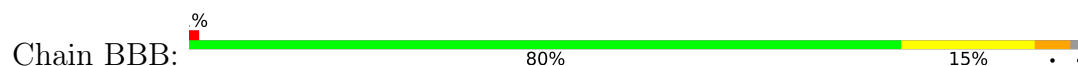
3 Residue-property plots [i](#)

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.

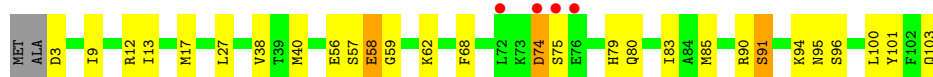
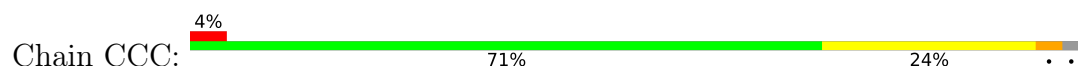
- Molecule 1: Ssr1698 protein



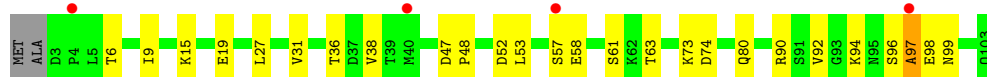
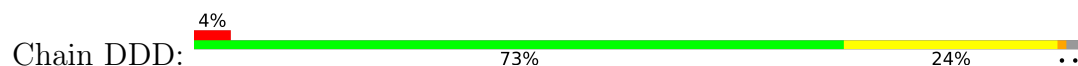
- Molecule 1: Ssr1698 protein



- Molecule 1: Ssr1698 protein



- Molecule 1: Ssr1698 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.72Å 87.23Å 57.24Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	29.50 – 2.35 29.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.50-2.35) 99.1 (29.50-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.247 0.202 , 0.254	Depositor DCC
R_{free} test set	1027 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3134	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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:
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	AAA	1.02	0/785	1.37	1/1060 (0.1%)
1	BBB	1.03	0/785	1.52	6/1060 (0.6%)
1	CCC	1.02	0/785	1.44	2/1060 (0.2%)
1	DDD	1.01	0/785	1.37	2/1060 (0.2%)
All	All	1.02	0/3140	1.43	11/4240 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	90	ARG	CA-C-N	6.56	128.97	120.44
1	BBB	90	ARG	C-N-CA	6.56	128.97	120.44
1	AAA	39	THR	CB-CA-C	5.96	120.70	110.86
1	BBB	103	GLN	CA-C-O	-5.82	110.90	120.80
1	CCC	103	GLN	CA-C-O	-5.67	111.17	120.80
1	DDD	74	ASP	CA-C-N	5.45	127.84	120.38
1	DDD	74	ASP	C-N-CA	5.45	127.84	120.38
1	BBB	93	GLY	CA-C-N	5.44	127.83	120.65
1	BBB	93	GLY	C-N-CA	5.44	127.83	120.65
1	CCC	101	TYR	CA-C-O	-5.34	115.38	121.58
1	BBB	19	GLU	CA-C-O	-5.09	115.11	120.55

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	AAA	774	0	753	14	0
1	BBB	774	0	753	5	0
1	CCC	774	0	753	10	0
1	DDD	774	0	753	12	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	13	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	3	0	0	1	0
3	DDD	13	0	0	0	0
All	All	3134	0	3012	38	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 6.

All (38) 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:AAA:3:ASP:HB3	1:AAA:4:PRO:HD3	1.62	0.79
1:DDD:15:LYS:HE2	1:DDD:19:GLU:OE2	2.01	0.61
1:AAA:40:MET:HE1	1:BBB:40:MET:CB	2.35	0.56
1:DDD:97:ALA:C	1:DDD:99:ASN:H	2.14	0.55
1:DDD:27:LEU:HD21	1:DDD:90:ARG:HG3	1.90	0.53
1:AAA:37:ASP:OD1	1:AAA:37:ASP:N	2.28	0.53
1:AAA:43:MET:HE1	1:AAA:82:LEU:HD22	1.91	0.53
1:AAA:3:ASP:HB3	1:AAA:4:PRO:CD	2.37	0.51
1:DDD:97:ALA:C	1:DDD:99:ASN:N	2.67	0.50
1:CCC:3:ASP:O	1:CCC:74:ASP:HB2	2.12	0.49
1:CCC:79:HIS:O	1:CCC:83:ILE:HG12	2.12	0.49
1:AAA:35:GLN:HB2	1:AAA:38:VAL:CG2	2.42	0.49
1:AAA:30:GLN:HA	1:AAA:35:GLN:O	2.13	0.49
1:CCC:95:ASN:HB2	3:CCC:301:HOH:O	2.13	0.49
1:DDD:31:VAL:HG13	1:DDD:92:VAL:HG21	1.94	0.49
1:DDD:96:SER:O	1:DDD:97:ALA:HB3	2.14	0.48
1:AAA:44:GLN:NE2	1:AAA:54:VAL:HG22	2.29	0.48
1:AAA:44:GLN:CD	1:AAA:54:VAL:HG22	2.40	0.46
1:CCC:27:LEU:HD21	1:CCC:90:ARG:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:6:THR:OG1	1:DDD:9:ILE:HG12	2.16	0.46
1:DDD:52:ASP:C	1:DDD:53:LEU:HD12	2.41	0.46
1:CCC:68:PHE:CE1	1:CCC:85:MET:HE1	2.52	0.46
1:CCC:80:GLN:NE2	1:CCC:80:GLN:HA	2.31	0.45
1:BBB:64:ILE:HA	1:DDD:99:ASN:HB3	1.99	0.45
1:BBB:3:ASP:HB3	1:BBB:4:PRO:HD3	2.00	0.44
1:AAA:35:GLN:OE1	1:AAA:62:LYS:HD2	2.18	0.44
1:AAA:94:LYS:O	1:AAA:95:ASN:C	2.61	0.44
1:AAA:3:ASP:O	1:AAA:74:ASP:HB2	2.19	0.43
1:DDD:96:SER:O	1:DDD:97:ALA:CB	2.66	0.42
1:AAA:3:ASP:CB	1:AAA:4:PRO:HD3	2.43	0.42
1:DDD:47:ASP:HB2	1:DDD:48:PRO:CD	2.49	0.42
1:BBB:29:ALA:O	1:BBB:33:GLY:HA3	2.20	0.41
1:BBB:56:GLU:HG3	1:BBB:61:SER:HB2	2.02	0.41
1:DDD:53:LEU:O	1:DDD:63:THR:HA	2.21	0.41
1:CCC:13:ILE:O	1:CCC:17:MET:HG2	2.21	0.41
1:CCC:91:SER:HA	1:CCC:94:LYS:HD2	2.02	0.41
1:AAA:63:THR:CG2	1:CCC:96:SER:HB3	2.51	0.40
1:CCC:57:SER:O	1:CCC:58:GLU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AAA	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
1	BBB	99/103 (96%)	93 (94%)	5 (5%)	1 (1%)	12	12
1	CCC	99/103 (96%)	91 (92%)	7 (7%)	1 (1%)	12	12
1	DDD	99/103 (96%)	92 (93%)	5 (5%)	2 (2%)	6	4
All	All	396/412 (96%)	370 (93%)	22 (6%)	4 (1%)	12	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	97	ALA
1	BBB	75	SER
1	DDD	98	GLU
1	CCC	59	GLY

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	AAA	84/85 (99%)	72 (86%)	12 (14%)	3	3
1	BBB	84/85 (99%)	74 (88%)	10 (12%)	5	4
1	CCC	84/85 (99%)	73 (87%)	11 (13%)	4	4
1	DDD	84/85 (99%)	76 (90%)	8 (10%)	8	7
All	All	336/340 (99%)	295 (88%)	41 (12%)	5	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	3	ASP
1	AAA	5	LEU
1	AAA	37	ASP
1	AAA	40	MET
1	AAA	53	LEU
1	AAA	54	VAL
1	AAA	61	SER
1	AAA	63	THR
1	AAA	80	GLN
1	AAA	94	LYS
1	AAA	98	GLU
1	AAA	100	LEU
1	BBB	3	ASP
1	BBB	5	LEU
1	BBB	38	VAL
1	BBB	40	MET

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Mol	Chain	Res	Type
1	BBB	44	GLN
1	BBB	61	SER
1	BBB	73	LYS
1	BBB	77	ASP
1	BBB	80	GLN
1	BBB	90	ARG
1	CCC	9	ILE
1	CCC	12	ARG
1	CCC	38	VAL
1	CCC	40	MET
1	CCC	56	GLU
1	CCC	58	GLU
1	CCC	62	LYS
1	CCC	74	ASP
1	CCC	75	SER
1	CCC	91	SER
1	CCC	100	LEU
1	DDD	36	THR
1	DDD	38	VAL
1	DDD	57	SER
1	DDD	58	GLU
1	DDD	61	SER
1	DDD	73	LYS
1	DDD	80	GLN
1	DDD	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	AAA	101/103 (98%)	0.23	5 (4%) 34 40	44, 57, 112, 152	0
1	BBB	101/103 (98%)	0.18	1 (0%) 79 83	46, 61, 100, 118	0
1	CCC	101/103 (98%)	0.42	4 (3%) 42 48	47, 65, 104, 174	0
1	DDD	101/103 (98%)	0.18	4 (3%) 42 48	44, 57, 107, 136	0
All	All	404/412 (98%)	0.25	14 (3%) 47 53	44, 61, 108, 174	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	96	SER	3.1
1	AAA	95	ASN	2.7
1	AAA	97	ALA	2.6
1	DDD	57	SER	2.6
1	CCC	75	SER	2.6
1	CCC	76	GLU	2.5
1	CCC	74	ASP	2.5
1	AAA	93	GLY	2.3
1	DDD	40	MET	2.2
1	DDD	4	PRO	2.2
1	BBB	95	ASN	2.1
1	AAA	98	GLU	2.1
1	CCC	72	LEU	2.1
1	DDD	97	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

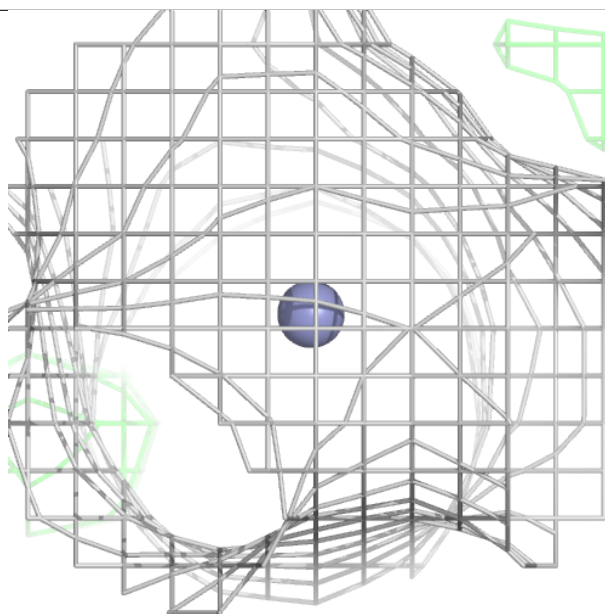
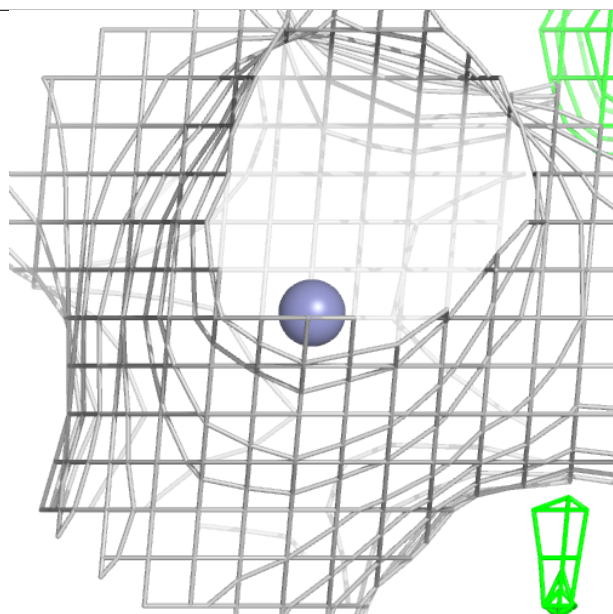
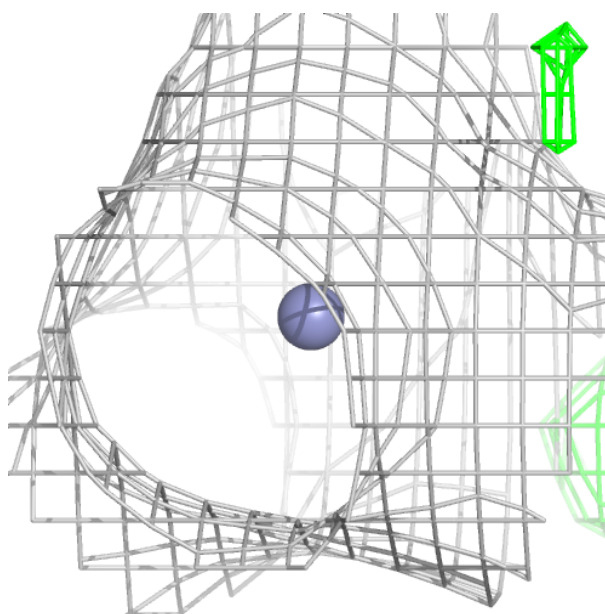
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	CCC	201	1/1	0.99	0.02	66,66,66,66	0
2	ZN	BBB	201	1/1	1.00	0.01	56,56,56,56	0
2	ZN	AAA	201	1/1	1.00	0.02	48,48,48,48	0
2	ZN	DDD	201	1/1	1.00	0.01	51,51,51,51	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.

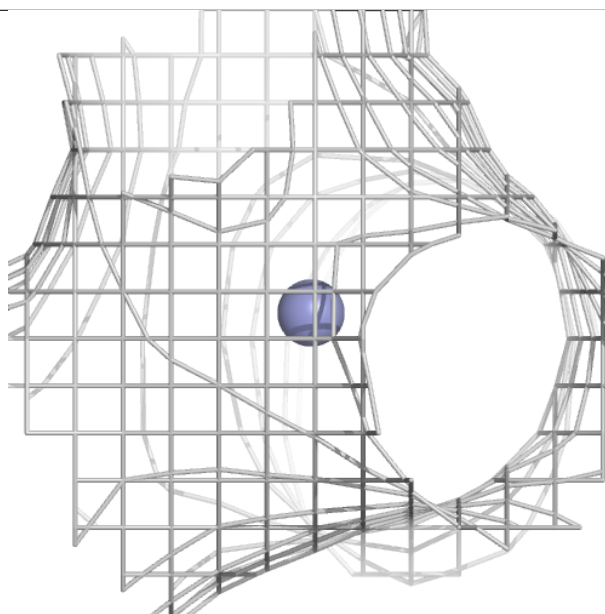
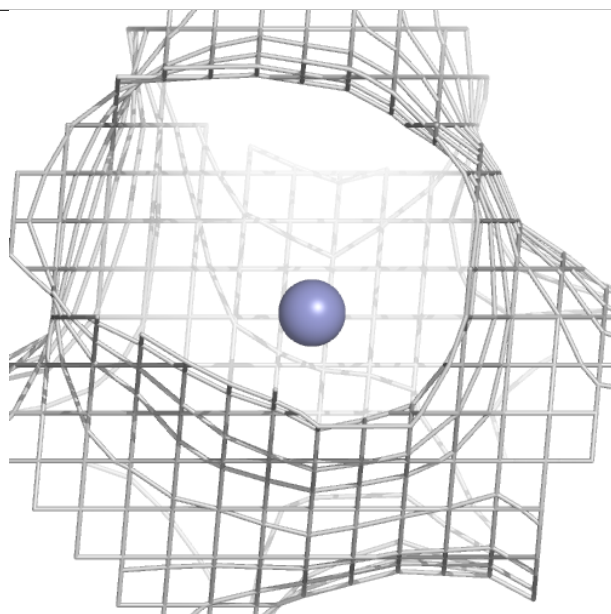
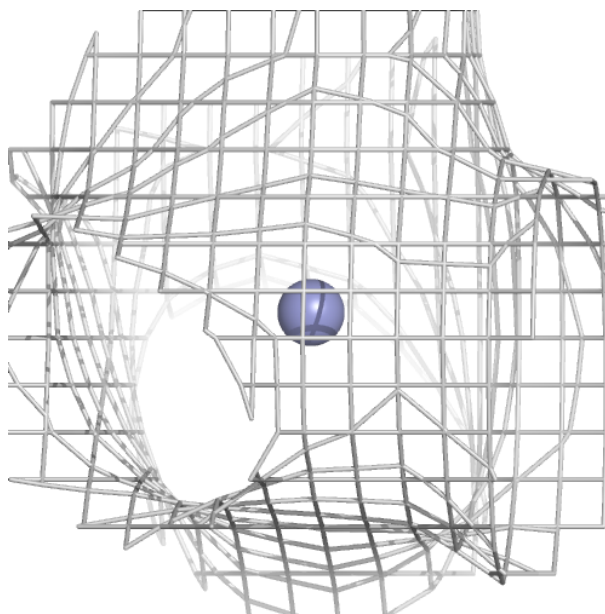
Electron density around ZN CCC 201:

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



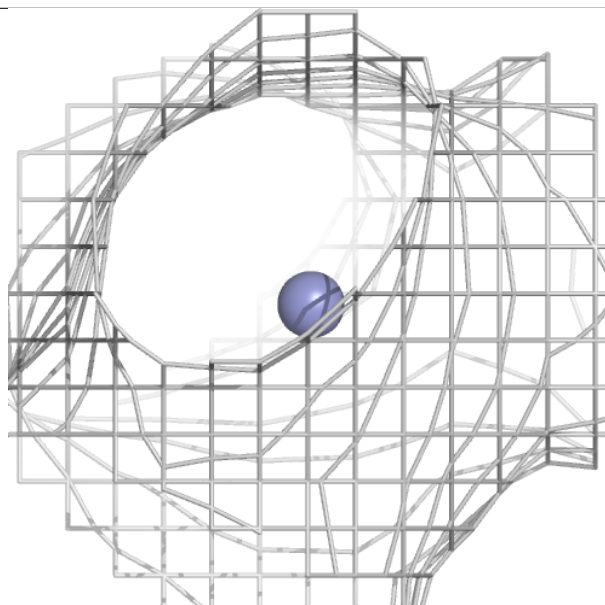
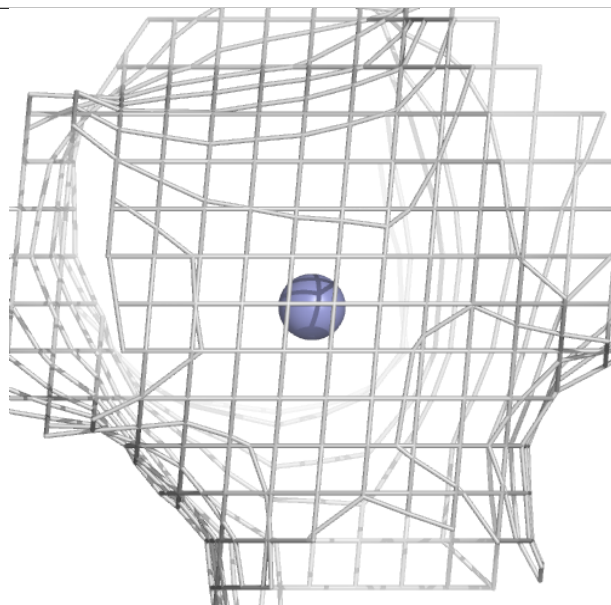
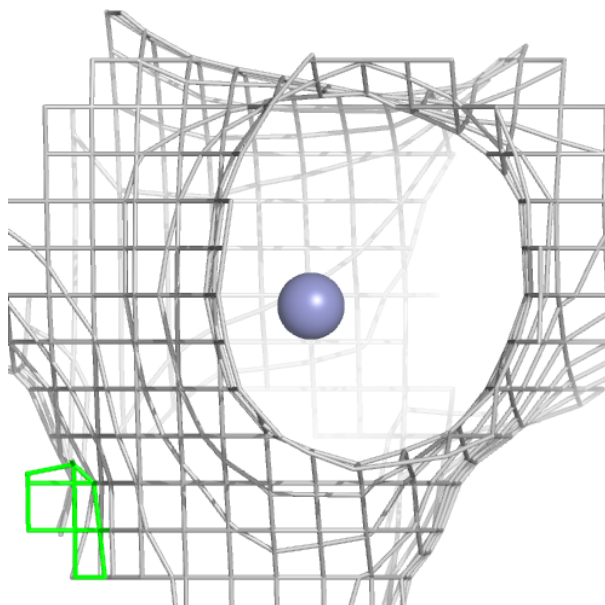
Electron density around ZN BBB 201:

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



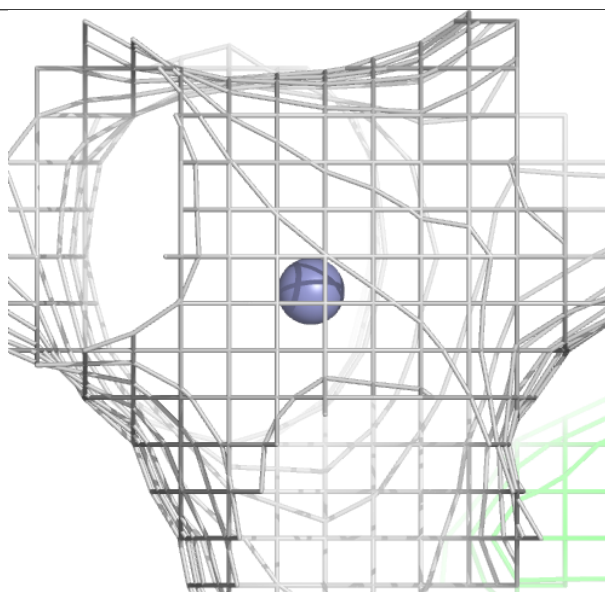
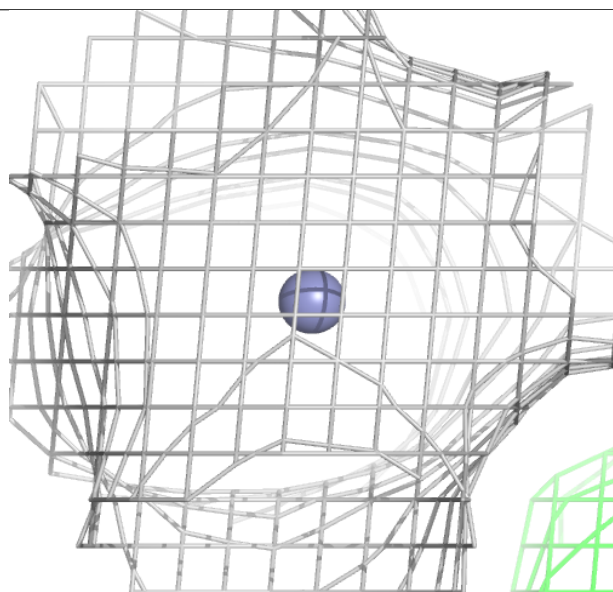
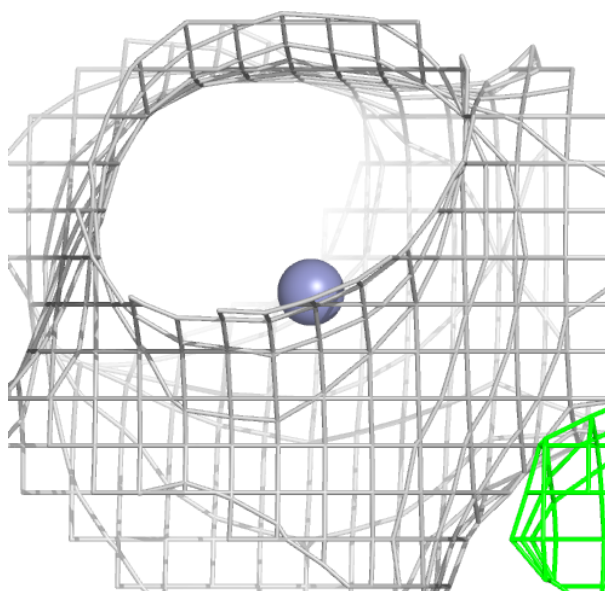
Electron density around ZN AAA 201:

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



Electron density around ZN DDD 201:

$2mF_o-DF_c$ (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.