



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 PM UTC

PDB ID : 5YI3 / pdb_00005yi3
Title : Structure of Lactococcus lactis ZitR, C30S mutant in complex with DNA
Authors : Song, Y.; Liu, H.; Zhu, R.; Yi, C.; Chen, P.
Deposited on : 2017-10-01
Resolution : 2.90 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

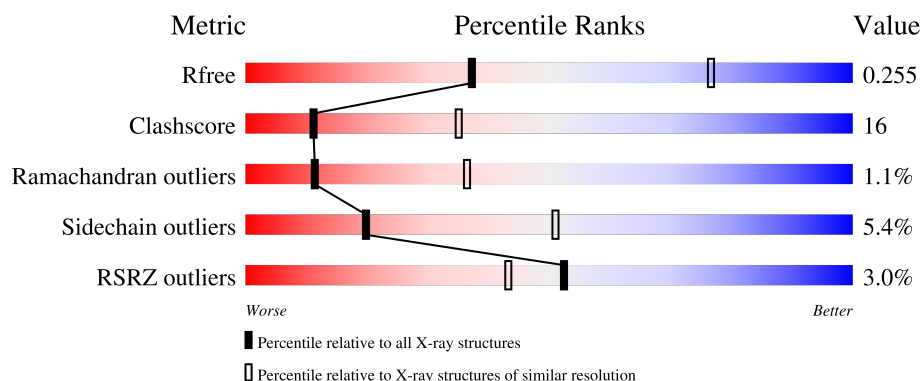
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	146	8% 55% 39% 5%
1	B	146	3% 58% 38% ..
1	E	146	% 65% 34% ..
1	F	146	% 64% 32% ..
1	I	146	3% 65% 32% ...

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Mol	Chain	Length	Quality of chain
1	J	146	
1	M	146	
1	N	146	
2	C	16	
2	D	16	
2	G	16	
2	H	16	
2	K	16	
2	L	16	
2	O	16	
2	P	16	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11717 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 Zinc transport transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1127	713	189	222	3			
1	B	144	Total	C	N	O	S	0	0	0
			1129	712	191	224	2			
1	E	145	Total	C	N	O	S	0	0	0
			1142	721	189	229	3			
1	F	145	Total	C	N	O	S	0	0	0
			1148	724	192	229	3			
1	I	145	Total	C	N	O	S	0	0	0
			1133	714	190	227	2			
1	J	145	Total	C	N	O	S	0	0	0
			1144	721	191	229	3			
1	M	144	Total	C	N	O	S	0	0	0
			1130	713	189	226	2			
1	N	144	Total	C	N	O	S	0	0	0
			1130	710	190	228	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9CDU5
A	30	SER	CYS	engineered mutation	UNP Q9CDU5
B	1	GLY	-	expression tag	UNP Q9CDU5
B	30	SER	CYS	engineered mutation	UNP Q9CDU5
E	1	GLY	-	expression tag	UNP Q9CDU5
E	30	SER	CYS	engineered mutation	UNP Q9CDU5
F	1	GLY	-	expression tag	UNP Q9CDU5
F	30	SER	CYS	engineered mutation	UNP Q9CDU5
I	1	GLY	-	expression tag	UNP Q9CDU5
I	30	SER	CYS	engineered mutation	UNP Q9CDU5
J	1	GLY	-	expression tag	UNP Q9CDU5
J	30	SER	CYS	engineered mutation	UNP Q9CDU5
M	1	GLY	-	expression tag	UNP Q9CDU5

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Chain	Residue	Modelled	Actual	Comment	Reference
M	30	SER	CYS	engineered mutation	UNP Q9CDU5
N	1	GLY	-	expression tag	UNP Q9CDU5
N	30	SER	CYS	engineered mutation	UNP Q9CDU5

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	G	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	K	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	O	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	P	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	L	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	H	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			
2	D	16	Total	C	N	O	P	0	0	0
			325	158	58	94	15			

- 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	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	M	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	1	Total 1	Zn 1	0	0

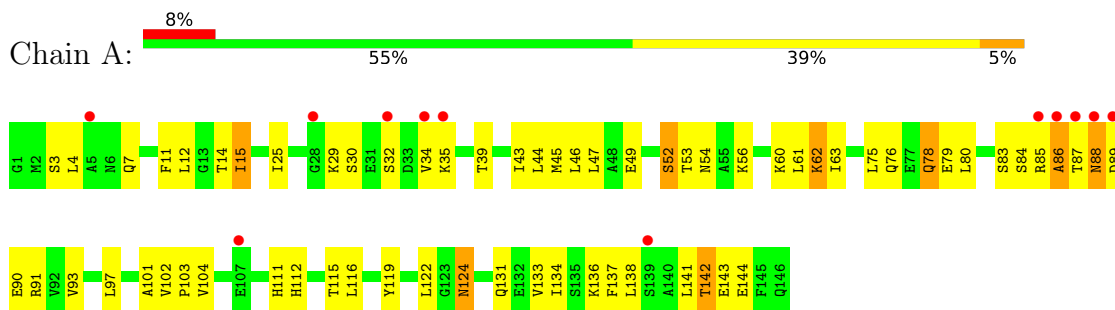
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	E	1	Total 1	O 1	0	0
4	F	3	Total 3	O 3	0	0
4	G	3	Total 3	O 3	0	0
4	I	4	Total 4	O 4	0	0
4	J	3	Total 3	O 3	0	0
4	K	1	Total 1	O 1	0	0
4	M	2	Total 2	O 2	0	0
4	N	1	Total 1	O 1	0	0
4	P	1	Total 1	O 1	0	0
4	L	3	Total 3	O 3	0	0
4	H	2	Total 2	O 2	0	0
4	D	1	Total 1	O 1	0	0

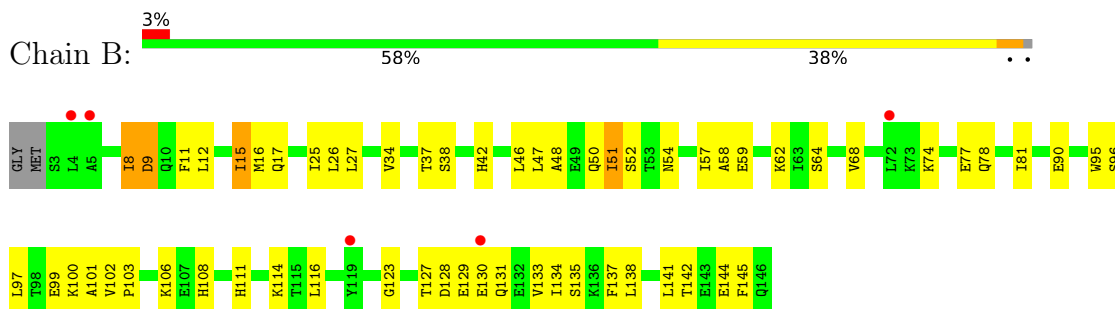
3 Residue-property plots

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.

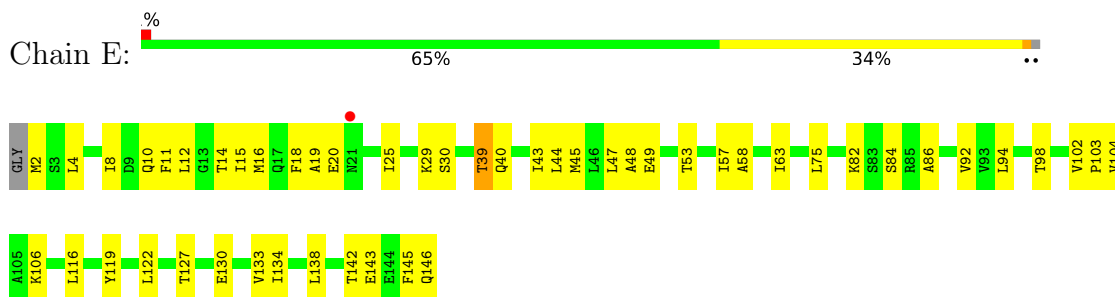
- Molecule 1: Zinc transport transcriptional regulator



- Molecule 1: Zinc transport transcriptional regulator

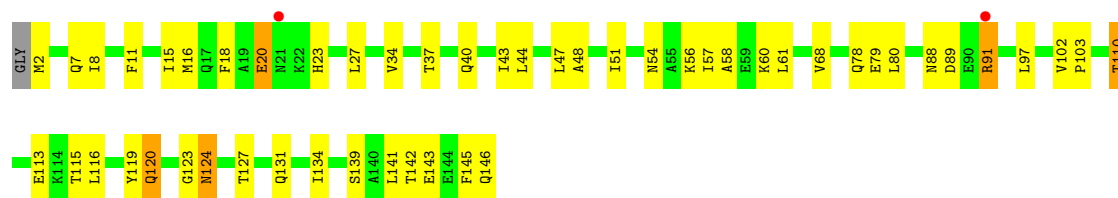


- Molecule 1: Zinc transport transcriptional regulator

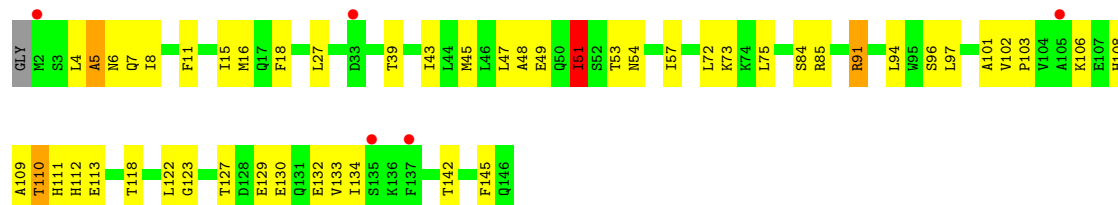


- Molecule 1: Zinc transport transcriptional regulator

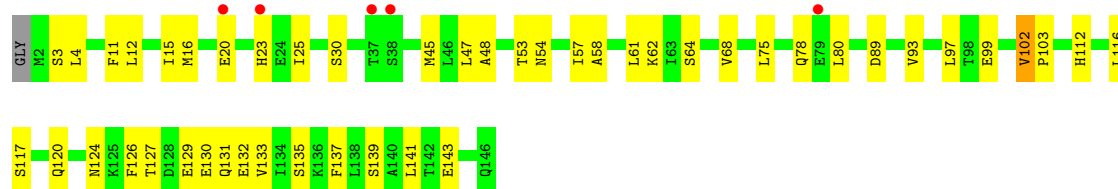




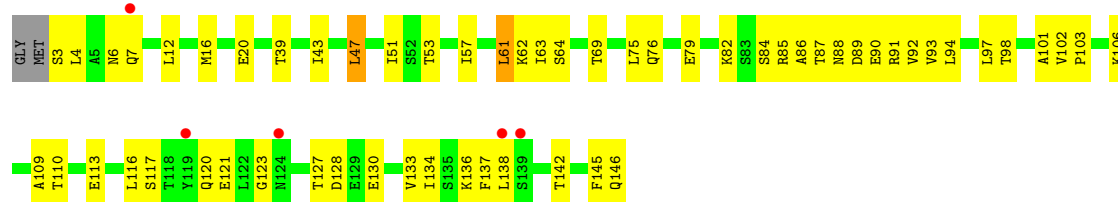
- Molecule 1: Zinc transport transcriptional regulator



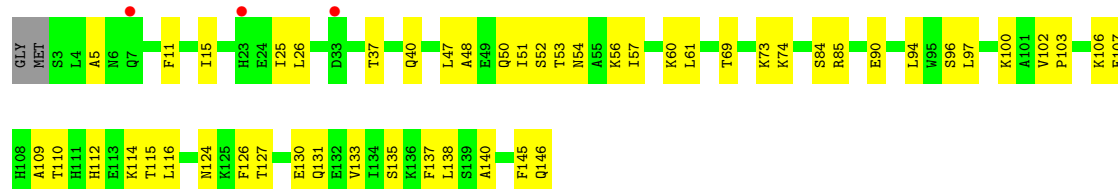
- Molecule 1: Zinc transport transcriptional regulator



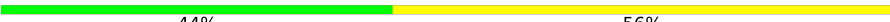
- Molecule 1: Zinc transport transcriptional regulator

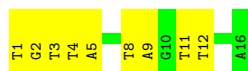


- Molecule 1: Zinc transport transcriptional regulator



- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain C:  44% 56%

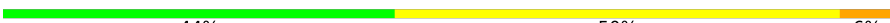


- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain G:  44% 50% 6%



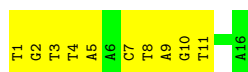
- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain K:  44% 50% 6%



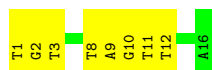
- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain O:  38% 62%



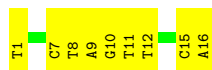
- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain P:  50% 50%



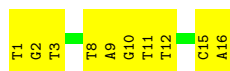
- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain L:  44% 56%



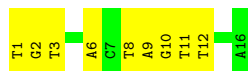
- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain H:  38% 62%



- Molecule 2: DNA (5'-D(*TP*GP*TP*TP*AP*AP*CP*TP*AP*GP*TP*TP*AP*AP*CP*A)-3')

Chain D:  44% 56%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.52Å 103.06Å 104.86Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	42.49 – 2.90 42.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (42.49-2.90) 90.7 (42.49-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.205 , 0.263 0.196 , 0.255	Depositor DCC
R_{free} test set	2034 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtrriage
Anisotropy	0.462	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9485e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/1141	0.94	4/1537 (0.3%)
1	B	0.51	0/1143	0.89	0/1540
1	E	0.54	0/1156	0.86	0/1557
1	F	0.56	0/1162	0.89	2/1564 (0.1%)
1	I	0.57	0/1147	0.91	1/1548 (0.1%)
1	J	0.57	0/1158	0.88	1/1560 (0.1%)
1	M	0.50	0/1144	0.85	1/1541 (0.1%)
1	N	0.50	0/1144	0.85	0/1542
2	C	0.42	0/364	1.17	0/560
2	D	0.42	0/364	1.22	2/560 (0.4%)
2	G	0.45	0/364	1.16	3/560 (0.5%)
2	H	0.42	0/364	1.12	2/560 (0.4%)
2	K	0.42	0/364	1.14	1/560 (0.2%)
2	L	0.41	0/364	1.09	0/560
2	O	0.42	0/364	1.17	1/560 (0.2%)
2	P	0.39	0/364	1.12	1/560 (0.2%)
All	All	0.51	0/12107	0.96	19/16869 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ALA	N-CA-C	-10.05	98.77	112.94
1	A	85	ARG	CB-CA-C	9.25	128.83	110.42
2	G	3	DT	N1-C1'-C2'	7.40	124.60	113.50
2	O	1	DT	N1-C1'-C2'	7.05	124.07	113.50
1	A	52	SER	N-CA-C	6.80	117.02	108.45
2	G	3	DT	O4'-C1'-N1	-6.66	98.41	108.40
2	H	3	DT	P-O5'-C5'	-6.46	110.30	120.00
2	D	3	DT	P-O5'-C5'	-6.21	110.69	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	84	SER	N-CA-C	-6.02	106.09	113.50
2	G	6	DA	O4'-C1'-N9	5.85	117.17	108.40
1	M	4	LEU	N-CA-C	-5.81	104.95	112.68
2	K	3	DT	O4'-C1'-N1	-5.79	99.72	108.40
2	D	6	DA	O4'-C1'-N9	5.44	116.56	108.40
1	F	20	GLU	CB-CA-C	-5.41	109.87	117.23
2	P	1	DT	N1-C1'-C2'	5.35	121.52	113.50
1	J	20	GLU	CB-CA-C	-5.22	110.13	117.23
1	A	86	ALA	N-CA-CB	5.02	119.27	110.98
2	H	2	DG	C3'-C2'-C1'	-5.01	94.09	101.60
1	F	8	ILE	CB-CA-C	-5.01	105.55	111.81

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	1127	0	1139	60	0
1	B	1129	0	1146	50	0
1	E	1142	0	1161	41	0
1	F	1148	0	1172	36	0
1	I	1133	0	1139	44	0
1	J	1144	0	1161	35	0
1	M	1130	0	1144	49	0
1	N	1130	0	1134	42	0
2	C	325	0	184	9	0
2	D	325	0	184	7	0
2	G	325	0	184	9	0
2	H	325	0	184	6	0
2	K	325	0	184	8	0
2	L	325	0	184	6	0
2	O	325	0	184	12	0
2	P	325	0	184	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	1	0
4	H	2	0	0	0	0
4	I	4	0	0	0	0
4	J	3	0	0	0	0
4	K	1	0	0	0	0
4	L	3	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	P	1	0	0	0	0
All	All	11717	0	10668	364	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 16.

All (364) 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:J:58:ALA:HB2	1:J:68:VAL:HG21	1.56	0.86
2:C:4:DT:H2''	2:C:5:DA:H5'	1.56	0.86
1:A:86:ALA:HB1	1:A:91:ARG:HA	1.54	0.85
1:E:29:LYS:HD3	1:E:30:SER:H	1.45	0.81
1:A:134:ILE:HD13	1:B:134:ILE:HD13	1.63	0.80
1:E:11:PHE:HD1	1:F:142:THR:HG22	1.46	0.80
1:A:102:VAL:HG23	1:A:103:PRO:HD3	1.64	0.79
1:E:10:GLN:O	1:E:14:THR:HG23	1.82	0.79
1:A:142:THR:HG23	1:B:11:PHE:HD1	1.48	0.79
1:B:25:ILE:O	1:B:26:LEU:HD23	1.85	0.77
1:F:48:ALA:HB2	1:F:97:LEU:HD11	1.68	0.75
1:F:27:LEU:HD11	1:F:119:TYR:CE1	2.22	0.74
1:B:51:ILE:HD11	1:B:96:SER:HB3	1.69	0.74
1:M:85:ARG:HH21	1:M:92:VAL:N	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:C	1:A:90:GLU:H	1.96	0.74
1:E:53:THR:HG21	2:D:1:DT:H5'	1.71	0.72
1:N:102:VAL:N	1:N:103:PRO:HD2	2.05	0.71
1:I:7:GLN:OE1	1:J:135:SER:HA	1.90	0.70
1:M:53:THR:HG21	2:L:1:DT:H5'	1.75	0.69
1:I:129:GLU:O	1:I:132:GLU:HB3	1.92	0.69
1:J:117:SER:O	1:J:120:GLN:HB3	1.93	0.69
1:A:12:LEU:HB3	1:B:25:ILE:HD12	1.75	0.68
1:M:145:PHE:O	1:M:146:GLN:HG3	1.93	0.68
2:C:2:DG:H2''	2:C:3:DT:H72	1.74	0.68
1:A:7:GLN:HG3	1:B:138:LEU:HD12	1.74	0.68
1:A:11:PHE:HD1	1:B:142:THR:HG22	1.56	0.68
1:A:101:ALA:O	1:A:104:VAL:HG22	1.93	0.68
2:P:11:DT:H2''	2:P:12:DT:H5'	1.77	0.67
1:A:143:GLU:CD	1:E:143:GLU:HG3	2.20	0.67
2:K:16:DA:H2''	1:M:90:GLU:HG2	1.77	0.66
1:J:102:VAL:N	1:J:103:PRO:HD2	2.10	0.66
1:M:102:VAL:N	1:M:103:PRO:HD2	2.10	0.66
1:F:89:ASP:OD1	1:F:91:ARG:HG3	1.96	0.65
1:J:47:LEU:HD21	1:J:57:ILE:HD11	1.77	0.65
1:A:44:LEU:HD22	1:A:97:LEU:CD2	2.26	0.65
1:A:15:ILE:HD12	1:B:12:LEU:HD22	1.79	0.65
1:B:130:GLU:O	1:B:133:VAL:HG12	1.97	0.64
2:O:2:DG:H2''	2:O:3:DT:H72	1.78	0.64
2:D:11:DT:H2''	2:D:12:DT:H5'	1.79	0.64
1:J:48:ALA:HB2	1:J:97:LEU:HD11	1.78	0.64
2:C:8:DT:H2''	2:C:9:DA:C8	2.32	0.64
1:N:127:THR:OG1	1:N:130:GLU:HG2	1.98	0.64
1:I:48:ALA:HB2	1:I:97:LEU:HD11	1.80	0.64
1:A:29:LYS:HG2	1:A:30:SER:H	1.62	0.64
1:A:39:THR:O	1:A:43:ILE:HG13	1.97	0.64
1:I:97:LEU:HB3	1:I:101:ALA:HB3	1.80	0.64
1:E:39:THR:O	1:E:43:ILE:HG13	1.97	0.63
1:I:53:THR:HG22	1:I:94:LEU:HD23	1.80	0.63
1:A:115:THR:HG22	1:A:119:TYR:CE2	2.34	0.63
1:E:127:THR:HG22	1:E:130:GLU:CG	2.28	0.63
2:G:8:DT:H2''	2:G:9:DA:C8	2.33	0.62
2:L:7:DC:H2'	2:L:8:DT:H71	1.80	0.62
1:F:120:GLN:NE2	1:F:124:ASN:HD22	1.98	0.62
1:N:40:GLN:HE22	1:N:74:LYS:NZ	1.97	0.62
1:F:18:PHE:O	1:F:20:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:ILE:HD13	1:J:137:PHE:CD1	2.35	0.62
1:M:101:ALA:C	1:M:103:PRO:HD2	2.25	0.62
2:L:15:DC:H4'	2:L:16:DA:OP1	2.00	0.61
1:A:61:LEU:O	1:A:63:ILE:HG23	2.01	0.61
2:L:8:DT:H2''	2:L:9:DA:C8	2.36	0.61
1:M:85:ARG:HD3	1:M:88:ASN:O	2.00	0.61
2:O:8:DT:H2''	2:O:9:DA:C8	2.35	0.61
1:A:45:MET:O	1:A:49:GLU:HG3	2.01	0.61
1:F:124:ASN:HA	1:F:131:GLN:OE1	2.01	0.60
2:D:8:DT:H2''	2:D:9:DA:C8	2.36	0.60
2:K:8:DT:H2''	2:K:9:DA:C8	2.36	0.60
1:M:134:ILE:O	1:M:137:PHE:HB3	2.02	0.60
1:B:11:PHE:CZ	1:B:15:ILE:HD11	2.37	0.60
1:B:127:THR:HG23	1:B:129:GLU:HB3	1.84	0.60
1:A:133:VAL:HG12	1:B:134:ILE:HD11	1.84	0.59
1:F:11:PHE:CZ	1:F:15:ILE:HD11	2.37	0.59
1:N:11:PHE:CZ	1:N:15:ILE:HD11	2.38	0.59
1:E:45:MET:O	1:E:49:GLU:HG3	2.03	0.59
1:M:136:LYS:HE2	1:N:126:PHE:HE1	1.67	0.59
1:N:48:ALA:HB2	1:N:97:LEU:HD11	1.85	0.59
1:I:45:MET:O	1:I:49:GLU:HG3	2.02	0.58
1:F:102:VAL:N	1:F:103:PRO:HD2	2.16	0.58
1:A:143:GLU:HG3	1:E:143:GLU:OE2	2.04	0.58
2:O:2:DG:H2''	2:O:3:DT:C7	2.32	0.58
1:A:11:PHE:CZ	1:B:141:LEU:HD23	2.38	0.58
1:F:110:THR:HA	1:F:113:GLU:HG2	1.84	0.58
1:M:85:ARG:HH21	1:M:92:VAL:H	1.50	0.58
2:H:8:DT:H2''	2:H:9:DA:C8	2.39	0.57
1:A:97:LEU:HD22	1:A:101:ALA:HB1	1.87	0.57
1:E:11:PHE:CD1	1:F:142:THR:HG22	2.34	0.57
1:M:3:SER:HB2	1:M:6:ASN:HB2	1.86	0.57
2:C:1:DT:H5''	2:C:1:DT:H6	1.70	0.56
1:M:16:MET:HE2	1:M:16:MET:HA	1.85	0.56
1:N:84:SER:O	1:N:85:ARG:HD3	2.05	0.56
1:F:47:LEU:HD21	1:F:57:ILE:HD11	1.88	0.56
1:M:90:GLU:HB2	1:M:92:VAL:HG12	1.88	0.56
2:O:7:DC:H2'	2:O:8:DT:H71	1.87	0.56
1:A:11:PHE:HD1	1:B:142:THR:CG2	2.19	0.56
1:F:54:ASN:HB3	2:G:2:DG:OP2	2.06	0.56
1:J:78:GLN:O	1:J:78:GLN:HG3	2.04	0.56
1:B:90:GLU:O	1:B:90:GLU:HG2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:107:GLU:O	1:N:110:THR:HB	2.06	0.55
1:F:37:THR:HG23	1:F:40:GLN:OE1	2.06	0.55
1:J:124:ASN:C	1:J:126:PHE:H	2.13	0.55
1:N:25:ILE:O	1:N:26:LEU:HD23	2.07	0.55
1:N:54:ASN:HB3	2:O:2:DG:OP2	2.07	0.55
1:B:141:LEU:O	1:B:144:GLU:HG2	2.06	0.55
1:N:100:LYS:O	1:N:100:LYS:HG2	2.05	0.55
1:B:51:ILE:HD11	1:B:96:SER:CB	2.36	0.55
2:C:2:DG:H2''	2:C:3:DT:C7	2.35	0.55
1:M:121:GLU:C	1:M:123:GLY:N	2.64	0.55
2:D:11:DT:H2'	2:D:12:DT:C6	2.42	0.55
1:A:141:LEU:O	1:A:144:GLU:N	2.33	0.55
1:A:83:SER:OG	1:A:84:SER:N	2.39	0.54
1:F:58:ALA:HB2	1:F:68:VAL:HG21	1.88	0.54
1:I:51:ILE:HG23	1:I:51:ILE:O	2.06	0.54
1:E:130:GLU:O	1:E:134:ILE:HG13	2.08	0.54
1:F:37:THR:HG23	1:F:40:GLN:CD	2.31	0.54
1:E:53:THR:O	1:E:57:ILE:HD12	2.07	0.54
1:A:102:VAL:CG2	1:A:103:PRO:HD3	2.37	0.54
1:I:16:MET:SD	1:J:25:ILE:HD11	2.48	0.54
1:N:11:PHE:CE2	1:N:15:ILE:HD11	2.43	0.54
1:N:84:SER:C	1:N:85:ARG:HD3	2.33	0.54
2:H:15:DC:H4'	2:H:16:DA:OP1	2.08	0.54
1:B:81:ILE:HD12	1:B:95:TRP:CE3	2.42	0.53
1:E:127:THR:HG23	1:E:130:GLU:H	1.72	0.53
1:I:102:VAL:HG23	1:I:103:PRO:HD3	1.90	0.53
1:E:119:TYR:O	1:E:122:LEU:HB3	2.08	0.53
1:N:102:VAL:N	1:N:103:PRO:CD	2.72	0.53
1:E:92:VAL:HG13	1:E:94:LEU:HG	1.91	0.53
1:I:122:LEU:C	1:I:122:LEU:HD23	2.34	0.53
1:A:88:ASN:C	1:A:90:GLU:N	2.65	0.53
1:A:32:SER:HB3	1:A:35:LYS:CD	2.39	0.53
1:A:54:ASN:HB3	2:D:2:DG:OP2	2.09	0.53
2:O:2:DG:C2'	2:O:3:DT:H72	2.38	0.53
1:M:47:LEU:HD21	1:M:57:ILE:HD11	1.91	0.53
1:E:18:PHE:CD2	1:F:145:PHE:HB3	2.44	0.52
1:B:99:GLU:C	1:B:101:ALA:H	2.16	0.52
1:J:139:SER:O	1:J:143:GLU:HG2	2.09	0.52
1:I:51:ILE:O	1:I:51:ILE:CG2	2.58	0.52
1:B:111:HIS:HA	1:B:114:LYS:HG2	1.92	0.52
1:A:78:GLN:O	1:A:80:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:THR:HG22	1:E:130:GLU:CD	2.34	0.52
1:E:127:THR:HG22	1:E:130:GLU:HG3	1.91	0.52
1:M:76:GLN:O	1:M:79:GLU:N	2.37	0.52
1:E:133:VAL:HG12	1:F:134:ILE:HD11	1.91	0.51
1:E:102:VAL:N	1:E:103:PRO:HD2	2.26	0.51
1:E:145:PHE:CE1	1:F:27:LEU:HD21	2.45	0.51
1:F:44:LEU:HD11	1:F:80:LEU:HD13	1.92	0.51
1:I:127:THR:HG22	1:I:130:GLU:OE1	2.10	0.51
1:I:127:THR:HG22	1:I:130:GLU:CG	2.41	0.51
1:F:43:ILE:HG13	1:F:61:LEU:HD11	1.92	0.51
1:B:47:LEU:HB2	1:B:97:LEU:HD21	1.91	0.51
1:B:127:THR:O	1:B:130:GLU:N	2.43	0.51
1:A:122:LEU:HD23	1:A:122:LEU:O	2.12	0.50
1:B:34:VAL:HG21	1:B:78:GLN:OE1	2.11	0.50
1:M:87:THR:HG22	1:M:87:THR:O	2.11	0.50
1:A:124:ASN:HA	1:A:131:GLN:NE2	2.26	0.50
1:E:4:LEU:HD23	1:F:123:GLY:HA3	1.92	0.50
1:A:142:THR:HG23	1:B:11:PHE:CD1	2.39	0.50
1:M:97:LEU:HD22	1:M:101:ALA:CB	2.42	0.50
2:G:8:DT:H5''	4:G:101:HOH:O	2.09	0.50
1:I:8:ILE:O	1:I:11:PHE:HB3	2.12	0.50
2:D:9:DA:C4	2:D:10:DG:C8	2.99	0.50
1:N:56:LYS:HE3	1:N:60:LYS:NZ	2.26	0.50
2:P:2:DG:H2''	2:P:3:DT:H71	1.93	0.50
1:M:84:SER:HB3	1:M:94:LEU:O	2.12	0.50
1:A:29:LYS:HG2	1:A:30:SER:N	2.27	0.50
1:B:8:ILE:O	1:B:9:ASP:C	2.54	0.50
1:B:51:ILE:CD1	1:B:96:SER:HB3	2.41	0.50
2:G:10:DG:H2'	2:G:11:DT:H6	1.76	0.50
1:I:39:THR:O	1:I:43:ILE:HG13	2.12	0.49
1:I:85:ARG:HG2	1:M:91:ARG:NH2	2.27	0.49
2:O:3:DT:H2''	2:O:4:DT:C6	2.47	0.49
2:G:10:DG:H2'	2:G:11:DT:C6	2.47	0.49
2:K:10:DG:H2'	2:K:11:DT:H6	1.77	0.49
1:E:19:ALA:O	1:E:20:GLU:HB2	2.12	0.49
2:H:9:DA:C4	2:H:10:DG:C8	3.01	0.49
1:A:142:THR:CG2	1:B:11:PHE:HD1	2.21	0.49
1:E:53:THR:HG22	1:E:94:LEU:CD2	2.42	0.49
2:K:2:DG:H2''	2:K:3:DT:H72	1.93	0.49
1:I:53:THR:O	1:I:57:ILE:HD12	2.13	0.49
1:M:85:ARG:NH2	1:M:91:ARG:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:THR:O	1:I:111:HIS:C	2.55	0.49
1:A:11:PHE:CD1	1:B:142:THR:HG22	2.42	0.48
2:O:2:DG:C8	2:O:3:DT:H72	2.48	0.48
1:B:97:LEU:HB3	1:B:101:ALA:HB3	1.95	0.48
1:E:29:LYS:HD3	1:E:30:SER:N	2.21	0.48
1:I:4:LEU:O	1:I:7:GLN:N	2.46	0.48
1:N:56:LYS:HE3	1:N:60:LYS:HZ2	1.78	0.48
1:I:110:THR:O	1:I:113:GLU:N	2.44	0.48
2:C:2:DG:C2'	2:C:3:DT:H72	2.40	0.48
1:A:32:SER:HB3	1:A:35:LYS:CE	2.44	0.48
1:I:127:THR:HG23	1:I:130:GLU:H	1.79	0.48
1:J:23:HIS:CE1	2:L:10:DG:H4'	2.48	0.48
2:O:10:DG:H2'	2:O:11:DT:H6	1.79	0.48
1:F:27:LEU:HD11	1:F:119:TYR:HE1	1.77	0.47
1:E:82:LYS:HD3	1:E:98:THR:HG22	1.96	0.47
1:M:85:ARG:HD2	1:M:89:ASP:HA	1.96	0.47
1:A:111:HIS:HD2	1:A:111:HIS:O	1.98	0.47
1:A:144:GLU:HG3	1:B:27:LEU:HD13	1.96	0.47
1:F:56:LYS:HE3	1:F:60:LYS:NZ	2.30	0.47
1:A:111:HIS:O	1:A:111:HIS:CD2	2.68	0.47
1:B:8:ILE:O	1:B:11:PHE:N	2.47	0.47
1:E:138:LEU:HD13	1:F:7:GLN:HG2	1.97	0.47
1:J:102:VAL:HG22	1:J:103:PRO:HD3	1.95	0.47
1:M:138:LEU:O	1:M:142:THR:HG23	2.14	0.47
1:B:138:LEU:N	1:B:138:LEU:HD23	2.30	0.47
1:F:146:GLN:OE1	1:F:146:GLN:HA	2.15	0.47
1:I:27:LEU:HD13	1:I:118:THR:HG21	1.97	0.47
1:J:99:GLU:O	1:J:102:VAL:HG13	2.14	0.47
1:M:61:LEU:HB3	1:M:63:ILE:HG12	1.97	0.47
1:M:120:GLN:HB2	1:N:5:ALA:HB2	1.97	0.47
1:F:80:LEU:HD23	1:F:80:LEU:HA	1.60	0.47
2:P:8:DT:H2''	2:P:9:DA:C8	2.50	0.47
1:A:141:LEU:O	1:A:143:GLU:N	2.48	0.47
1:B:59:GLU:O	1:B:62:LYS:HD2	2.14	0.47
1:B:64:SER:O	1:B:68:VAL:HG23	2.14	0.47
1:M:39:THR:O	1:M:43:ILE:HG13	2.15	0.47
1:B:103:PRO:O	1:B:106:LYS:HB2	2.15	0.46
1:I:51:ILE:HD12	1:I:96:SER:HB3	1.97	0.46
1:N:69:THR:O	1:N:73:LYS:HG2	2.15	0.46
1:B:134:ILE:O	1:B:137:PHE:HB3	2.15	0.46
1:J:75:LEU:HA	1:J:75:LEU:HD23	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:ASN:C	1:J:126:PHE:N	2.74	0.46
1:B:42:HIS:HA	1:B:108:HIS:CD2	2.50	0.46
1:J:130:GLU:O	1:J:133:VAL:N	2.49	0.46
2:K:15:DC:H2''	2:K:16:DA:C8	2.50	0.46
1:F:18:PHE:CD1	1:F:18:PHE:C	2.94	0.46
1:N:47:LEU:HD21	1:N:57:ILE:HD11	1.97	0.46
1:B:47:LEU:HD21	1:B:57:ILE:HD11	1.98	0.46
1:B:99:GLU:C	1:B:101:ALA:N	2.73	0.46
1:I:15:ILE:HG22	1:I:16:MET:N	2.31	0.46
1:N:40:GLN:HE22	1:N:74:LYS:HZ3	1.64	0.45
2:O:4:DT:H2''	2:O:5:DA:H5'	1.98	0.45
1:A:143:GLU:OE1	1:E:143:GLU:HG3	2.16	0.45
1:B:48:ALA:HB2	1:B:97:LEU:HD11	1.97	0.45
1:E:40:GLN:HG2	1:E:75:LEU:HG	1.98	0.45
1:I:53:THR:HG22	1:I:94:LEU:CD2	2.46	0.45
1:I:142:THR:HG22	1:J:11:PHE:HD1	1.80	0.45
1:M:85:ARG:NH2	1:M:91:ARG:CA	2.80	0.45
1:M:92:VAL:O	1:M:92:VAL:HG13	2.15	0.45
2:L:11:DT:H2''	2:L:12:DT:H5'	1.98	0.45
1:E:44:LEU:HD21	1:E:75:LEU:HD13	1.97	0.45
1:J:64:SER:O	1:J:68:VAL:HG23	2.17	0.45
1:A:7:GLN:HG2	1:B:135:SER:OG	2.16	0.45
1:J:12:LEU:HA	1:J:12:LEU:HD23	1.72	0.45
1:M:121:GLU:C	1:M:123:GLY:H	2.24	0.45
1:A:44:LEU:HD22	1:A:97:LEU:HD23	1.98	0.45
1:E:8:ILE:O	1:E:12:LEU:HG	2.17	0.45
1:I:106:LYS:O	1:I:109:ALA:HB3	2.16	0.45
1:N:110:THR:HG22	1:N:114:LYS:HD3	1.98	0.45
1:E:134:ILE:O	1:E:138:LEU:HG	2.16	0.45
1:I:127:THR:HG22	1:I:130:GLU:CD	2.42	0.45
1:M:51:ILE:HD11	1:M:94:LEU:HD13	1.98	0.45
1:M:133:VAL:HG11	1:N:133:VAL:HG21	1.98	0.45
1:A:32:SER:HB3	1:A:35:LYS:HE3	1.98	0.45
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.76	0.45
1:I:11:PHE:CZ	1:J:141:LEU:HD23	2.52	0.45
1:B:16:MET:HE3	1:B:16:MET:HA	1.99	0.44
1:E:145:PHE:O	1:E:146:GLN:HB3	2.18	0.44
1:I:91:ARG:HE	1:M:85:ARG:CZ	2.29	0.44
1:E:58:ALA:HB1	1:E:63:ILE:O	2.18	0.44
1:M:134:ILE:HD12	1:N:137:PHE:CG	2.52	0.44
1:N:51:ILE:HG22	1:N:96:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:10:DG:H2'	2:P:11:DT:C6	2.53	0.44
1:A:12:LEU:O	1:A:15:ILE:HG22	2.17	0.44
1:A:34:VAL:O	1:A:34:VAL:HG12	2.18	0.44
1:I:72:LEU:O	1:I:73:LYS:C	2.61	0.44
1:B:37:THR:O	1:B:38:SER:C	2.60	0.44
1:E:53:THR:CG2	2:D:1:DT:H5'	2.45	0.44
1:I:102:VAL:N	1:I:103:PRO:HD2	2.32	0.44
1:M:86:ALA:C	1:M:88:ASN:H	2.26	0.44
1:N:145:PHE:C	1:N:146:GLN:HG2	2.43	0.44
2:O:7:DC:C2'	2:O:8:DT:H71	2.47	0.44
1:N:106:LYS:O	1:N:109:ALA:HB3	2.18	0.43
1:A:56:LYS:HD2	1:A:56:LYS:HA	1.73	0.43
1:B:145:PHE:CD1	1:B:145:PHE:N	2.85	0.43
1:B:128:ASP:HA	1:B:131:GLN:HB2	2.00	0.43
2:G:4:DT:H2''	2:G:5:DA:C5'	2.47	0.43
1:I:145:PHE:CE2	1:J:15:ILE:HG22	2.53	0.43
1:M:137:PHE:CE2	1:N:138:LEU:HD21	2.53	0.43
1:A:46:LEU:HD13	1:A:60:LYS:HG2	1.99	0.43
1:J:12:LEU:O	1:J:16:MET:HB2	2.19	0.43
1:A:4:LEU:HD23	1:B:123:GLY:HA3	2.00	0.43
1:A:136:LYS:HD2	1:A:136:LYS:HA	1.83	0.43
1:J:61:LEU:HA	1:J:61:LEU:HD23	1.67	0.43
1:M:102:VAL:N	1:M:103:PRO:CD	2.79	0.43
1:A:141:LEU:C	1:A:143:GLU:N	2.77	0.43
1:E:29:LYS:CD	1:E:30:SER:H	2.25	0.43
1:N:124:ASN:HA	1:N:131:GLN:NE2	2.34	0.43
1:A:53:THR:HG21	2:H:1:DT:H5'	1.99	0.43
2:K:10:DG:H2'	2:K:11:DT:C6	2.54	0.43
2:G:4:DT:H2''	2:G:5:DA:H5'	2.00	0.43
1:I:145:PHE:CD2	1:J:15:ILE:HG22	2.53	0.43
1:B:58:ALA:HB2	1:B:68:VAL:HG21	2.00	0.43
1:F:89:ASP:OD1	1:F:89:ASP:C	2.61	0.43
1:M:116:LEU:O	1:M:117:SER:C	2.62	0.43
1:F:48:ALA:HB2	1:F:97:LEU:CD1	2.42	0.42
2:P:11:DT:H2'	2:P:12:DT:C6	2.54	0.42
1:A:137:PHE:O	1:A:138:LEU:C	2.61	0.42
1:E:15:ILE:HG22	1:E:16:MET:HE2	2.01	0.42
1:I:4:LEU:O	1:I:5:ALA:C	2.60	0.42
1:J:54:ASN:HB3	2:K:2:DG:OP2	2.19	0.42
1:M:142:THR:HG22	1:N:11:PHE:HD1	1.83	0.42
1:I:18:PHE:CD1	1:I:18:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3:DT:C2'	2:K:4:DT:C6	3.02	0.42
1:I:142:THR:CG2	1:J:11:PHE:HD1	2.32	0.42
1:J:15:ILE:HG13	1:J:16:MET:N	2.33	0.42
1:A:47:LEU:HB3	1:A:97:LEU:HG	2.01	0.42
1:J:130:GLU:C	1:J:132:GLU:N	2.76	0.42
1:N:56:LYS:HE3	1:N:60:LYS:HG3	2.01	0.42
1:I:75:LEU:HA	1:I:75:LEU:HD23	1.76	0.42
1:M:61:LEU:O	1:M:62:LYS:C	2.61	0.42
1:M:130:GLU:O	1:M:134:ILE:HG12	2.18	0.42
1:A:76:GLN:O	1:A:79:GLU:N	2.52	0.42
1:E:12:LEU:HD22	1:F:15:ILE:HD13	2.01	0.42
1:E:19:ALA:HB2	1:E:25:ILE:HD11	2.01	0.42
1:I:108:HIS:CD2	1:I:112:HIS:HD2	2.37	0.42
1:J:127:THR:HG22	1:J:129:GLU:HG3	2.01	0.42
1:M:12:LEU:HD22	1:N:15:ILE:HD13	2.01	0.42
1:M:7:GLN:HE22	1:N:135:SER:CB	2.32	0.42
1:N:137:PHE:O	1:N:140:ALA:HB3	2.20	0.42
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.74	0.42
1:N:50:GLN:HG2	1:N:51:ILE:O	2.19	0.42
1:F:78:GLN:C	1:F:79:GLU:HG2	2.45	0.41
1:N:51:ILE:HG22	1:N:96:SER:HB3	2.01	0.41
1:I:123:GLY:HA3	1:J:4:LEU:HD23	2.02	0.41
1:N:53:THR:HG22	1:N:94:LEU:HD23	2.01	0.41
1:B:54:ASN:OD1	1:B:54:ASN:C	2.63	0.41
1:E:84:SER:O	1:E:86:ALA:N	2.53	0.41
1:M:85:ARG:CD	1:M:88:ASN:O	2.67	0.41
1:N:90:GLU:O	1:N:90:GLU:HG3	2.19	0.41
1:N:116:LEU:HD23	1:N:116:LEU:HA	1.96	0.41
1:I:47:LEU:HD21	1:I:57:ILE:HD11	2.02	0.41
1:N:47:LEU:HA	1:N:50:GLN:O	2.20	0.41
1:E:47:LEU:O	1:E:48:ALA:C	2.62	0.41
1:J:53:THR:HG22	1:J:93:VAL:O	2.21	0.41
1:M:82:LYS:HB2	1:M:82:LYS:HE3	1.90	0.41
1:A:44:LEU:HD21	1:A:75:LEU:HD13	2.03	0.41
1:F:47:LEU:HB2	1:F:97:LEU:HD21	2.03	0.41
1:J:45:MET:HE2	1:J:45:MET:HB3	1.87	0.41
1:F:139:SER:O	1:F:143:GLU:HG2	2.20	0.41
1:M:85:ARG:CD	1:M:89:ASP:HA	2.51	0.41
1:I:53:THR:O	1:I:54:ASN:C	2.64	0.41
1:J:80:LEU:HD23	1:J:80:LEU:HA	1.89	0.41
1:M:106:LYS:O	1:M:109:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:127:THR:CG2	1:M:128:ASP:N	2.84	0.41
1:N:37:THR:OG1	1:N:40:GLN:HG3	2.20	0.41
1:N:127:THR:O	1:N:130:GLU:N	2.54	0.41
2:H:1:DT:O5'	2:H:1:DT:H2'	2.21	0.41
1:A:45:MET:HE2	1:A:45:MET:HB3	1.87	0.41
1:A:61:LEU:O	1:A:62:LYS:C	2.63	0.41
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.85	0.41
2:C:1:DT:H5''	2:C:1:DT:C6	2.52	0.41
1:F:141:LEU:O	1:F:142:THR:C	2.64	0.41
1:M:75:LEU:HD23	1:M:75:LEU:HA	1.86	0.41
1:I:51:ILE:CD1	1:I:96:SER:HB3	2.50	0.41
2:H:11:DT:H2'	2:H:12:DT:C6	2.56	0.41
1:M:110:THR:HG22	1:M:113:GLU:OE1	2.21	0.40
1:F:120:GLN:NE2	1:F:120:GLN:HA	2.35	0.40
2:O:3:DT:H2'	2:O:4:DT:H72	2.03	0.40
2:C:11:DT:H2'	2:C:12:DT:C6	2.55	0.40
2:G:4:DT:H2''	2:G:5:DA:O5'	2.21	0.40
2:C:4:DT:H2'	2:C:5:DA:C8	2.56	0.40
2:G:2:DG:H2''	2:G:3:DT:H72	2.03	0.40
1:J:61:LEU:O	1:J:62:LYS:C	2.65	0.40
1:B:74:LYS:O	1:B:77:GLU:HB2	2.21	0.40
1:N:61:LEU:N	1:N:61:LEU:HD12	2.36	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	144/146 (99%)	123 (85%)	16 (11%)	5 (4%)	3	12
1	B	142/146 (97%)	130 (92%)	9 (6%)	3 (2%)	5	21
1	E	143/146 (98%)	132 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	143/146 (98%)	134 (94%)	8 (6%)	1 (1%)	18	48
1	I	143/146 (98%)	129 (90%)	12 (8%)	2 (1%)	9	30
1	J	143/146 (98%)	134 (94%)	7 (5%)	2 (1%)	9	30
1	M	142/146 (97%)	124 (87%)	18 (13%)	0	100	100
1	N	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
All	All	1142/1168 (98%)	1038 (91%)	91 (8%)	13 (1%)	11	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	89	ASP
1	A	142	THR
1	I	51	ILE
1	A	87	THR
1	J	131	GLN
1	B	9	ASP
1	B	100	LYS
1	A	3	SER
1	F	88	ASN
1	J	89	ASP
1	B	8	ILE
1	I	5	ALA

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	122/129 (95%)	113 (93%)	9 (7%)	13	38
1	B	125/129 (97%)	118 (94%)	7 (6%)	19	50
1	E	128/129 (99%)	122 (95%)	6 (5%)	23	56
1	F	129/129 (100%)	117 (91%)	12 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	125/129 (97%)	120 (96%)	5 (4%)	28	62
1	J	128/129 (99%)	123 (96%)	5 (4%)	28	63
1	M	125/129 (97%)	118 (94%)	7 (6%)	19	50
1	N	125/129 (97%)	122 (98%)	3 (2%)	43	75
All	All	1007/1032 (98%)	953 (95%)	54 (5%)	20	51

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	15	ILE
1	A	25	ILE
1	A	52	SER
1	A	62	LYS
1	A	78	GLN
1	A	93	VAL
1	A	112	HIS
1	A	124	ASN
1	B	15	ILE
1	B	17	GLN
1	B	46	LEU
1	B	50	GLN
1	B	51	ILE
1	B	52	SER
1	B	102	VAL
1	E	2	MET
1	E	39	THR
1	E	104	VAL
1	E	106	LYS
1	E	116	LEU
1	E	142	THR
1	F	2	MET
1	F	16	MET
1	F	23	HIS
1	F	34	VAL
1	F	51	ILE
1	F	91	ARG
1	F	110	THR
1	F	115	THR
1	F	116	LEU
1	F	120	GLN

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Mol	Chain	Res	Type
1	F	124	ASN
1	F	127	THR
1	I	6	ASN
1	I	51	ILE
1	I	91	ARG
1	I	110	THR
1	I	133	VAL
1	J	3	SER
1	J	30	SER
1	J	102	VAL
1	J	112	HIS
1	J	116	LEU
1	M	20	GLU
1	M	47	LEU
1	M	61	LEU
1	M	64	SER
1	M	69	THR
1	M	93	VAL
1	M	98	THR
1	N	52	SER
1	N	112	HIS
1	N	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	23	HIS
1	A	111	HIS
1	A	120	GLN
1	A	124	ASN
1	E	6	ASN
1	F	120	GLN
1	F	124	ASN
1	F	131	GLN
1	I	6	ASN
1	I	21	ASN
1	I	111	HIS
1	I	120	GLN
1	J	78	GLN
1	M	6	ASN
1	M	7	GLN

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Mol	Chain	Res	Type
1	M	17	GLN
1	N	10	GLN
1	N	40	GLN

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 8 ligands modelled in this entry, 8 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, 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	146/146 (100%)	0.72	12 (8%) 17 14	58, 104, 142, 165	0
1	B	144/146 (98%)	0.42	5 (3%) 47 38	62, 96, 127, 136	0
1	E	145/146 (99%)	0.29	1 (0%) 84 79	56, 87, 115, 142	0
1	F	145/146 (99%)	0.35	2 (1%) 73 65	58, 85, 115, 126	0
1	I	145/146 (99%)	0.37	5 (3%) 48 39	52, 78, 107, 116	0
1	J	145/146 (99%)	0.37	5 (3%) 48 39	56, 82, 111, 121	0
1	M	144/146 (98%)	0.58	5 (3%) 47 38	59, 103, 132, 162	0
1	N	144/146 (98%)	0.42	3 (2%) 63 54	64, 100, 127, 144	0
2	C	16/16 (100%)	-0.25	0 100 100	60, 71, 76, 78	0
2	D	16/16 (100%)	-0.48	0 100 100	55, 69, 75, 77	0
2	G	16/16 (100%)	0.07	0 100 100	63, 73, 95, 100	0
2	H	16/16 (100%)	-0.08	0 100 100	60, 72, 84, 88	0
2	K	16/16 (100%)	-0.09	0 100 100	59, 69, 88, 91	0
2	L	16/16 (100%)	-0.14	0 100 100	60, 70, 80, 80	0
2	O	16/16 (100%)	-0.09	0 100 100	61, 69, 76, 76	0
2	P	16/16 (100%)	-0.39	0 100 100	51, 66, 75, 78	0
All	All	1286/1296 (99%)	0.38	38 (2%) 52 43	51, 89, 126, 165	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	139	SER	4.2
1	A	87	THR	3.9
1	A	85	ARG	3.7
1	A	88	ASN	3.7
1	B	5	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	3.2
1	M	7	GLN	3.2
1	N	7	GLN	3.2
1	A	35	LYS	3.0
1	J	37	THR	3.0
1	A	5	ALA	3.0
1	A	139	SER	3.0
1	E	21	ASN	2.9
1	M	119	TYR	2.8
1	B	4	LEU	2.8
1	N	33	ASP	2.8
1	I	2	MET	2.7
1	I	33	ASP	2.6
1	B	72	LEU	2.6
1	M	124	ASN	2.6
1	J	79	GLU	2.5
1	J	23	HIS	2.5
1	A	28	GLY	2.4
1	A	32	SER	2.3
1	I	105	ALA	2.2
1	J	20	GLU	2.2
1	A	34	VAL	2.2
1	A	107	GLU	2.2
1	N	23	HIS	2.2
1	J	38	SER	2.2
1	I	135	SER	2.1
1	F	21	ASN	2.1
1	M	138	LEU	2.1
1	B	130	GLU	2.1
1	F	91	ARG	2.1
1	I	137	PHE	2.1
1	A	89	ASP	2.0
1	B	119	TYR	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

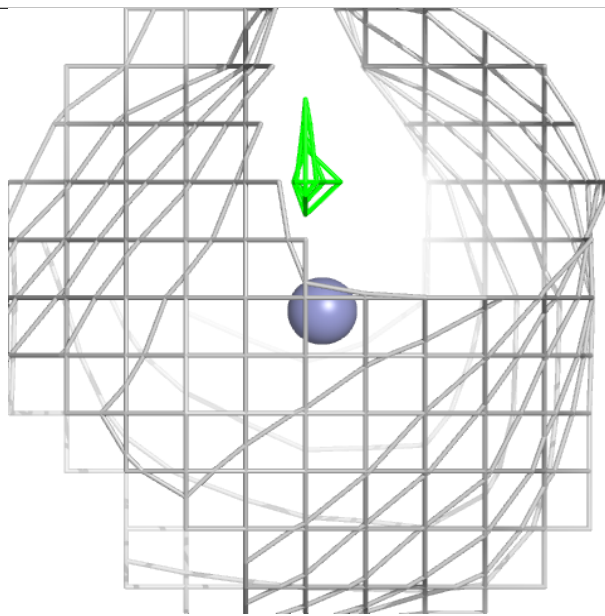
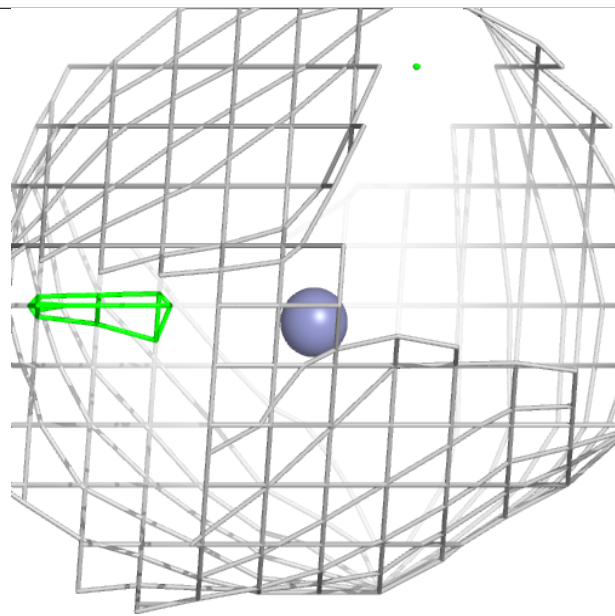
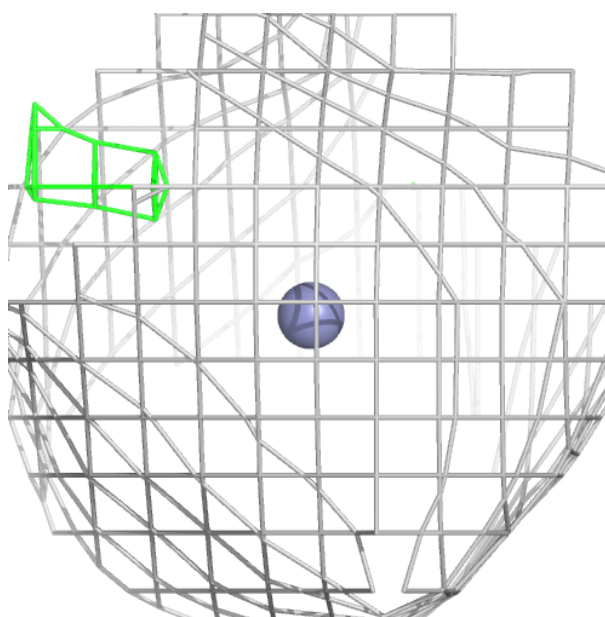
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	201	1/1	0.99	0.07	88,88,88,88	0
3	ZN	F	201	1/1	0.99	0.06	76,76,76,76	0
3	ZN	I	201	1/1	0.99	0.05	70,70,70,70	0
3	ZN	J	201	1/1	0.99	0.05	74,74,74,74	0
3	ZN	M	201	1/1	0.99	0.09	91,91,91,91	0
3	ZN	N	201	1/1	0.99	0.07	81,81,81,81	0
3	ZN	E	201	1/1	1.00	0.06	77,77,77,77	0
3	ZN	B	201	1/1	1.00	0.03	79,79,79,79	0

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

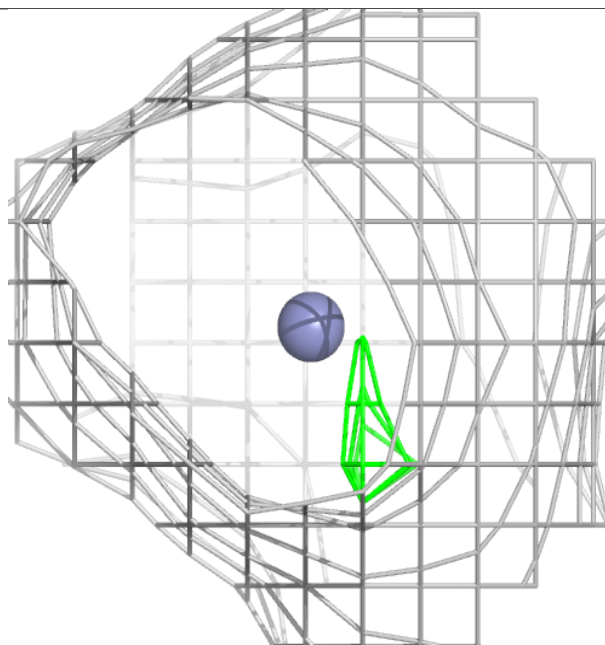
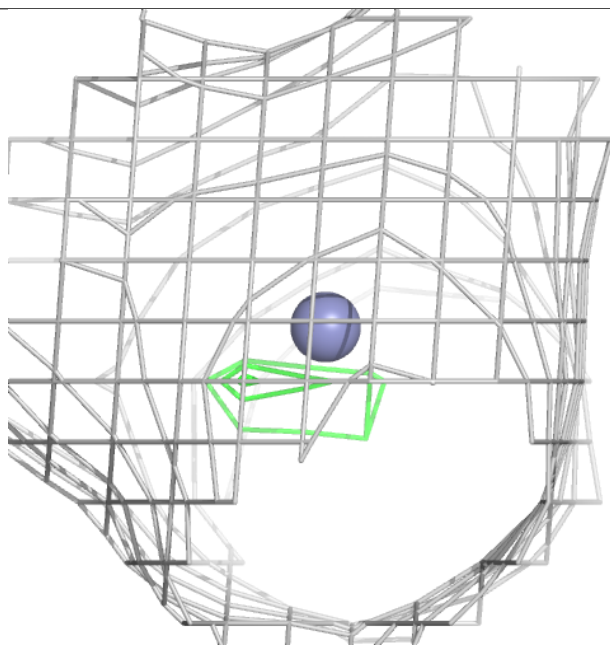
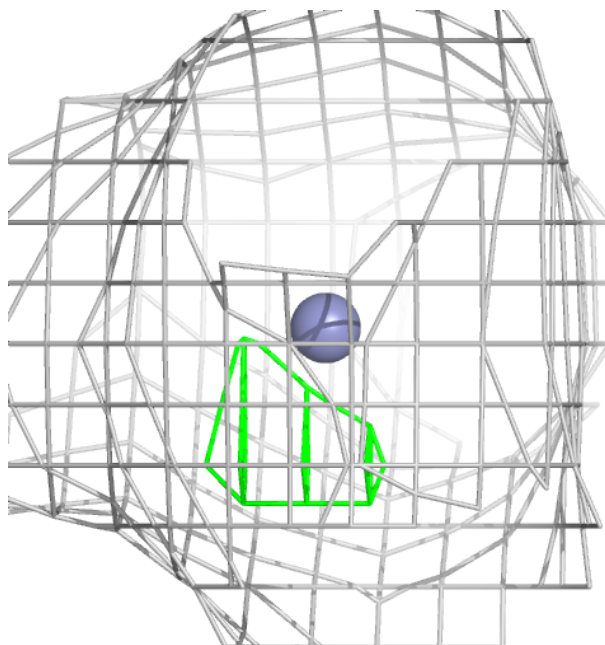
Electron density around ZN A 201:

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



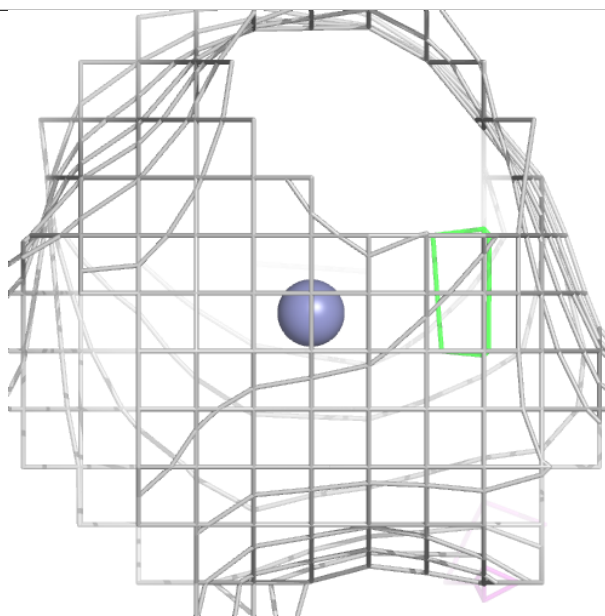
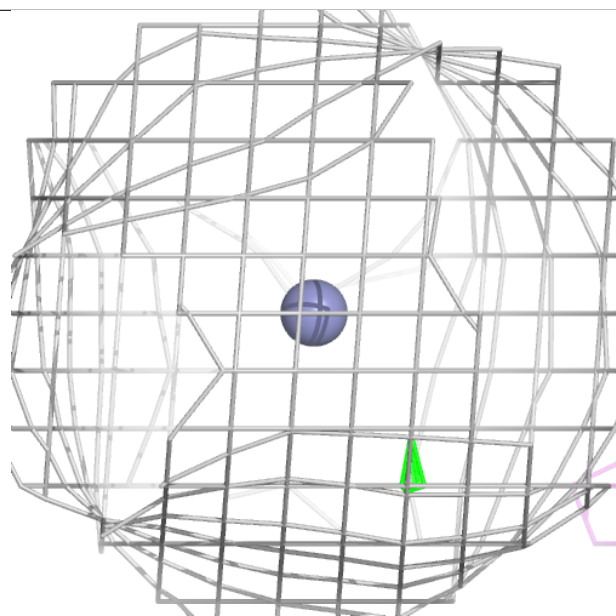
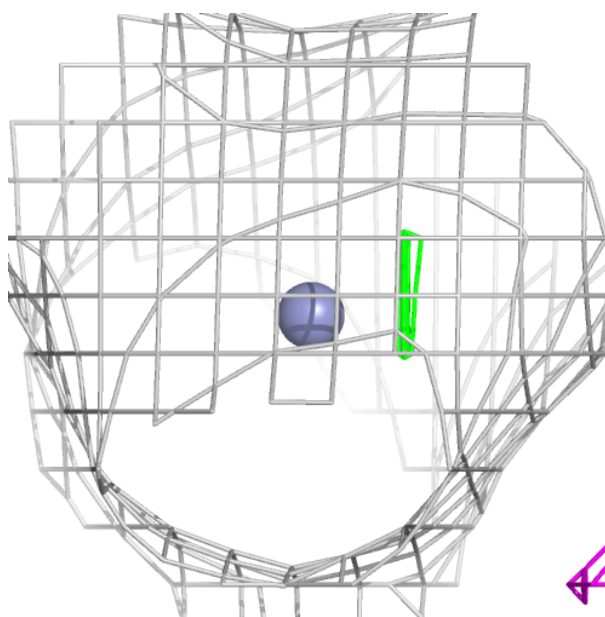
Electron density around ZN F 201:

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



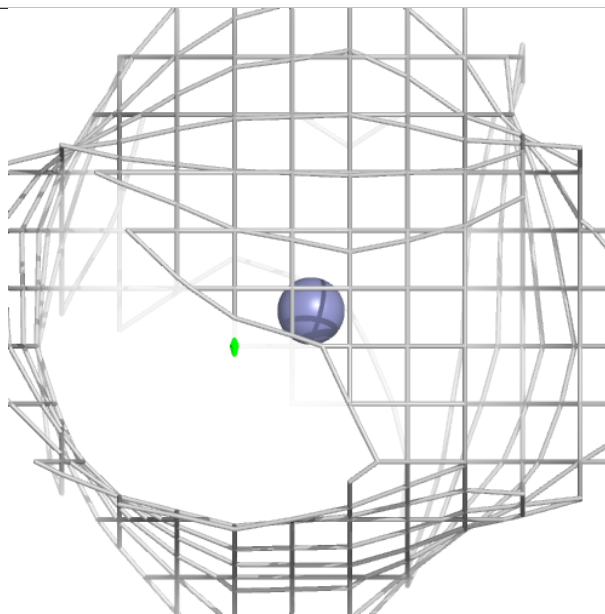
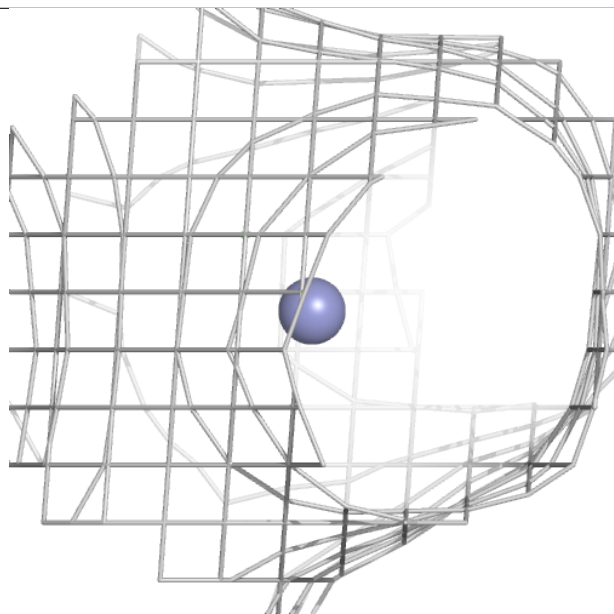
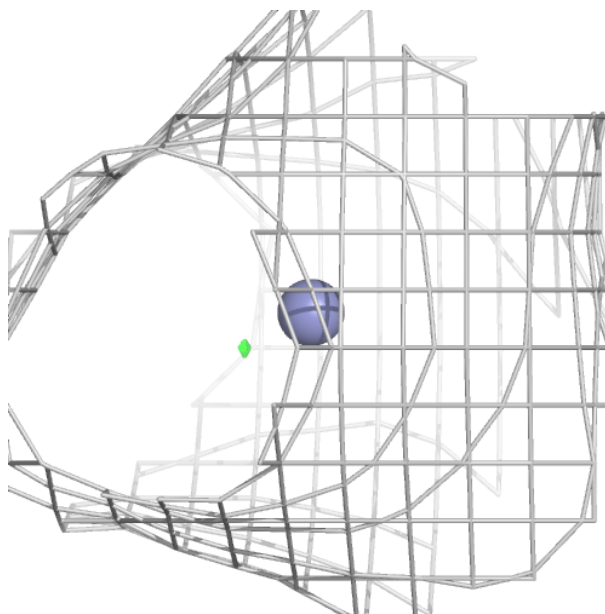
Electron density around ZN I 201:

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



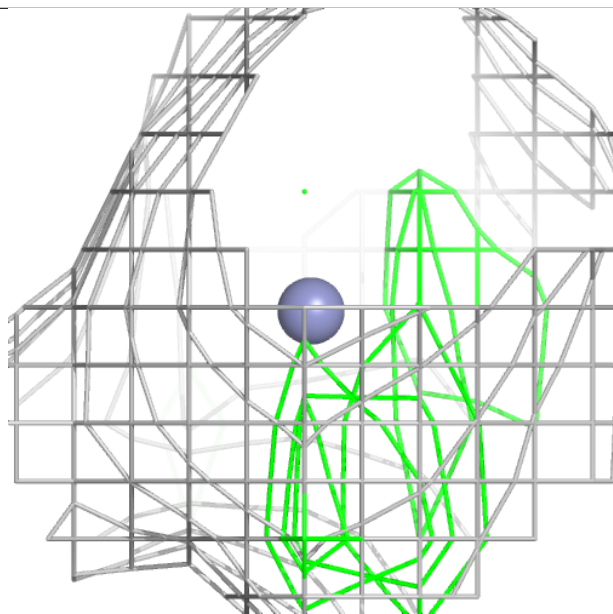
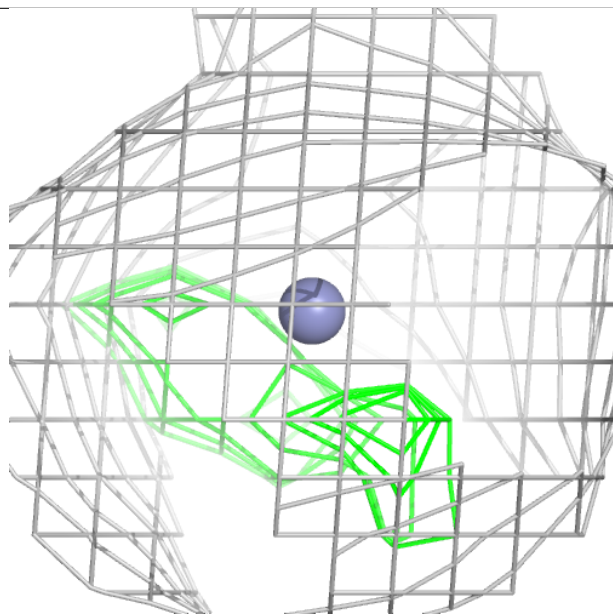
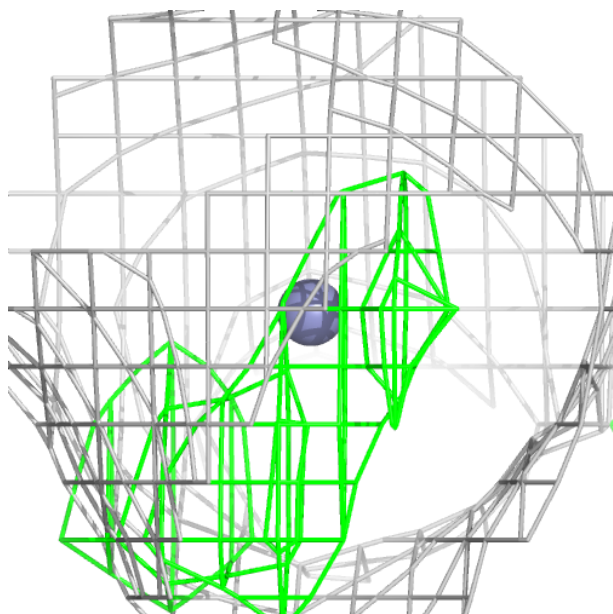
Electron density around ZN J 201:

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



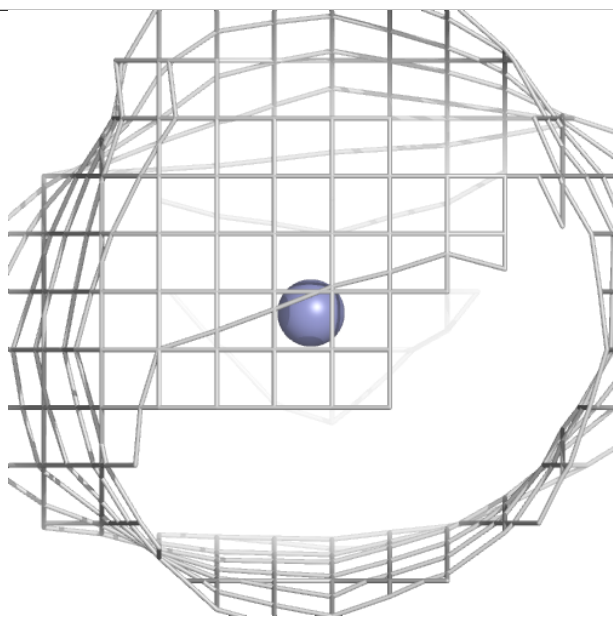
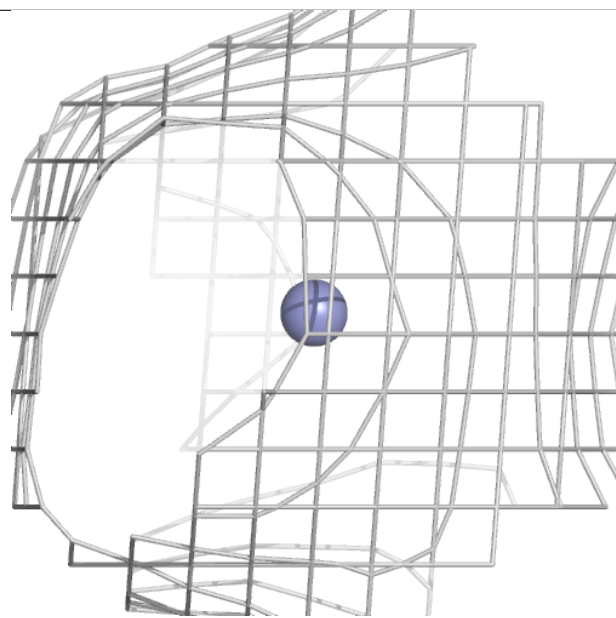
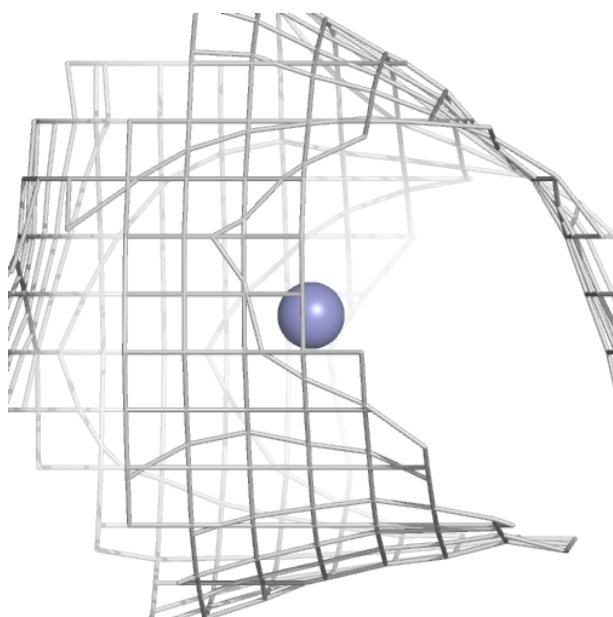
Electron density around ZN M 201:

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



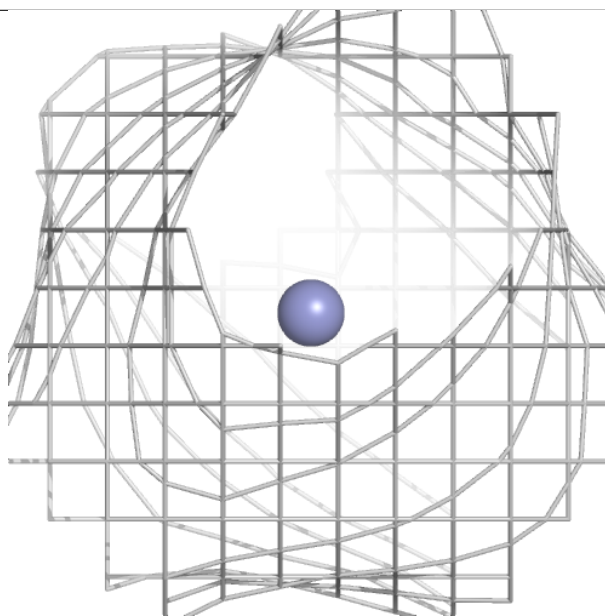
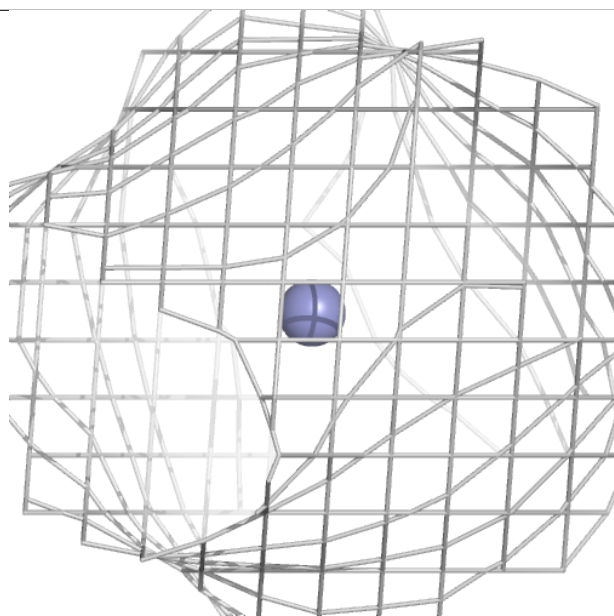
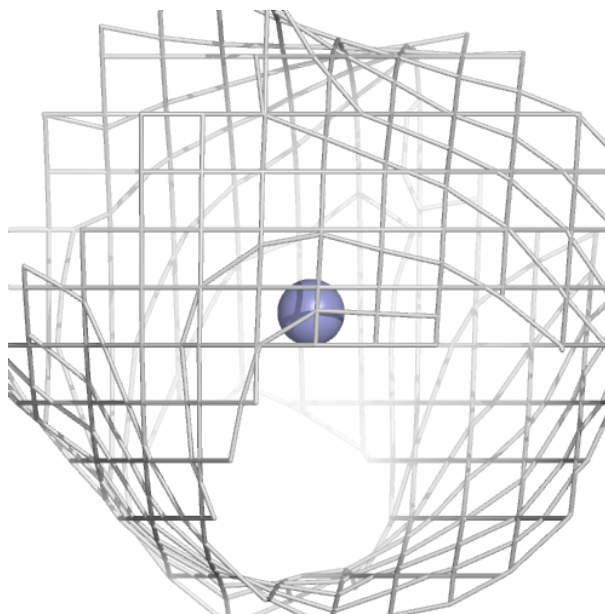
Electron density around ZN N 201:

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



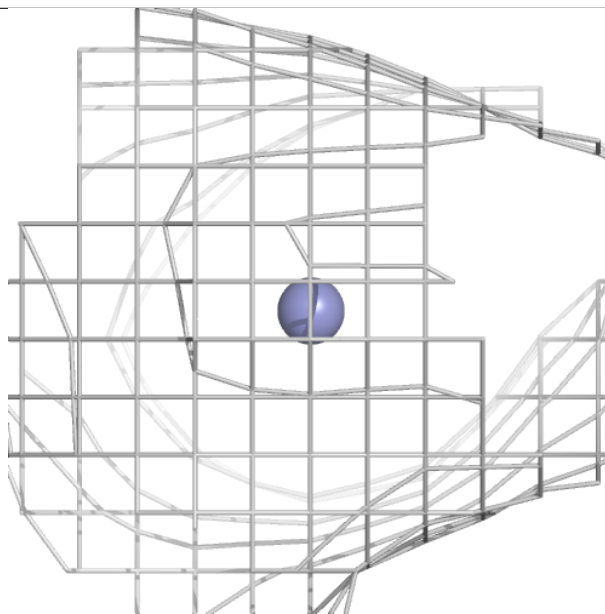
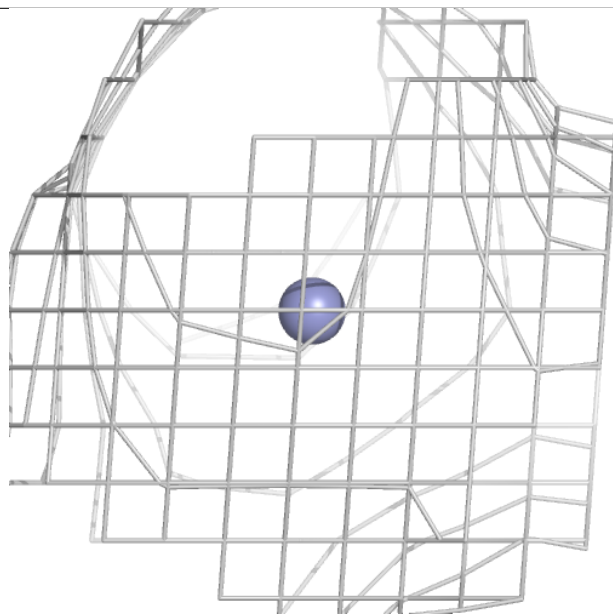
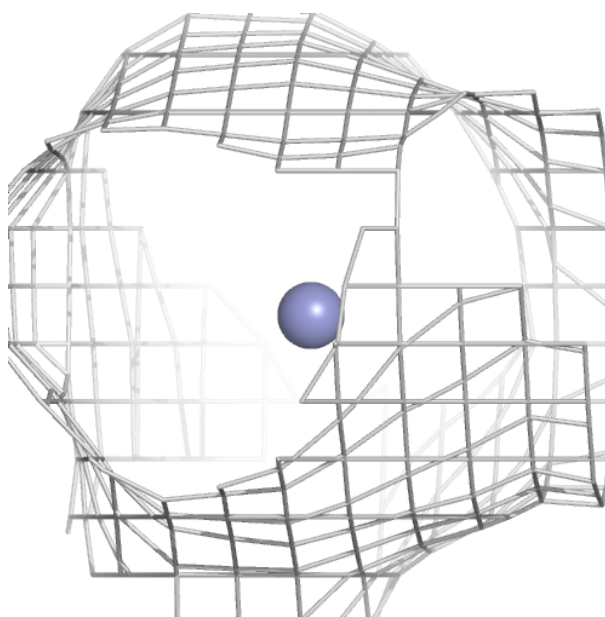
Electron density around ZN E 201:

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



Electron density around ZN B 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.