



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2025 – 06:34 PM JST

PDB ID : 9KBO / pdb\_00009kbo  
Title : Crystal structure of human Shiftless (SFL) containing phosphorylation sites Ser249, Thr250, Thr253 and Ser256  
Authors : Li, Z.; Hao, W.; Zhang, Y.; Hou, P.; Cui, S.  
Deposited on : 2024-10-31  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

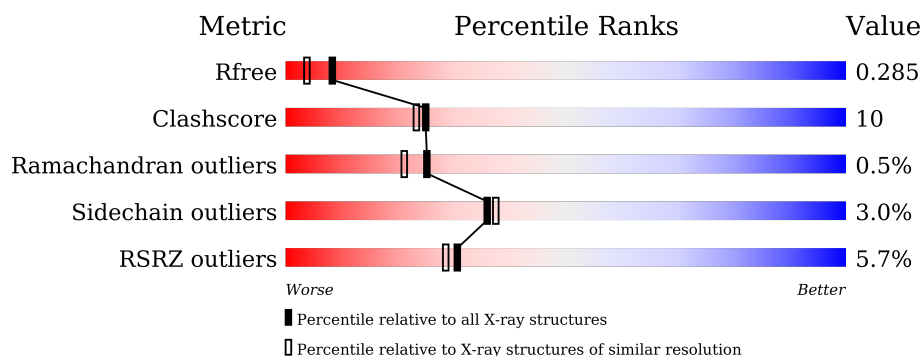
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	291	<div> <div>3%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div>
1	B	291	<div> <div>3%</div> <div>78%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	291	<div> <div>8%</div> <div>68%</div> <div>24%</div> <div>• 5%</div> </div>
1	D	291	<div> <div>6%</div> <div>45%</div> <div>18%</div> <div>• 35%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16681 atoms, of which 7949 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 Shiftless antiviral inhibitor of ribosomal frameshifting protein.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	278	Total	C	H	N	O	P	S		0	4	0
			4429	1381	2174	428	425	4	17				
1	B	277	Total	C	H	N	O	P	S		0	2	0
			4349	1359	2125	423	421	4	17				
1	C	276	Total	C	H	N	O	P	S		0	4	0
			4399	1367	2166	425	420	4	17				
1	D	188	Total	C	H	N	O	P	S		0	1	0
			2994	920	1484	279	298	4	9				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NUL5
B	1	GLY	-	expression tag	UNP Q9NUL5
C	1	GLY	-	expression tag	UNP Q9NUL5
D	1	GLY	-	expression tag	UNP Q9NUL5

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		
2	D	2	Total	Zn	0	0
			2	2		

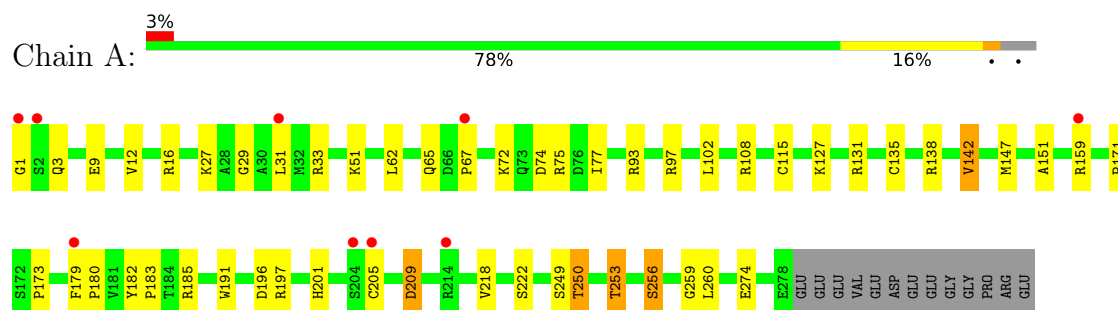
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total 152	O 152	0	0
3	B	159	Total 159	O 159	0	0
3	C	133	Total 133	O 133	0	0
3	D	55	Total 55	O 55	0	0

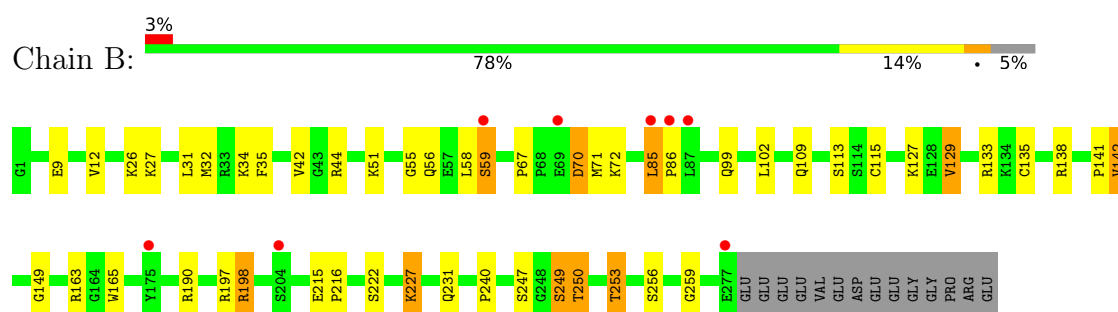
### 3 Residue-property plots [i](#)

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.

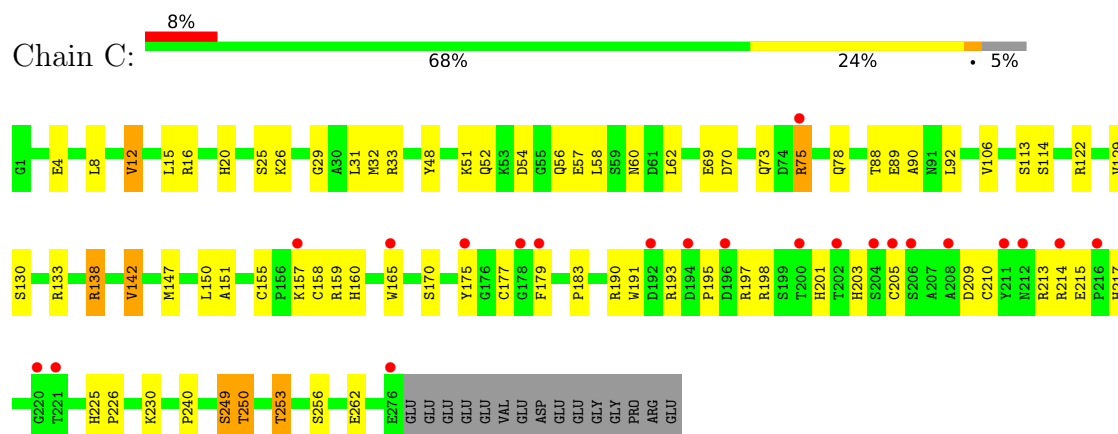
- Molecule 1: Shiftless antiviral inhibitor of ribosomal frameshifting protein



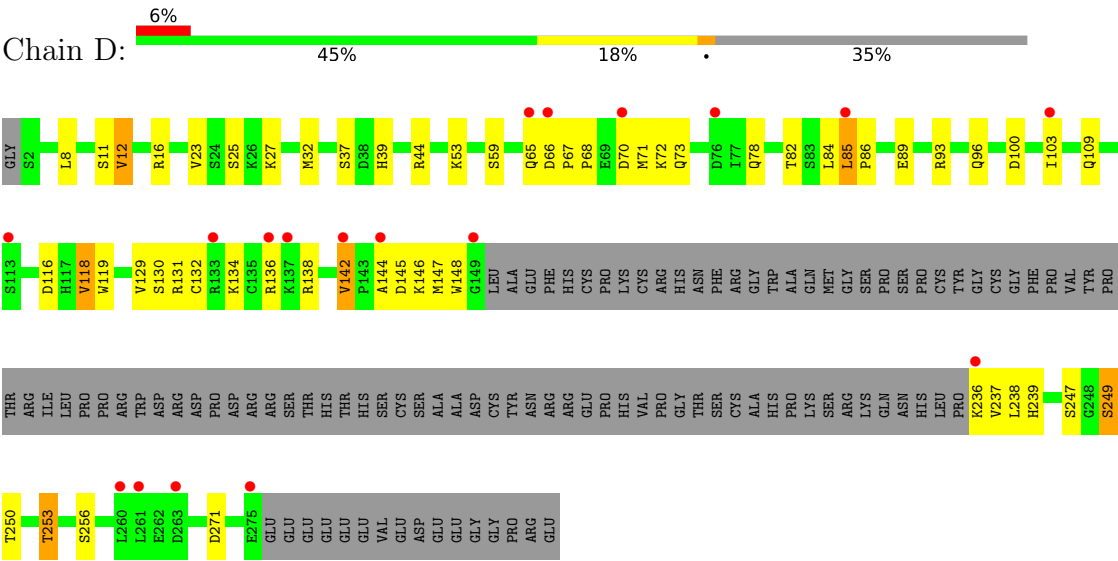
- Molecule 1: Shiftless antiviral inhibitor of ribosomal frameshifting protein



- Molecule 1: Shiftless antiviral inhibitor of ribosomal frameshifting protein



- Molecule 1: Shiftless antiviral inhibitor of ribosomal frameshifting protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.72Å 89.41Å 82.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.00 39.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.28-2.00) 97.7 (39.28-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, $R_{free}$	0.222 , 0.286 0.222 , 0.285	Depositor DCC
$R_{free}$ test set	5271 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, SEP, 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	0.63	0/2278	0.76	1/3069 (0.0%)
1	B	0.69	0/2239	0.77	1/3018 (0.0%)
1	C	0.61	0/2254	0.73	0/3037
1	D	0.47	0/1492	0.65	0/1998
All	All	0.62	0/8263	0.73	2/11122 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ARG	CB-CG-CD	-6.37	96.66	111.30
1	A	205	CYS	CB-CA-C	-5.02	98.42	109.56

There are no chirality outliers.

All (5) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	A	209	ASP	Peptide
1	B	163	ARG	Sidechain
1	C	138	ARG	Sidechain
1	D	84	LEU	Peptide

## 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	2255	2174	2175	29	0
1	B	2224	2125	2142	32	0
1	C	2233	2166	2166	51	0
1	D	1510	1484	1480	46	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	152	0	0	5	0
3	B	159	0	0	5	1
3	C	133	0	0	10	1
3	D	55	0	0	8	0
All	All	8732	7949	7963	156	1

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 10.

All (156) 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:127:LYS:NZ	1:B:250:TPO:O2P	1.95	0.98
1:B:198:ARG:NH1	3:B:401:HOH:O	1.99	0.95
1:D:86:PRO:O	3:D:401:HOH:O	1.88	0.90
1:C:88:THR:HG22	1:C:90:ALA:H	1.39	0.87
1:D:27:LYS:NZ	3:D:404:HOH:O	2.07	0.86
1:A:159[B]:ARG:NH1	3:A:401:HOH:O	2.12	0.80
1:B:85:LEU:HB3	1:B:86:PRO:HD3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:TPO:O3P	3:D:403:HOH:O	2.06	0.72
1:D:32:MET:HE1	1:D:39:HIS:N	2.06	0.71
1:D:100:ASP:OD1	3:D:402:HOH:O	2.06	0.71
1:D:144:ALA:HA	1:D:147:MET:HE2	1.71	0.71
1:A:27:LYS:O	1:A:31:LEU:HD23	1.93	0.69
1:D:253:TPO:P	3:D:403:HOH:O	2.50	0.69
1:A:173:PRO:HG2	1:A:218:VAL:HG21	1.76	0.68
1:B:247:SER:OG	1:B:249:SEP:O3P	2.09	0.67
1:B:70:ASP:N	1:B:70:ASP:OD1	2.27	0.67
1:C:230:LYS:O	3:C:401:HOH:O	2.13	0.67
1:D:16:ARG:HD2	1:D:23:VAL:O	1.94	0.67
1:B:85:LEU:CB	1:B:86:PRO:CD	2.74	0.65
1:B:222:SER:OG	3:B:402:HOH:O	2.14	0.64
1:B:227:LYS:NZ	3:B:405:HOH:O	2.26	0.64
1:C:160:HIS:NE2	3:C:407:HOH:O	2.30	0.63
1:B:129:VAL:HG11	1:B:138:ARG:HD3	1.80	0.63
1:A:1:GLY:N	3:A:403:HOH:O	2.30	0.63
1:B:85:LEU:HB3	1:B:86:PRO:CD	2.27	0.63
1:D:68:PRO:HD2	1:D:71:MET:HB2	1.81	0.61
1:A:253:TPO:HG22	3:A:405:HOH:O	2.00	0.60
1:B:133:ARG:NH2	1:B:253:TPO:O2P	2.35	0.59
1:C:51:LYS:HE2	1:C:62:LEU:O	2.03	0.58
1:C:155:CYS:SG	1:C:158:CYS:N	2.75	0.58
1:A:256:SEP:HB2	3:A:497:HOH:O	2.05	0.57
1:A:171:PRO:HD3	1:A:182:TYR:CE2	2.40	0.56
1:C:75[A]:ARG:NE	1:C:78:GLN:OE1	2.37	0.56
1:C:205:CYS:O	1:C:214:ARG:N	2.37	0.56
1:B:141:PRO:O	3:B:403:HOH:O	2.18	0.55
1:C:113:SER:HB2	1:C:240:PRO:HB3	1.87	0.55
1:D:68:PRO:HG2	1:D:71:MET:HE3	1.87	0.55
1:C:129:VAL:CG2	1:C:138:ARG:HD3	2.37	0.55
1:D:93:ARG:HD2	1:D:96:GLN:OE1	2.06	0.55
1:C:4[A]:GLU:HG3	3:C:427:HOH:O	2.05	0.54
1:D:32:MET:HE3	1:D:37:SER:C	2.32	0.54
1:D:65:GLN:O	1:D:67:PRO:HD3	2.07	0.54
1:B:109:GLN:O	1:B:142:VAL:HG12	2.07	0.54
1:C:20:HIS:HE1	3:C:516:HOH:O	1.91	0.53
1:C:177:CYS:HB2	1:C:179:PHE:H	1.73	0.53
1:D:247:SER:OG	1:D:249:SEP:O3P	2.16	0.53
1:A:72:LYS:O	1:A:72:LYS:HD3	2.08	0.53
1:D:118:VAL:HG11	1:D:148:TRP:HZ2	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD12	1:D:85:LEU:O	2.08	0.53
1:C:122:ARG:NH1	3:C:404:HOH:O	2.24	0.53
1:B:27:LYS:O	1:B:31:LEU:HD23	2.10	0.52
1:A:115:CYS:SG	1:A:135:CYS:HB3	2.49	0.52
1:D:11:SER:HB2	1:D:32:MET:CE	2.41	0.51
1:C:197:ARG:HD2	3:C:434:HOH:O	2.10	0.51
1:D:130:SER:HA	3:D:403:HOH:O	2.11	0.51
1:A:12:VAL:O	1:A:16:ARG:HG3	2.11	0.50
1:A:185:ARG:NH1	1:D:89[B]:GLU:OE1	2.45	0.50
1:D:146:LYS:HE3	1:D:239:HIS:CD2	2.47	0.50
1:B:42:VAL:HG23	1:B:71:MET:HE2	1.93	0.50
1:C:249:SEP:O1P	3:C:403:HOH:O	2.20	0.50
1:C:69:GLU:O	1:C:73[B]:GLN:OE1	2.29	0.49
1:A:142:VAL:CG2	1:A:147:MET:HG2	2.42	0.49
1:D:32:MET:HE3	1:D:37:SER:HA	1.93	0.49
1:C:262:GLU:OE1	3:C:402:HOH:O	2.19	0.49
1:B:51:LYS:NZ	1:B:59:SER:O	2.42	0.49
1:D:53:LYS:HB3	1:D:85:LEU:HD21	1.95	0.49
1:D:11:SER:HB2	1:D:32:MET:HE2	1.94	0.49
1:D:32:MET:HE2	1:D:39:HIS:HB3	1.94	0.48
1:D:131:ARG:NH2	1:D:271:ASP:OD2	2.42	0.48
1:C:54:ASP:OD1	1:C:56:GLN:HB2	2.14	0.48
1:C:129:VAL:HG22	1:C:138:ARG:HD3	1.95	0.48
1:C:190:ARG:HD3	1:C:193:ARG:HG3	1.95	0.48
1:D:109:GLN:HB3	1:D:142:VAL:CG1	2.43	0.47
1:C:230:LYS:HA	1:C:230:LYS:HD2	1.74	0.47
1:D:119:TRP:CH2	1:D:132:CYS:HA	2.50	0.47
1:A:209:ASP:HB2	1:A:222:SER:HA	1.96	0.47
1:B:85:LEU:CB	1:B:86:PRO:HD3	2.34	0.47
1:D:32:MET:CE	1:D:39:HIS:HB3	2.44	0.47
1:A:9:GLU:O	1:A:12:VAL:HG22	2.15	0.46
1:A:74:ASP:HB3	1:A:77:ILE:HD13	1.98	0.46
1:C:75[A]:ARG:CZ	1:C:78:GLN:OE1	2.63	0.46
1:B:190:ARG:HA	1:B:259:GLY:O	2.16	0.46
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.83	0.45
1:C:29:GLY:O	1:C:33:ARG:HG3	2.16	0.45
1:C:203:HIS:CE1	1:C:205:CYS:HB2	2.51	0.45
1:D:16:ARG:HD3	1:D:25:SER:HA	1.97	0.45
1:A:127:LYS:HD3	1:A:250:TPO:OG1	2.17	0.44
1:B:215:GLU:HA	1:B:216:PRO:C	2.42	0.44
1:B:32:MET:HA	1:B:32:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HD3	1:D:65:GLN:NE2	2.33	0.44
1:B:231:GLN:NE2	3:B:411:HOH:O	2.38	0.44
1:C:15:LEU:HD22	1:C:32:MET:HE3	1.98	0.44
1:C:150:LEU:HD23	1:C:197:ARG:HG2	2.00	0.44
1:D:70:ASP:N	1:D:70:ASP:OD1	2.50	0.44
1:B:9:GLU:O	1:B:12:VAL:HG22	2.18	0.44
1:B:67:PRO:HG2	1:B:72:LYS:HB2	2.00	0.43
1:A:151:ALA:HB1	1:A:183:PRO:HB3	2.01	0.43
1:C:26:LYS:HA	3:C:519:HOH:O	2.18	0.43
1:C:195:PRO:HB2	1:C:201:HIS:CD2	2.53	0.43
1:C:133:ARG:NH2	1:C:262:GLU:OE1	2.51	0.43
1:C:57:GLU:O	1:C:60:ASN:HB2	2.18	0.43
1:D:132:CYS:SG	1:D:134:LYS:HB2	2.58	0.43
1:C:142:VAL:HG23	1:C:147:MET:HG3	2.00	0.43
1:B:44:ARG:HD3	1:B:99:GLN:O	2.18	0.43
1:B:55:GLY:O	1:B:56:GLN:HB2	2.18	0.43
1:D:32:MET:HE3	1:D:37:SER:CA	2.49	0.43
1:D:118:VAL:HG12	1:D:237:VAL:HG22	2.01	0.43
1:C:75[A]:ARG:HA	1:C:78:GLN:HG2	2.00	0.43
1:D:116:ASP:OD2	1:D:236:LYS:N	2.52	0.43
1:C:88:THR:HG22	1:C:89:GLU:N	2.34	0.43
1:C:138:ARG:CZ	1:C:250:TPO:HG21	2.49	0.43
1:C:213:ARG:HD2	1:C:217:HIS:CG	2.54	0.42
1:A:51:LYS:HE2	1:A:62:LEU:O	2.20	0.42
1:B:113:SER:HB2	1:B:240:PRO:HB3	2.01	0.42
1:D:85:LEU:N	1:D:86:PRO:CD	2.82	0.42
1:C:58:LEU:HD22	1:C:92:LEU:HD22	2.01	0.42
1:A:3:GLN:OE1	1:B:26:LYS:CE	2.67	0.42
1:D:72:LYS:O	1:D:78:GLN:NE2	2.53	0.42
1:A:191:TRP:NE1	1:A:259:GLY:HA2	2.34	0.42
1:B:115:CYS:SG	1:B:135:CYS:HB3	2.59	0.42
1:C:70:ASP:HA	1:C:73[B]:GLN:HE22	1.85	0.42
1:C:8:LEU:O	1:C:12:VAL:HG13	2.19	0.42
1:D:132:CYS:O	1:D:136:ARG:N	2.51	0.42
1:A:196:ASP:HA	1:A:201:HIS:CG	2.55	0.42
1:D:82:THR:HA	1:D:85:LEU:HD22	2.01	0.42
1:D:86:PRO:HB2	3:D:401:HOH:O	2.20	0.42
1:A:93:ARG:HG2	3:D:402:HOH:O	2.19	0.41
1:C:130:SER:OG	1:C:253:TPO:O3P	2.37	0.41
1:A:108:ARG:HD2	3:A:492:HOH:O	2.20	0.41
1:C:165:TRP:HB2	1:C:203:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HA	1:A:138:ARG:HA	2.03	0.41
1:C:32:MET:HA	1:C:32:MET:HE2	2.02	0.41
1:C:48:TYR:CE1	1:C:52:GLN:OE1	2.73	0.41
1:B:34:LYS:HD3	1:B:35:PHE:CZ	2.56	0.41
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.91	0.41
1:D:146:LYS:HE3	1:D:239:HIS:HD2	1.84	0.41
1:C:209:ASP:O	1:C:210:CYS:C	2.64	0.41
1:A:65:GLN:O	1:A:67:PRO:HD3	2.21	0.41
1:A:179[B]:PHE:CD1	1:A:180:PRO:HD2	2.56	0.41
1:B:149:GLY:HA2	1:B:165:TRP:CE2	2.56	0.41
1:C:16:ARG:HD2	1:C:25:SER:HA	2.02	0.41
1:C:151:ALA:HB1	1:C:183:PRO:HB3	2.03	0.41
1:C:225:HIS:ND1	1:C:226:PRO:HD2	2.35	0.41
1:A:93:ARG:O	1:A:97:ARG:HG3	2.21	0.41
1:C:215:GLU:OE1	1:C:217:HIS:HD2	2.04	0.41
1:D:8:LEU:O	1:D:12:VAL:HG13	2.21	0.41
1:D:78:GLN:O	1:D:82:THR:HG23	2.21	0.41
1:D:131:ARG:HG3	1:D:138:ARG:HG2	2.03	0.41
1:A:29:GLY:O	1:A:33:ARG:HG3	2.21	0.40
1:D:148:TRP:NE1	1:D:238:LEU:HD13	2.37	0.40
1:C:129:VAL:HG21	1:C:138:ARG:HD3	2.02	0.40
1:C:170:SER:O	1:C:183:PRO:HD3	2.21	0.40
1:A:75:ARG:HB3	1:A:75:ARG:CZ	2.52	0.40
1:B:109:GLN:HB3	1:B:142:VAL:CG1	2.52	0.40
1:C:175:TYR:HD2	3:C:407:HOH:O	2.05	0.40
1:D:145:ASP:OD1	1:D:146:LYS:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:HOH:O	3:C:507:HOH:O[3_545]	2.17	0.03

## 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	276/291 (95%)	270 (98%)	6 (2%)	0	100	100
1	B	273/291 (94%)	260 (95%)	11 (4%)	2 (1%)	19	14
1	C	274/291 (94%)	261 (95%)	11 (4%)	2 (1%)	19	14
1	D	181/291 (62%)	169 (93%)	11 (6%)	1 (1%)	22	17
All	All	1004/1164 (86%)	960 (96%)	39 (4%)	5 (0%)	25	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	LEU
1	B	59	SER
1	C	157	LYS
1	C	191	TRP
1	D	66	ASP

### 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	244/251 (97%)	240 (98%)	4 (2%)	58	64
1	B	240/251 (96%)	234 (98%)	6 (2%)	42	45
1	C	242/251 (96%)	233 (96%)	9 (4%)	29	29
1	D	162/251 (64%)	154 (95%)	8 (5%)	21	18
All	All	888/1004 (88%)	861 (97%)	27 (3%)	36	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	142	VAL
1	A	260	LEU

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Mol	Chain	Res	Type
1	A	274	GLU
1	B	70	ASP
1	B	102	LEU
1	B	129	VAL
1	B	142	VAL
1	B	198	ARG
1	B	227	LYS
1	C	12	VAL
1	C	31	LEU
1	C	75[A]	ARG
1	C	75[B]	ARG
1	C	106	VAL
1	C	114	SER
1	C	142	VAL
1	C	159	ARG
1	C	198	ARG
1	D	12	VAL
1	D	59	SER
1	D	73	GLN
1	D	85	LEU
1	D	103	ILE
1	D	118	VAL
1	D	129	VAL
1	D	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	242	ASN
1	B	20	HIS
1	C	20	HIS
1	C	201	HIS
1	C	232	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	D	253	1	8,10,11	1.15	0	10,14,16	1.87	2 (20%)
1	SEP	A	249	1	8,9,10	1.64	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	D	249	1	8,9,10	1.66	1 (12%)	8,12,14	1.12	1 (12%)
1	TPO	C	253	1	8,10,11	1.61	2 (25%)	10,14,16	1.09	1 (10%)
1	SEP	B	249	1	8,9,10	1.72	1 (12%)	8,12,14	1.93	2 (25%)
1	TPO	B	250	1	8,10,11	1.25	1 (12%)	10,14,16	1.28	1 (10%)
1	TPO	B	253	1	8,10,11	0.88	0	10,14,16	1.31	1 (10%)
1	TPO	C	250	1	8,10,11	1.36	1 (12%)	10,14,16	1.71	2 (20%)
1	SEP	B	256	1	8,9,10	1.44	2 (25%)	8,12,14	1.66	1 (12%)
1	TPO	A	253	1	8,10,11	1.50	2 (25%)	10,14,16	1.59	2 (20%)
1	TPO	D	250	1	8,10,11	1.21	0	10,14,16	1.32	1 (10%)
1	SEP	D	256	1	8,9,10	1.57	2 (25%)	8,12,14	0.94	0
1	TPO	A	250	1	8,10,11	0.90	0	10,14,16	1.32	1 (10%)
1	SEP	C	249	1	8,9,10	1.45	1 (12%)	8,12,14	1.22	0
1	SEP	C	256	1	8,9,10	1.78	3 (37%)	8,12,14	2.66	5 (62%)
1	SEP	A	256	1	8,9,10	1.53	2 (25%)	8,12,14	1.26	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	D	253	1	-	1/9/11/13	-
1	SEP	A	249	1	-	0/5/8/10	-
1	SEP	D	249	1	-	0/5/8/10	-
1	TPO	C	253	1	-	2/9/11/13	-
1	SEP	B	249	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	250	1	-	0/9/11/13	-
1	TPO	B	253	1	-	1/9/11/13	-
1	TPO	C	250	1	-	1/9/11/13	-
1	SEP	B	256	1	-	0/5/8/10	-
1	TPO	A	253	1	-	5/9/11/13	-
1	TPO	D	250	1	-	0/9/11/13	-
1	SEP	D	256	1	-	0/5/8/10	-
1	TPO	A	250	1	-	1/9/11/13	-
1	SEP	C	249	1	-	1/5/8/10	-
1	SEP	C	256	1	-	0/5/8/10	-
1	SEP	A	256	1	-	0/5/8/10	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	SEP	P-O1P	4.14	1.63	1.50
1	A	249	SEP	P-O1P	3.72	1.62	1.50
1	C	256	SEP	P-O1P	3.67	1.62	1.50
1	D	249	SEP	P-O1P	3.57	1.62	1.50
1	C	253	TPO	CB-CA	3.40	1.61	1.53
1	D	256	SEP	P-O1P	3.24	1.61	1.50
1	C	249	SEP	P-O1P	3.09	1.60	1.50
1	A	256	SEP	P-O1P	2.87	1.59	1.50
1	A	253	TPO	CB-CA	2.72	1.59	1.53
1	B	256	SEP	P-O1P	2.69	1.59	1.50
1	B	256	SEP	P-O2P	2.57	1.64	1.54
1	B	250	TPO	P-O3P	2.34	1.63	1.54
1	A	256	SEP	P-O3P	2.32	1.63	1.54
1	C	256	SEP	P-O3P	2.28	1.63	1.54
1	C	253	TPO	P-OG1	2.25	1.63	1.59
1	A	253	TPO	P-O3P	2.21	1.63	1.54
1	C	256	SEP	P-O2P	2.18	1.63	1.54
1	D	256	SEP	P-O2P	2.07	1.62	1.54
1	C	250	TPO	P-OG1	2.02	1.63	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	TPO	P-OG1-CB	-4.48	109.68	123.21
1	C	250	TPO	P-OG1-CB	-4.17	110.61	123.21
1	A	249	SEP	P-OG-CB	-4.14	106.89	118.30
1	C	256	SEP	O2P-P-OG	-3.85	96.48	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	TPO	P-OG1-CB	-3.56	112.46	123.21
1	D	250	TPO	P-OG1-CB	-3.54	112.51	123.21
1	B	249	SEP	P-OG-CB	-3.38	108.98	118.30
1	B	256	SEP	OG-P-O1P	-3.34	97.12	106.47
1	B	249	SEP	O3P-P-O2P	3.32	120.32	107.64
1	C	256	SEP	O3P-P-O2P	3.28	120.19	107.64
1	B	250	TPO	P-OG1-CB	-3.25	113.39	123.21
1	A	253	TPO	O3P-P-OG1	3.14	120.07	105.99
1	C	256	SEP	O3P-P-OG	3.04	114.81	106.73
1	C	256	SEP	O3P-P-O1P	-2.96	99.09	110.68
1	B	253	TPO	CG2-CB-CA	-2.95	107.34	113.16
1	C	256	SEP	OG-CB-CA	-2.90	105.32	108.14
1	A	253	TPO	CG2-CB-CA	-2.88	107.47	113.16
1	A	256	SEP	OG-CB-CA	-2.77	105.45	108.14
1	D	253	TPO	O2P-P-OG1	2.66	117.90	105.99
1	D	249	SEP	P-OG-CB	-2.46	111.52	118.30
1	A	249	SEP	O3P-P-O2P	2.17	115.92	107.64
1	C	253	TPO	CG2-CB-CA	-2.11	109.00	113.16
1	C	250	TPO	O-C-CA	-2.08	119.34	124.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	250	TPO	O-C-CA-CB
1	A	253	TPO	N-CA-CB-CG2
1	A	253	TPO	N-CA-CB-OG1
1	A	253	TPO	C-CA-CB-CG2
1	A	253	TPO	CG2-CB-OG1-P
1	A	253	TPO	CB-OG1-P-O1P
1	C	253	TPO	CB-OG1-P-O3P
1	C	253	TPO	CB-OG1-P-O1P
1	B	249	SEP	CA-CB-OG-P
1	B	253	TPO	CB-OG1-P-O3P
1	C	249	SEP	CA-CB-OG-P
1	D	253	TPO	CB-OG1-P-O3P
1	C	250	TPO	O-C-CA-CB

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	253	TPO	2	0
1	D	249	SEP	1	0
1	C	253	TPO	1	0
1	B	249	SEP	1	0
1	B	250	TPO	1	0
1	B	253	TPO	1	0
1	C	250	TPO	1	0
1	A	253	TPO	1	0
1	A	250	TPO	1	0
1	C	249	SEP	1	0
1	A	256	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	274/291 (94%)	0.23	9 (3%)	49	47	22, 58, 90, 122	4 (1%)
1	B	273/291 (93%)	0.12	8 (2%)	54	52	29, 51, 87, 118	2 (0%)
1	C	272/291 (93%)	0.44	22 (8%)	19	18	25, 58, 106, 129	4 (1%)
1	D	184/291 (63%)	0.74	18 (9%)	14	13	31, 70, 109, 121	1 (0%)
All	All	1003/1164 (86%)	0.35	57 (5%)	30	28	22, 59, 99, 129	11 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	LEU	6.9
1	D	85	LEU	5.6
1	B	175	TYR	5.0
1	D	149	GLY	4.8
1	C	175	TYR	4.2
1	B	69[A]	GLU	4.2
1	B	86	PRO	3.9
1	C	75[A]	ARG	3.9
1	C	208	ALA	3.8
1	C	214	ARG	3.8
1	C	212	ASN	3.7
1	A	205	CYS	3.6
1	D	70	ASP	3.4
1	A	2	SER	3.1
1	A	179[A]	PHE	2.9
1	C	179	PHE	2.9
1	C	200	THR	2.8
1	A	1	GLY	2.7
1	D	103	ILE	2.7
1	D	261	LEU	2.7
1	C	196	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	202	THR	2.7
1	D	65	GLN	2.6
1	D	142	VAL	2.6
1	B	59	SER	2.6
1	D	113	SER	2.6
1	C	194	ASP	2.5
1	B	277	GLU	2.5
1	C	220	GLY	2.5
1	D	136	ARG	2.5
1	C	206	SER	2.5
1	C	205	CYS	2.5
1	D	137	LYS	2.5
1	D	133	ARG	2.4
1	A	159[A]	ARG	2.4
1	C	276	GLU	2.3
1	D	66	ASP	2.3
1	B	87	LEU	2.3
1	A	204	SER	2.3
1	C	192	ASP	2.3
1	D	76	ASP	2.3
1	C	178	GLY	2.2
1	C	157	LYS	2.2
1	D	275	GLU	2.2
1	C	216	PRO	2.2
1	D	144	ALA	2.2
1	C	211	TYR	2.2
1	C	221	THR	2.2
1	A	214	ARG	2.2
1	D	260	LEU	2.1
1	C	204	SER	2.1
1	D	263	ASP	2.1
1	A	67	PRO	2.1
1	A	31	LEU	2.1
1	D	236	LYS	2.1
1	B	204	SER	2.0
1	C	165	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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
1	SEP	C	256	10/11	0.91	0.09	33,50,59,70	0
1	SEP	A	256	10/11	0.94	0.09	35,47,56,63	0
1	TPO	A	253	11/12	0.95	0.10	41,56,75,75	0
1	TPO	B	253	11/12	0.96	0.09	32,46,51,53	0
1	TPO	D	253	11/12	0.96	0.08	49,59,70,70	0
1	SEP	D	256	10/11	0.96	0.07	54,60,72,73	0
1	TPO	C	253	11/12	0.97	0.08	34,43,51,51	0
1	SEP	A	249	10/11	0.97	0.07	43,51,59,66	0
1	SEP	D	249	10/11	0.97	0.06	53,59,66,71	0
1	TPO	D	250	11/12	0.97	0.07	46,56,68,68	0
1	SEP	B	256	10/11	0.97	0.05	33,40,47,54	0
1	SEP	C	249	10/11	0.97	0.06	40,50,55,60	0
1	TPO	B	250	11/12	0.98	0.06	39,49,58,64	0
1	TPO	C	250	11/12	0.98	0.06	39,46,53,61	0
1	TPO	A	250	11/12	0.98	0.06	41,50,59,60	0
1	SEP	B	249	10/11	0.98	0.06	39,49,59,62	0

### 6.3 Carbohydrates

There are no oligosaccharides in this entry.

### 6.4 Ligands

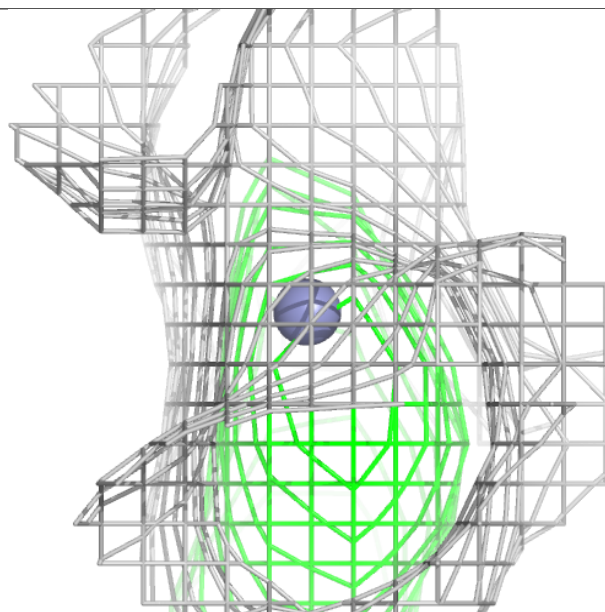
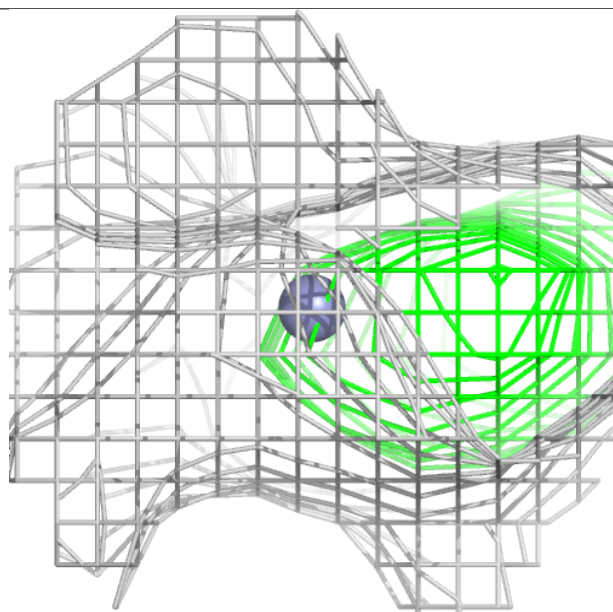
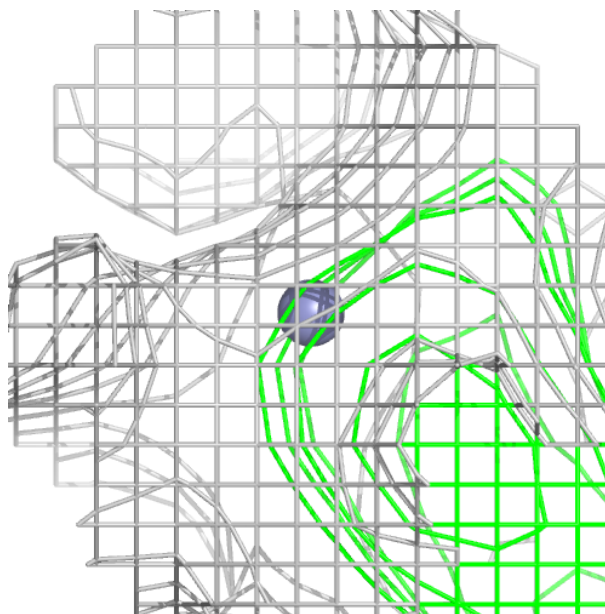
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	D	302	1/1	-0.30	0.22	207,207,207,207	0
2	ZN	C	301	1/1	0.98	0.04	76,76,76,76	0
2	ZN	A	303	1/1	0.99	0.03	39,39,39,39	0
2	ZN	B	301	1/1	0.99	0.03	40,40,40,40	0
2	ZN	B	302	1/1	0.99	0.02	39,39,39,39	0
2	ZN	B	303	1/1	0.99	0.05	60,60,60,60	0
2	ZN	A	301	1/1	0.99	0.03	45,45,45,45	0
2	ZN	C	303	1/1	0.99	0.03	82,82,82,82	0
2	ZN	D	301	1/1	0.99	0.05	80,80,80,80	0
2	ZN	A	302	1/1	0.99	0.04	52,52,52,52	0
2	ZN	C	302	1/1	1.00	0.04	54,54,54,54	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 D 302:**

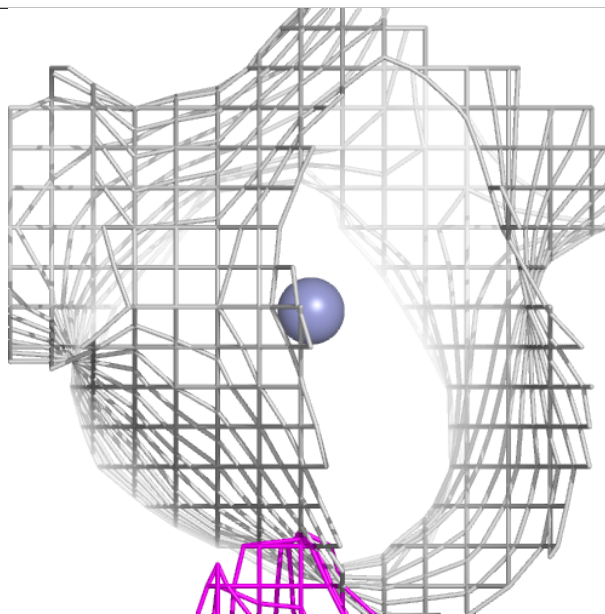
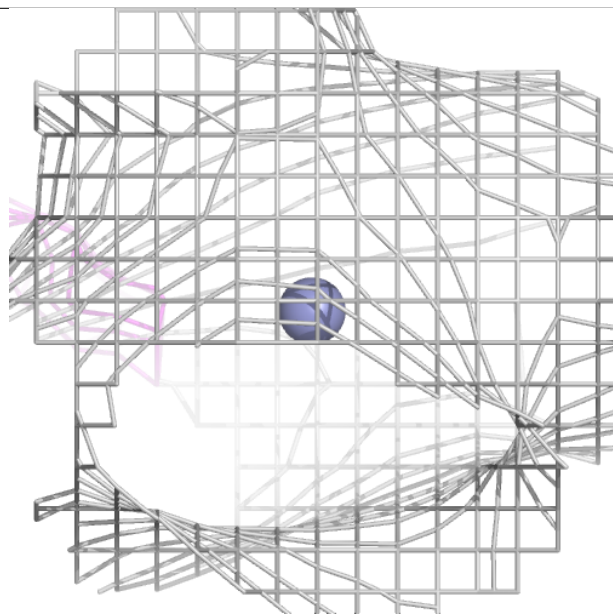
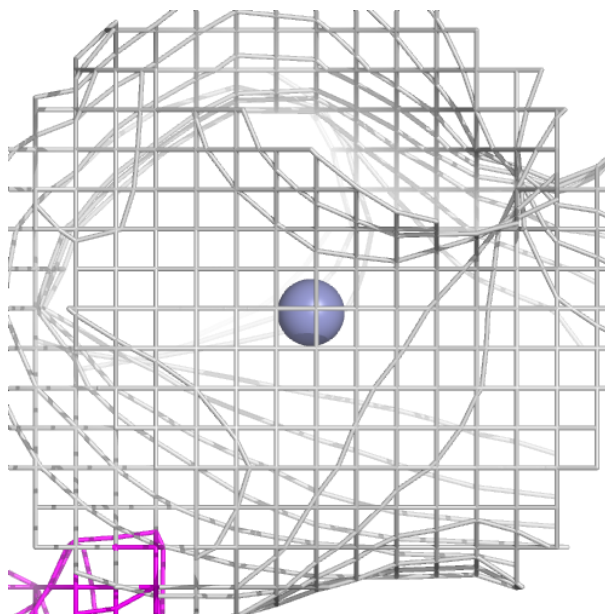
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN C 301:**

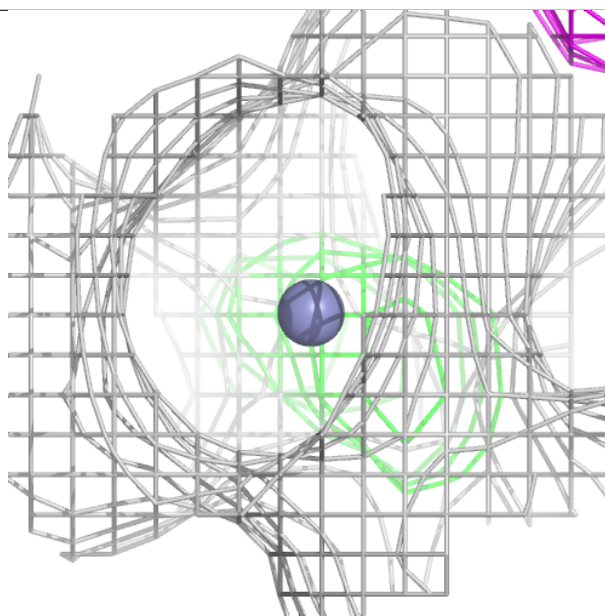
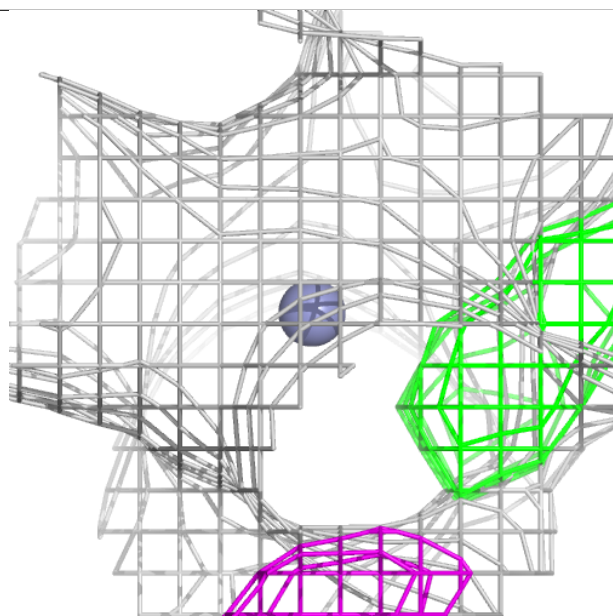
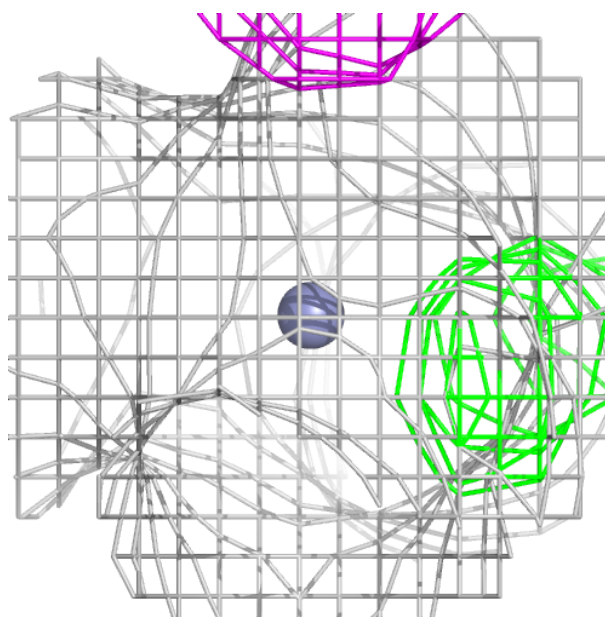
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





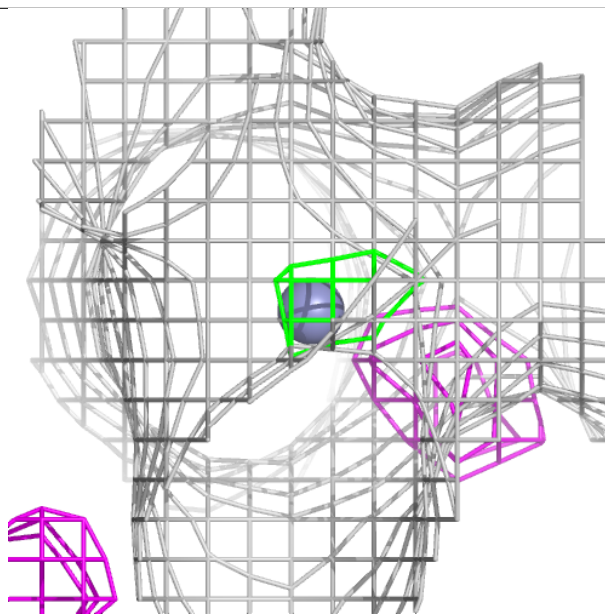
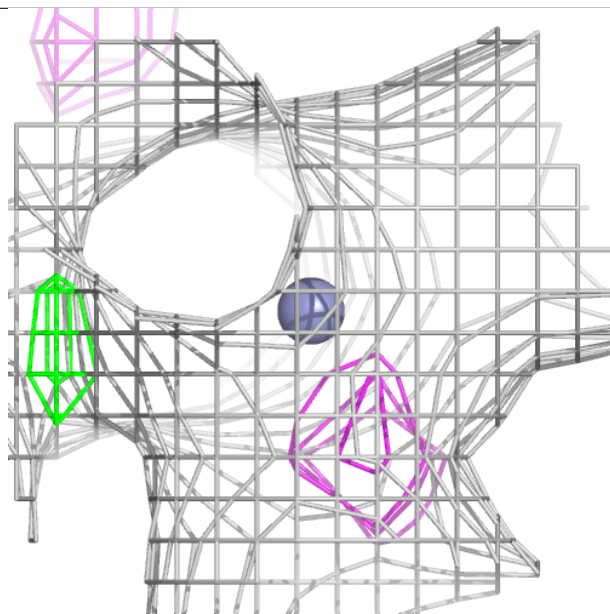
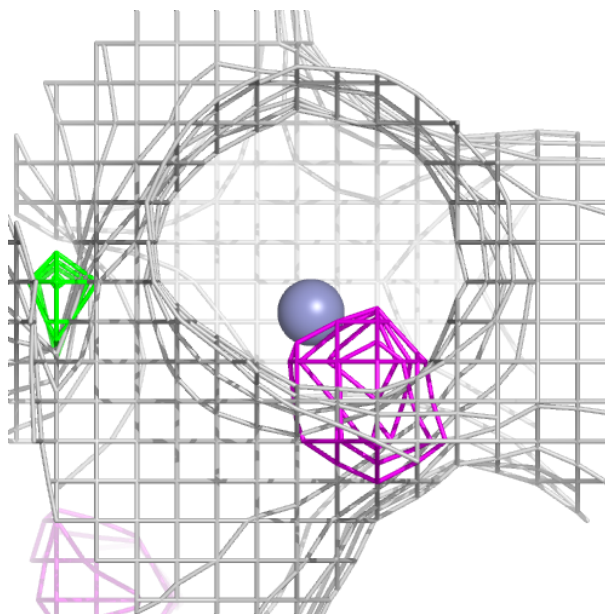
**Electron density around ZN A 303:**

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



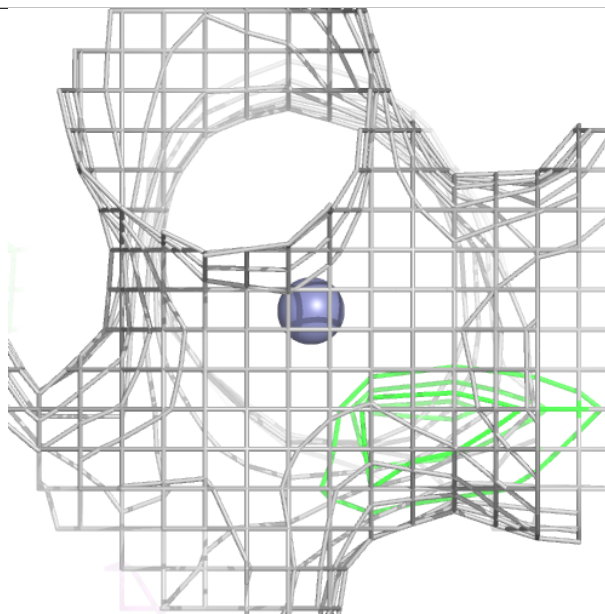
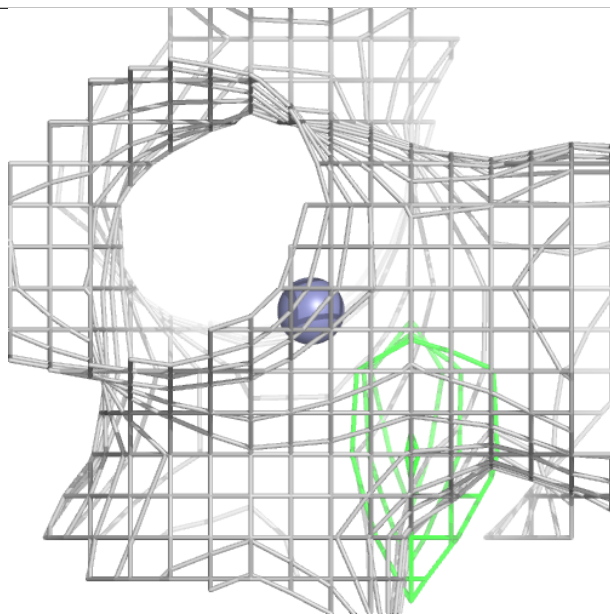
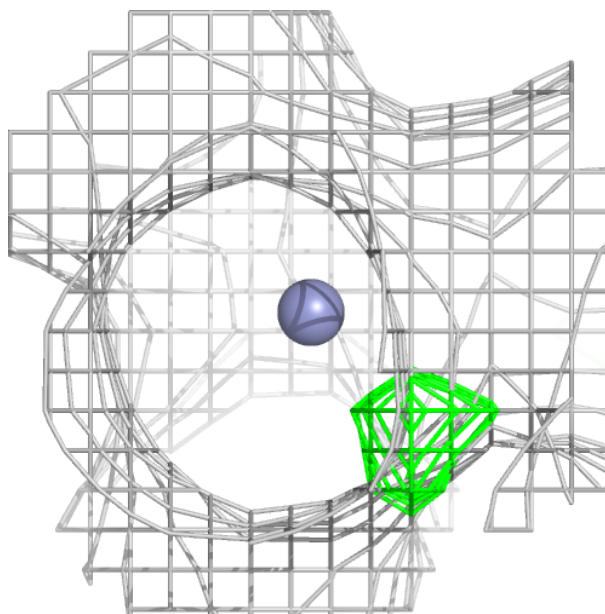
**Electron density around ZN B 301:**

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



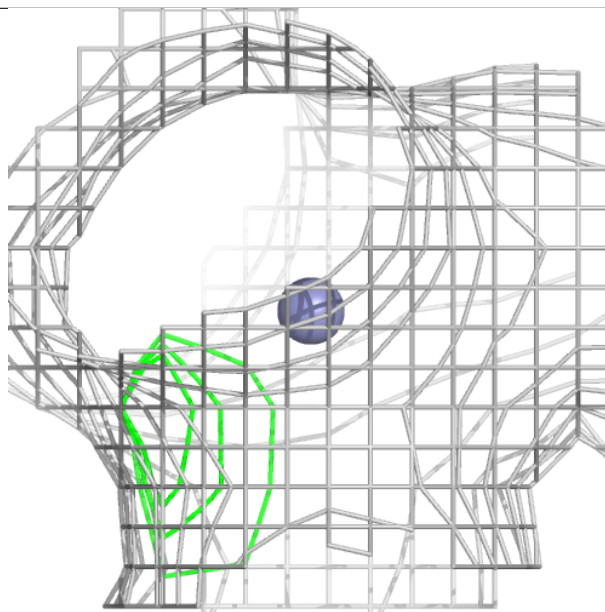
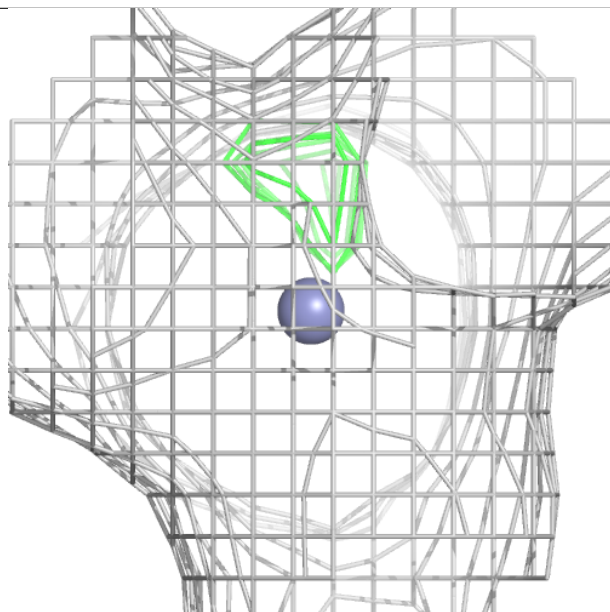
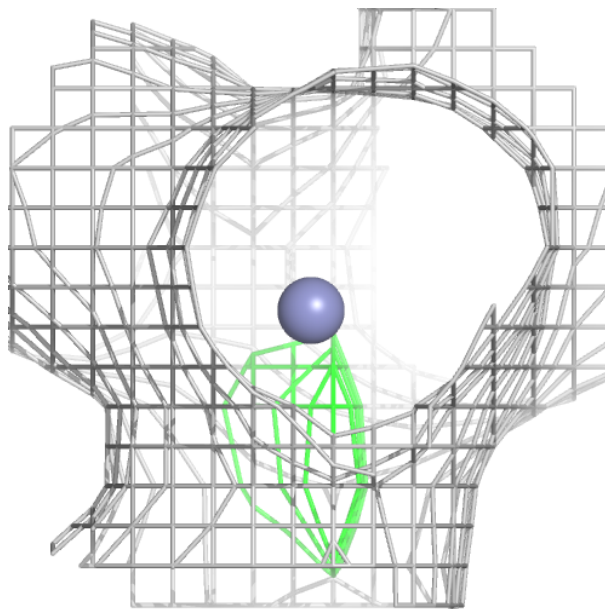
**Electron density around ZN B 302:**

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



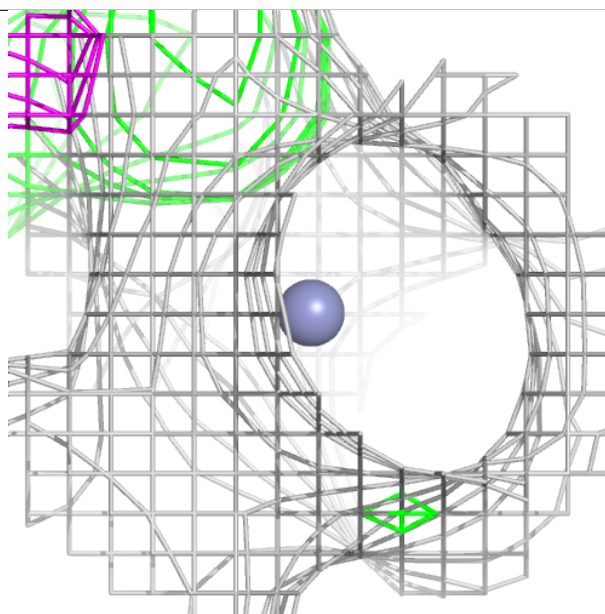
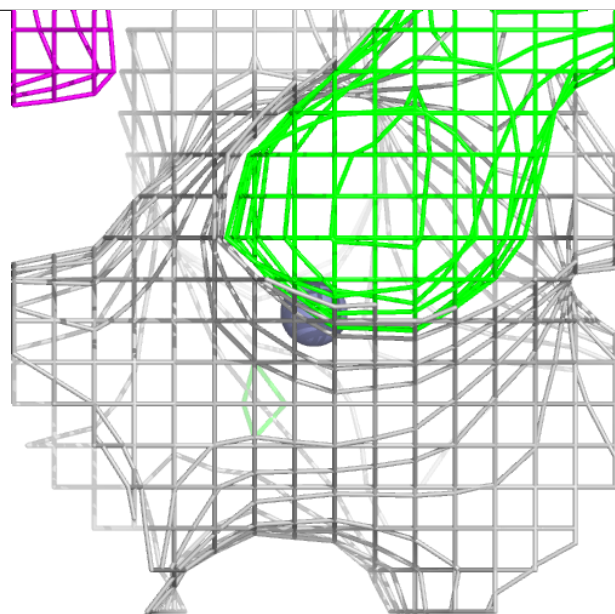
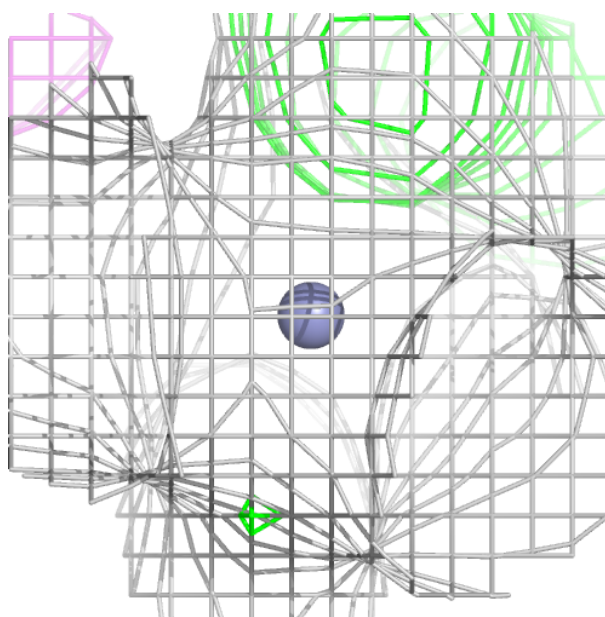
**Electron density around ZN B 303:**

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



**Electron density around ZN A 301:**

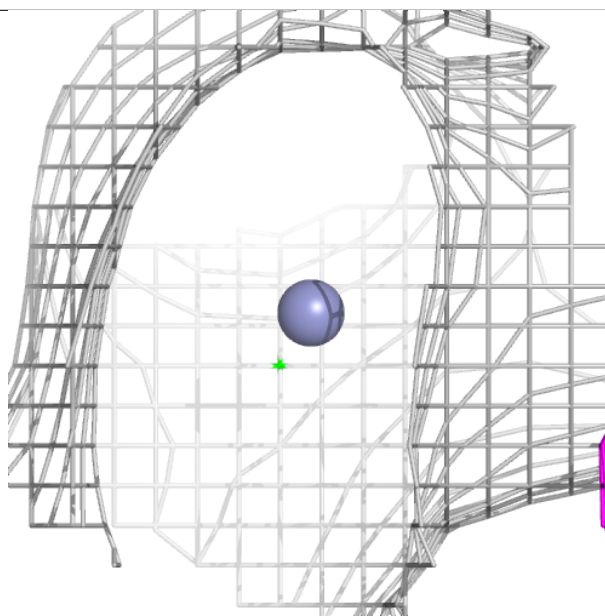
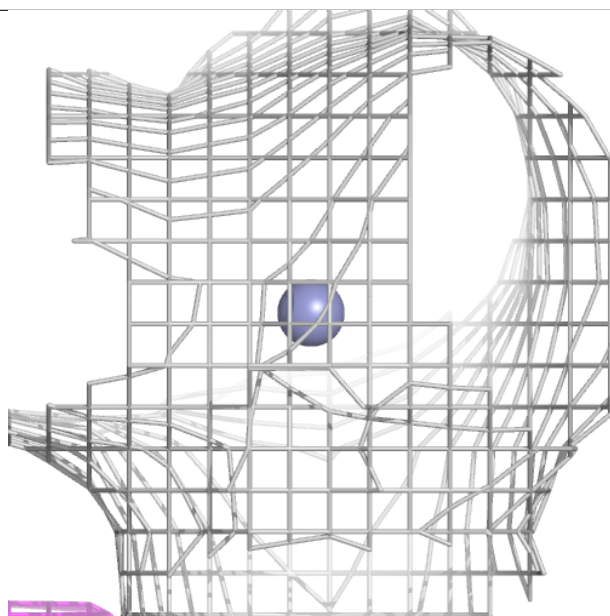
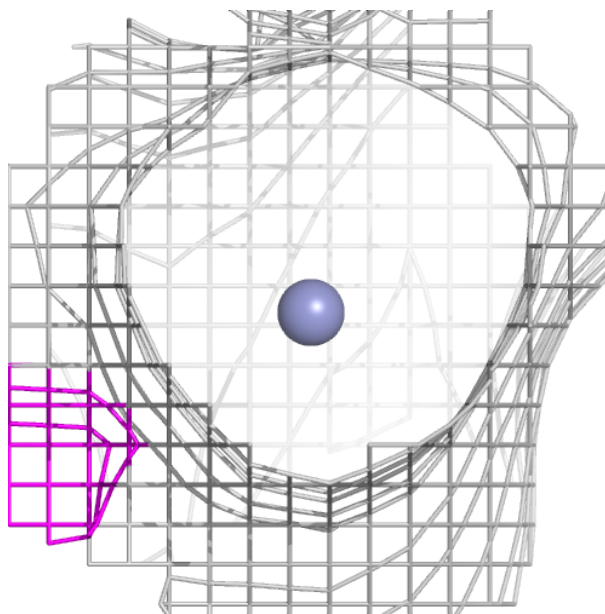
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





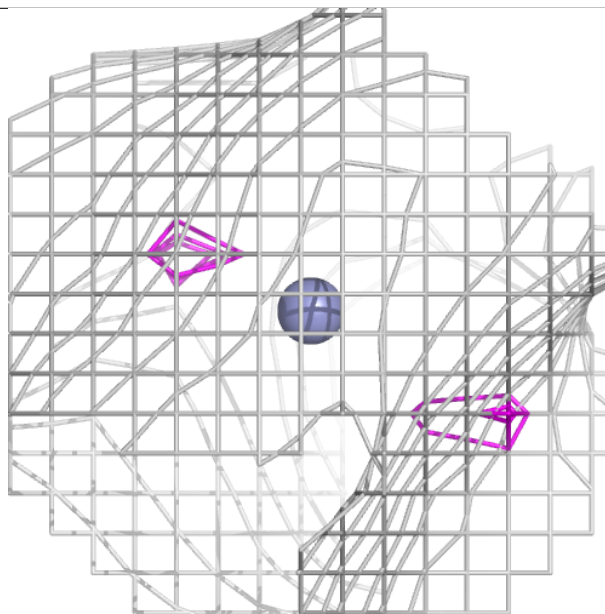
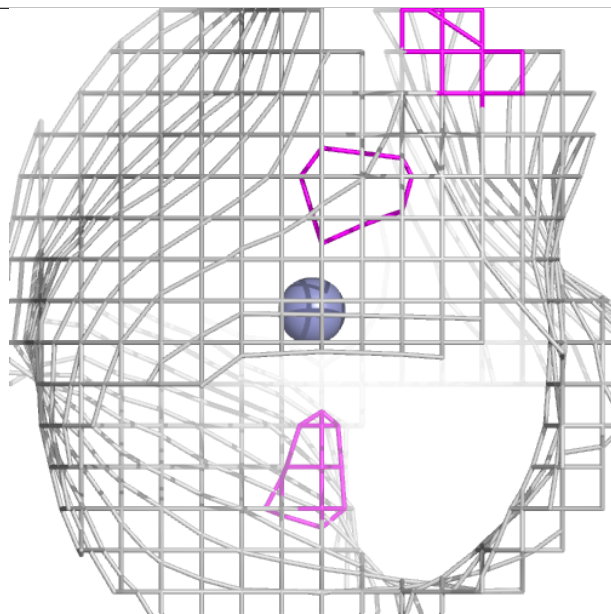
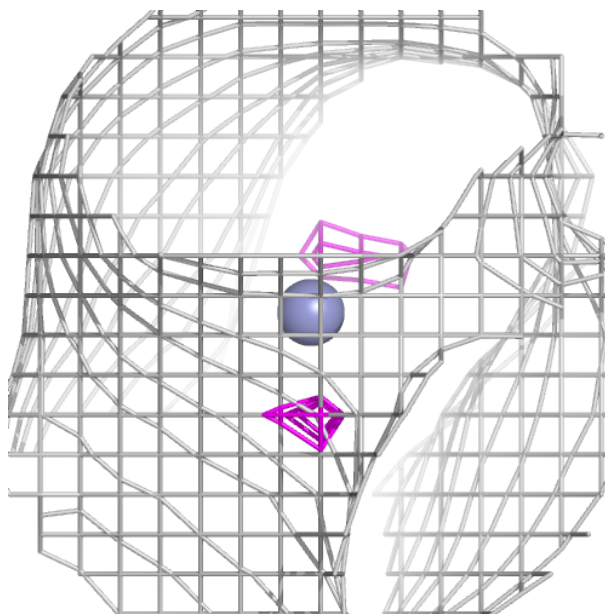
**Electron density around ZN C 303:**

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



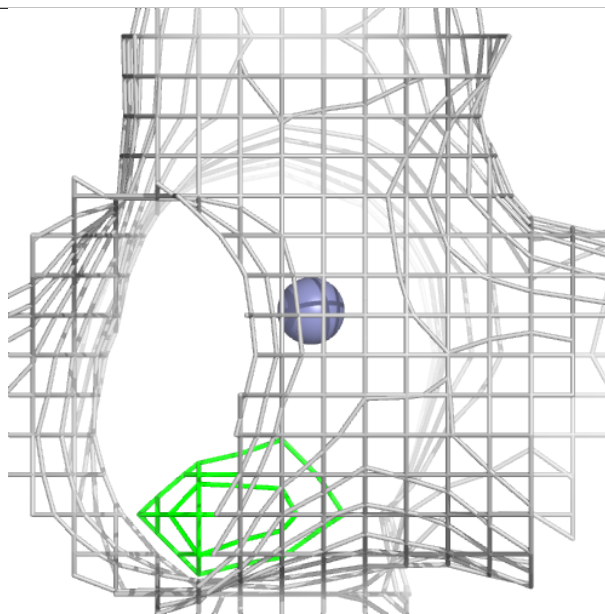
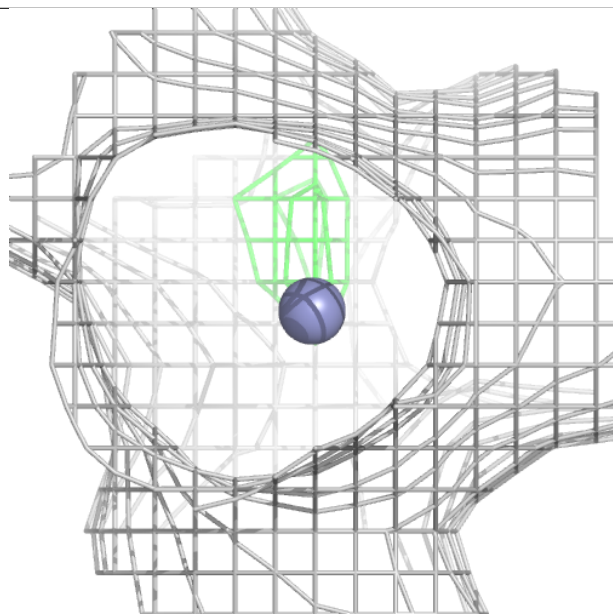
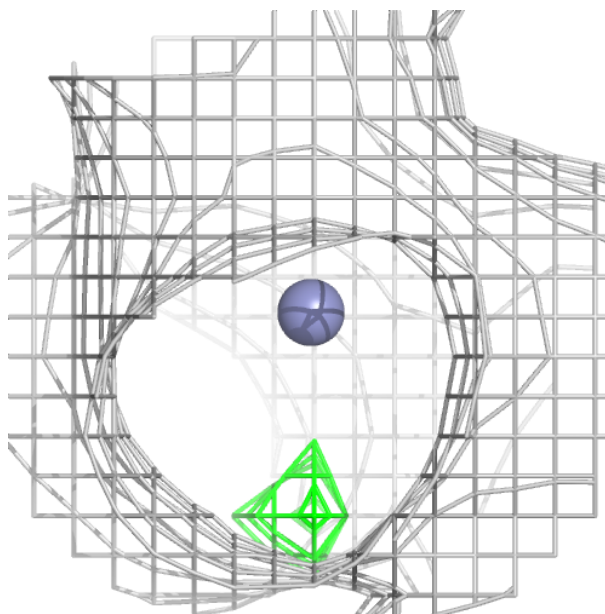
**Electron density around ZN D 301:**

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



**Electron density around ZN A 302:**

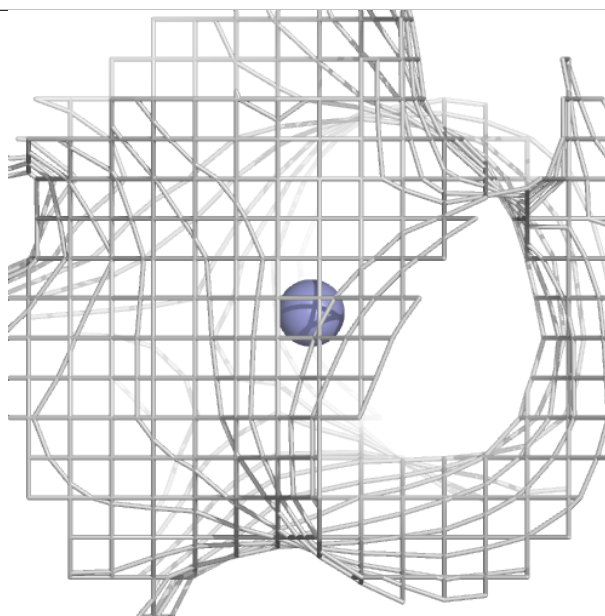
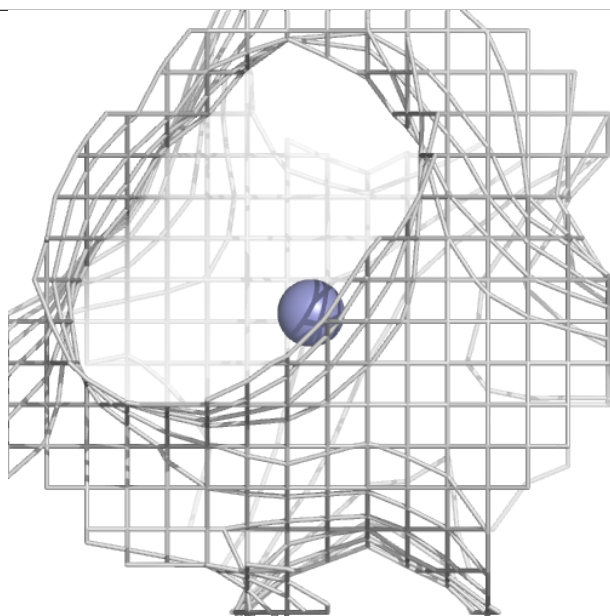
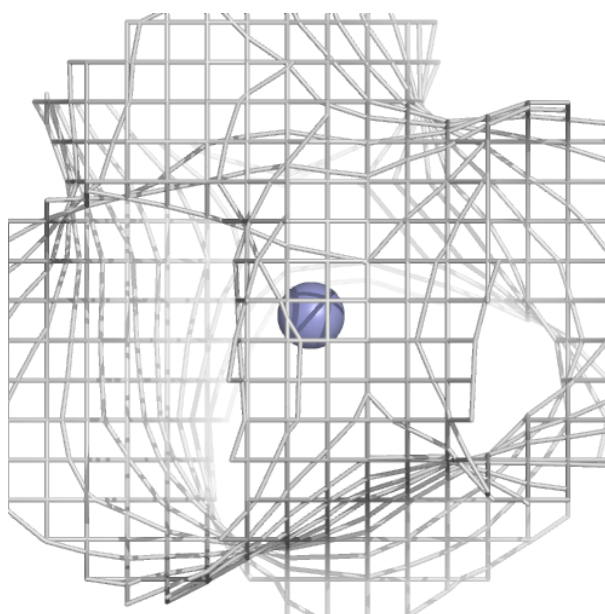
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN C 302:**

$2mF_o-DF_c$  (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.