



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 AM UTC

PDB ID : 7ZJ3 / pdb_00007zj3
Title : Structure of TRIM2 RING domain in complex with UBE2D1 Ub conjugate
Authors : Esposito, D.; Garza-Garcia, A.; Dudley-Fraser, J.; Rittinger, K.
Deposited on : 2022-04-08
Resolution : 2.53 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:

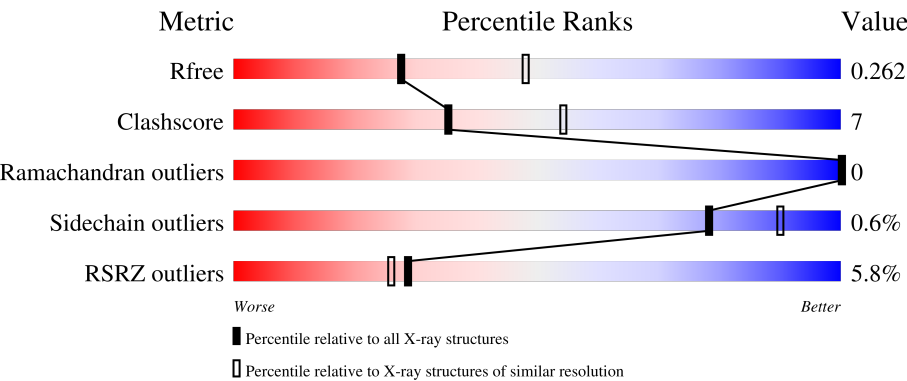
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	97	70%19%11%
1	D	97	3% 65%23%12%
1	G	97	4% 70%18%12%
1	J	97	7% 68%20%12%
2	B	150	% 85%13%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	150	% 85%13% .
2	H	150	% 86%14%
2	K	150	14% 81%15% ..
3	C	80	2% 75%20%5%
3	F	80	% 82%14% .
3	I	80	20% 66%25% .8%
3	L	80	18% 66%29% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9950 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 Tripartite motif-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	85	Total	C	N	O	S	0	0	0
			677	432	119	118	8			
1	G	85	Total	C	N	O	S	0	0	0
			677	432	119	118	8			
1	J	85	Total	C	N	O	S	0	0	0
			677	432	119	118	8			
1	A	86	Total	C	N	O	S	0	0	0
			684	437	120	119	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9C040
D	0	PRO	-	expression tag	UNP Q9C040
D	1	GLY	-	expression tag	UNP Q9C040
G	-1	GLY	-	expression tag	UNP Q9C040
G	0	PRO	-	expression tag	UNP Q9C040
G	1	GLY	-	expression tag	UNP Q9C040
J	-1	GLY	-	expression tag	UNP Q9C040
J	0	PRO	-	expression tag	UNP Q9C040
J	1	GLY	-	expression tag	UNP Q9C040
A	-1	GLY	-	expression tag	UNP Q9C040
A	0	PRO	-	expression tag	UNP Q9C040
A	1	GLY	-	expression tag	UNP Q9C040

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	147	Total	C	N	O	S	0	0	0
			1171	753	201	213	4			
2	H	150	Total	C	N	O	S	0	0	0
			1190	766	204	216	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	145	Total	C	N	O	S	0	0	0
			1162	748	199	211	4			
2	B	147	Total	C	N	O	S	0	0	0
			1171	753	201	213	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P51668
E	-2	PRO	-	expression tag	UNP P51668
E	-1	LEU	-	expression tag	UNP P51668
E	0	GLY	-	expression tag	UNP P51668
E	1	SER	-	expression tag	UNP P51668
E	22	ARG	SER	engineered mutation	UNP P51668
E	85	LYS	CYS	engineered mutation	UNP P51668
H	-3	GLY	-	expression tag	UNP P51668
H	-2	PRO	-	expression tag	UNP P51668
H	-1	LEU	-	expression tag	UNP P51668
H	0	GLY	-	expression tag	UNP P51668
H	1	SER	-	expression tag	UNP P51668
H	22	ARG	SER	engineered mutation	UNP P51668
H	85	LYS	CYS	engineered mutation	UNP P51668
K	-3	GLY	-	expression tag	UNP P51668
K	-2	PRO	-	expression tag	UNP P51668
K	-1	LEU	-	expression tag	UNP P51668
K	0	GLY	-	expression tag	UNP P51668
K	1	SER	-	expression tag	UNP P51668
K	22	ARG	SER	engineered mutation	UNP P51668
K	85	LYS	CYS	engineered mutation	UNP P51668
B	-3	GLY	-	expression tag	UNP P51668
B	-2	PRO	-	expression tag	UNP P51668
B	-1	LEU	-	expression tag	UNP P51668
B	0	GLY	-	expression tag	UNP P51668
B	1	SER	-	expression tag	UNP P51668
B	22	ARG	SER	engineered mutation	UNP P51668
B	85	LYS	CYS	engineered mutation	UNP P51668

- Molecule 3 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	77	Total	C	N	O	S	0	0	0
			605	380	106	118	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	74	Total	C	N	O	0	0	0
			584	368	102	114			
3	L	77	Total	C	N	O	0	0	0
			605	380	106	118			
3	C	76	Total	C	N	O	0	0	0
			601	378	105	117			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P0CG48
F	-2	ALA	-	expression tag	UNP P0CG48
F	-1	MET	-	expression tag	UNP P0CG48
I	-3	GLY	-	expression tag	UNP P0CG48
I	-2	ALA	-	expression tag	UNP P0CG48
I	-1	MET	-	expression tag	UNP P0CG48
L	-3	GLY	-	expression tag	UNP P0CG48
L	-2	ALA	-	expression tag	UNP P0CG48
L	-1	MET	-	expression tag	UNP P0CG48
C	-3	GLY	-	expression tag	UNP P0CG48
C	-2	ALA	-	expression tag	UNP P0CG48
C	-1	MET	-	expression tag	UNP P0CG48

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	J	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	5	Total	O	0	0
			5	5		

Continued on next page...

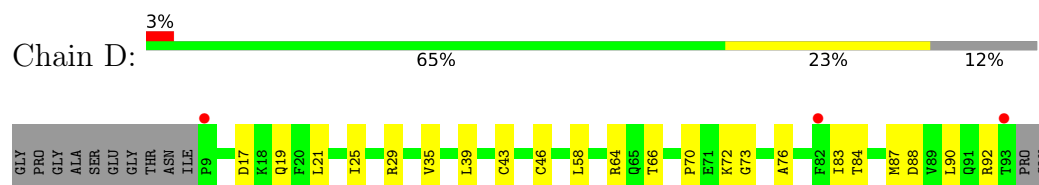
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	13	Total 13	O 13	0	0
5	F	8	Total 8	O 8	0	0
5	G	8	Total 8	O 8	0	0
5	H	25	Total 25	O 25	0	0
5	I	2	Total 2	O 2	0	0
5	J	7	Total 7	O 7	0	0
5	K	10	Total 10	O 10	0	0
5	L	2	Total 2	O 2	0	0
5	A	13	Total 13	O 13	0	0
5	C	7	Total 7	O 7	0	0
5	B	38	Total 38	O 38	0	0

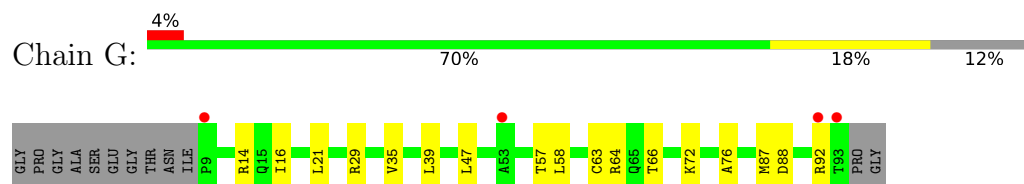
3 Residue-property plots [i](#)

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.

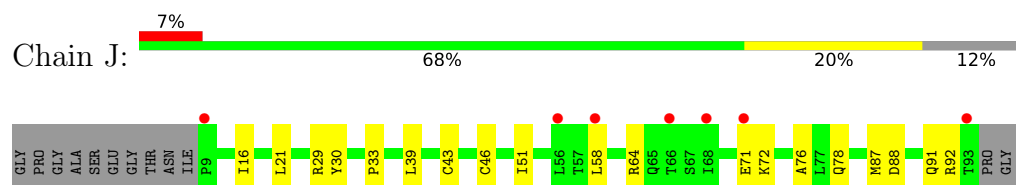
- Molecule 1: Tripartite motif-containing protein 2



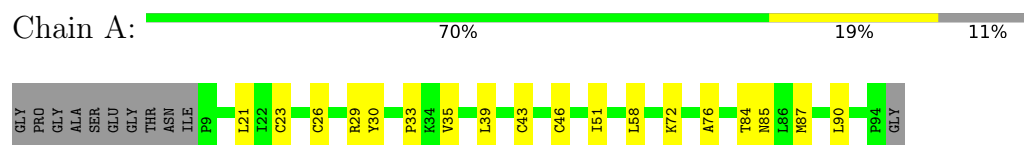
- Molecule 1: Tripartite motif-containing protein 2



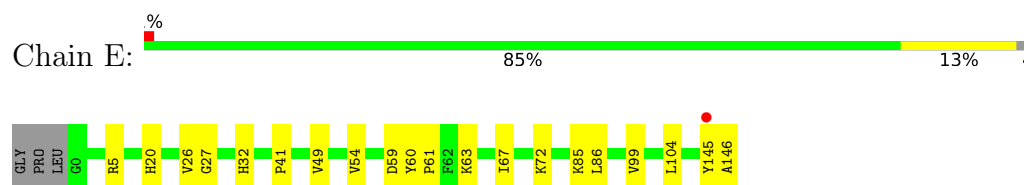
- Molecule 1: Tripartite motif-containing protein 2



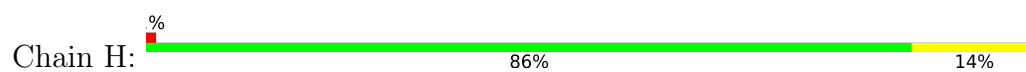
- Molecule 1: Tripartite motif-containing protein 2



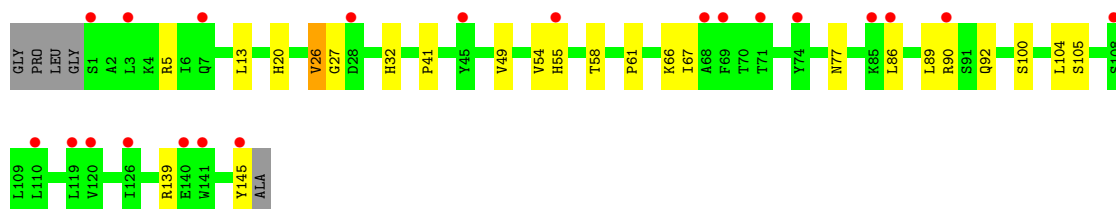
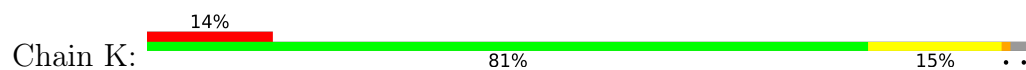
- Molecule 2: Ubiquitin-conjugating enzyme E2 D1



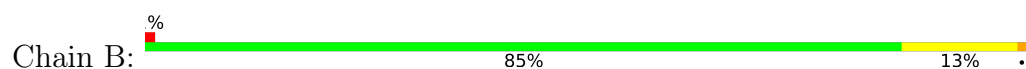
- Molecule 2: Ubiquitin-conjugating enzyme E2 D1



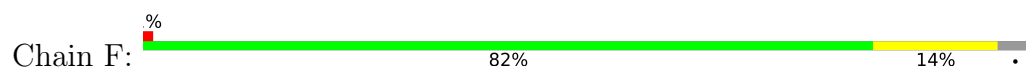
• Molecule 2: Ubiquitin-conjugating enzyme E2 D1



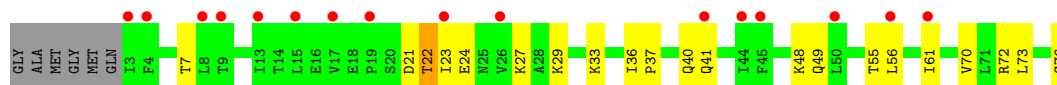
• Molecule 2: Ubiquitin-conjugating enzyme E2 D1



• Molecule 3: Polyubiquitin-C



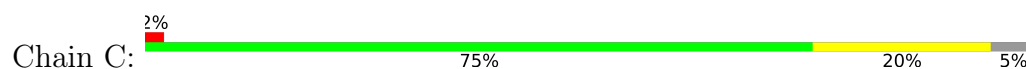
• Molecule 3: Polyubiquitin-C

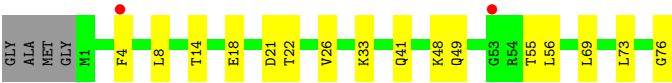


• Molecule 3: Polyubiquitin-C



• Molecule 3: Polyubiquitin-C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.32Å 123.66Å 112.47Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	54.97 – 2.53 54.97 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.97-2.53) 100.0 (54.97-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032, PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.210 , 0.258 0.227 , 0.262	Depositor DCC
R_{free} test set	2565 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9950	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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	A	0.26	0/699	0.46	0/950
1	D	0.26	0/691	0.48	0/938
1	G	0.25	0/691	0.48	0/938
1	J	0.30	0/691	0.47	0/938
2	B	0.28	0/1208	0.49	0/1647
2	E	0.23	0/1208	0.44	0/1647
2	H	0.26	0/1228	0.49	0/1675
2	K	0.20	0/1199	0.44	0/1635
3	C	0.25	0/607	0.50	0/816
3	F	0.27	0/611	0.51	0/821
3	I	0.21	0/590	0.43	0/794
3	L	0.22	0/611	0.52	0/821
All	All	0.25	0/10034	0.47	0/13620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	684	0	701	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	677	0	694	16	0
1	G	677	0	694	12	0
1	J	677	0	694	16	0
2	B	1171	0	1159	13	0
2	E	1171	0	1159	15	0
2	H	1190	0	1180	19	0
2	K	1162	0	1151	17	0
3	C	601	0	629	13	0
3	F	605	0	632	10	0
3	I	584	0	609	18	0
3	L	605	0	632	18	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
5	A	13	0	0	0	0
5	B	38	0	0	0	0
5	C	7	0	0	0	0
5	D	5	0	0	0	0
5	E	13	0	0	0	0
5	F	8	0	0	0	0
5	G	8	0	0	1	0
5	H	25	0	0	3	0
5	I	2	0	0	1	0
5	J	7	0	0	1	0
5	K	10	0	0	4	0
5	L	2	0	0	1	0
All	All	9950	0	9934	146	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 7.

All (146) 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)
3:C:76:GLY:O	2:B:85:LYS:NZ	1.98	0.96
1:D:92:ARG:NH1	3:L:14:THR:OG1	2.04	0.91
3:I:36:ILE:HB	3:I:41:GLN:HE21	1.40	0.86
3:L:38:PRO:HA	3:L:41:GLN:HE21	1.41	0.86
3:C:41:GLN:HB2	3:C:69:LEU:HD11	1.62	0.82
1:G:88:ASP:OD1	1:G:92:ARG:NH2	2.13	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:16:GLU:O	3:L:29:LYS:NZ	2.16	0.79
3:F:14:THR:O	3:F:33:LYS:NZ	2.17	0.78
2:K:66:LYS:O	5:K:201:HOH:O	2.03	0.77
1:J:64:ARG:NH1	2:K:92:GLN:O	2.18	0.77
1:G:35:VAL:HG11	1:A:39:LEU:HD11	1.68	0.76
2:H:127:TYR:O	5:H:201:HOH:O	2.05	0.74
2:K:55:HIS:N	5:K:201:HOH:O	2.19	0.72
1:D:25:ILE:O	2:E:5:ARG:NH1	2.23	0.72
2:H:54:VAL:HG22	2:H:67:ILE:HG12	1.71	0.71
2:E:26:VAL:HG23	2:E:27:GLY:H	1.56	0.70
2:K:41:PRO:O	3:L:48:LYS:NZ	2.26	0.69
1:G:39:LEU:HD11	1:A:35:VAL:HG11	1.74	0.68
1:J:29:ARG:NH1	1:J:91:GLN:OE1	2.26	0.67
2:K:54:VAL:HG22	2:K:67:ILE:HG12	1.75	0.67
3:I:22:THR:HG23	3:I:24:GLU:H	1.61	0.66
1:D:17:ASP:OD1	1:D:29:ARG:NH1	2.29	0.65
3:C:22:THR:HG22	3:C:55:THR:HG22	1.77	0.65
2:B:26:VAL:HG23	2:B:27:GLY:H	1.61	0.65
2:B:54:VAL:HG22	2:B:67:ILE:HG12	1.79	0.65
1:G:14:ARG:NH2	5:G:201:HOH:O	2.27	0.64
1:J:29:ARG:HH11	1:J:87:MET:HE3	1.62	0.64
2:K:90:ARG:O	5:K:202:HOH:O	2.13	0.64
2:E:54:VAL:HG22	2:E:67:ILE:HG12	1.81	0.62
1:J:72:LYS:HB2	1:J:76:ALA:HB2	1.82	0.61
2:E:41:PRO:O	3:F:48:LYS:NZ	2.33	0.61
2:H:5:ARG:NH2	2:H:9:GLU:OE1	2.34	0.61
3:I:22:THR:HA	3:I:55:THR:HA	1.83	0.61
3:L:27:LYS:HD2	3:L:41:GLN:HG3	1.83	0.61
1:G:72:LYS:HB2	1:G:76:ALA:HB2	1.83	0.60
1:A:51:ILE:HD11	1:A:58:LEU:HG	1.82	0.60
2:E:26:VAL:HG21	2:E:32:HIS:HD2	1.66	0.60
2:K:139:ARG:NH1	5:K:205:HOH:O	2.34	0.59
2:H:55:HIS:HB2	2:H:66:LYS:HB3	1.85	0.59
1:A:72:LYS:HB2	1:A:76:ALA:HB2	1.85	0.59
3:L:11:LYS:NZ	5:L:101:HOH:O	2.36	0.58
3:C:22:THR:HA	3:C:55:THR:HA	1.85	0.58
1:D:19:GLN:HE22	3:F:12:THR:H	1.52	0.58
2:E:59:ASP:OD1	2:E:63:LYS:HD3	2.01	0.58
3:I:22:THR:HG23	3:I:24:GLU:N	2.18	0.58
1:D:35:VAL:HG11	1:J:39:LEU:HD11	1.86	0.57
1:J:51:ILE:HD11	1:J:58:LEU:HG	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:LEU:HD11	3:I:73:LEU:HD13	1.85	0.57
2:H:-1:LEU:HD22	2:H:3:LEU:HD23	1.87	0.57
2:K:49:VAL:H	2:K:145:TYR:HE1	1.52	0.56
1:A:30:TYR:HB3	1:A:33:PRO:HG3	1.88	0.56
2:K:26:VAL:HG23	2:K:27:GLY:H	1.72	0.54
1:A:21:LEU:HD22	1:A:87:MET:HG3	1.89	0.54
1:G:21:LEU:HD22	1:G:87:MET:HG3	1.90	0.54
1:J:21:LEU:HD22	1:J:87:MET:HG3	1.90	0.53
3:L:22:THR:HG22	3:L:25:ASN:OD1	2.08	0.53
2:B:11:SER:O	2:B:15:ARG:HD3	2.08	0.53
2:E:26:VAL:HG21	2:E:32:HIS:CD2	2.43	0.53
3:C:22:THR:CG2	3:C:55:THR:HG22	2.39	0.52
1:A:23:CYS:HB3	1:A:26:CYS:SG	2.49	0.52
1:D:21:LEU:HD22	1:D:87:MET:HG3	1.91	0.52
1:D:83:ILE:HG22	1:D:87:MET:HE2	1.92	0.52
2:E:20:HIS:CE1	2:E:104:LEU:HD12	2.45	0.52
3:I:23:ILE:O	3:I:27:LYS:HG3	2.10	0.52
3:F:63:LYS:HB3	3:F:64:GLU:OE1	2.10	0.51
3:I:21:ASP:OD2	3:I:29:LYS:NZ	2.41	0.51
2:H:112:ASP:OD2	3:I:49:GLN:HG2	2.10	0.51
3:L:27:LYS:HB3	3:L:41:GLN:NE2	2.25	0.51
1:G:16:ILE:HD11	1:A:90:LEU:HD11	1.92	0.51
3:I:36:ILE:HB	3:I:41:GLN:NE2	2.19	0.51
1:A:43:CYS:HB2	1:A:46:CYS:SG	2.51	0.51
2:K:5:ARG:HD2	2:K:61:PRO:HG3	1.93	0.50
2:B:72:LYS:HD3	2:B:146:ALA:HA	1.94	0.50
2:B:86:LEU:HD13	2:B:109:LEU:HD22	1.92	0.50
3:C:14:THR:O	3:C:33:LYS:NZ	2.44	0.50
2:E:85:LYS:HZ2	3:F:76:GLY:C	2.20	0.49
1:J:43:CYS:HB2	1:J:46:CYS:SG	2.51	0.49
2:E:60:TYR:CD1	2:E:61:PRO:HA	2.47	0.49
2:K:77:ASN:ND2	3:L:76:GLY:HA2	2.27	0.49
2:E:5:ARG:HH11	2:E:61:PRO:HG3	1.79	0.48
2:H:117:ASP:O	3:I:76:GLY:HA2	2.13	0.48
3:I:56:LEU:HD22	3:I:61:ILE:HD12	1.95	0.48
3:L:24:GLU:O	3:L:28:ALA:N	2.41	0.48
1:J:29:ARG:NH1	1:J:87:MET:HE3	2.27	0.47
3:C:73:LEU:HD22	2:B:105:SER:HB3	1.97	0.47
2:K:86:LEU:HB3	2:K:89:LEU:HD13	1.96	0.47
1:D:72:LYS:HB2	1:D:76:ALA:HB2	1.96	0.47
2:K:32:HIS:HD2	2:K:55:HIS:NE2	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:ARG:NH2	5:I:101:HOH:O	2.46	0.47
1:D:64:ARG:HD2	3:F:40:GLN:OE1	2.16	0.46
3:C:18:GLU:O	3:C:21:ASP:HB2	2.15	0.46
3:C:8:LEU:HD23	3:C:8:LEU:HA	1.82	0.46
1:D:39:LEU:HD23	1:J:78:GLN:HG2	1.98	0.46
1:G:47:LEU:HD22	1:G:58:LEU:HD11	1.98	0.46
1:D:58:LEU:O	1:D:66:THR:HA	2.16	0.45
3:L:27:LYS:HE2	3:L:52:ASP:OD1	2.15	0.45
3:L:45:PHE:HB2	3:L:50:LEU:HD11	1.98	0.45
3:C:26:VAL:HG21	3:C:56:LEU:HD11	1.98	0.45
2:B:33:TRP:HB2	2:B:54:VAL:HB	1.97	0.45
3:L:61:ILE:HD13	3:L:67:LEU:HD11	1.98	0.45
3:C:49:GLN:HG2	2:B:112:ASP:OD2	2.16	0.45
1:G:63:CYS:HB2	3:I:37:PRO:HD2	1.98	0.45
2:E:72:LYS:HB3	2:E:146:ALA:HA	1.99	0.45
2:H:-1:LEU:HG	1:J:71:GLU:OE1	2.17	0.45
2:B:72:LYS:HE3	2:B:141:TRP:CZ3	2.52	0.44
1:D:88:ASP:CG	3:L:33:LYS:HZ1	2.25	0.44
1:D:70:PRO:HG2	1:D:73:GLY:O	2.17	0.44
3:L:26:VAL:O	3:L:30:ILE:HG13	2.18	0.44
2:K:32:HIS:HA	2:K:54:VAL:O	2.16	0.44
2:B:5:ARG:NH2	2:B:95:PRO:O	2.51	0.44
1:A:84:THR:HA	1:A:87:MET:HE2	1.99	0.44
1:A:21:LEU:O	1:A:29:ARG:HA	2.19	0.43
3:C:48:LYS:NZ	2:B:41:PRO:O	2.43	0.43
2:E:59:ASP:CG	2:E:63:LYS:HD3	2.43	0.43
3:L:23:ILE:HG12	3:L:54:ARG:O	2.17	0.43
2:E:86:LEU:HD11	3:F:73:LEU:HD13	2.01	0.43
3:F:33:LYS:NZ	1:J:88:ASP:OD2	2.40	0.43
2:H:-1:LEU:HD23	2:H:-1:LEU:HA	1.86	0.43
2:H:26:VAL:HA	5:H:219:HOH:O	2.18	0.43
1:G:57:THR:HG23	1:G:66:THR:HG23	2.01	0.43
2:H:41:PRO:O	3:I:48:LYS:NZ	2.52	0.43
1:D:90:LEU:HD11	1:J:16:ILE:HD11	2.01	0.43
1:G:64:ARG:HD2	3:I:40:GLN:OE1	2.18	0.42
2:H:131:LYS:HE2	2:H:135:ASN:HD21	1.84	0.42
2:H:105:SER:HB3	3:I:73:LEU:HD22	2.00	0.42
2:H:131:LYS:HA	5:H:201:HOH:O	2.18	0.42
1:G:21:LEU:O	1:G:29:ARG:HA	2.20	0.42
3:C:4:PHE:CD1	3:C:14:THR:HG22	2.55	0.42
3:I:33:LYS:O	1:A:85:ASN:ND2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:20:HIS:CE1	2:K:104:LEU:HB2	2.54	0.42
2:E:49:VAL:H	2:E:145:TYR:HE1	1.68	0.41
1:J:21:LEU:HD13	1:J:87:MET:HG2	2.02	0.41
1:J:92:ARG:NH2	5:J:203:HOH:O	2.52	0.41
2:B:32:HIS:CD2	2:B:55:HIS:NE2	2.89	0.41
3:F:8:LEU:HD23	3:F:8:LEU:HA	1.84	0.41
2:H:60:TYR:CD1	2:H:61:PRO:HA	2.55	0.41
2:H:101:LYS:HD2	3:I:70:VAL:HG12	2.03	0.41
2:K:105:SER:HB3	3:L:73:LEU:HD22	2.03	0.41
1:D:84:THR:HA	1:D:87:MET:HE3	2.03	0.41
3:F:43:LEU:HD23	3:F:43:LEU:HA	1.93	0.41
3:L:23:ILE:HD12	3:L:50:LEU:HD23	2.03	0.41
2:H:9:GLU:OE1	2:H:60:TYR:OH	2.33	0.40
1:D:43:CYS:HB2	1:D:46:CYS:SG	2.61	0.40
1:J:30:TYR:HB3	1:J:33:PRO:HG3	2.03	0.40
2:K:13:LEU:HD21	2:K:100:SER:HB2	2.04	0.40
2:H:28:ASP:OD2	2:H:28:ASP:N	2.52	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	A	84/97 (87%)	84 (100%)	0	0	100	100
1	D	83/97 (86%)	83 (100%)	0	0	100	100
1	G	83/97 (86%)	83 (100%)	0	0	100	100
1	J	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
2	B	145/150 (97%)	142 (98%)	3 (2%)	0	100	100
2	E	145/150 (97%)	142 (98%)	3 (2%)	0	100	100
2	H	148/150 (99%)	145 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	143/150 (95%)	140 (98%)	3 (2%)	0	100	100
3	C	74/80 (92%)	71 (96%)	3 (4%)	0	100	100
3	F	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
3	I	72/80 (90%)	70 (97%)	2 (3%)	0	100	100
3	L	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
All	All	1210/1308 (92%)	1186 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	82/88 (93%)	82 (100%)	0	100	100
1	D	81/88 (92%)	81 (100%)	0	100	100
1	G	81/88 (92%)	81 (100%)	0	100	100
1	J	81/88 (92%)	81 (100%)	0	100	100
2	B	130/132 (98%)	129 (99%)	1 (1%)	73	88
2	E	130/132 (98%)	129 (99%)	1 (1%)	73	88
2	H	132/132 (100%)	132 (100%)	0	100	100
2	K	130/132 (98%)	128 (98%)	2 (2%)	57	79
3	C	68/69 (99%)	68 (100%)	0	100	100
3	F	68/69 (99%)	68 (100%)	0	100	100
3	I	66/69 (96%)	64 (97%)	2 (3%)	36	62
3	L	68/69 (99%)	67 (98%)	1 (2%)	57	79
All	All	1117/1156 (97%)	1110 (99%)	7 (1%)	78	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	99	VAL
3	I	7	THR
3	I	22	THR
2	K	26	VAL
2	K	58	THR
3	L	14	THR
2	B	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	GLN
1	D	49	ASN
1	D	65	GLN
1	D	78	GLN
3	F	49	GLN
1	G	48	GLN
1	G	78	GLN
2	H	46	GLN
2	H	135	ASN
3	I	41	GLN
3	I	68	HIS
1	J	15	GLN
2	K	32	HIS
2	K	34	GLN
3	L	41	GLN
1	A	49	ASN
3	C	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	86/97 (88%)	0.04	0	100	100	28, 45, 68, 93	0
1	D	85/97 (87%)	0.10	3 (3%)	47	43	33, 47, 74, 88	0
1	G	85/97 (87%)	0.10	4 (4%)	36	33	26, 47, 79, 94	0
1	J	85/97 (87%)	0.51	7 (8%)	17	15	38, 60, 110, 124	0
2	B	147/150 (98%)	-0.18	1 (0%)	84	82	27, 37, 58, 81	0
2	E	147/150 (98%)	0.11	1 (0%)	84	82	36, 50, 75, 109	0
2	H	150/150 (100%)	0.07	2 (1%)	75	72	29, 47, 78, 97	0
2	K	145/150 (96%)	1.12	21 (14%)	6	5	48, 78, 103, 124	0
3	C	76/80 (95%)	0.46	2 (2%)	57	53	31, 59, 96, 104	0
3	F	77/80 (96%)	0.03	1 (1%)	75	72	35, 52, 65, 80	0
3	I	74/80 (92%)	1.42	16 (21%)	2	2	57, 91, 125, 129	0
3	L	77/80 (96%)	1.36	14 (18%)	3	3	71, 99, 123, 131	0
All	All	1234/1308 (94%)	0.38	72 (5%)	29	26	26, 55, 110, 131	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	9	THR	3.7
1	G	93	THR	3.7
2	K	145	TYR	3.7
2	K	120	VAL	3.5
1	J	9	PRO	3.3
1	J	71	GLU	3.2
2	K	110	LEU	3.1
2	K	86	LEU	3.1
1	J	68	ILE	3.0
3	L	8	LEU	3.0
3	L	47	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	61	ILE	2.9
2	K	141	TRP	2.9
3	L	76	GLY	2.9
3	I	17	VAL	2.8
3	I	4	PHE	2.8
3	I	15	LEU	2.8
1	J	93	THR	2.8
3	I	41	GLN	2.8
3	L	1	MET	2.7
3	I	44	ILE	2.7
1	D	9	PRO	2.7
3	L	43	LEU	2.7
3	I	19	PRO	2.6
3	I	8	LEU	2.5
3	L	57	SER	2.5
3	I	23	ILE	2.5
2	H	146	ALA	2.5
2	K	55	HIS	2.5
1	J	58	LEU	2.4
2	K	3	LEU	2.4
3	L	5	VAL	2.4
2	K	28	ASP	2.4
3	L	56	LEU	2.4
2	K	119	LEU	2.4
2	K	69	PHE	2.4
3	I	45	PHE	2.4
3	C	4	PHE	2.3
3	I	26	VAL	2.3
3	F	0	GLY	2.3
2	E	145	TYR	2.3
1	J	66	THR	2.3
1	J	56	LEU	2.3
3	I	3	ILE	2.3
1	G	53	ALA	2.2
2	K	68	ALA	2.2
3	I	13	ILE	2.2
1	G	92	ARG	2.2
3	I	56	LEU	2.2
1	G	9	PRO	2.2
2	K	90	ARG	2.2
2	K	71	THR	2.2
3	C	53	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	126	ILE	2.2
3	L	3	ILE	2.2
3	L	4	PHE	2.2
3	L	50	LEU	2.1
2	K	85	LYS	2.1
2	H	-2	PRO	2.1
3	L	44	ILE	2.1
2	K	108	SER	2.1
1	D	82	PHE	2.1
2	K	7	GLN	2.1
1	D	93	THR	2.1
2	K	140	GLU	2.1
2	K	1	SER	2.1
3	I	50	LEU	2.0
2	K	45	TYR	2.0
2	K	74	TYR	2.0
3	L	71	LEU	2.0
3	L	13	ILE	2.0
2	B	42	ASP	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
4	ZN	A	101	1/1	0.97	0.07	48,48,48,48	0
4	ZN	D	102	1/1	0.99	0.07	53,53,53,53	0
4	ZN	G	101	1/1	0.99	0.07	45,45,45,45	0
4	ZN	G	102	1/1	0.99	0.10	56,56,56,56	0

Continued on next page...

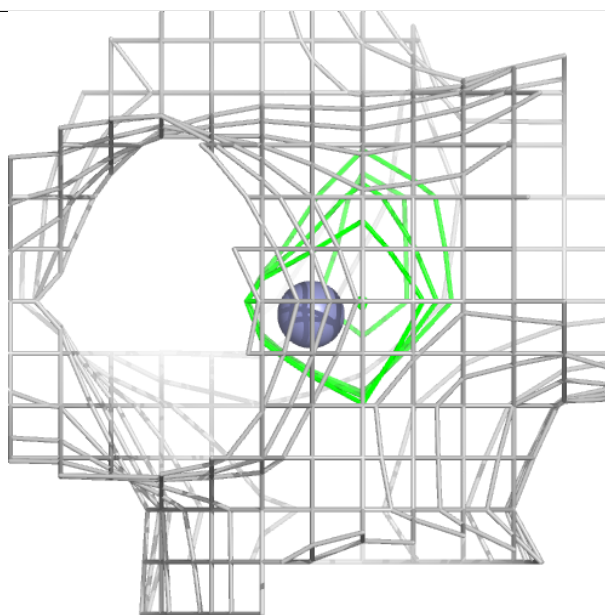
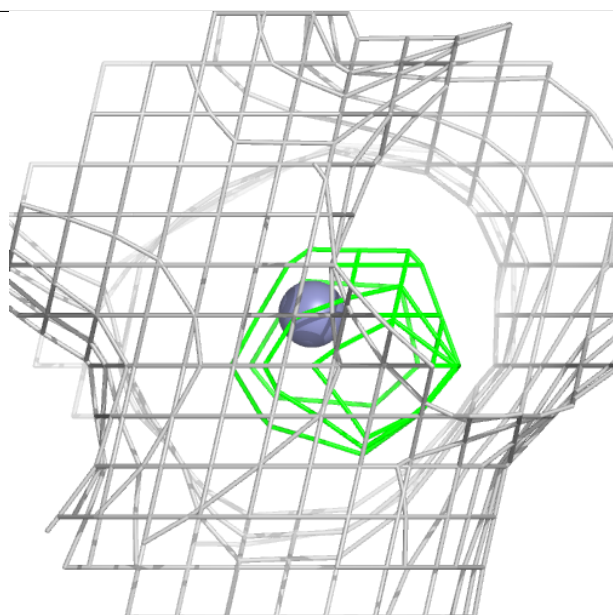
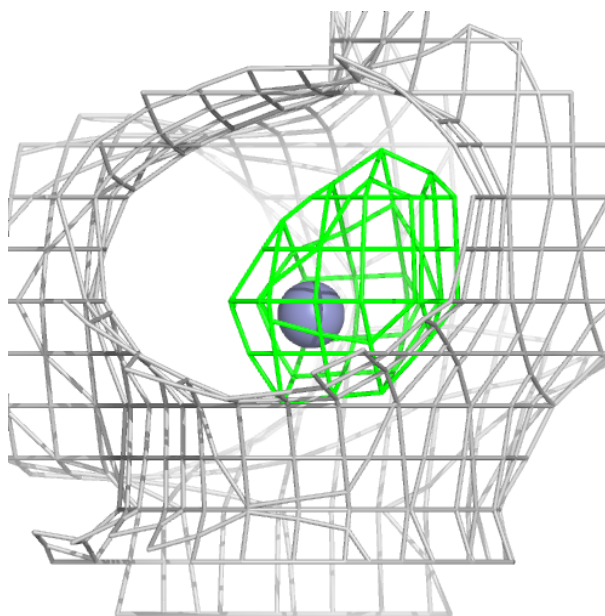
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	J	101	1/1	0.99	0.05	70,70,70,70	0
4	ZN	J	102	1/1	0.99	0.06	73,73,73,73	0
4	ZN	D	101	1/1	0.99	0.05	55,55,55,55	0
4	ZN	A	102	1/1	0.99	0.07	52,52,52,52	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.

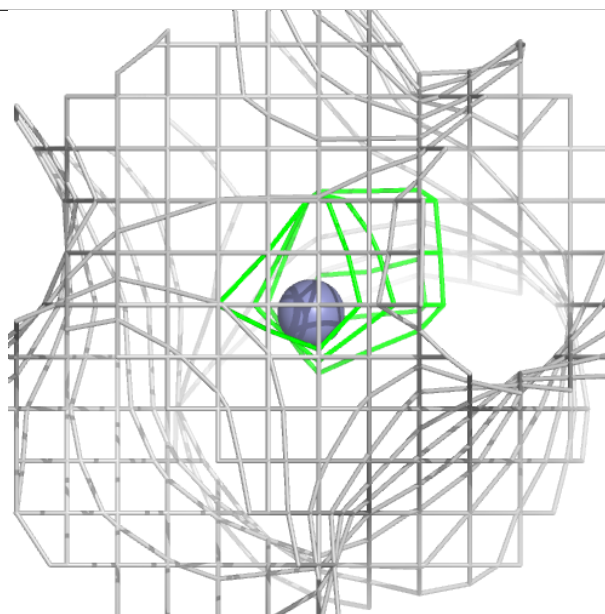
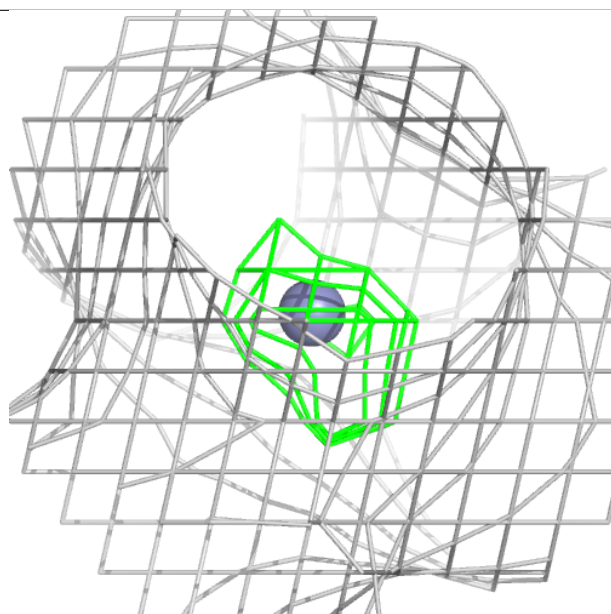
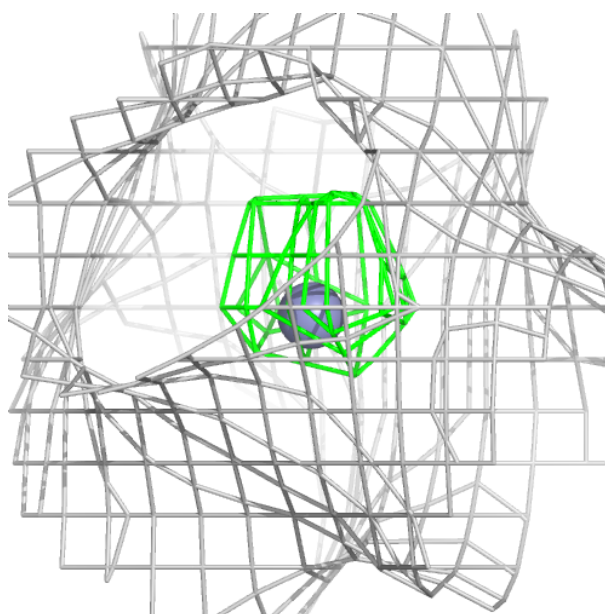
Electron density around ZN A 101:

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



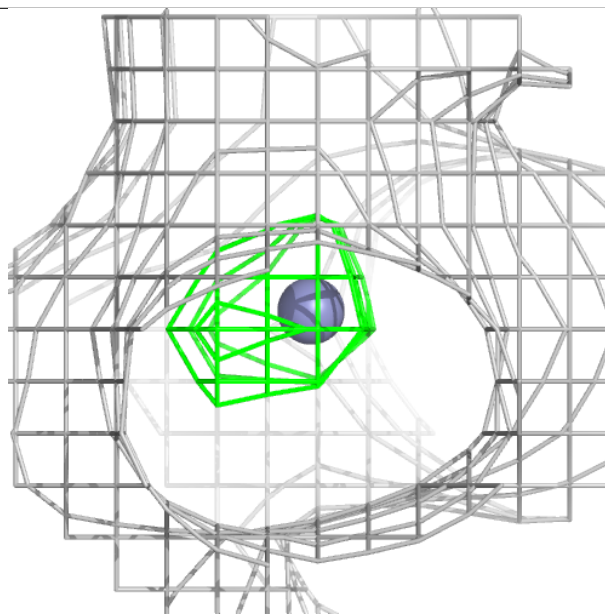
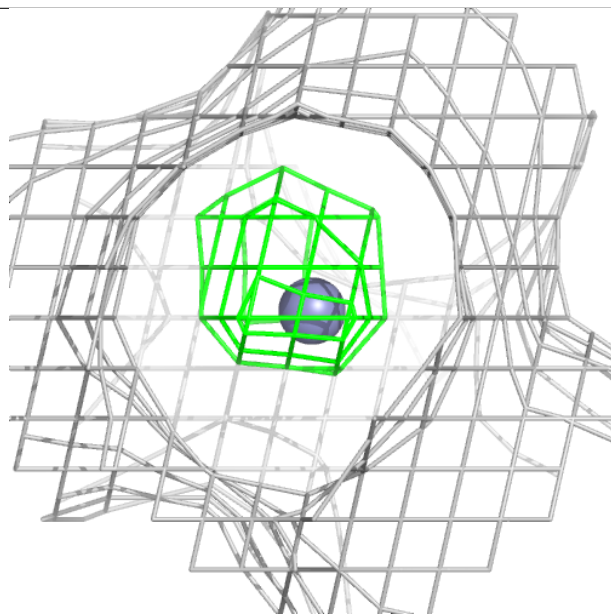
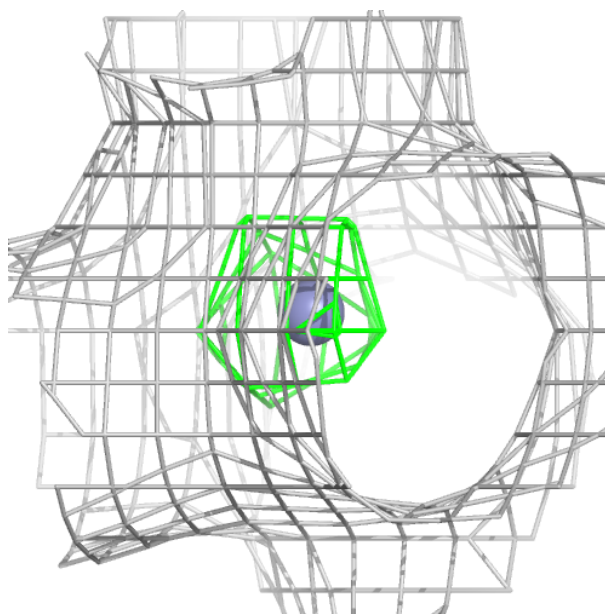
Electron density around ZN D 102:

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



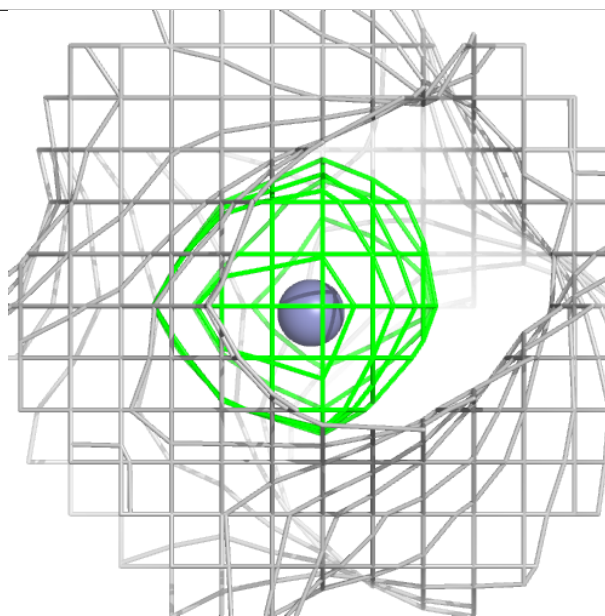
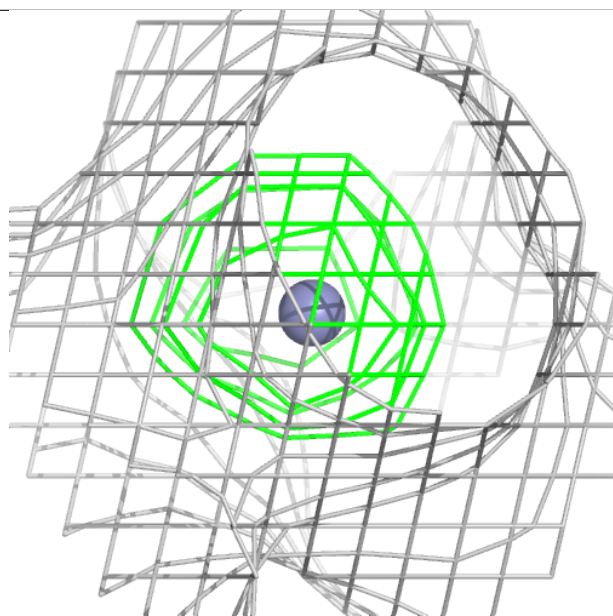
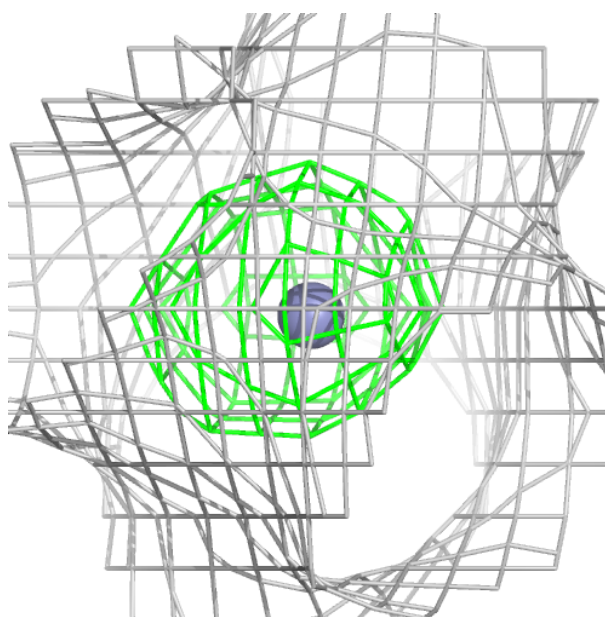
Electron density around ZN G 101:

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



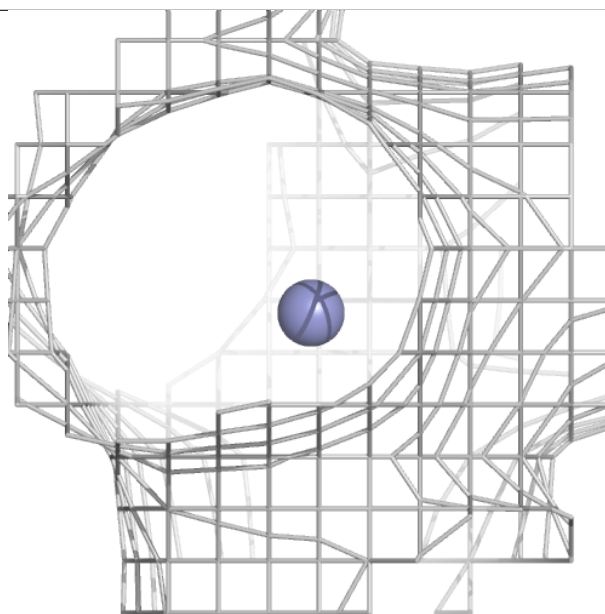
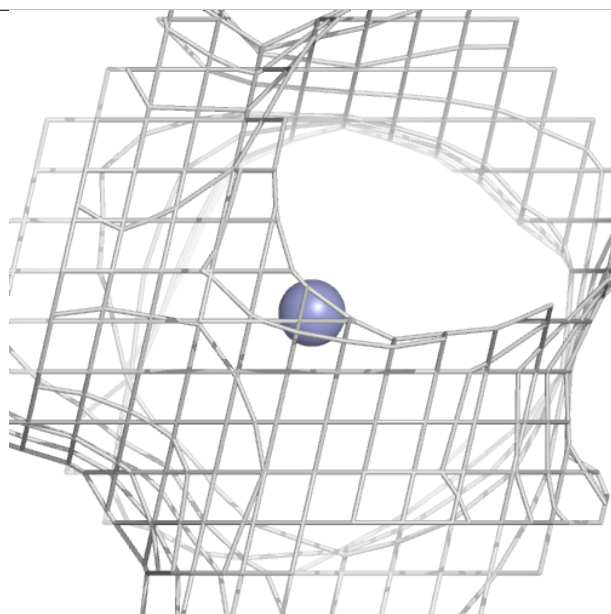
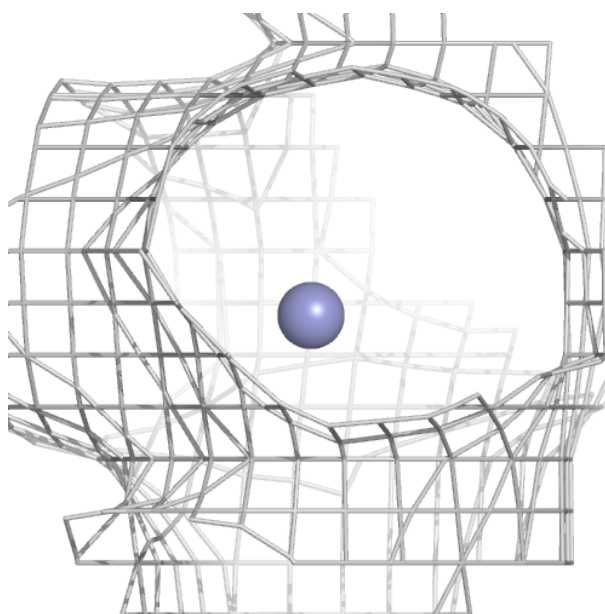
Electron density around ZN G 102:

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



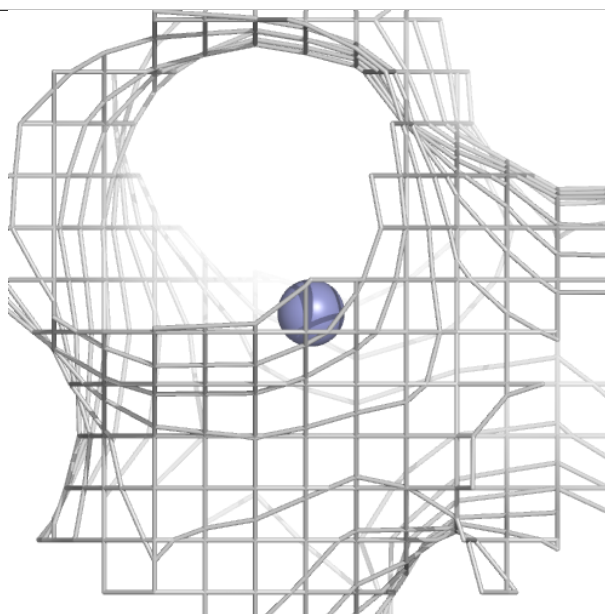
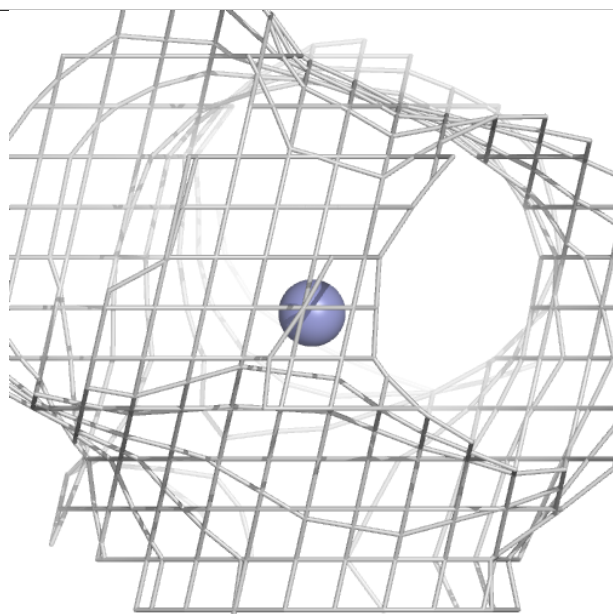
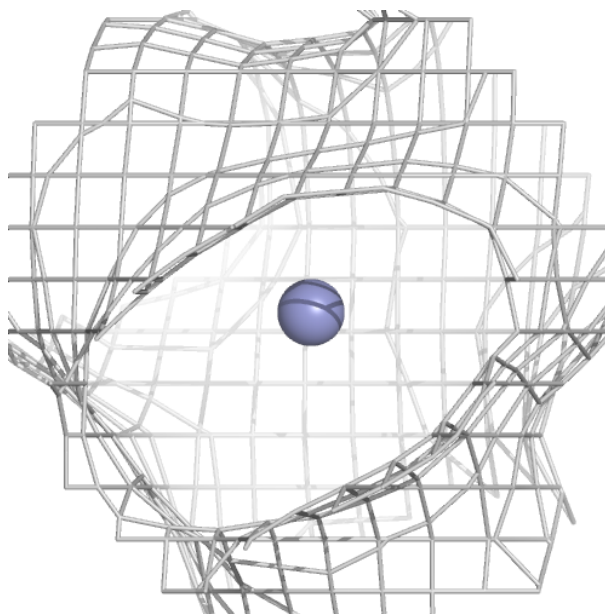
Electron density around ZN J 101:

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



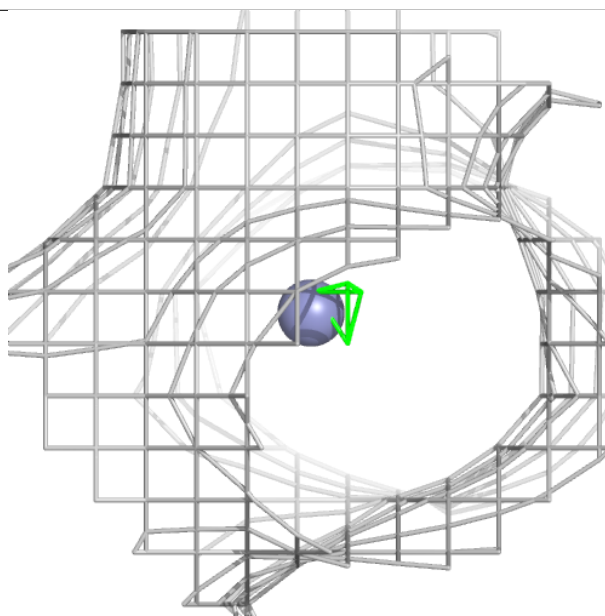
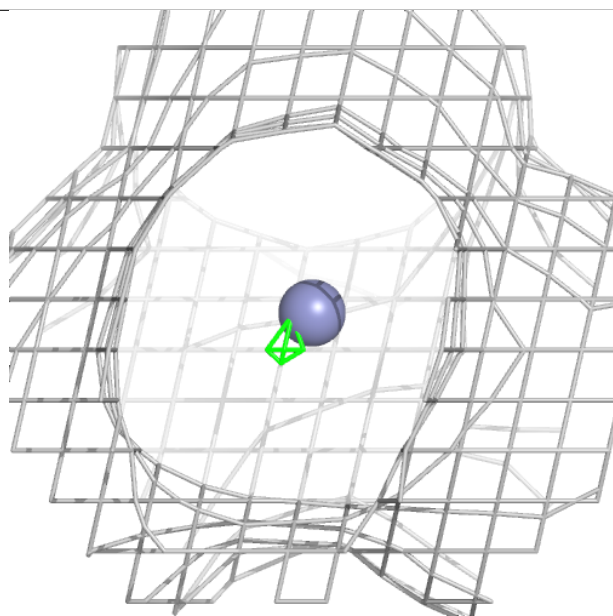
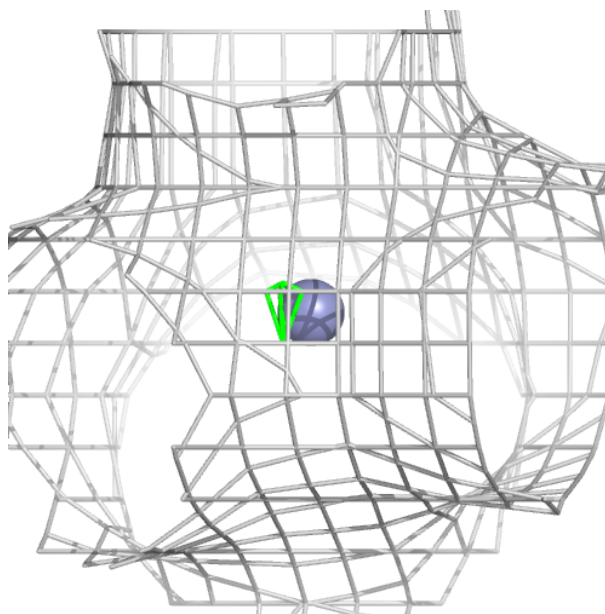
Electron density around ZN J 102:

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



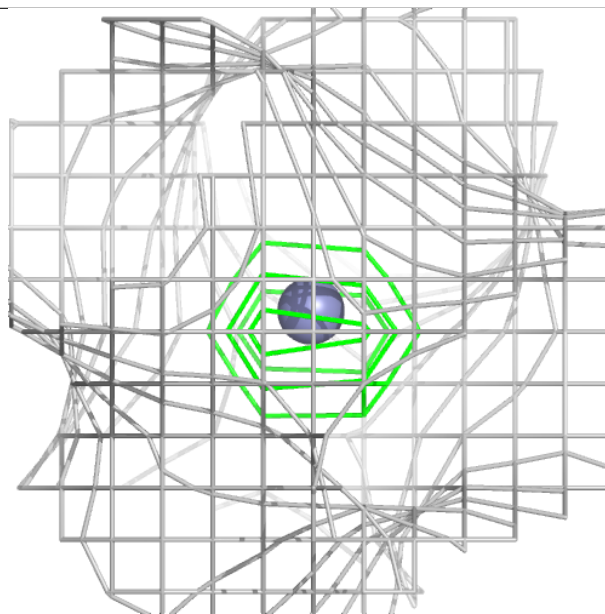
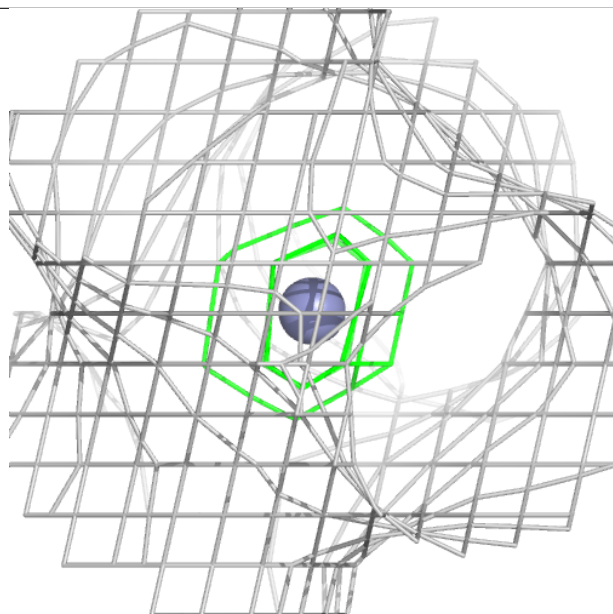
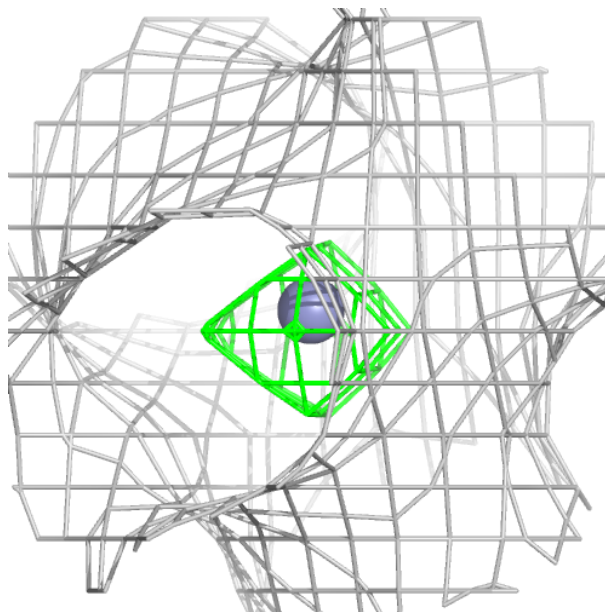
Electron density around ZN D 101:

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



Electron density around ZN A 102:

$2mF_o-DF_c$ (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.