



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 PM UTC

PDB ID : 7Z6E / pdb_00007z6e
Title : Structure of the C1-PH-CNH regulatory module of MRCK1
Authors : Truebestein, L.; Leonard, T.A.
Deposited on : 2022-03-11
Resolution : 2.14 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

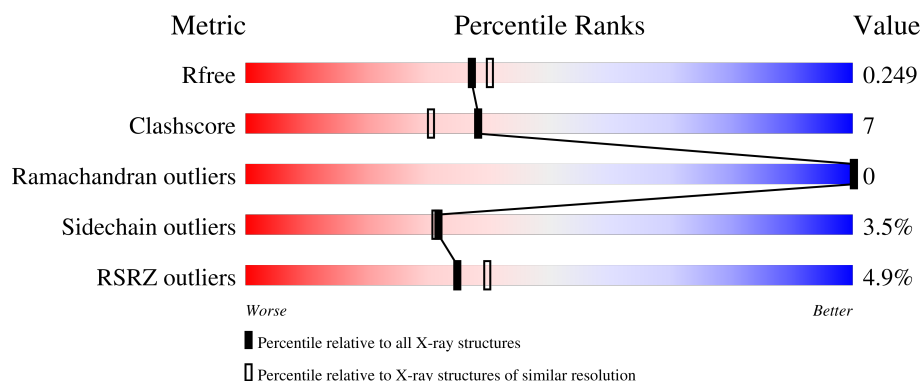
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	582	 3% 74% 15% 11%
1	B	582	 4% 77% 13% 9%
1	C	582	 5% 71% 20% 8%
1	D	582	 4% 71% 18% 10%
1	E	582	 5% 79% 10% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21821 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 Serine/threonine-protein kinase mrck-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4095	2606	708	753	28			
1	B	530	Total	C	N	O	S	0	0	0
			4188	2659	725	776	28			
1	C	534	Total	C	N	O	S	0	0	0
			4208	2672	729	778	29			
1	D	525	Total	C	N	O	S	0	0	0
			4140	2632	714	766	28			
1	E	517	Total	C	N	O	S	0	0	0
			4085	2596	702	758	29			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	953	ALA	-	expression tag	UNP O01583
A	954	ARG	-	expression tag	UNP O01583
B	953	ALA	-	expression tag	UNP O01583
B	954	ARG	-	expression tag	UNP O01583
C	953	ALA	-	expression tag	UNP O01583
C	954	ARG	-	expression tag	UNP O01583
D	953	ALA	-	expression tag	UNP O01583
D	954	ARG	-	expression tag	UNP O01583
E	953	ALA	-	expression tag	UNP O01583
E	954	ARG	-	expression tag	UNP O01583

- 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	2	Total	Zn	0	0
			2	2		

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

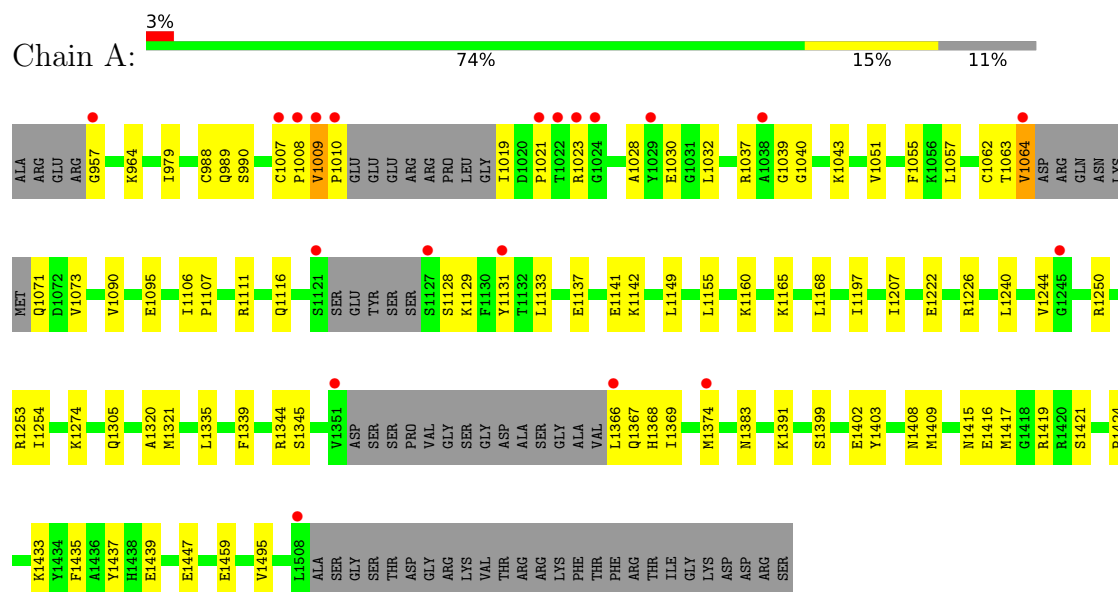
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	298	Total 298	O 298	0	0
3	B	268	Total 268	O 268	0	0
3	C	180	Total 180	O 180	0	0
3	D	168	Total 168	O 168	0	0
3	E	181	Total 181	O 181	0	0

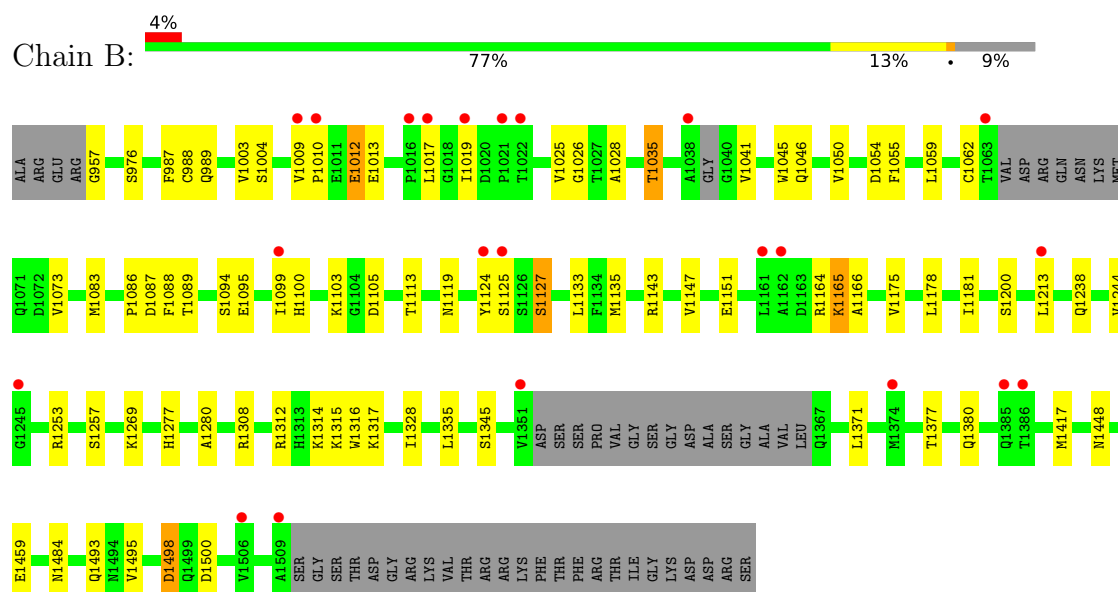
3 Residue-property plots [i](#)

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.

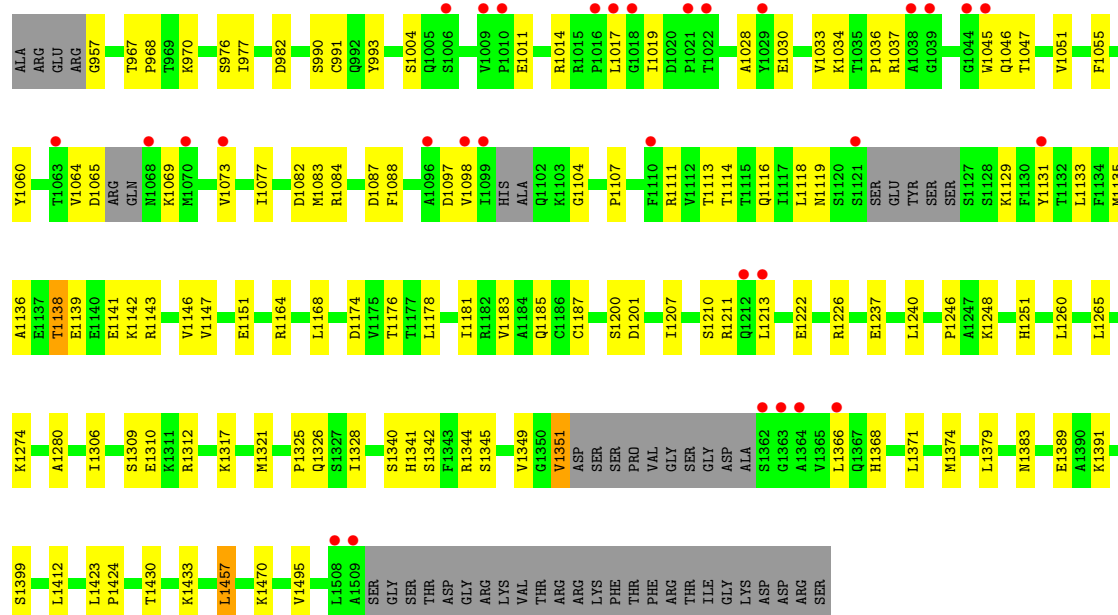
- Molecule 1: Serine/threonine-protein kinase mrck-1



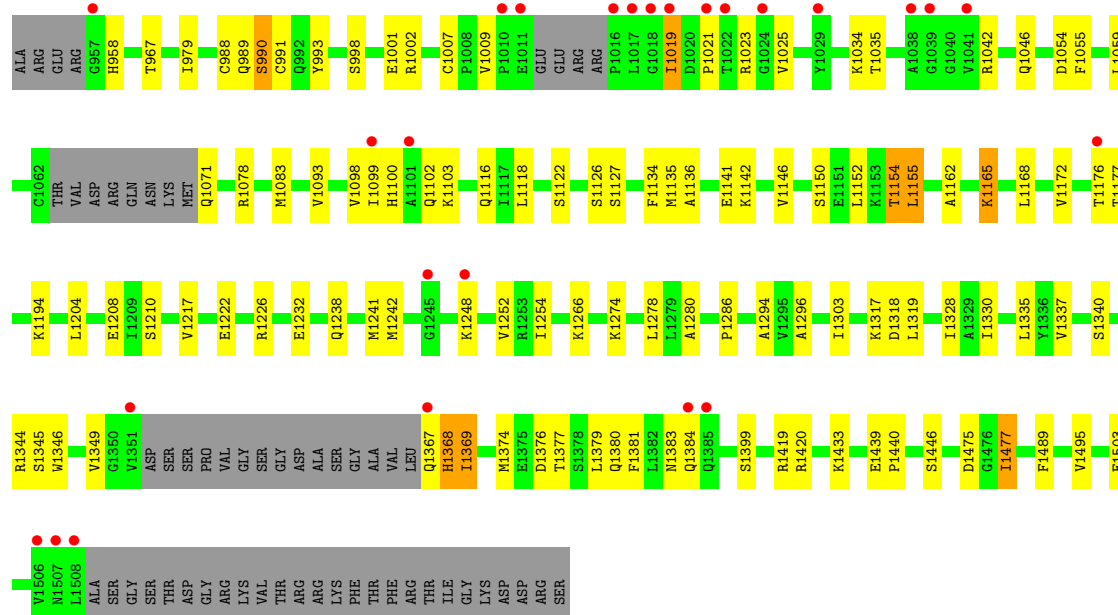
- Molecule 1: Serine/threonine-protein kinase mrck-1



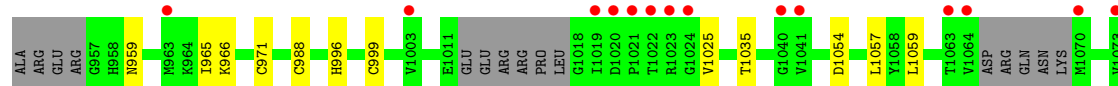
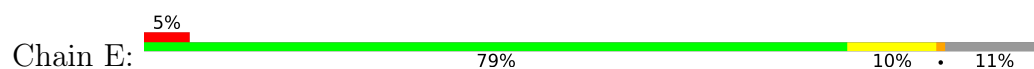
- Molecule 1: Serine/threonine-protein kinase mrck-1

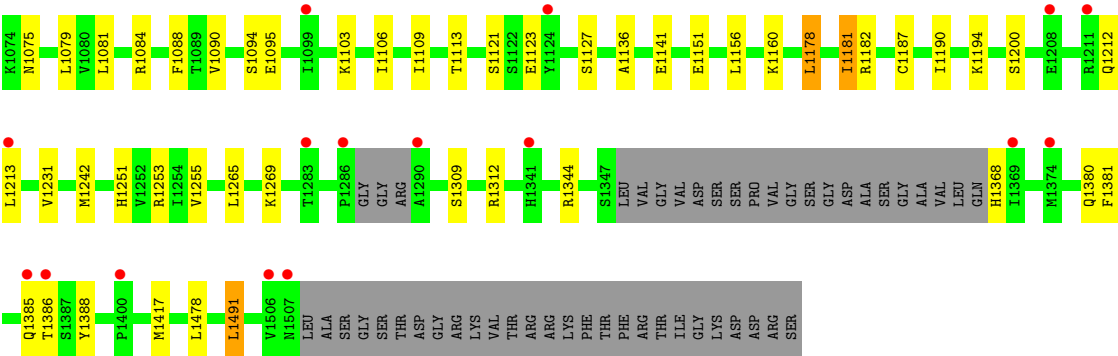


- Molecule 1: Serine/threonine-protein kinase mrck-1



- Molecule 1: Serine/threonine-protein kinase mrck-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.14Å 97.47Å 131.41Å 81.38° 77.77° 80.39°	Depositor
Resolution (Å)	49.60 – 2.14 49.60 – 2.14	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.60-2.14) 94.0 (49.60-2.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.194 , 0.244 0.204 , 0.249	Depositor DCC
R_{free} test set	8482 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21821	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

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	0.38	0/4174	0.59	1/5645 (0.0%)
1	B	0.37	0/4270	0.57	0/5775
1	C	0.33	0/4287	0.52	1/5795 (0.0%)
1	D	0.31	0/4222	0.51	0/5710
1	E	0.31	0/4165	0.52	0/5632
All	All	0.34	0/21118	0.54	2/28557 (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	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1457	LEU	CB-CG-CD1	-6.33	91.70	110.70
1	A	1040	GLY	N-CA-C	5.31	117.48	111.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1244	VAL	Peptide
1	B	1244	VAL	Peptide
1	D	990	SER	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	4095	0	4125	57	0
1	B	4188	0	4203	53	1
1	C	4208	0	4237	75	0
1	D	4140	0	4157	73	0
1	E	4085	0	4092	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	298	0	0	9	0
3	B	268	0	0	10	0
3	C	180	0	0	12	0
3	D	168	0	0	4	0
3	E	181	0	0	5	0
All	All	21821	0	20814	287	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 7.

All (287) 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:D:1344:ARG:HD2	1:D:1368:HIS:HE1	1.46	0.81
1:C:1164:ARG:NH2	3:C:1704:HOH:O	2.15	0.80
1:C:1470:LYS:NZ	3:C:1703:HOH:O	2.14	0.79
1:D:1204:LEU:HD23	1:D:1217:VAL:HG11	1.64	0.79
1:A:1417:MET:HE3	1:A:1419:ARG:HD3	1.65	0.79
1:D:1433:LYS:HD3	1:D:1446:SER:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1071:GLN:NE2	3:D:1701:HOH:O	2.20	0.73
1:E:1253:ARG:HH22	1:E:1269:LYS:HE3	1.53	0.73
1:C:1136:ALA:HB1	1:C:1141:GLU:HB3	1.70	0.72
1:A:1023:ARG:NH1	3:A:1707:HOH:O	2.23	0.70
1:D:1019:ILE:HD11	1:D:1055:PHE:H	1.55	0.70
1:A:1459:GLU:OE2	3:A:1701:HOH:O	2.09	0.69
1:B:1099:ILE:HG23	1:B:1100:HIS:HD2	1.58	0.69
1:C:1237:GLU:HG3	1:C:1306:ILE:HG21	1.74	0.69
1:C:1222:GLU:OE2	3:C:1701:HOH:O	2.11	0.68
1:C:991:CYS:N	3:C:1709:HOH:O	2.25	0.68
1:D:1376:ASP:HB2	1:D:1419:ARG:HE	1.58	0.68
1:B:1087:ASP:OD1	3:B:1701:HOH:O	2.11	0.68
1:E:1151:GLU:O	3:E:1701:HOH:O	2.11	0.68
1:C:982:ASP:OD2	3:C:1702:HOH:O	2.12	0.67
1:C:1034:LYS:HB2	1:C:1135:MET:HB3	1.77	0.67
1:B:1164:ARG:NH1	1:B:1459:GLU:OE2	2.28	0.66
1:D:1248:LYS:H	1:D:1248:LYS:HD3	1.59	0.65
1:B:1417:MET:HE2	1:C:1341:HIS:CE1	2.30	0.65
1:A:1007:CYS:HB3	1:A:1008:PRO:HD3	1.79	0.65
1:B:1046:GLN:NE2	3:B:1706:HOH:O	2.30	0.65
1:B:1238:GLN:HB3	1:B:1257:SER:HB2	1.79	0.65
1:C:1210:SER:OG	1:C:1211:ARG:NH1	2.28	0.65
1:E:1269:LYS:NZ	3:E:1705:HOH:O	2.28	0.65
1:A:1111:ARG:HD2	1:A:1131:TYR:CD2	2.32	0.64
1:A:1111:ARG:HD2	1:A:1131:TYR:HD2	1.62	0.64
1:B:1099:ILE:HG23	1:B:1100:HIS:CD2	2.32	0.64
1:D:1280:ALA:HB2	1:D:1328:ILE:HG23	1.78	0.64
1:E:1075:ASN:ND2	3:E:1709:HOH:O	2.31	0.64
1:A:1095:GLU:HG2	1:A:1106:ILE:HG13	1.80	0.64
1:B:1062:CYS:HB3	1:B:1073:VAL:HG22	1.80	0.63
1:C:957:GLY:N	3:C:1712:HOH:O	2.31	0.63
1:C:1344:ARG:HG2	1:C:1368:HIS:NE2	2.13	0.63
1:D:1248:LYS:HD3	1:D:1248:LYS:N	2.14	0.63
1:D:1116:GLN:HG2	1:D:1118:LEU:HD23	1.79	0.62
1:D:1021:PRO:HB3	1:D:1155:LEU:HD11	1.81	0.62
1:E:1255:VAL:HG23	1:E:1265:LEU:HD22	1.81	0.62
1:A:1064:VAL:HG12	1:A:1071:GLN:HG2	1.80	0.62
1:A:1415:ASN:HD21	1:A:1417:MET:HE2	1.64	0.62
1:C:1326:GLN:OE1	1:C:1389:GLU:HB2	2.01	0.61
1:D:1475:ASP:OD1	1:D:1477:ILE:HG22	2.00	0.61
1:A:1037:ARG:HB2	1:A:1037:ARG:NH1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:THR:HG22	1:B:1133:LEU:O	2.01	0.61
1:C:1019:ILE:HG13	1:C:1028:ALA:HB2	1.83	0.61
1:A:1374:MET:HE3	1:A:1383:ASN:ND2	2.16	0.61
1:A:1439:GLU:OE2	3:A:1702:HOH:O	2.16	0.60
1:D:988:CYS:SG	1:D:991:CYS:HB3	2.40	0.60
1:D:1099:ILE:HG13	1:D:1100:HIS:CD2	2.36	0.60
1:C:1251:HIS:HB3	1:C:1274:LYS:HD2	1.83	0.60
1:D:1162:ALA:N	3:D:1704:HOH:O	2.34	0.60
1:C:991:CYS:SG	1:C:993:TYR:HB2	2.42	0.60
1:D:958:HIS:ND1	1:D:1007:CYS:HB2	2.17	0.60
1:D:1059:LEU:HD11	1:D:1134:PHE:CE1	2.37	0.59
1:D:1046:GLN:OE1	1:D:1078:ARG:NH1	2.33	0.59
1:D:1286:PRO:HG2	1:D:1349:VAL:HG21	1.85	0.59
1:D:1367:GLN:OE1	1:D:1369:ILE:HG12	2.03	0.59
1:A:1019:ILE:HD13	1:A:1055:PHE:H	1.67	0.59
1:B:1147:VAL:O	1:B:1151:GLU:HG3	2.02	0.59
1:C:1077:ILE:O	1:C:1430:THR:HB	2.02	0.59
1:E:1136:ALA:HB1	1:E:1141:GLU:HG2	1.85	0.58
1:B:1019:ILE:HD13	1:B:1055:PHE:H	1.68	0.58
1:A:1402:GLU:OE2	1:A:1421:SER:OG	2.20	0.58
1:D:1222:GLU:OE2	1:D:1226:ARG:NH2	2.35	0.58
1:B:1253:ARG:HH11	1:B:1269:LYS:HB2	1.68	0.58
1:D:1136:ALA:HB1	1:D:1141:GLU:HG3	1.86	0.57
1:A:1116:GLN:HG3	1:A:1129:LYS:HG3	1.86	0.57
1:A:1433:LYS:HE2	1:A:1447:GLU:OE2	2.04	0.57
1:A:1374:MET:HE3	1:A:1383:ASN:HD21	1.69	0.57
1:B:1380:GLN:NE2	3:B:1711:HOH:O	2.38	0.56
1:A:1111:ARG:HG3	1:A:1133:LEU:HD23	1.87	0.56
1:B:1019:ILE:HG13	1:B:1028:ALA:HB2	1.88	0.56
1:C:970:LYS:HE3	1:C:1030:GLU:OE2	2.06	0.56
1:D:1172:VAL:HB	1:D:1489:PHE:HD1	1.69	0.56
1:B:1095:GLU:OE2	1:B:1103:LYS:HG3	2.06	0.55
1:A:1019:ILE:HG13	1:A:1028:ALA:HB2	1.88	0.55
1:C:1034:LYS:HG2	1:C:1047:THR:HG22	1.88	0.55
1:D:991:CYS:SG	1:D:993:TYR:HB2	2.47	0.55
1:C:1222:GLU:OE1	1:C:1226:ARG:NH2	2.40	0.54
1:C:1178:LEU:HD23	1:C:1181:ILE:HB	1.88	0.54
1:E:1253:ARG:CZ	1:E:1269:LYS:HG2	2.38	0.54
1:C:1055:PHE:O	1:C:1083:MET:HG3	2.07	0.54
1:D:1150:SER:O	1:D:1154:THR:HG23	2.07	0.54
1:E:1380:GLN:NE2	3:E:1702:HOH:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1204:LEU:O	1:D:1217:VAL:HG12	2.08	0.54
1:C:1168:LEU:HD12	1:C:1495:VAL:HG12	1.89	0.54
1:B:988:CYS:O	1:B:989:GLN:HB3	2.07	0.53
1:A:1339:PHE:CE1	1:A:1344:ARG:HD2	2.43	0.53
1:B:1105:ASP:OD1	3:B:1702:HOH:O	2.19	0.53
1:C:1309:SER:O	1:C:1312:ARG:HD2	2.09	0.53
1:C:1111:ARG:HD2	1:C:1131:TYR:CD2	2.42	0.52
1:C:1280:ALA:HB2	1:C:1328:ILE:HG23	1.91	0.52
1:A:1021:PRO:HG2	1:B:1124:TYR:CE2	2.44	0.52
1:A:1039:GLY:HA3	1:A:1043:LYS:NZ	2.25	0.52
1:B:1025:VAL:HA	1:B:1054:ASP:OD1	2.10	0.52
1:C:1011:GLU:OE1	1:C:1014:ARG:NH1	2.42	0.52
1:A:1368:HIS:O	1:A:1369:ILE:HD13	2.09	0.52
1:E:959:ASN:O	1:E:988:CYS:HA	2.09	0.52
1:B:1105:ASP:HB3	1:B:1135:MET:HE2	1.91	0.52
1:C:1248:LYS:H	1:C:1248:LYS:HD3	1.74	0.52
1:E:1344:ARG:HD2	1:E:1368:HIS:NE2	2.25	0.52
1:B:1498:ASP:OD1	1:B:1498:ASP:N	2.41	0.52
1:C:1138:THR:OG1	1:C:1139:GLU:N	2.39	0.52
1:D:1034:LYS:HB2	1:D:1135:MET:HB3	1.90	0.51
1:B:1086:PRO:O	1:D:1102:GLN:HG2	2.10	0.51
1:D:1042:ARG:HG3	1:D:1100:HIS:ND1	2.26	0.51
1:D:1042:ARG:CZ	1:D:1100:HIS:HE1	2.23	0.51
1:D:1001:GLU:OE1	1:D:1002:ARG:HG3	2.10	0.51
1:B:1316:TRP:O	1:B:1317:LYS:HD2	2.11	0.51
1:C:1423:LEU:HB2	1:C:1424:PRO:HD3	1.93	0.51
1:E:996:HIS:HB2	1:E:999:CYS:HB2	1.92	0.50
1:C:1034:LYS:HD3	1:C:1135:MET:HE3	1.92	0.50
1:D:1222:GLU:OE1	1:D:1266:LYS:HD2	2.12	0.50
1:D:1278:LEU:HB2	1:D:1296:ALA:HB3	1.94	0.50
1:B:1178:LEU:HD23	1:B:1181:ILE:HB	1.94	0.50
1:B:1377:THR:HA	1:B:1380:GLN:OE1	2.12	0.49
1:A:1197:ILE:HD12	1:A:1207:ILE:HD12	1.95	0.49
1:C:1139:GLU:HG2	1:C:1143:ARG:HE	1.77	0.49
1:E:971:CYS:HB2	1:E:996:HIS:CE1	2.47	0.49
1:B:1166:ALA:O	1:B:1495:VAL:HG22	2.13	0.49
1:C:1379:LEU:HD22	1:C:1412:LEU:HD21	1.94	0.49
1:D:1346:TRP:HA	1:D:1367:GLN:O	2.13	0.49
1:C:1321:MET:HG3	1:C:1325:PRO:HG3	1.95	0.49
1:C:1457:LEU:HD11	3:C:1826:HOH:O	2.12	0.49
1:C:1433:LYS:NZ	3:C:1706:HOH:O	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:PRO:HG2	1:B:1124:TYR:HE2	1.77	0.49
1:A:1408:ASN:ND2	1:A:1409:MET:HE3	2.27	0.48
1:C:990:SER:HB2	3:C:1709:HOH:O	2.13	0.48
1:D:1335:LEU:O	1:D:1345:SER:HA	2.13	0.48
1:D:1344:ARG:HH11	1:D:1368:HIS:CE1	2.31	0.48
1:C:1129:LYS:HB2	1:C:1131:TYR:HE1	1.78	0.48
1:D:1210:SER:HB3	1:D:1503:GLU:OE2	2.13	0.48
1:D:1238:GLN:NE2	3:D:1713:HOH:O	2.46	0.48
1:D:1374:MET:HE3	1:D:1383:ASN:OD1	2.13	0.48
3:B:1701:HOH:O	1:D:1103:LYS:HG2	2.13	0.47
1:C:1019:ILE:HD13	1:C:1055:PHE:H	1.79	0.47
1:E:1057:LEU:HB2	1:E:1081:LEU:HB2	1.96	0.47
1:E:1160:LYS:NZ	3:E:1718:HOH:O	2.46	0.47
1:E:1385:GLN:HB3	1:E:1388:TYR:CD1	2.49	0.47
1:D:1059:LEU:HD11	1:D:1134:PHE:HE1	1.76	0.47
1:E:1088:PHE:HA	1:E:1113:THR:O	2.15	0.47
1:A:1403:TYR:OH	1:A:1416:GLU:OE2	2.26	0.47
1:A:1415:ASN:ND2	1:A:1417:MET:HE2	2.27	0.47
1:A:957:GLY:N	3:A:1728:HOH:O	2.48	0.47
1:A:1437:TYR:OH	3:A:1705:HOH:O	2.20	0.47
1:B:1143:ARG:HG3	3:B:1918:HOH:O	2.15	0.47
1:A:1253:ARG:NH1	3:A:1726:HOH:O	2.47	0.47
1:E:1025:VAL:HA	1:E:1054:ASP:OD1	2.15	0.47
1:A:1250:ARG:O	1:A:1274:LYS:HA	2.14	0.47
1:A:964:LYS:NZ	3:A:1729:HOH:O	2.48	0.47
1:A:1021:PRO:HG3	1:A:1155:LEU:HD21	1.97	0.47
1:A:1160:LYS:HD2	1:A:1160:LYS:HA	1.65	0.47
1:C:968:PRO:HG3	1:C:1060:TYR:CE2	2.49	0.46
1:B:1253:ARG:NH1	1:B:1269:LYS:HB2	2.30	0.46
1:B:1417:MET:HE2	1:C:1341:HIS:HE1	1.76	0.46
1:D:1374:MET:HE1	1:D:1379:LEU:O	2.15	0.46
1:B:1277:HIS:ND1	3:B:1709:HOH:O	2.36	0.46
1:C:1389:GLU:HG3	1:C:1391:LYS:HE2	1.98	0.46
1:B:1269:LYS:NZ	3:B:1713:HOH:O	2.39	0.46
1:C:970:LYS:HE2	1:C:1017:LEU:HD21	1.96	0.46
1:C:1111:ARG:HG3	1:C:1133:LEU:HD23	1.98	0.46
1:C:1065:ASP:OD2	1:C:1069:LYS:HB3	2.15	0.46
1:E:1478:LEU:HD23	1:E:1491:LEU:HD23	1.98	0.46
1:D:1204:LEU:HB3	1:D:1217:VAL:CG1	2.46	0.46
1:C:1142:LYS:O	1:C:1146:VAL:HG23	2.16	0.46
1:C:1240:LEU:HD11	1:C:1260:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1328:ILE:CD1	1:D:1337:VAL:HG22	2.46	0.46
1:D:1303:ILE:HD11	1:D:1319:LEU:HD12	1.98	0.45
1:B:1335:LEU:O	1:B:1345:SER:HA	2.17	0.45
1:D:1083:MET:HE1	1:D:1152:LEU:HB3	1.98	0.45
1:E:1095:GLU:OE2	1:E:1103:LYS:HG3	2.16	0.45
1:A:1131:TYR:OH	3:A:1703:HOH:O	2.17	0.45
1:B:1010:PRO:HG2	1:B:1013:GLU:OE1	2.16	0.45
1:D:1344:ARG:HD2	1:D:1368:HIS:CE1	2.37	0.45
1:D:1439:GLU:HA	1:D:1440:PRO:HA	1.85	0.45
1:E:1136:ALA:HB1	1:E:1141:GLU:CG	2.45	0.45
1:B:1050:VAL:HG22	1:B:1059:LEU:HD13	1.98	0.45
1:B:1119:ASN:ND2	3:B:1724:HOH:O	2.48	0.45
1:B:1127:SER:HB2	1:B:1484:ASN:OD1	2.17	0.45
1:C:1034:LYS:HE3	1:C:1047:THR:HG23	1.97	0.45
1:D:958:HIS:CE1	1:D:1007:CYS:HB2	2.50	0.45
1:E:1231:VAL:HG23	1:E:1242:MET:HG2	1.99	0.45
1:A:1043:LYS:HB3	1:A:1043:LYS:HE2	1.58	0.45
1:B:1493:GLN:NE2	1:B:1500:ASP:HA	2.32	0.45
1:D:1204:LEU:HB3	1:D:1217:VAL:HG11	1.98	0.45
1:E:1160:LYS:HA	1:E:1160:LYS:HD2	1.75	0.45
1:C:977:ILE:HG13	1:C:1051:VAL:HG11	1.99	0.44
1:C:1246:PRO:HG2	1:C:1248:LYS:HE2	1.99	0.44
1:D:1025:VAL:HA	1:D:1054:ASP:OD1	2.17	0.44
1:E:1178:LEU:HD23	1:E:1181:ILE:HB	1.97	0.44
1:A:1391:LYS:HG3	1:A:1435:PHE:CE1	2.52	0.44
1:C:1111:ARG:HD2	1:C:1131:TYR:HD2	1.81	0.44
1:E:1417:MET:HE3	1:E:1417:MET:HB2	1.89	0.44
1:C:1088:PHE:HA	1:C:1113:THR:O	2.17	0.44
1:A:1320:ALA:O	1:A:1321:MET:HE2	2.18	0.44
1:C:1037:ARG:NH1	1:C:1046:GLN:OE1	2.51	0.44
1:D:1023:ARG:HD2	1:D:1023:ARG:HA	1.82	0.44
1:A:988:CYS:O	1:A:989:GLN:HB3	2.17	0.44
1:C:1082:ASP:OD1	1:C:1084:ARG:NH1	2.51	0.44
1:C:1183:VAL:HB	1:C:1200:SER:OG	2.18	0.44
1:B:1010:PRO:O	1:B:1012:GLU:N	2.47	0.44
1:C:1351:VAL:HG21	1:C:1366:LEU:HD22	1.99	0.44
1:B:1045:TRP:CE2	1:B:1135:MET:HE3	2.54	0.43
1:C:1174:ASP:OD2	1:C:1176:THR:N	2.50	0.43
1:D:1433:LYS:HD2	1:D:1433:LYS:N	2.33	0.43
1:C:1119:ASN:ND2	1:C:1119:ASN:O	2.50	0.43
1:C:1147:VAL:O	1:C:1151:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1146:VAL:O	1:D:1150:SER:OG	2.22	0.43
1:A:988:CYS:SG	1:A:990:SER:HB2	2.58	0.43
1:C:1118:LEU:HD11	1:C:1168:LEU:HD22	2.00	0.43
1:D:1242:MET:O	1:D:1252:VAL:HA	2.18	0.43
1:D:1034:LYS:HB2	1:D:1034:LYS:HE2	1.75	0.43
1:A:1062:CYS:HB3	1:A:1073:VAL:HG22	1.99	0.43
1:D:1165:LYS:NZ	3:D:1727:HOH:O	2.52	0.43
1:A:1037:ARG:HB2	1:A:1037:ARG:CZ	2.49	0.43
1:C:1213:LEU:HD23	1:C:1213:LEU:HA	1.81	0.43
1:B:1019:ILE:HG12	1:B:1026:GLY:O	2.19	0.43
1:B:1055:PHE:O	1:B:1083:MET:HG3	2.18	0.43
1:A:1030:GLU:HG2	1:A:1051:VAL:HG22	2.00	0.42
1:A:1335:LEU:O	1:A:1345:SER:HA	2.19	0.42
1:C:967:THR:HG22	1:C:1073:VAL:O	2.18	0.42
1:D:1317:LYS:HD3	1:D:1318:ASP:N	2.34	0.42
1:A:1222:GLU:OE1	1:A:1226:ARG:NH2	2.53	0.42
1:E:966:LYS:HD2	1:E:966:LYS:HA	1.79	0.42
1:B:987:PHE:CE2	1:B:989:GLN:HA	2.53	0.42
1:C:1317:LYS:HE2	3:C:1793:HOH:O	2.20	0.42
1:A:1057:LEU:HD11	1:A:1149:LEU:HD22	2.01	0.42
1:E:1190:ILE:HG21	1:E:1194:LYS:HE2	2.00	0.42
1:E:1381:PHE:O	1:E:1385:GLN:HG2	2.19	0.42
1:A:1009:VAL:HG12	1:A:1010:PRO:HD2	2.02	0.42
1:B:1086:PRO:HG3	1:B:1165:LYS:HE2	2.01	0.42
1:A:1142:LYS:HD2	1:A:1142:LYS:C	2.44	0.42
1:C:1036:PRO:HD3	1:C:1045:TRP:CZ3	2.54	0.42
1:D:1194:LYS:HG2	1:D:1208:GLU:HG2	2.02	0.42
1:A:1424:PRO:HG2	3:A:1984:HOH:O	2.20	0.42
1:B:1088:PHE:HA	1:B:1113:THR:O	2.20	0.42
1:C:1116:GLN:HB2	1:C:1129:LYS:HG2	2.01	0.42
1:D:1142:LYS:HE2	1:D:1142:LYS:HB3	1.86	0.42
1:D:1346:TRP:NE1	1:D:1368:HIS:HB2	2.35	0.42
1:D:1379:LEU:HD21	1:D:1420:ARG:HB2	2.01	0.42
1:B:1010:PRO:C	1:B:1012:GLU:H	2.27	0.41
1:B:1280:ALA:HB2	1:B:1328:ILE:HG23	2.01	0.41
1:B:1314:LYS:HD2	1:B:1315:LYS:O	2.20	0.41
1:E:1084:ARG:HG3	1:E:1156:LEU:HD21	2.02	0.41
1:E:1121:SER:C	1:E:1123:GLU:H	2.28	0.41
1:D:1099:ILE:HG13	1:D:1100:HIS:HD2	1.83	0.41
1:D:1168:LEU:HG	1:D:1495:VAL:HG12	2.02	0.41
1:D:1294:ALA:HB2	1:D:1330:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:TYR:CG	1:B:1125:SER:N	2.88	0.41
1:C:1097:ASP:OD2	1:C:1111:ARG:NH1	2.53	0.41
1:D:1103:LYS:HA	1:D:1103:LYS:HD3	1.78	0.41
1:D:1241:MET:HG3	1:D:1254:ILE:HG13	2.02	0.41
1:A:1168:LEU:HG	1:A:1495:VAL:HG12	2.02	0.41
1:B:1448:ASN:ND2	3:B:1728:HOH:O	2.53	0.41
1:A:1111:ARG:CD	1:A:1131:TYR:HD2	2.30	0.41
1:C:1274:LYS:HD3	3:C:1827:HOH:O	2.20	0.41
1:D:1381:PHE:O	1:D:1384:GLN:HG2	2.20	0.41
1:E:1251:HIS:NE2	1:E:1253:ARG:HD2	2.35	0.41
1:B:1493:GLN:CD	1:B:1500:ASP:HA	2.46	0.41
1:C:1087:ASP:HB2	1:C:1114:THR:O	2.20	0.41
1:C:1185:GLN:NE2	1:C:1200:SER:HB3	2.35	0.41
1:D:1369:ILE:HD13	1:D:1369:ILE:HA	1.87	0.41
1:E:1127:SER:O	1:E:1127:SER:OG	2.36	0.41
1:A:1137:GLU:HG3	1:A:1141:GLU:HG3	2.01	0.41
1:C:1344:ARG:CG	1:C:1368:HIS:NE2	2.83	0.41
1:C:1374:MET:HE3	1:C:1383:ASN:CG	2.45	0.41
1:A:1019:ILE:CD1	1:A:1055:PHE:H	2.31	0.41
1:A:1240:LEU:O	1:A:1254:ILE:HA	2.20	0.41
1:C:1069:LYS:HA	1:C:1069:LYS:HD3	1.94	0.41
1:C:1104:GLY:O	1:C:1107:PRO:HD2	2.20	0.41
1:C:1129:LYS:HB2	1:C:1129:LYS:HE3	1.81	0.41
1:A:1106:ILE:HB	1:A:1107:PRO:HD3	2.03	0.41
1:A:1197:ILE:HD12	1:A:1207:ILE:CD1	2.50	0.41
1:B:976:SER:OG	1:B:1054:ASP:OD1	2.39	0.41
1:C:1310:GLU:O	3:C:1705:HOH:O	2.22	0.41
1:E:1309:SER:O	1:E:1312:ARG:HD2	2.20	0.41
1:E:1106:ILE:HD13	1:E:1109:ILE:HD12	2.04	0.40
1:B:1312:ARG:HA	1:B:1312:ARG:HD2	1.91	0.40
1:D:1274:LYS:HD3	1:D:1274:LYS:HA	1.95	0.40
1:E:1059:LEU:HD12	1:E:1079:LEU:HD23	2.04	0.40
1:D:1377:THR:HA	1:D:1380:GLN:HG3	2.02	0.40
1:D:1419:ARG:N	1:D:1419:ARG:HD2	2.36	0.40
1:D:1376:ASP:HA	1:D:1419:ARG:HH21	1.87	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)
1:B:957:GLY:O	1:B:1308:ARG:NH2[1 _655]	2.08	0.12

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	421/582 (72%)	408 (97%)	13 (3%)	0	100	100
1	B	522/582 (90%)	500 (96%)	22 (4%)	0	100	100
1	C	524/582 (90%)	511 (98%)	13 (2%)	0	100	100
1	D	517/582 (89%)	501 (97%)	16 (3%)	0	100	100
1	E	507/582 (87%)	484 (96%)	23 (4%)	0	100	100
All	All	2491/2910 (86%)	2404 (96%)	87 (4%)	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	459/511 (90%)	447 (97%)	12 (3%)	40	42
1	B	469/511 (92%)	453 (97%)	16 (3%)	32	32
1	C	471/511 (92%)	454 (96%)	17 (4%)	31	30
1	D	464/511 (91%)	440 (95%)	24 (5%)	21	16
1	E	459/511 (90%)	446 (97%)	13 (3%)	38	39
All	All	2322/2555 (91%)	2240 (96%)	82 (4%)	32	31

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	979	ILE
1	A	1009	VAL
1	A	1032	LEU
1	A	1063	THR
1	A	1064	VAL
1	A	1090	VAL
1	A	1128	SER
1	A	1165	LYS
1	A	1305	GLN
1	A	1366	LEU
1	A	1367	GLN
1	A	1399	SER
1	B	1003	VAL
1	B	1004	SER
1	B	1009	VAL
1	B	1012	GLU
1	B	1017	LEU
1	B	1035	THR
1	B	1041	VAL
1	B	1089	THR
1	B	1094	SER
1	B	1127	SER
1	B	1165	LYS
1	B	1175	VAL
1	B	1200	SER
1	B	1213	LEU
1	B	1371	LEU
1	B	1498	ASP
1	C	976	SER
1	C	1004	SER
1	C	1033	VAL
1	C	1064	VAL
1	C	1098	VAL
1	C	1138	THR
1	C	1187	CYS
1	C	1201	ASP
1	C	1207	ILE
1	C	1265	LEU
1	C	1340	SER
1	C	1342	SER
1	C	1345	SER
1	C	1349	VAL
1	C	1351	VAL

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Mol	Chain	Res	Type
1	C	1371	LEU
1	C	1399	SER
1	D	967	THR
1	D	979	ILE
1	D	989	GLN
1	D	990	SER
1	D	998	SER
1	D	1009	VAL
1	D	1019	ILE
1	D	1035	THR
1	D	1093	VAL
1	D	1098	VAL
1	D	1122	SER
1	D	1126	SER
1	D	1127	SER
1	D	1154	THR
1	D	1155	LEU
1	D	1165	LYS
1	D	1176	THR
1	D	1177	THR
1	D	1232	GLU
1	D	1340	SER
1	D	1368	HIS
1	D	1369	ILE
1	D	1399	SER
1	D	1477	ILE
1	E	965	ILE
1	E	1035	THR
1	E	1090	VAL
1	E	1094	SER
1	E	1178	LEU
1	E	1181	ILE
1	E	1182	ARG
1	E	1187	CYS
1	E	1200	SER
1	E	1212	GLN
1	E	1213	LEU
1	E	1386	THR
1	E	1491	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1305	GLN
1	A	1341	HIS
1	A	1383	ASN
1	A	1384	GLN
1	A	1415	ASN
1	B	959	ASN
1	B	1185	GLN
1	B	1285	ASN
1	B	1431	GLN
1	B	1448	ASN
1	B	1507	ASN
1	C	989	GLN
1	C	1116	GLN
1	C	1185	GLN
1	C	1284	ASN
1	C	1285	ASN
1	C	1431	GLN
1	D	1100	HIS
1	D	1185	GLN
1	D	1225	GLN
1	D	1368	HIS
1	D	1385	GLN
1	E	973	HIS
1	E	1075	ASN
1	E	1285	ASN

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 10 ligands modelled in this entry, 10 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

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	519/582 (89%)	-0.02	20 (3%) 43 48	24, 38, 79, 121	0
1	B	530/582 (91%)	0.05	22 (4%) 40 46	26, 41, 81, 141	0
1	C	534/582 (91%)	0.36	31 (5%) 29 33	27, 51, 108, 143	0
1	D	525/582 (90%)	0.36	26 (4%) 34 39	30, 53, 88, 133	0
1	E	517/582 (88%)	0.31	30 (5%) 29 33	27, 50, 90, 120	0
All	All	2625/2910 (90%)	0.21	129 (4%) 35 40	24, 46, 94, 143	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1351	VAL	6.1
1	A	1366	LEU	5.4
1	D	1508	LEU	4.8
1	A	1010	PRO	4.7
1	C	1044	GLY	4.3
1	D	1017	LEU	4.2
1	A	1064	VAL	4.2
1	B	1017	LEU	4.0
1	A	1351	VAL	4.0
1	D	1016	PRO	4.0
1	A	1038	ALA	3.8
1	E	1374	MET	3.8
1	D	1367	GLN	3.8
1	C	1021	PRO	3.7
1	E	1022	THR	3.7
1	E	1021	PRO	3.6
1	D	1010	PRO	3.6
1	C	1099	ILE	3.4
1	A	1508	LEU	3.4
1	D	1099	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	957	GLY	3.4
1	C	1017	LEU	3.4
1	D	1245	GLY	3.4
1	B	1124	TYR	3.3
1	C	1016	PRO	3.3
1	E	1064	VAL	3.3
1	E	1019	ILE	3.3
1	C	1068	ASN	3.3
1	B	1021	PRO	3.3
1	C	1366	LEU	3.2
1	A	1008	PRO	3.2
1	B	1351	VAL	3.2
1	D	1039	GLY	3.2
1	D	1038	ALA	3.1
1	B	1038	ALA	3.1
1	B	1016	PRO	3.1
1	C	1508	LEU	3.1
1	C	1363	GLY	3.0
1	C	1098	VAL	3.0
1	B	1099	ILE	3.0
1	E	1020	ASP	3.0
1	C	1364	ALA	3.0
1	C	1213	LEU	2.9
1	B	1009	VAL	2.9
1	E	1385	GLN	2.9
1	E	1400	PRO	2.9
1	A	1245	GLY	2.9
1	A	1021	PRO	2.8
1	E	1070	MET	2.8
1	E	1290	ALA	2.8
1	E	1213	LEU	2.8
1	E	963	MET	2.8
1	C	1038	ALA	2.8
1	B	1509	ALA	2.8
1	D	1506	VAL	2.8
1	B	1019	ILE	2.8
1	E	1506	VAL	2.7
1	C	1212	GLN	2.6
1	B	1063	THR	2.6
1	E	1041	VAL	2.6
1	B	1213	LEU	2.6
1	C	1006	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1099	ILE	2.6
1	E	1124	TYR	2.6
1	E	1208	GLU	2.6
1	C	1070	MET	2.5
1	E	1386	THR	2.5
1	C	1039	GLY	2.5
1	D	1022	THR	2.5
1	D	1176	THR	2.5
1	C	1009	VAL	2.5
1	C	1010	PRO	2.5
1	A	1029	TYR	2.4
1	C	1131	TYR	2.4
1	D	1101	ALA	2.4
1	D	1385	GLN	2.4
1	B	1022	THR	2.4
1	E	1286	PRO	2.4
1	C	1096	ALA	2.4
1	E	1024	GLY	2.4
1	C	1073	VAL	2.3
1	C	1362	SER	2.3
1	A	1022	THR	2.3
1	C	1018	GLY	2.3
1	E	1283	THR	2.3
1	D	1029	TYR	2.3
1	B	1125	SER	2.3
1	D	1384	GLN	2.3
1	D	1021	PRO	2.3
1	A	957	GLY	2.3
1	B	1010	PRO	2.2
1	B	1386	THR	2.2
1	A	1023	ARG	2.2
1	B	1245	GLY	2.2
1	E	1211	ARG	2.2
1	D	1019	ILE	2.2
1	C	1022	THR	2.2
1	D	1041	VAL	2.2
1	D	1018	GLY	2.2
1	D	1024	GLY	2.2
1	E	1507	ASN	2.2
1	A	1374	MET	2.2
1	E	1063	THR	2.2
1	B	1506	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1341	HIS	2.1
1	D	1011	GLU	2.1
1	C	1110	PHE	2.1
1	E	1040	GLY	2.1
1	B	1162	ALA	2.1
1	C	1509	ALA	2.1
1	A	1121	SER	2.1
1	A	1127	SER	2.1
1	B	1374	MET	2.1
1	E	1023	ARG	2.1
1	E	1369	ILE	2.1
1	A	1009	VAL	2.1
1	E	1003	VAL	2.1
1	D	1507	ASN	2.1
1	A	1131	TYR	2.1
1	C	1063	THR	2.1
1	D	1248	LYS	2.1
1	C	1045	TRP	2.1
1	C	1121	SER	2.1
1	A	1007	CYS	2.0
1	E	1073	VAL	2.0
1	B	1161	LEU	2.0
1	B	1385	GLN	2.0
1	A	1024	GLY	2.0
1	C	1029	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

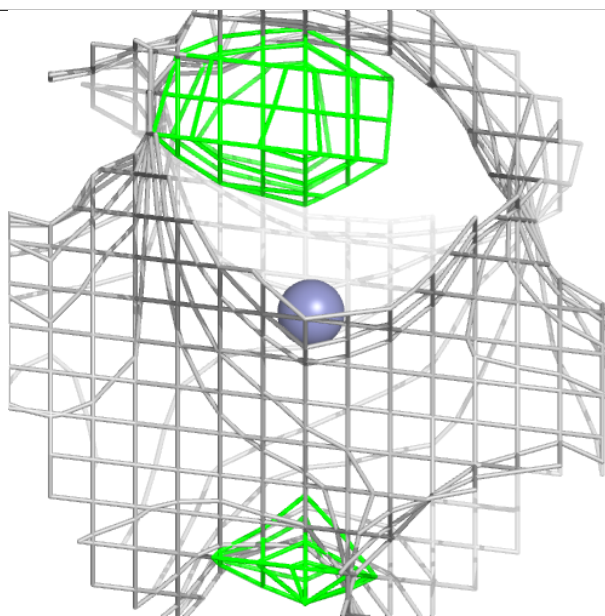
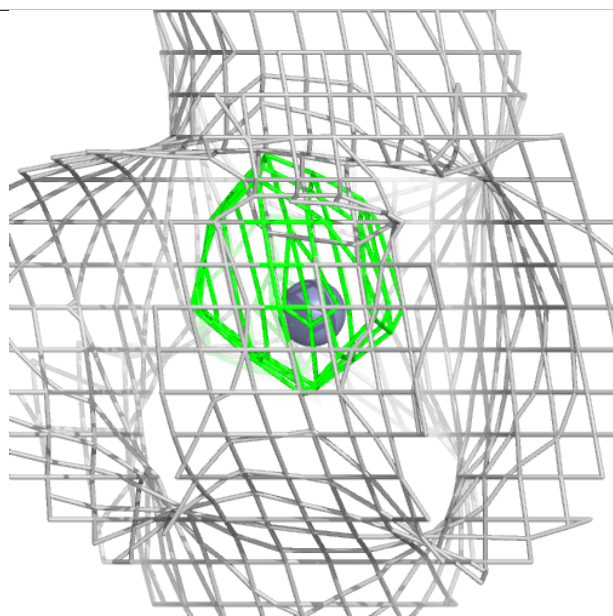
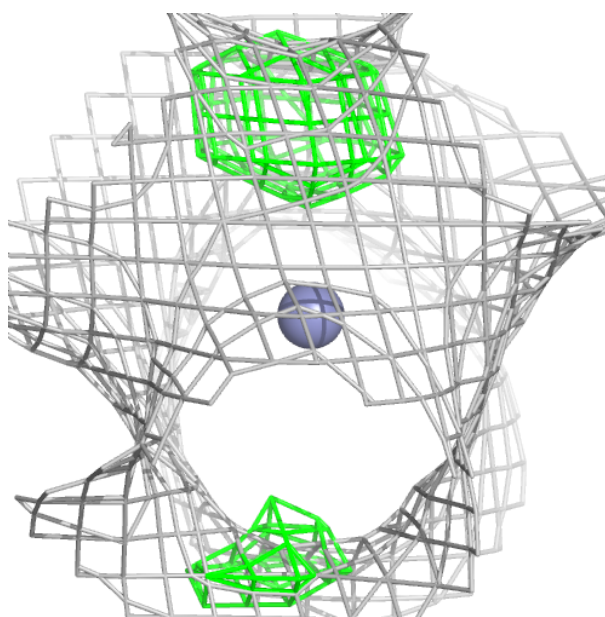
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	1602	1/1	0.98	0.03	42,42,42,42	0
2	ZN	A	1602	1/1	0.99	0.04	40,40,40,40	0
2	ZN	B	1601	1/1	0.99	0.03	53,53,53,53	0
2	ZN	A	1601	1/1	0.99	0.04	40,40,40,40	0
2	ZN	C	1601	1/1	0.99	0.04	48,48,48,48	0
2	ZN	C	1602	1/1	0.99	0.03	44,44,44,44	0
2	ZN	D	1601	1/1	0.99	0.03	41,41,41,41	0
2	ZN	D	1602	1/1	0.99	0.03	57,57,57,57	0
2	ZN	E	1601	1/1	0.99	0.03	50,50,50,50	0
2	ZN	E	1602	1/1	0.99	0.03	50,50,50,50	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.

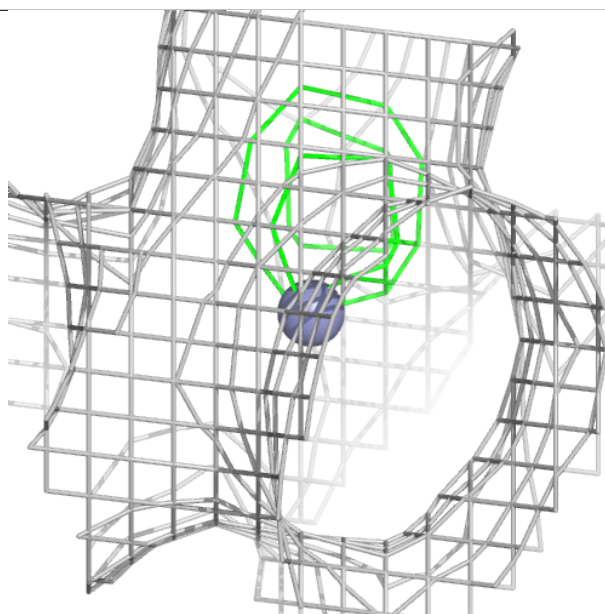
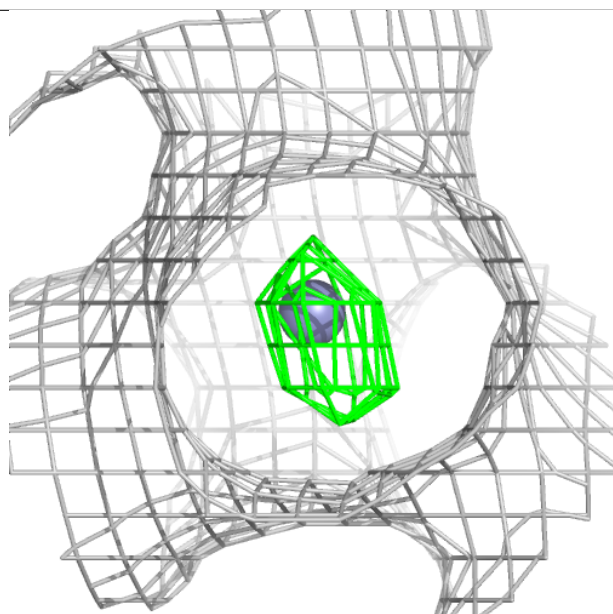
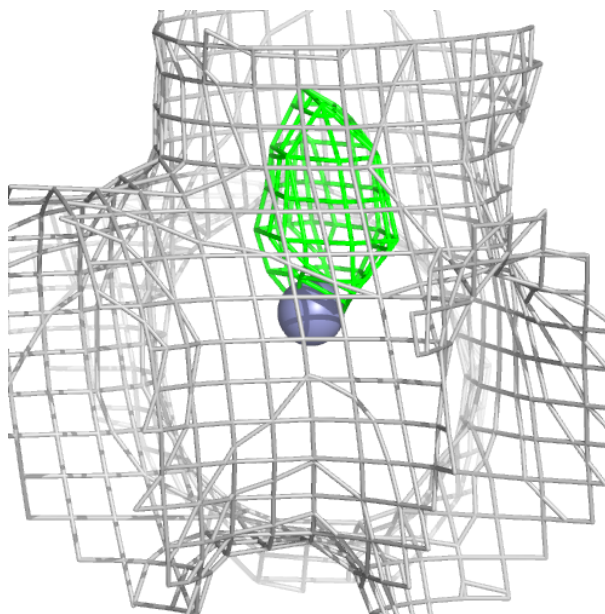
Electron density around ZN B 1602:

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



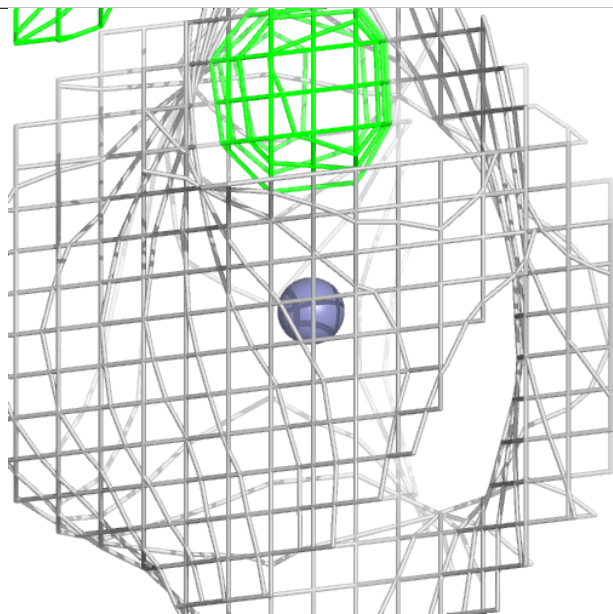
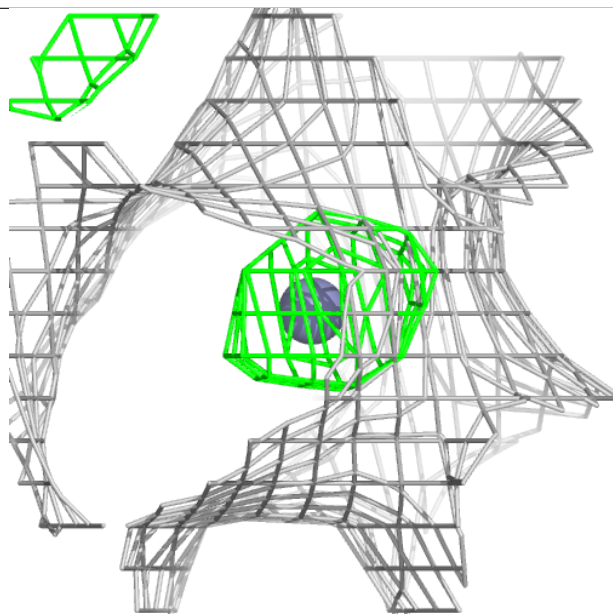
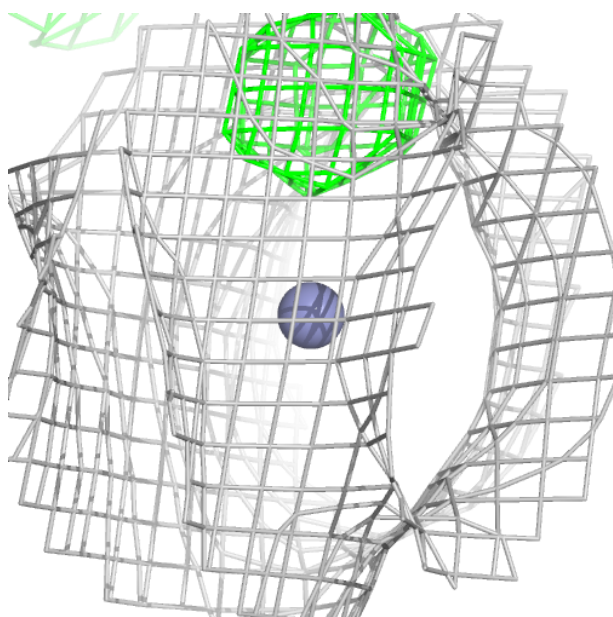
Electron density around ZN A 1602:

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



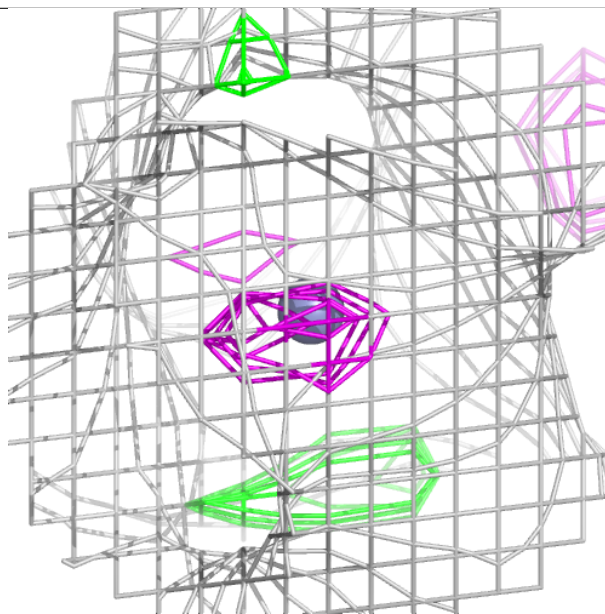
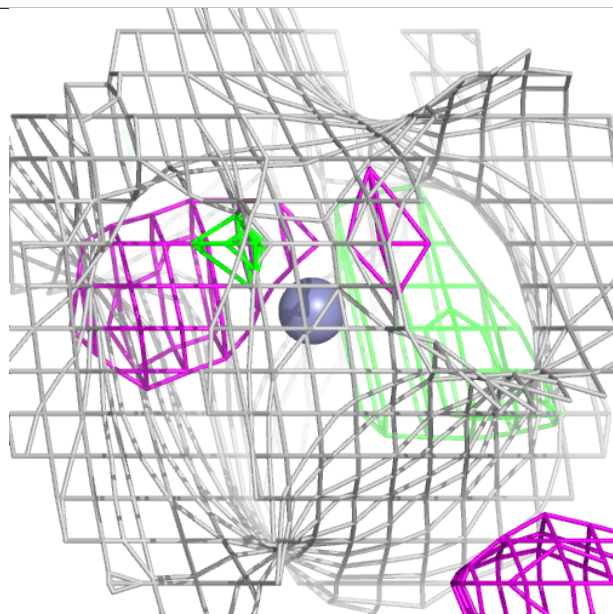
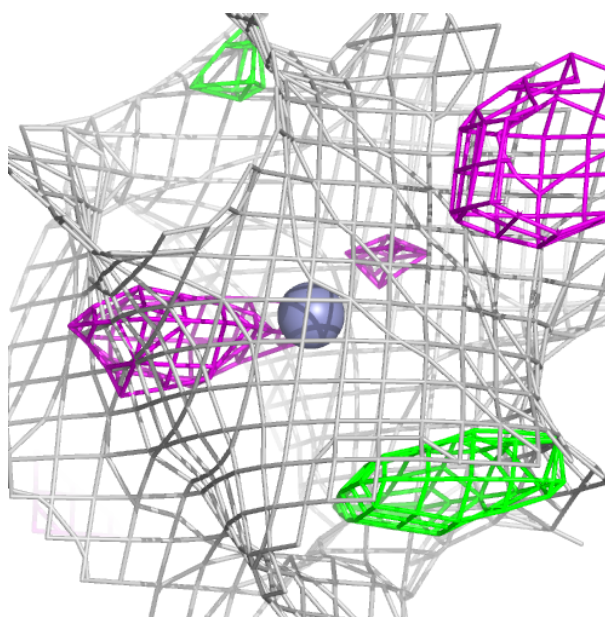
Electron density around ZN B 1601:

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



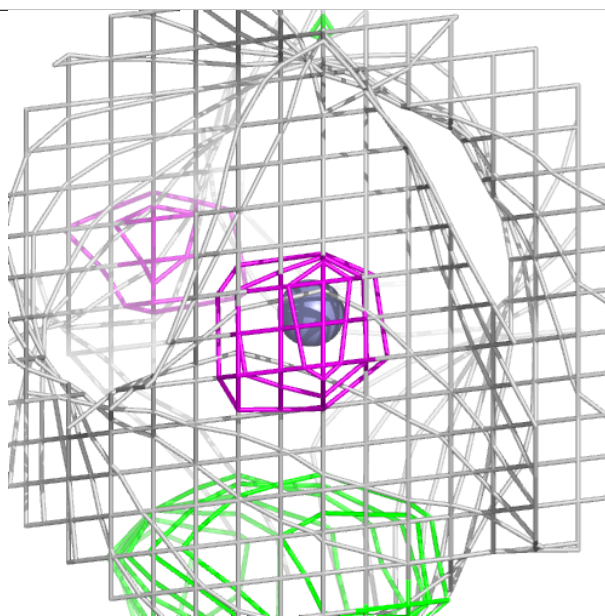
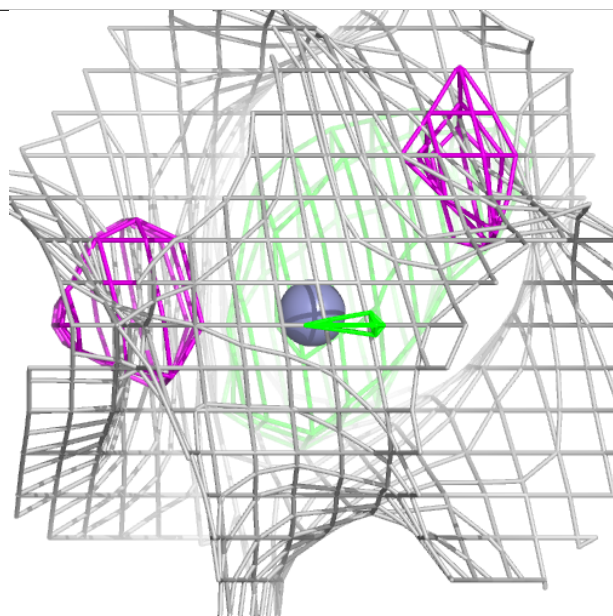
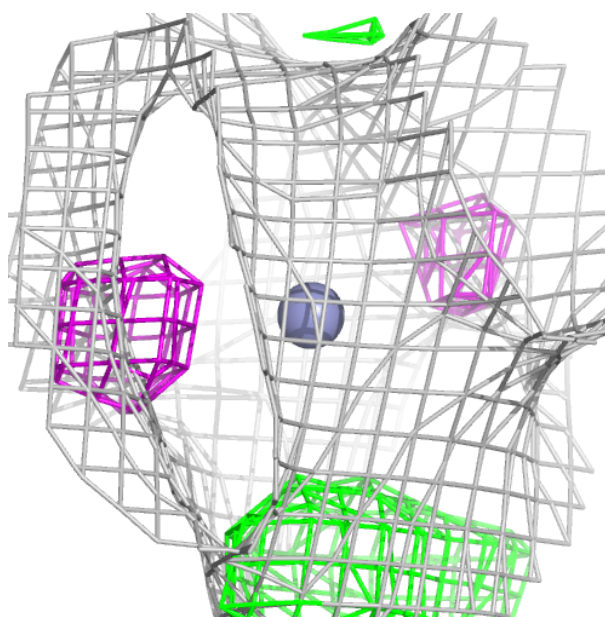
Electron density around ZN A 1601:

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



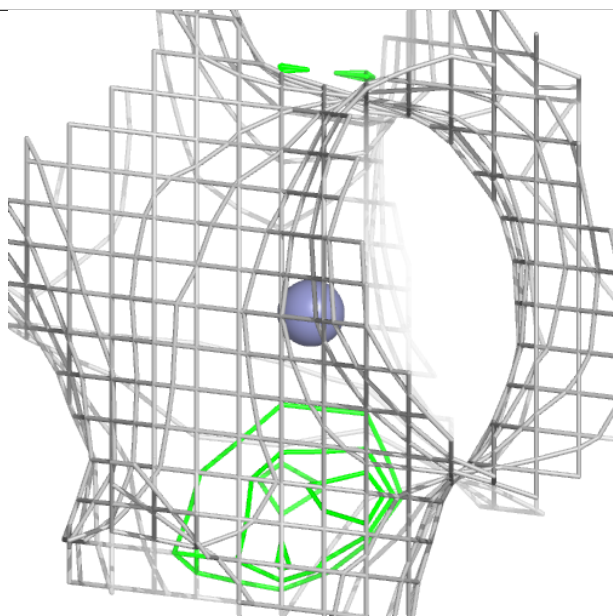
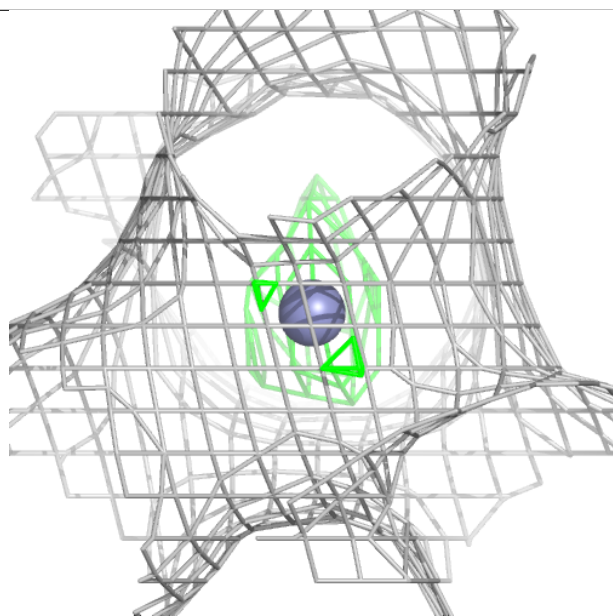
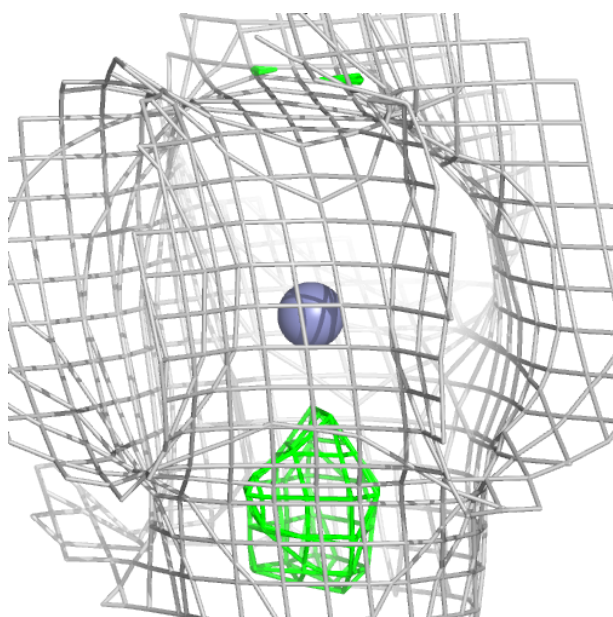
Electron density around ZN C 1601:

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



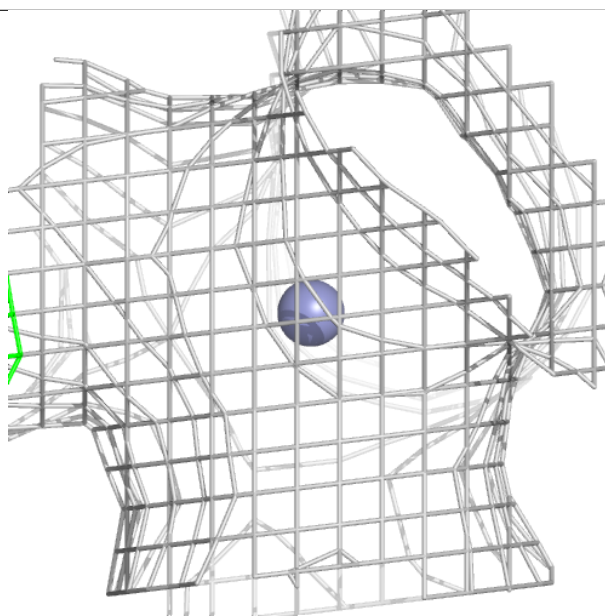
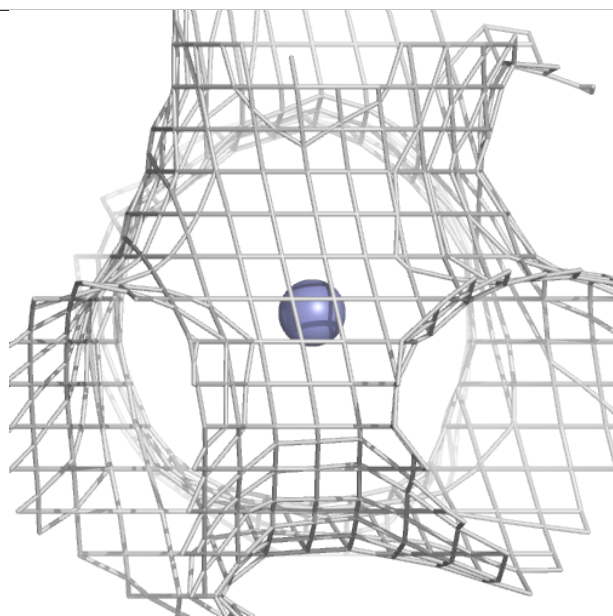
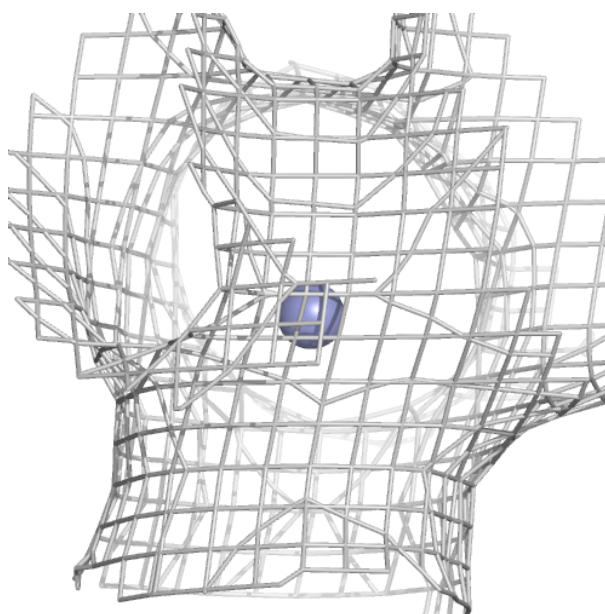
Electron density around ZN C 1602:

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



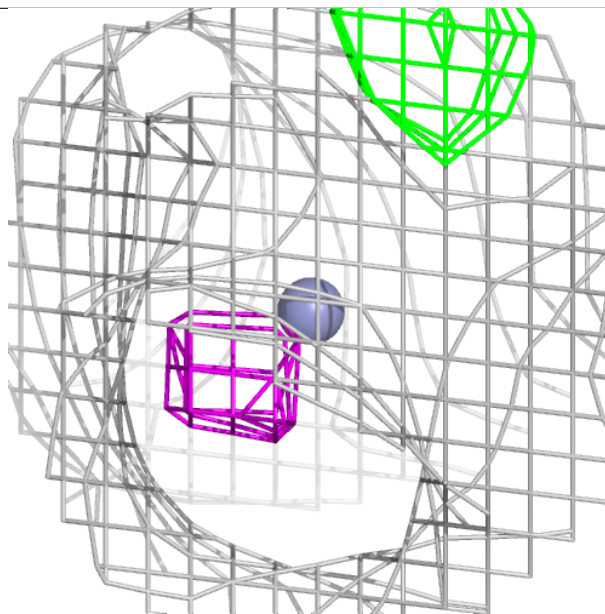
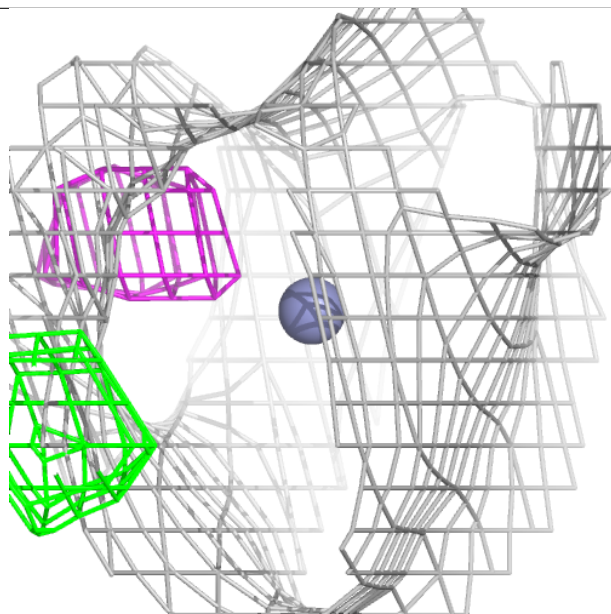
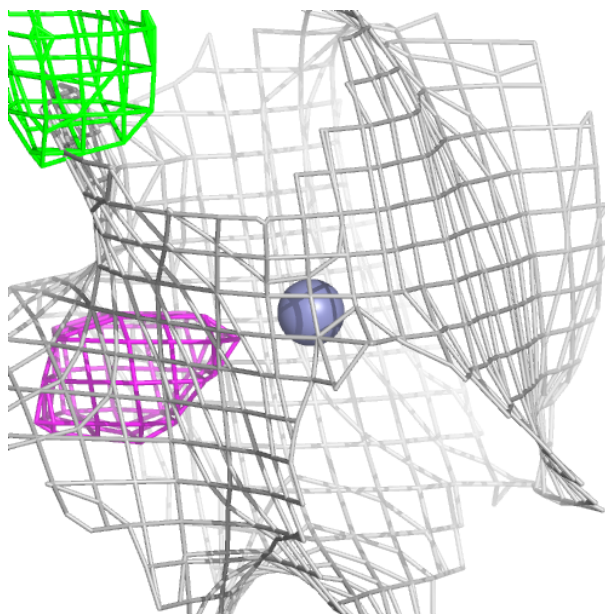
Electron density around ZN D 1601:

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



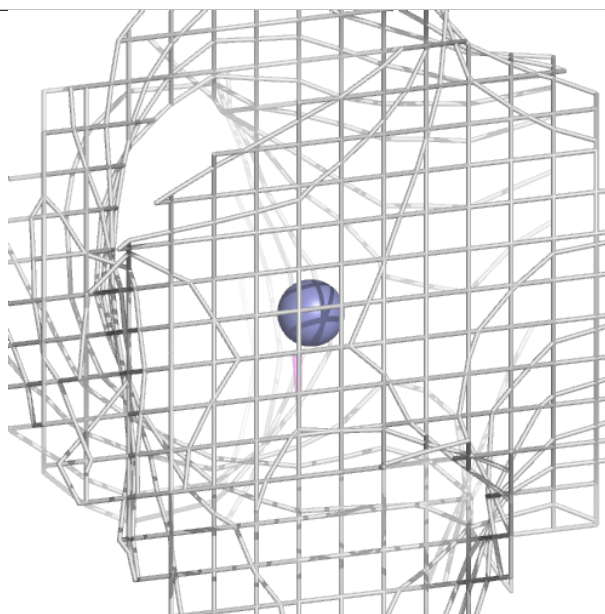
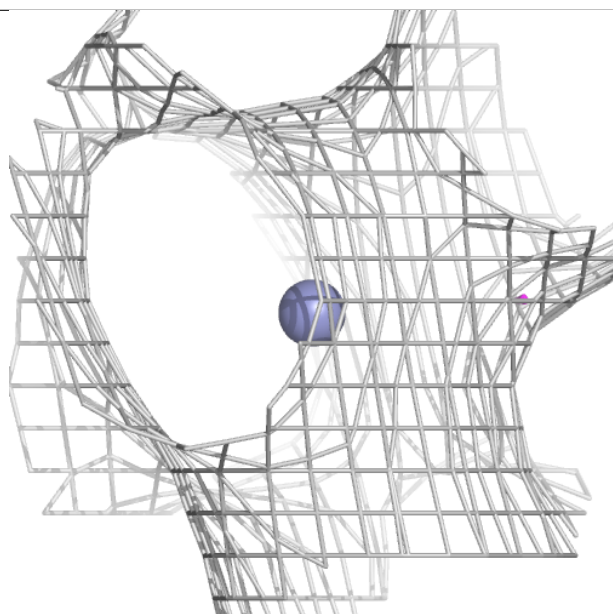
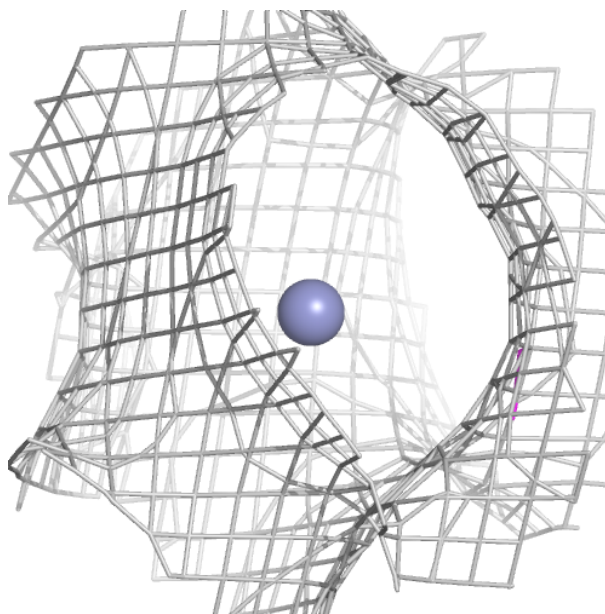
Electron density around ZN D 1602:

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



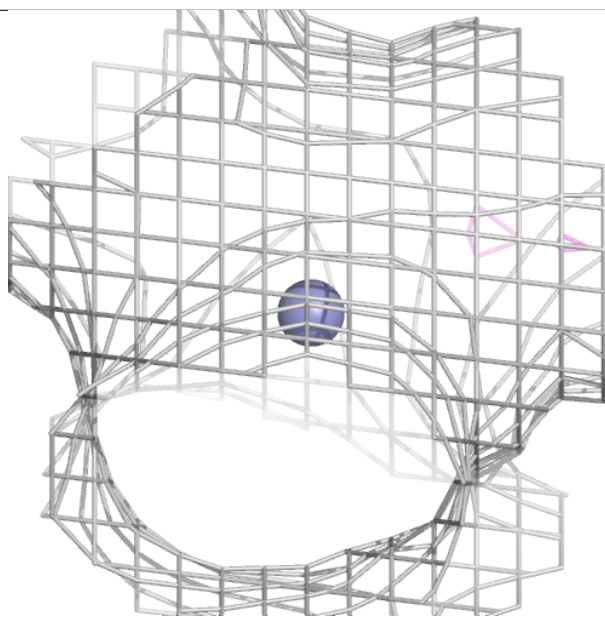
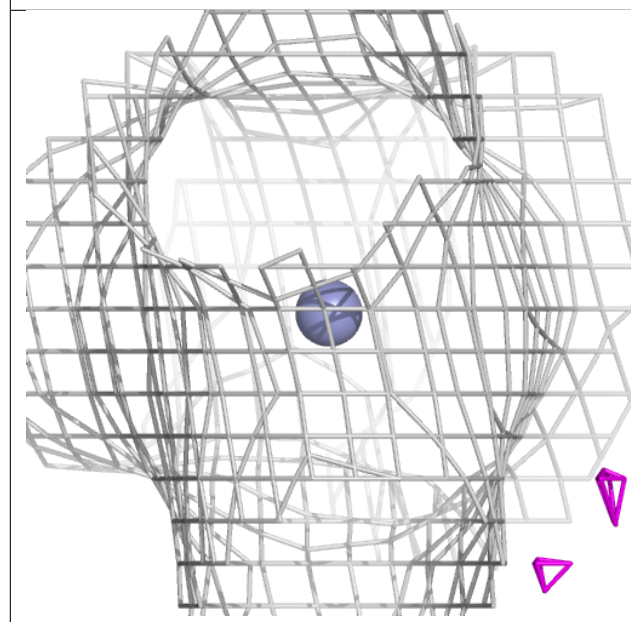
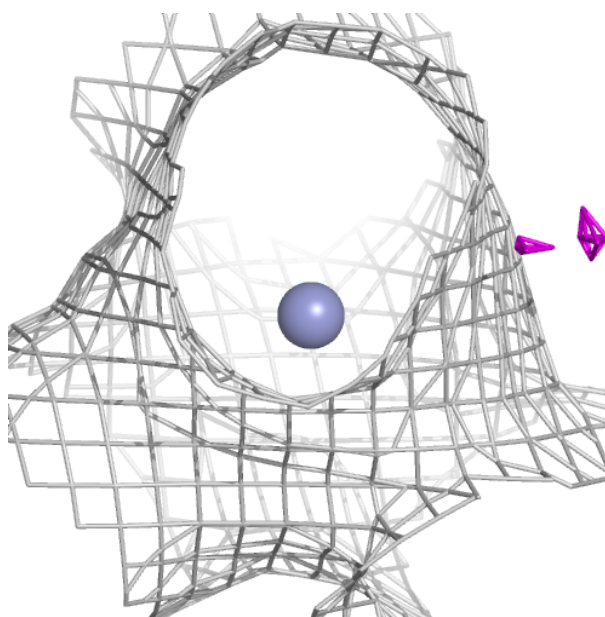
Electron density around ZN E 1601:

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



Electron density around ZN E 1602:

$2mF_o - DF_c$ (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.