



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:18 AM UTC

PDB ID : 7BZI / pdb_00007bzi
Title : The mutant variant of PNGM-1. H91 was substituted for alanine to study metal coordination.
Authors : Park, Y.S.; Kang, L.W.; Lee, J.H.
Deposited on : 2020-04-28
Resolution : 1.94 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

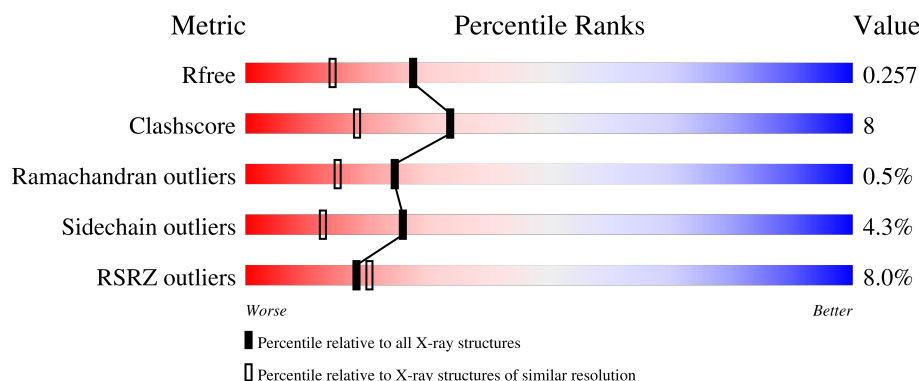
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	372	5% 81%15%..
1	B	372	8% 78%18%..
1	C	372	8% 81%13%..
1	D	372	8% 81%15%..
1	E	372	8% 79%16%..

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Mol	Chain	Length	Quality of chain
1	F	372	9% 80% 16% ..
1	G	372	9% 79% 17% ...
1	H	372	6% 78% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24617 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 Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	366	Total	C	N	O	S	0	0	0
			2874	1818	497	539	20			
1	B	365	Total	C	N	O	S	0	0	0
			2869	1815	496	538	20			
1	C	357	Total	C	N	O	S	0	0	0
			2818	1787	484	527	20			
1	F	363	Total	C	N	O	S	0	0	0
			2848	1805	490	533	20			
1	E	359	Total	C	N	O	S	0	0	0
			2831	1794	487	530	20			
1	D	360	Total	C	N	O	S	0	0	0
			2836	1797	488	531	20			
1	A	360	Total	C	N	O	S	0	0	0
			2836	1797	488	531	20			
1	H	357	Total	C	N	O	S	0	0	0
			2818	1787	484	527	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
F	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
E	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
A	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
H	91	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

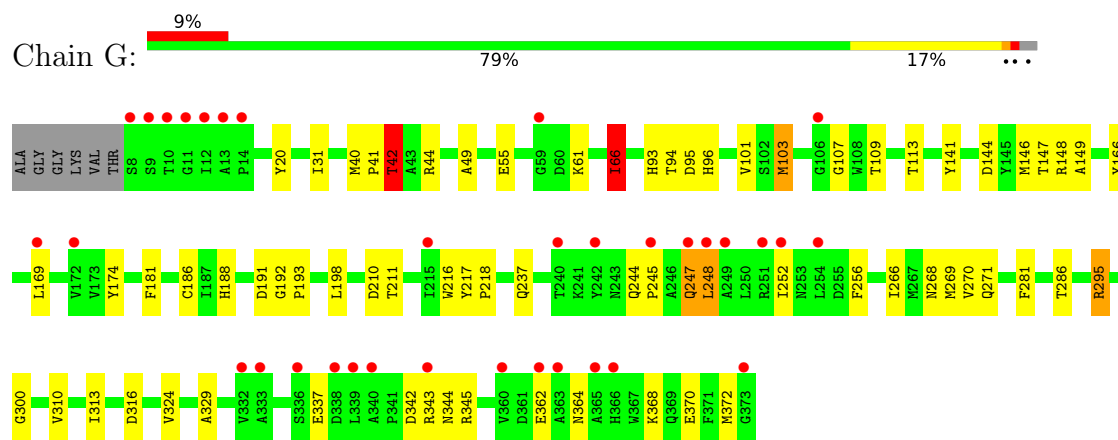
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	213	Total O 213 213	0	0
3	B	209	Total O 209 209	0	0
3	C	257	Total O 257 257	0	0
3	F	268	Total O 268 268	0	0
3	E	229	Total O 229 229	0	0
3	D	218	Total O 218 218	0	0
3	A	251	Total O 251 251	0	0
3	H	234	Total O 234 234	0	0

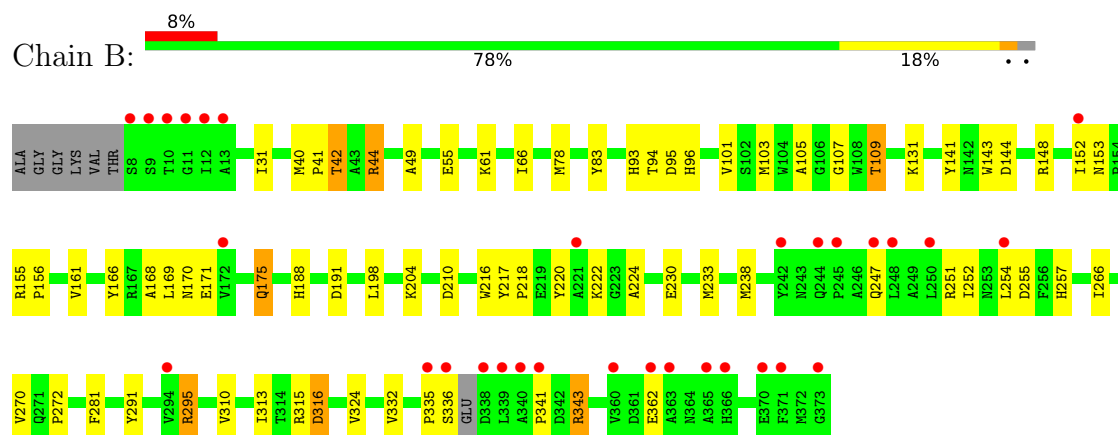
3 Residue-property plots [i](#)

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.

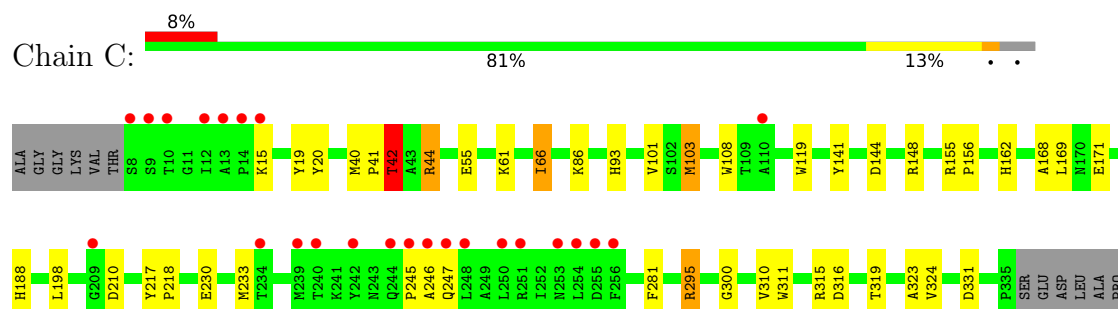
• Molecule 1: Metallo-beta-lactamase PNGM-1

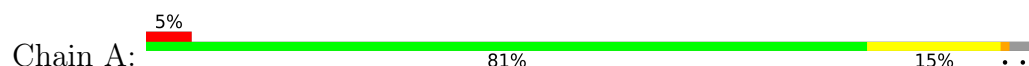


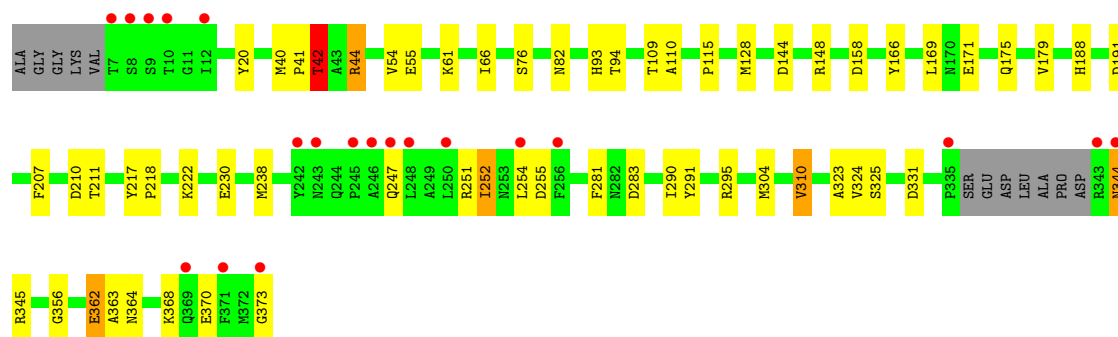
• Molecule 1: Metallo-beta-lactamase PNGM-1



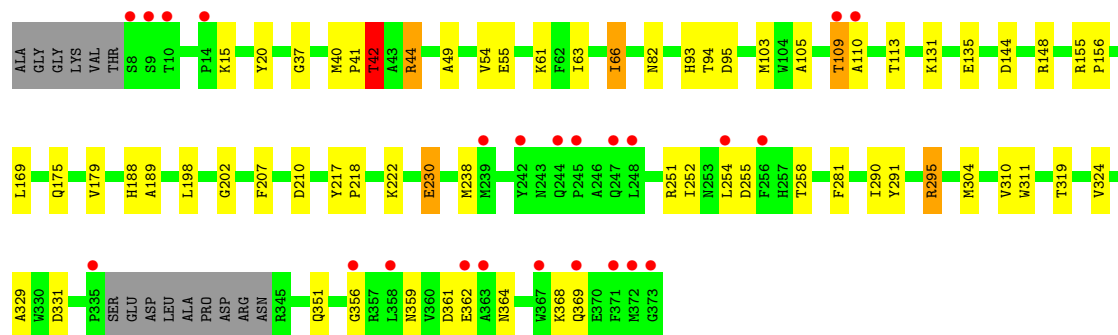
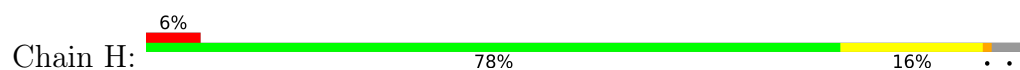
• Molecule 1: Metallo-beta-lactamase PNGM-1







● Molecule 1: Metallo-beta-lactamase PNGM-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.38Å 83.06Å 163.58Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	49.04 – 1.94 49.04 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.04-1.94) 95.4 (49.04-1.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.210 , 0.255 0.216 , 0.257	Depositor DCC
R_{free} test set	10778 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24617	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0365e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: 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	1.02	0/2919	1.33	1/3979 (0.0%)
1	B	1.04	0/2953	1.35	0/4026
1	C	1.01	0/2901	1.31	3/3954 (0.1%)
1	D	1.03	0/2919	1.37	5/3979 (0.1%)
1	E	1.03	0/2914	1.36	4/3972 (0.1%)
1	F	1.02	1/2931 (0.0%)	1.32	2/3996 (0.1%)
1	G	1.05	0/2959	1.39	3/4036 (0.1%)
1	H	1.01	0/2901	1.34	1/3954 (0.0%)
All	All	1.03	1/23397 (0.0%)	1.35	19/31896 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	271	GLN	N-CA	5.46	1.50	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ILE	CA-C-N	7.13	126.88	120.10
1	D	66	ILE	C-N-CA	7.13	126.88	120.10
1	D	42	THR	CB-CA-C	7.09	122.68	109.71
1	F	341	PRO	N-CA-CB	6.46	110.11	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	THR	CB-CA-C	6.29	120.12	109.75
1	H	42	THR	CB-CA-C	6.21	119.92	109.48
1	F	42	THR	CB-CA-C	6.01	120.12	109.72
1	D	207	PHE	CA-C-N	5.76	126.33	119.94
1	D	207	PHE	C-N-CA	5.76	126.33	119.94
1	A	42	THR	CB-CA-C	5.59	119.95	109.71
1	E	127	ASP	CA-CB-CG	5.36	117.96	112.60
1	G	66	ILE	CA-C-N	5.27	126.18	120.44
1	G	66	ILE	C-N-CA	5.27	126.18	120.44
1	C	66	ILE	CA-C-N	5.24	126.15	120.44
1	C	66	ILE	C-N-CA	5.24	126.15	120.44
1	G	42	THR	CB-CA-C	5.17	118.17	109.48
1	E	42	THR	CB-CA-C	5.12	118.09	109.48
1	E	362	GLU	CA-C-N	5.01	126.99	120.28
1	E	362	GLU	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	THR	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	2836	0	2649	42	0
1	B	2869	0	2671	53	0
1	C	2818	0	2639	39	0
1	D	2836	0	2649	43	0
1	E	2831	0	2647	44	0
1	F	2848	0	2651	43	0
1	G	2874	0	2674	59	0
1	H	2818	0	2639	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	251	0	0	13	1
3	B	209	0	0	5	1
3	C	257	0	0	6	0
3	D	218	0	0	15	0
3	E	229	0	0	11	0
3	F	268	0	0	5	0
3	G	213	0	0	4	0
3	H	234	0	0	11	0
All	All	24617	0	21219	338	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 8.

All (338) 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:A:93:HIS:HE1	1:A:188:HIS:NE2	1.60	1.00
1:E:93:HIS:HE1	1:E:188:HIS:NE2	1.63	0.95
1:E:42:THR:CG2	3:E:577:HOH:O	2.14	0.95
1:H:93:HIS:HE1	1:H:188:HIS:NE2	1.68	0.92
1:C:315:ARG:HD2	3:C:548:HOH:O	1.69	0.92
1:G:146:MET:SD	3:G:599:HOH:O	2.28	0.92
1:A:247:GLN:HB2	3:A:518:HOH:O	1.69	0.92
1:F:210:ASP:N	3:F:501:HOH:O	2.04	0.90
1:D:93:HIS:HE1	1:D:188:HIS:NE2	1.69	0.90
1:B:42:THR:CG2	3:A:550:HOH:O	2.19	0.89
1:C:315:ARG:CD	3:C:548:HOH:O	2.22	0.85
1:G:93:HIS:HE1	1:G:188:HIS:NE2	1.74	0.84
1:H:42:THR:CG2	3:H:595:HOH:O	2.24	0.84
1:A:93:HIS:CE1	1:A:188:HIS:NE2	2.47	0.83
1:G:42:THR:CG2	3:H:585:HOH:O	2.26	0.82
1:D:175:GLN:NE2	3:D:501:HOH:O	2.13	0.82
1:C:42:THR:CG2	3:D:612:HOH:O	2.28	0.81
1:D:210:ASP:N	3:D:502:HOH:O	2.13	0.81
1:B:42:THR:HG22	3:A:550:HOH:O	1.80	0.81
1:F:40:MET:HE2	1:F:233:MET:HE2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG23	3:A:579:HOH:O	1.82	0.80
1:A:373:GLY:HA2	3:A:707:HOH:O	1.82	0.79
1:A:344:ASN:HB3	3:A:729:HOH:O	1.83	0.79
1:B:93:HIS:HE1	1:B:188:HIS:NE2	1.82	0.77
1:B:44:ARG:HD3	1:B:281:PHE:CZ	2.20	0.77
1:F:42:THR:CG2	3:E:642:HOH:O	2.33	0.76
1:F:93:HIS:HE1	1:F:188:HIS:NE2	1.85	0.75
1:H:42:THR:HG22	3:H:595:HOH:O	1.86	0.74
1:C:359:ASN:ND2	1:C:361:ASP:OD2	2.21	0.74
1:A:210:ASP:N	3:A:502:HOH:O	2.20	0.73
1:F:42:THR:HG23	3:E:642:HOH:O	1.89	0.73
1:B:44:ARG:HD3	1:B:281:PHE:CE1	2.24	0.73
1:A:44:ARG:HD3	1:A:281:PHE:CZ	2.24	0.72
1:C:93:HIS:HE1	1:C:188:HIS:NE2	1.87	0.72
1:G:166:TYR:OH	1:G:191:ASP:OD2	2.04	0.71
1:F:40:MET:CE	1:F:233:MET:HE2	2.21	0.71
1:H:93:HIS:CE1	1:H:188:HIS:NE2	2.56	0.70
1:C:42:THR:HG22	3:D:612:HOH:O	1.90	0.70
1:G:368:LYS:O	1:G:372:MET:HG3	1.94	0.68
1:E:42:THR:HG23	3:E:577:HOH:O	1.88	0.67
1:E:291:TYR:CZ	1:E:295:ARG:HD2	2.28	0.67
1:D:42:THR:HG23	3:D:555:HOH:O	1.93	0.67
1:C:55:GLU:OE1	1:C:61:LYS:HE2	1.95	0.66
1:E:93:HIS:CE1	1:E:188:HIS:NE2	2.55	0.66
1:E:42:THR:HG22	3:E:577:HOH:O	1.86	0.66
1:D:101:VAL:HG21	1:D:141:TYR:CE2	2.32	0.65
1:H:131:LYS:HE2	3:H:580:HOH:O	1.95	0.65
1:G:174:TYR:HB3	1:G:181:PHE:HB2	1.80	0.64
1:G:42:THR:HG23	3:H:585:HOH:O	1.95	0.64
1:G:93:HIS:CE1	1:G:188:HIS:NE2	2.63	0.64
1:B:216:TRP:CH2	1:A:356:GLY:HA3	2.33	0.64
1:C:44:ARG:HD3	1:C:281:PHE:CZ	2.33	0.63
1:C:364:ASN:O	1:C:368:LYS:HB2	1.97	0.63
1:D:42:THR:CG2	3:D:555:HOH:O	2.46	0.63
1:G:144:ASP:OD1	1:H:93:HIS:HD2	1.81	0.63
1:G:266:ILE:O	1:G:270:VAL:HG23	1.99	0.62
1:E:107:GLY:HA3	3:E:562:HOH:O	1.97	0.62
1:A:290:ILE:HG22	1:A:304:MET:HE1	1.82	0.62
1:G:42:THR:HG21	3:H:618:HOH:O	1.99	0.62
1:G:44:ARG:HD3	1:G:281:PHE:CE1	2.35	0.61
1:D:44:ARG:HD3	1:D:281:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:HG22	1:B:148:ARG:NE	2.16	0.61
1:D:295:ARG:NH2	1:D:300:GLY:O	2.33	0.61
1:C:210:ASP:N	3:C:505:HOH:O	2.34	0.61
1:A:44:ARG:HD3	1:A:281:PHE:CE1	2.35	0.60
1:G:329:ALA:O	1:H:44:ARG:HD2	2.01	0.60
1:H:55:GLU:OE1	1:H:61:LYS:HE2	2.02	0.60
1:G:113:THR:HG21	1:G:337:GLU:H	1.66	0.59
1:B:316:ASP:OD1	1:B:316:ASP:N	2.30	0.59
1:C:93:HIS:CE1	1:C:188:HIS:NE2	2.71	0.58
1:D:93:HIS:CE1	1:D:188:HIS:NE2	2.61	0.58
1:B:144:ASP:OD1	1:A:93:HIS:HD2	1.86	0.58
1:E:101:VAL:HG21	1:E:141:TYR:CE2	2.38	0.58
1:G:101:VAL:HG22	1:H:94:THR:HG21	1.86	0.58
1:F:295:ARG:NH2	1:F:300:GLY:O	2.33	0.58
1:E:198:LEU:C	1:E:198:LEU:HD23	2.28	0.58
1:B:93:HIS:CE1	1:B:188:HIS:NE2	2.69	0.57
1:D:44:ARG:HD3	1:D:281:PHE:CE1	2.40	0.57
1:F:44:ARG:HD3	1:F:281:PHE:CZ	2.40	0.57
1:A:291:TYR:CZ	1:A:295:ARG:HD2	2.40	0.57
1:H:210:ASP:C	3:H:511:HOH:O	2.47	0.57
1:F:55:GLU:OE1	1:F:61:LYS:HE2	2.05	0.57
1:C:295:ARG:NH2	1:C:300:GLY:O	2.37	0.57
1:G:55:GLU:OE1	1:G:61:LYS:HE2	2.04	0.56
1:F:209:GLY:C	3:F:501:HOH:O	2.42	0.56
1:G:44:ARG:HG2	1:H:329:ALA:H	1.71	0.56
1:F:238:MET:HE2	1:F:252:ILE:HD13	1.87	0.56
1:E:40:MET:HB3	1:E:41:PRO:HD2	1.87	0.56
1:A:42:THR:CG2	3:A:579:HOH:O	2.48	0.56
1:H:44:ARG:HD3	1:H:281:PHE:CE1	2.40	0.56
1:B:198:LEU:HD23	1:B:198:LEU:C	2.31	0.56
1:F:364:ASN:O	1:F:368:LYS:HB2	2.05	0.56
3:G:639:HOH:O	1:H:42:THR:HG21	2.04	0.56
1:C:168:ALA:HB1	1:C:171:GLU:HG3	1.87	0.56
1:H:359:ASN:ND2	1:H:361:ASP:OD2	2.34	0.56
1:G:295:ARG:NH2	1:G:300:GLY:O	2.30	0.55
1:F:144:ASP:OD1	1:E:93:HIS:HD2	1.89	0.55
1:A:251:ARG:HD3	1:A:255:ASP:OD2	2.06	0.55
3:C:616:HOH:O	1:D:42:THR:HG21	2.05	0.55
1:A:364:ASN:O	1:A:368:LYS:HB2	2.06	0.55
1:E:243:ASN:ND2	3:E:507:HOH:O	2.40	0.55
1:H:210:ASP:N	3:H:511:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:TRP:HA	1:C:319:THR:O	2.06	0.55
1:E:49:ALA:HB1	1:E:95:ASP:HB2	1.87	0.55
1:G:217:TYR:HB3	1:G:218:PRO:HD3	1.89	0.55
1:B:168:ALA:HB1	1:B:171:GLU:HG3	1.89	0.54
1:E:174:TYR:HB3	1:E:181:PHE:HB2	1.89	0.54
1:G:44:ARG:HD2	1:H:329:ALA:O	2.07	0.54
1:C:40:MET:HE2	1:C:233:MET:HE2	1.89	0.54
1:C:315:ARG:HD3	3:C:548:HOH:O	1.98	0.54
1:H:40:MET:HB3	1:H:41:PRO:HD2	1.90	0.54
1:G:144:ASP:OD1	1:H:93:HIS:CD2	2.61	0.54
1:B:175:GLN:HE21	1:B:175:GLN:HA	1.72	0.54
1:C:324:VAL:HG12	1:A:324:VAL:HG12	1.90	0.54
1:B:105:ALA:O	1:B:109:THR:HG23	2.07	0.54
1:D:209:GLY:C	3:D:502:HOH:O	2.48	0.54
1:G:40:MET:HB3	1:G:41:PRO:HD2	1.91	0.53
1:C:101:VAL:HG21	1:C:141:TYR:CE2	2.44	0.53
1:H:44:ARG:HD3	1:H:281:PHE:CZ	2.44	0.53
1:H:290:ILE:HG22	1:H:304:MET:HE1	1.91	0.53
1:G:44:ARG:HD3	1:G:281:PHE:CZ	2.44	0.52
1:F:93:HIS:CE1	1:F:188:HIS:NE2	2.72	0.52
1:E:210:ASP:N	3:E:508:HOH:O	2.41	0.52
1:F:324:VAL:HG12	1:H:324:VAL:HG12	1.91	0.52
1:H:63:ILE:CD1	1:H:103:MET:HE3	2.38	0.52
1:G:198:LEU:HD23	1:G:198:LEU:C	2.35	0.52
1:B:257:HIS:CE1	3:B:569:HOH:O	2.62	0.52
1:C:93:HIS:HE1	1:C:188:HIS:CD2	2.28	0.52
1:E:44:ARG:HD3	1:E:281:PHE:CZ	2.45	0.52
1:A:42:THR:HB	3:A:711:HOH:O	2.10	0.52
1:B:251:ARG:HD3	1:B:255:ASP:OD2	2.10	0.52
1:B:93:HIS:HE1	1:B:188:HIS:CD2	2.26	0.52
1:B:144:ASP:OD1	1:A:93:HIS:CD2	2.63	0.51
1:G:20:TYR:HB3	1:E:20:TYR:CD2	2.45	0.51
1:B:166:TYR:CE2	1:B:191:ASP:HB3	2.46	0.51
1:C:93:HIS:HD2	1:D:144:ASP:OD1	1.94	0.51
1:C:198:LEU:C	1:C:198:LEU:HD23	2.36	0.51
1:G:252:ILE:HA	1:G:256:PHE:HD2	1.74	0.51
1:B:40:MET:HB3	1:B:41:PRO:HD2	1.92	0.51
1:C:40:MET:CE	1:C:233:MET:HE2	2.40	0.51
1:H:109:THR:HG22	1:H:148:ARG:NE	2.26	0.51
1:E:308:MET:HB3	1:E:323:ALA:HB3	1.93	0.50
1:H:105:ALA:O	1:H:109:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:CYS:HB3	1:G:211:THR:HB	1.93	0.50
1:C:42:THR:HG21	3:D:655:HOH:O	2.11	0.50
1:D:84:LEU:HA	3:D:635:HOH:O	2.10	0.50
1:C:40:MET:HB3	1:C:41:PRO:HD2	1.93	0.50
1:G:247:GLN:HE21	1:G:248:LEU:HD12	1.77	0.50
1:A:210:ASP:C	3:A:502:HOH:O	2.54	0.50
1:D:109:THR:HG22	1:D:148:ARG:HE	1.76	0.50
1:F:311:TRP:HA	1:F:319:THR:O	2.12	0.50
1:G:66:ILE:CD1	1:G:103:MET:HE3	2.42	0.49
1:F:44:ARG:HD3	1:F:281:PHE:CE1	2.47	0.49
1:A:171:GLU:OE1	3:A:501:HOH:O	2.20	0.49
1:F:144:ASP:OD2	1:E:94:THR:HG23	2.12	0.49
1:D:188:HIS:HA	3:D:518:HOH:O	2.12	0.49
1:B:204:LYS:NZ	1:B:222:LYS:O	2.45	0.49
1:D:163:GLU:OE2	3:D:503:HOH:O	2.20	0.49
1:F:93:HIS:HE1	1:F:188:HIS:CD2	2.31	0.49
1:H:82:ASN:HD21	1:H:113:THR:HG1	1.60	0.49
1:G:324:VAL:HG12	1:E:324:VAL:HG12	1.94	0.49
1:G:316:ASP:HB2	3:G:629:HOH:O	2.11	0.48
1:G:364:ASN:O	1:G:368:LYS:HB2	2.13	0.48
1:F:40:MET:HB3	1:F:41:PRO:CD	2.42	0.48
1:G:20:TYR:CD2	1:E:20:TYR:HB3	2.48	0.48
1:B:61:LYS:NZ	1:D:9:SER:O	2.46	0.48
1:C:144:ASP:OD1	1:D:93:HIS:HD2	1.96	0.48
1:G:245:PRO:HG2	1:G:248:LEU:HB2	1.96	0.48
1:G:342:ASP:OD1	1:G:344:ASN:HB2	2.14	0.48
1:A:110:ALA:HB1	1:A:331:ASP:CG	2.39	0.48
1:H:311:TRP:HA	1:H:319:THR:O	2.13	0.48
1:F:40:MET:HB3	1:F:41:PRO:HD2	1.95	0.48
1:B:40:MET:HE2	1:B:233:MET:HE2	1.96	0.48
1:F:101:VAL:HG21	1:F:141:TYR:CE1	2.48	0.48
1:G:44:ARG:HG2	1:H:329:ALA:N	2.28	0.48
1:H:93:HIS:HB3	1:H:95:ASP:OD1	2.13	0.48
1:C:93:HIS:CD2	1:D:144:ASP:OD1	2.66	0.47
1:E:78:MET:C	1:E:332:VAL:HG11	2.38	0.47
1:F:216:TRP:CH2	1:E:356:GLY:HA3	2.50	0.47
1:A:44:ARG:NH2	1:A:283:ASP:OD1	2.39	0.47
1:G:147:THR:HB	1:H:189:ALA:HB1	1.94	0.47
1:B:96:HIS:CE1	1:B:210:ASP:OD1	2.68	0.47
1:D:37:GLY:HA3	1:D:49:ALA:O	2.14	0.47
1:A:217:TYR:HB3	1:A:218:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ARG:HD3	1:E:281:PHE:CE1	2.50	0.47
1:E:37:GLY:HA3	1:E:49:ALA:O	2.14	0.47
1:H:291:TYR:CZ	1:H:295:ARG:HD2	2.50	0.47
1:G:101:VAL:HG21	1:G:141:TYR:CE2	2.49	0.47
1:H:110:ALA:HB1	1:H:331:ASP:CG	2.40	0.47
1:F:108:TRP:CE3	1:F:148:ARG:HD2	2.50	0.47
1:D:217:TYR:HB3	1:D:218:PRO:HD3	1.96	0.47
1:A:210:ASP:CA	3:A:502:HOH:O	2.62	0.47
1:C:217:TYR:HB3	1:C:218:PRO:HD3	1.98	0.46
1:H:42:THR:HG23	3:H:595:HOH:O	2.04	0.46
1:H:54:VAL:HG21	1:H:207:PHE:HZ	1.79	0.46
1:H:238:MET:HE2	1:H:252:ILE:HD13	1.97	0.46
1:F:42:THR:HG22	1:F:281:PHE:HZ	1.80	0.46
1:D:166:TYR:CE2	1:D:191:ASP:HB3	2.51	0.46
1:D:181:PHE:CZ	1:D:198:LEU:HD12	2.51	0.46
1:H:210:ASP:CA	3:H:511:HOH:O	2.63	0.46
1:B:335:PRO:O	1:B:336:SER:C	2.59	0.46
1:G:42:THR:HG22	3:H:585:HOH:O	2.03	0.46
1:F:107:GLY:HA3	3:F:629:HOH:O	2.15	0.46
1:F:20:TYR:HB3	1:H:20:TYR:CD2	2.49	0.46
1:E:155:ARG:HB3	1:E:156:PRO:HD3	1.98	0.45
1:D:79:ILE:HB	3:D:564:HOH:O	2.16	0.45
1:H:54:VAL:HG21	1:H:207:PHE:CZ	2.51	0.45
1:C:86:LYS:HD3	3:C:622:HOH:O	2.15	0.45
1:B:55:GLU:OE1	1:B:61:LYS:HE3	2.16	0.45
1:B:141:TYR:OH	3:B:501:HOH:O	2.18	0.45
1:B:324:VAL:HG12	1:D:324:VAL:HG12	1.98	0.45
1:B:238:MET:HE2	1:B:252:ILE:HD13	1.98	0.45
1:D:198:LEU:C	1:D:198:LEU:HD23	2.41	0.45
3:B:646:HOH:O	1:A:42:THR:HG21	2.15	0.45
1:C:103:MET:HE3	1:C:103:MET:HB2	1.91	0.45
1:C:356:GLY:HA3	1:D:216:TRP:CH2	2.51	0.45
1:B:217:TYR:HB3	1:B:218:PRO:HD3	1.97	0.45
1:B:101:VAL:HG21	1:B:141:TYR:CE2	2.52	0.45
1:F:20:TYR:CD2	1:H:20:TYR:HB3	2.52	0.45
1:E:93:HIS:HB3	1:E:95:ASP:OD1	2.16	0.45
1:B:107:GLY:HA3	3:B:590:HOH:O	2.17	0.45
1:F:291:TYR:CZ	1:F:295:ARG:HD2	2.52	0.45
1:H:109:THR:HG22	1:H:148:ARG:HE	1.82	0.45
1:F:245:PRO:O	1:F:247:GLN:N	2.50	0.45
1:E:166:TYR:CZ	1:E:191:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:ARG:HB3	1:H:156:PRO:HD3	1.99	0.45
1:G:93:HIS:HE1	1:G:188:HIS:CD2	2.34	0.44
1:G:166:TYR:CZ	1:G:191:ASP:HB3	2.52	0.44
1:C:108:TRP:CE3	1:C:148:ARG:HD2	2.52	0.44
1:D:49:ALA:HB1	1:D:95:ASP:HB2	1.99	0.44
1:H:198:LEU:C	1:H:198:LEU:HD23	2.42	0.44
1:G:101:VAL:HG22	1:H:94:THR:CG2	2.46	0.44
1:D:210:ASP:C	3:D:502:HOH:O	2.60	0.44
1:G:268:ASN:O	1:G:271:GLN:HG2	2.17	0.44
1:A:238:MET:HE2	1:A:252:ILE:HD13	2.00	0.44
1:F:72:ALA:HB3	3:F:530:HOH:O	2.17	0.44
1:H:37:GLY:HA3	1:H:49:ALA:O	2.17	0.44
1:B:291:TYR:CZ	1:B:295:ARG:HD2	2.52	0.44
1:E:108:TRP:CE3	1:E:148:ARG:HD2	2.53	0.44
1:A:345:ARG:HD3	3:A:549:HOH:O	2.17	0.44
1:B:152:ILE:O	1:B:153:ASN:C	2.61	0.44
1:B:166:TYR:CZ	1:B:191:ASP:HB3	2.53	0.44
1:C:44:ARG:HD3	1:C:281:PHE:CE1	2.52	0.44
1:E:311:TRP:HA	1:E:319:THR:O	2.17	0.44
1:G:218:PRO:HB3	1:G:269:MET:HE2	2.00	0.44
1:B:266:ILE:O	1:B:270:VAL:HG23	2.17	0.44
1:C:119:TRP:HA	1:C:162:HIS:O	2.17	0.44
1:C:20:TYR:CD2	1:A:20:TYR:HB3	2.52	0.44
1:D:131:LYS:HD2	3:D:581:HOH:O	2.18	0.44
1:H:66:ILE:HG23	1:H:66:ILE:O	2.18	0.44
1:G:149:ALA:O	1:G:345:ARG:HD2	2.18	0.43
1:D:166:TYR:CZ	1:D:191:ASP:HB3	2.54	0.43
1:G:181:PHE:CZ	1:G:198:LEU:HD12	2.53	0.43
1:D:290:ILE:HG22	1:D:304:MET:HE1	1.99	0.43
1:E:42:THR:HB	3:E:665:HOH:O	2.18	0.43
1:E:9:SER:CB	3:E:522:HOH:O	2.66	0.43
1:D:115:PRO:HB3	1:D:158:ASP:HB2	2.00	0.43
1:B:155:ARG:N	1:B:156:PRO:HD2	2.34	0.43
1:F:210:ASP:C	3:F:501:HOH:O	2.61	0.43
1:E:63:ILE:CD1	1:E:103:MET:HE3	2.48	0.43
1:D:245:PRO:HG2	1:D:248:LEU:HD13	2.01	0.43
1:A:362:GLU:CD	1:A:363:ALA:H	2.27	0.43
1:H:251:ARG:HD3	1:H:255:ASP:OD2	2.18	0.43
1:F:200:TRP:CE2	1:F:201:ASN:HB2	2.54	0.43
1:E:110:ALA:HB1	1:E:331:ASP:CG	2.44	0.43
1:H:230:GLU:HG2	1:H:258:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:THR:HG22	1:G:148:ARG:NE	2.34	0.42
1:G:342:ASP:HB3	1:G:345:ARG:HG3	2.01	0.42
1:F:329:ALA:O	1:E:44:ARG:HD2	2.19	0.42
1:E:251:ARG:NH1	1:E:255:ASP:OD1	2.52	0.42
1:D:155:ARG:N	1:D:156:PRO:HD2	2.33	0.42
1:H:54:VAL:CG2	1:H:207:PHE:HZ	2.32	0.42
1:A:55:GLU:OE1	1:A:61:LYS:HE2	2.19	0.42
1:H:217:TYR:HB3	1:H:218:PRO:HD3	2.01	0.42
1:B:315:ARG:HG3	1:H:202:GLY:HA2	2.01	0.42
1:F:94:THR:HG21	1:E:105:ALA:HB2	2.02	0.42
1:D:20:TYR:HB2	1:D:23:SER:OG	2.19	0.42
1:D:174:TYR:HB3	1:D:181:PHE:HB2	2.02	0.42
1:B:170:ASN:HB2	1:B:220:TYR:CD1	2.54	0.42
1:B:103:MET:HE3	1:B:103:MET:HB2	1.93	0.42
1:G:237:GLN:NE2	1:G:286:THR:HA	2.35	0.42
1:G:66:ILE:HD11	1:G:103:MET:HE3	2.02	0.42
1:G:96:HIS:CE1	1:G:210:ASP:OD1	2.73	0.42
1:G:192:GLY:N	1:G:193:PRO:CD	2.83	0.42
1:E:266:ILE:O	1:E:270:VAL:HG23	2.20	0.42
1:A:115:PRO:HB3	1:A:158:ASP:HB2	2.02	0.42
1:H:364:ASN:O	1:H:368:LYS:HB2	2.20	0.42
1:F:166:TYR:CE2	1:F:191:ASP:HB3	2.54	0.42
1:E:237:GLN:NE2	1:E:286:THR:HA	2.34	0.42
1:E:263:PHE:CD1	1:E:263:PHE:C	2.98	0.42
1:A:76:SER:HB2	1:A:325:SER:HB2	2.02	0.42
1:B:143:TRP:CD1	1:A:128:MET:HE3	2.55	0.42
1:F:174:TYR:HB3	1:F:181:PHE:HB2	2.02	0.42
1:B:94:THR:HG23	1:A:144:ASP:OD2	2.20	0.41
1:B:341:PRO:HG3	3:B:652:HOH:O	2.20	0.41
1:C:144:ASP:OD2	1:D:94:THR:HG23	2.20	0.41
1:G:93:HIS:HD2	1:H:144:ASP:OD1	2.02	0.41
1:G:107:GLY:HA3	3:G:630:HOH:O	2.19	0.41
1:B:31:ILE:HB	1:B:313:ILE:HB	2.02	0.41
1:B:49:ALA:HB1	1:B:95:ASP:O	2.20	0.41
1:C:245:PRO:O	1:C:247:GLN:N	2.52	0.41
1:D:210:ASP:CA	3:D:502:HOH:O	2.66	0.41
1:B:224:ALA:O	1:B:272:PRO:HA	2.21	0.41
1:B:131:LYS:HA	1:B:161:VAL:HG11	2.01	0.41
1:H:175:GLN:HA	1:H:179:VAL:O	2.21	0.41
1:B:170:ASN:ND2	1:B:220:TYR:CD1	2.89	0.41
1:D:101:VAL:HG21	1:D:141:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:TYR:O	1:C:323:ALA:HA	2.20	0.41
1:A:40:MET:HB3	1:A:41:PRO:CD	2.50	0.41
1:G:44:ARG:CD	1:G:281:PHE:CE1	3.04	0.41
1:G:216:TRP:CH2	1:H:356:GLY:HA3	2.56	0.41
1:F:290:ILE:HG22	1:F:304:MET:HE1	2.02	0.41
1:D:31:ILE:HB	1:D:313:ILE:HB	2.02	0.41
1:D:40:MET:HB3	1:D:41:PRO:HD2	2.01	0.41
1:F:250:LEU:O	1:F:254:LEU:HD23	2.20	0.41
1:E:40:MET:HB3	1:E:41:PRO:CD	2.50	0.41
1:A:310:VAL:HG11	1:A:323:ALA:HB2	2.02	0.41
1:G:31:ILE:HB	1:G:313:ILE:HB	2.03	0.41
1:B:343:ARG:HA	1:B:343:ARG:NE	2.35	0.41
1:E:291:TYR:OH	1:E:295:ARG:HD2	2.21	0.41
1:G:49:ALA:HB1	1:G:95:ASP:HB2	2.03	0.41
1:B:78:MET:O	1:B:332:VAL:HG11	2.21	0.41
1:B:101:VAL:HG22	1:A:94:THR:HG21	2.01	0.41
1:E:13:ALA:HB1	3:E:649:HOH:O	2.21	0.41
1:C:369:GLN:HG3	1:C:370:GLU:N	2.36	0.40
1:F:217:TYR:HB3	1:F:218:PRO:HD3	2.03	0.40
1:A:109:THR:HG22	1:A:148:ARG:NE	2.37	0.40
1:B:61:LYS:HD2	1:B:83:TYR:HB3	2.04	0.40
1:F:198:LEU:HD23	1:F:198:LEU:C	2.47	0.40
1:A:54:VAL:HG21	1:A:207:PHE:CZ	2.57	0.40
1:A:166:TYR:CE2	1:A:191:ASP:HB3	2.56	0.40
1:C:155:ARG:N	1:C:156:PRO:HD2	2.37	0.40
1:F:78:MET:O	1:F:332:VAL:HG11	2.22	0.40
1:B:155:ARG:HB3	1:B:156:PRO:HD3	2.02	0.40
1:E:217:TYR:HB3	1:E:218:PRO:HD3	2.04	0.40
1:A:175:GLN:HA	1:A:179:VAL:O	2.21	0.40
1:G:94:THR:HG21	1:H:105:ALA:HB2	2.02	0.40
1:F:105:ALA:O	1:F:109:THR:HG23	2.21	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:570:HOH:O	3:A:729:HOH:O[2_655]	2.13	0.07

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	356/372 (96%)	342 (96%)	13 (4%)	1 (0%)	36	30
1	B	361/372 (97%)	342 (95%)	18 (5%)	1 (0%)	36	30
1	C	353/372 (95%)	336 (95%)	15 (4%)	2 (1%)	21	11
1	D	356/372 (96%)	343 (96%)	10 (3%)	3 (1%)	16	7
1	E	355/372 (95%)	344 (97%)	9 (2%)	2 (1%)	21	11
1	F	359/372 (96%)	342 (95%)	15 (4%)	2 (1%)	21	11
1	G	364/372 (98%)	342 (94%)	21 (6%)	1 (0%)	36	30
1	H	353/372 (95%)	339 (96%)	13 (4%)	1 (0%)	36	30
All	All	2857/2976 (96%)	2730 (96%)	114 (4%)	13 (0%)	24	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	246	ALA
1	B	66	ILE
1	F	246	ALA
1	G	66	ILE
1	E	279	HIS
1	D	65	ASP
1	D	279	HIS
1	F	66	ILE
1	D	66	ILE
1	H	66	ILE
1	E	66	ILE
1	C	66	ILE
1	A	66	ILE

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	288/301 (96%)	276 (96%)	12 (4%)	26	13
1	B	290/301 (96%)	277 (96%)	13 (4%)	24	11
1	C	287/301 (95%)	274 (96%)	13 (4%)	24	11
1	D	288/301 (96%)	278 (96%)	10 (4%)	32	18
1	E	288/301 (96%)	276 (96%)	12 (4%)	26	13
1	F	287/301 (95%)	274 (96%)	13 (4%)	24	11
1	G	290/301 (96%)	279 (96%)	11 (4%)	29	15
1	H	287/301 (95%)	273 (95%)	14 (5%)	22	9
All	All	2305/2408 (96%)	2207 (96%)	98 (4%)	26	13

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	42	THR
1	G	103	MET
1	G	169	LEU
1	G	244	GLN
1	G	247	GLN
1	G	248	LEU
1	G	295	ARG
1	G	310	VAL
1	G	343	ARG
1	G	362	GLU
1	G	370	GLU
1	B	42	THR
1	B	44	ARG
1	B	109	THR
1	B	169	LEU
1	B	175	GLN
1	B	230	GLU
1	B	247	GLN
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	295	ARG
1	B	310	VAL
1	B	316	ASP
1	B	343	ARG
1	B	362	GLU
1	C	15	LYS
1	C	42	THR
1	C	44	ARG
1	C	103	MET
1	C	169	LEU
1	C	230	GLU
1	C	295	ARG
1	C	310	VAL
1	C	316	ASP
1	C	331	ASP
1	C	362	GLU
1	C	368	LYS
1	C	369	GLN
1	F	15	LYS
1	F	42	THR
1	F	44	ARG
1	F	131	LYS
1	F	152	ILE
1	F	169	LEU
1	F	219	GLU
1	F	230	GLU
1	F	252	ILE
1	F	254	LEU
1	F	310	VAL
1	F	362	GLU
1	F	369	GLN
1	E	42	THR
1	E	44	ARG
1	E	169	LEU
1	E	199	GLU
1	E	219	GLU
1	E	230	GLU
1	E	247	GLN
1	E	254	LEU
1	E	295	ARG
1	E	310	VAL
1	E	362	GLU

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Mol	Chain	Res	Type
1	E	370	GLU
1	D	42	THR
1	D	44	ARG
1	D	169	LEU
1	D	230	GLU
1	D	247	GLN
1	D	254	LEU
1	D	295	ARG
1	D	310	VAL
1	D	362	GLU
1	D	370	GLU
1	A	42	THR
1	A	44	ARG
1	A	82	ASN
1	A	169	LEU
1	A	222	LYS
1	A	230	GLU
1	A	252	ILE
1	A	254	LEU
1	A	310	VAL
1	A	344	ASN
1	A	362	GLU
1	A	370	GLU
1	H	15	LYS
1	H	42	THR
1	H	44	ARG
1	H	109	THR
1	H	135	GLU
1	H	169	LEU
1	H	222	LYS
1	H	230	GLU
1	H	254	LEU
1	H	295	ARG
1	H	310	VAL
1	H	351	GLN
1	H	362	GLU
1	H	369	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	93	HIS

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Mol	Chain	Res	Type
1	G	247	GLN
1	G	344	ASN
1	G	369	GLN
1	B	93	HIS
1	B	170	ASN
1	B	175	GLN
1	B	344	ASN
1	B	369	GLN
1	C	93	HIS
1	C	170	ASN
1	C	175	GLN
1	F	93	HIS
1	F	247	GLN
1	E	93	HIS
1	E	243	ASN
1	E	257	HIS
1	E	268	ASN
1	E	344	ASN
1	E	369	GLN
1	D	93	HIS
1	D	175	GLN
1	D	271	GLN
1	A	93	HIS
1	A	170	ASN
1	A	247	GLN
1	A	369	GLN
1	H	93	HIS
1	H	170	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 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	360/372 (96%)	0.14	20 (5%)	30 33	12, 21, 59, 80	0
1	B	365/372 (98%)	0.62	31 (8%)	16 18	15, 28, 58, 83	0
1	C	357/372 (95%)	0.14	31 (8%)	16 18	11, 21, 57, 95	0
1	D	360/372 (96%)	0.39	28 (7%)	19 21	14, 27, 56, 73	0
1	E	359/372 (96%)	0.29	29 (8%)	18 20	14, 25, 53, 75	0
1	F	363/372 (97%)	0.16	33 (9%)	15 16	11, 20, 59, 90	0
1	G	366/372 (98%)	0.79	34 (9%)	14 16	17, 30, 59, 80	0
1	H	357/372 (95%)	0.15	24 (6%)	24 27	12, 22, 58, 84	0
All	All	2887/2976 (97%)	0.34	230 (7%)	18 20	11, 24, 58, 95	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	THR	7.7
1	B	338	ASP	6.5
1	F	7	THR	6.1
1	F	8	SER	5.7
1	F	6	VAL	5.6
1	D	342	ASP	5.3
1	G	373	GLY	5.0
1	E	8	SER	4.5
1	A	8	SER	4.5
1	F	248	LEU	4.2
1	G	339	LEU	4.0
1	C	254	LEU	4.0
1	B	336	SER	4.0
1	E	10	THR	3.9
1	D	373	GLY	3.8
1	G	242	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	9	SER	3.7
1	B	242	TYR	3.7
1	A	245	PRO	3.7
1	A	344	ASN	3.6
1	G	362	GLU	3.6
1	B	10	THR	3.6
1	B	13	ALA	3.6
1	G	12	ILE	3.5
1	A	254	LEU	3.5
1	A	248	LEU	3.5
1	D	9	SER	3.5
1	F	242	TYR	3.5
1	B	254	LEU	3.5
1	F	246	ALA	3.5
1	F	341	PRO	3.4
1	F	13	ALA	3.4
1	C	10	THR	3.4
1	F	10	THR	3.4
1	G	13	ALA	3.4
1	C	246	ALA	3.4
1	G	254	LEU	3.4
1	D	110	ALA	3.4
1	B	248	LEU	3.4
1	H	254	LEU	3.4
1	C	245	PRO	3.4
1	D	332	VAL	3.3
1	G	363	ALA	3.3
1	B	340	ALA	3.3
1	D	10	THR	3.3
1	F	14	PRO	3.3
1	A	335	PRO	3.3
1	B	373	GLY	3.3
1	G	10	THR	3.2
1	G	8	SER	3.2
1	G	336	SER	3.2
1	F	245	PRO	3.2
1	E	245	PRO	3.2
1	E	12	ILE	3.2
1	C	234	THR	3.2
1	H	358	LEU	3.2
1	C	14	PRO	3.1
1	C	9	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	244	GLN	3.1
1	D	13	ALA	3.1
1	G	11	GLY	3.1
1	G	248	LEU	3.0
1	E	368	LYS	3.0
1	G	338	ASP	3.0
1	B	360	VAL	3.0
1	C	256	PHE	3.0
1	G	240	THR	3.0
1	G	215	ILE	3.0
1	A	242	TYR	3.0
1	F	209	GLY	3.0
1	A	373	GLY	3.0
1	E	14	PRO	3.0
1	G	365	ALA	3.0
1	B	339	LEU	2.9
1	F	373	GLY	2.9
1	C	242	TYR	2.9
1	G	245	PRO	2.9
1	F	363	ALA	2.9
1	H	363	ALA	2.9
1	C	248	LEU	2.9
1	D	248	LEU	2.9
1	G	340	ALA	2.9
1	C	372	MET	2.9
1	H	256	PHE	2.8
1	A	10	THR	2.8
1	C	13	ALA	2.8
1	H	371	PHE	2.8
1	C	244	GLN	2.8
1	C	250	LEU	2.8
1	D	12	ILE	2.8
1	B	8	SER	2.8
1	D	246	ALA	2.8
1	C	251	ARG	2.8
1	G	360	VAL	2.8
1	F	239	MET	2.7
1	E	367	TRP	2.7
1	A	247	GLN	2.7
1	H	244	GLN	2.7
1	B	362	GLU	2.7
1	G	252	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	9	SER	2.7
1	B	366	HIS	2.7
1	C	110	ALA	2.7
1	E	110	ALA	2.7
1	C	8	SER	2.7
1	F	252	ILE	2.7
1	H	373	GLY	2.6
1	D	367	TRP	2.6
1	H	369	GLN	2.6
1	F	256	PHE	2.6
1	G	169	LEU	2.6
1	G	366	HIS	2.6
1	D	363	ALA	2.6
1	F	250	LEU	2.6
1	A	371	PHE	2.6
1	E	254	LEU	2.6
1	D	152	ILE	2.6
1	D	11	GLY	2.6
1	D	109	THR	2.6
1	D	245	PRO	2.5
1	F	342	ASP	2.5
1	B	12	ILE	2.5
1	G	343	ARG	2.5
1	C	247	GLN	2.5
1	B	371	PHE	2.5
1	E	248	LEU	2.5
1	C	209	GLY	2.5
1	G	249	ALA	2.5
1	B	294	VAL	2.5
1	E	372	MET	2.5
1	B	335	PRO	2.5
1	H	245	PRO	2.5
1	C	255	ASP	2.5
1	D	254	LEU	2.5
1	F	372	MET	2.5
1	E	246	ALA	2.5
1	C	240	THR	2.5
1	E	109	THR	2.5
1	G	251	ARG	2.4
1	F	371	PHE	2.4
1	B	9	SER	2.4
1	E	332	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	209	GLY	2.4
1	B	244	GLN	2.4
1	H	8	SER	2.4
1	E	360	VAL	2.4
1	C	369	GLN	2.4
1	C	373	GLY	2.4
1	H	9	SER	2.4
1	E	152	ILE	2.4
1	E	251	ARG	2.4
1	F	369	GLN	2.4
1	H	335	PRO	2.4
1	A	243	ASN	2.4
1	A	250	LEU	2.3
1	D	111	GLY	2.3
1	F	368	LYS	2.3
1	A	369	GLN	2.3
1	H	248	LEU	2.3
1	H	242	TYR	2.3
1	G	14	PRO	2.3
1	B	245	PRO	2.3
1	C	360	VAL	2.3
1	B	250	LEU	2.3
1	D	371	PHE	2.3
1	B	341	PRO	2.3
1	F	110	ALA	2.3
1	A	343	ARG	2.3
1	G	247	GLN	2.3
1	B	172	VAL	2.3
1	C	253	ASN	2.3
1	E	243	ASN	2.3
1	D	368	LYS	2.3
1	C	371	PHE	2.2
1	E	371	PHE	2.2
1	B	152	ILE	2.2
1	C	239	MET	2.2
1	H	239	MET	2.2
1	H	109	THR	2.2
1	F	335	PRO	2.2
1	E	9	SER	2.2
1	E	331	ASP	2.2
1	D	360	VAL	2.2
1	F	247	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	250	LEU	2.2
1	B	11	GLY	2.2
1	F	9	SER	2.2
1	H	356	GLY	2.2
1	H	14	PRO	2.2
1	B	365	ALA	2.2
1	A	12	ILE	2.2
1	H	367	TRP	2.2
1	F	362	GLU	2.2
1	G	332	VAL	2.2
1	G	106	GLY	2.2
1	E	335	PRO	2.2
1	F	343	ARG	2.2
1	D	251	ARG	2.2
1	E	364	ASN	2.1
1	A	256	PHE	2.1
1	C	12	ILE	2.1
1	G	172	VAL	2.1
1	H	10	THR	2.1
1	E	11	GLY	2.1
1	E	373	GLY	2.1
1	F	241	LYS	2.1
1	E	362	GLU	2.1
1	B	221	ALA	2.1
1	A	246	ALA	2.1
1	H	110	ALA	2.1
1	H	362	GLU	2.1
1	E	366	HIS	2.1
1	F	344	ASN	2.1
1	G	333	ALA	2.1
1	B	247	GLN	2.1
1	B	363	ALA	2.1
1	D	242	TYR	2.1
1	C	15	LYS	2.1
1	F	240	THR	2.1
1	H	372	MET	2.1
1	C	363	ALA	2.1
1	C	362	GLU	2.0
1	G	59	GLY	2.0
1	D	244	GLN	2.0
1	H	247	GLN	2.0
1	D	333	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLU	2.0
1	E	111	GLY	2.0
1	E	244	GLN	2.0
1	D	247	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

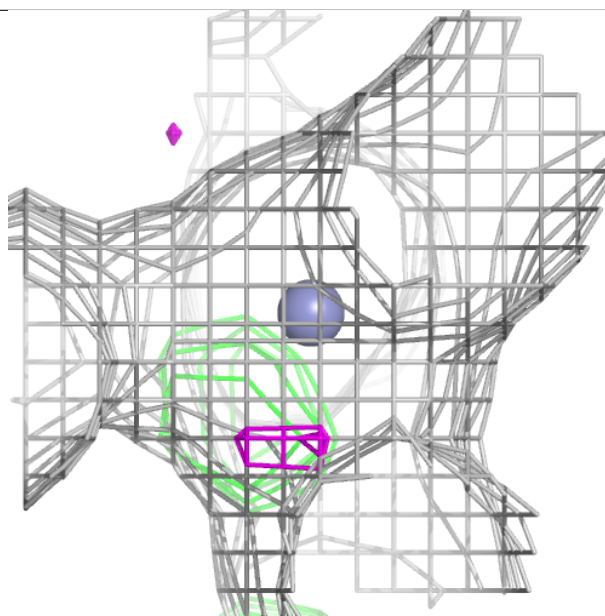
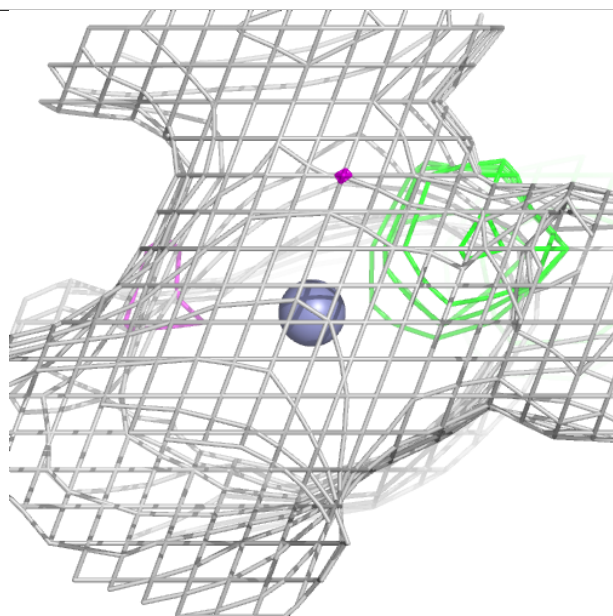
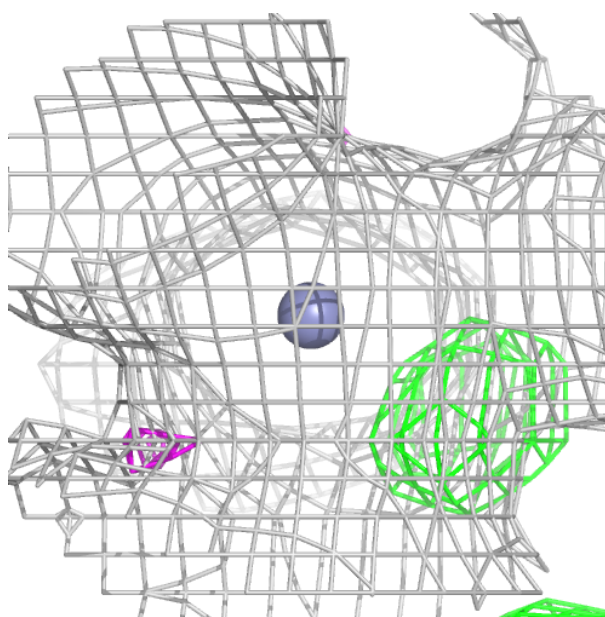
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	G	401	1/1	0.99	0.02	25,25,25,25	0
2	ZN	B	401	1/1	1.00	0.02	23,23,23,23	0
2	ZN	C	401	1/1	1.00	0.02	20,20,20,20	0
2	ZN	F	401	1/1	1.00	0.02	18,18,18,18	0
2	ZN	E	401	1/1	1.00	0.01	20,20,20,20	0
2	ZN	D	401	1/1	1.00	0.02	22,22,22,22	0
2	ZN	A	401	1/1	1.00	0.02	19,19,19,19	0
2	ZN	H	401	1/1	1.00	0.01	21,21,21,21	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.

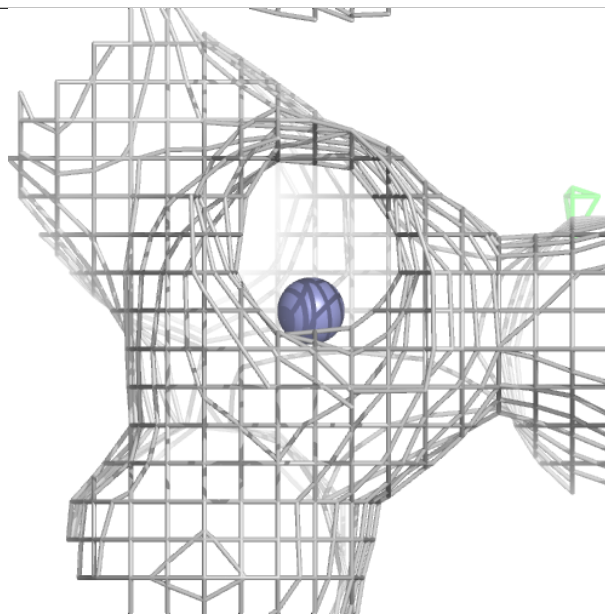
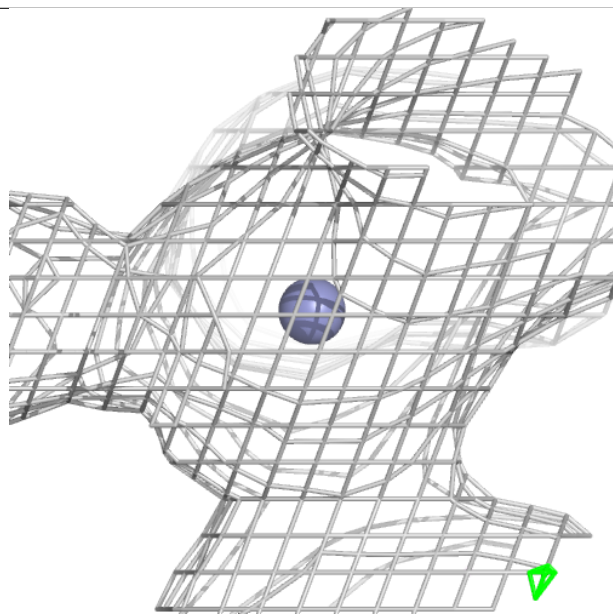
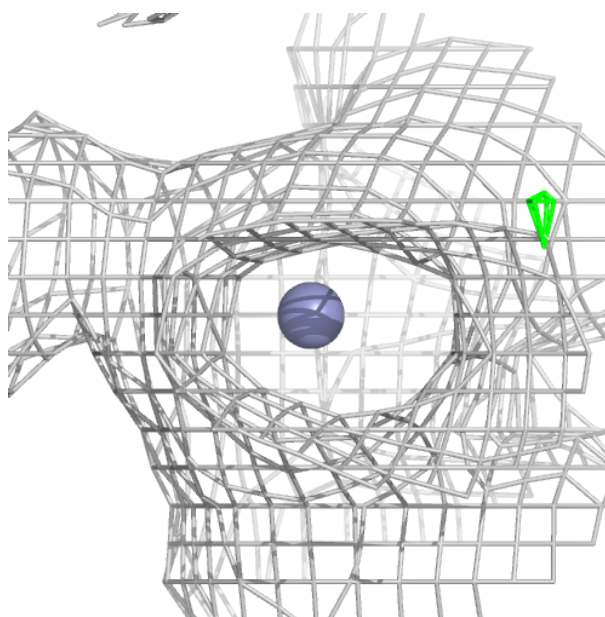
Electron density around ZN G 401:

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



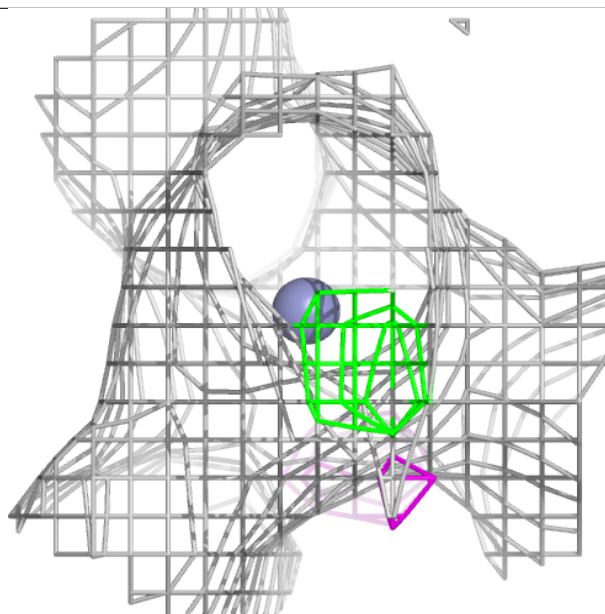
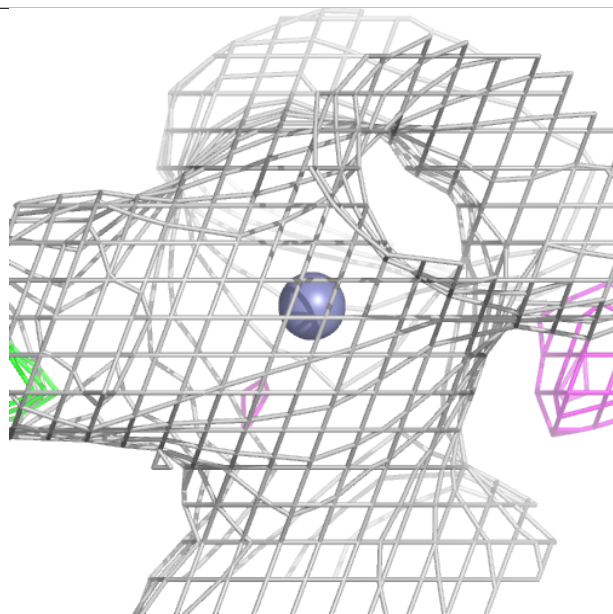
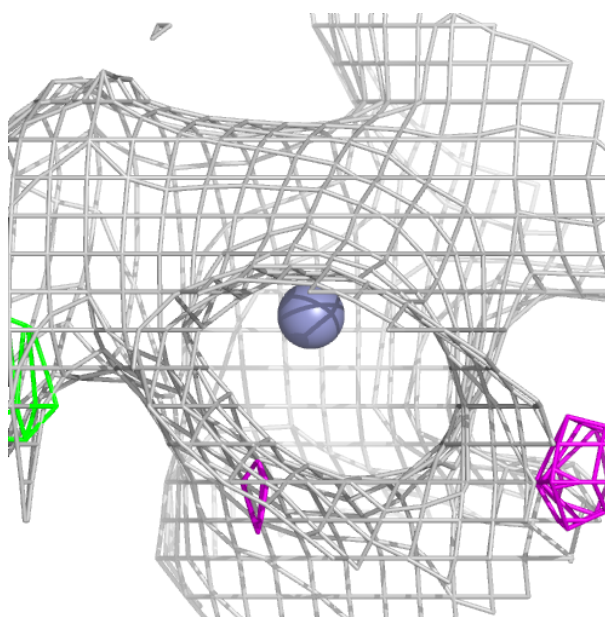
Electron density around ZN B 401:

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



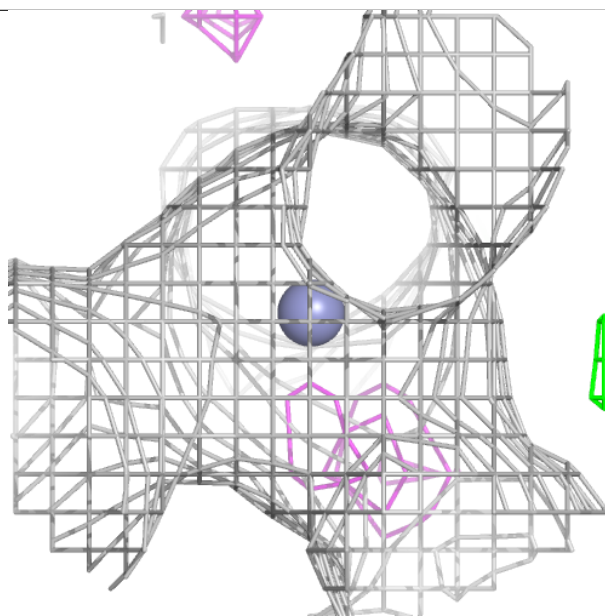
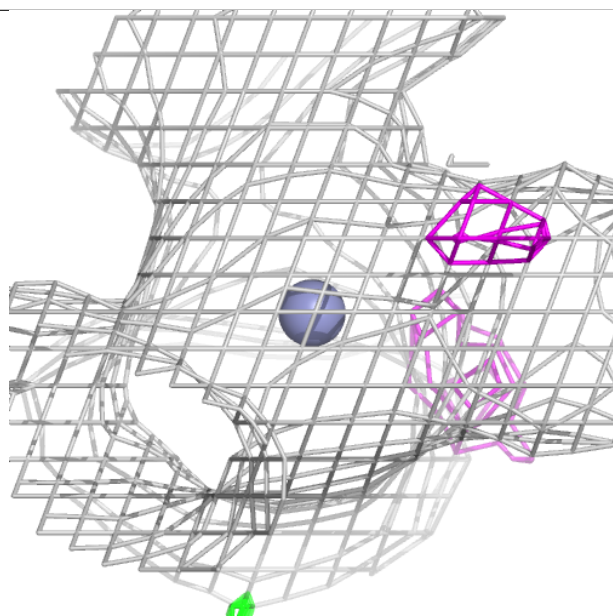
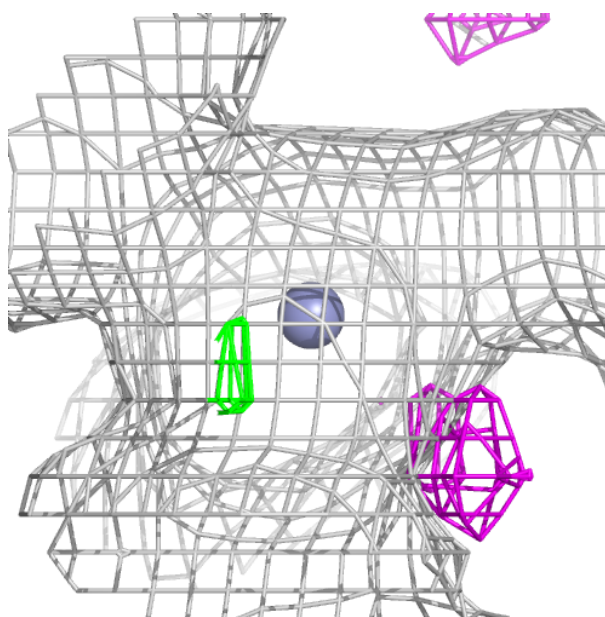
Electron density around ZN C 401:

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



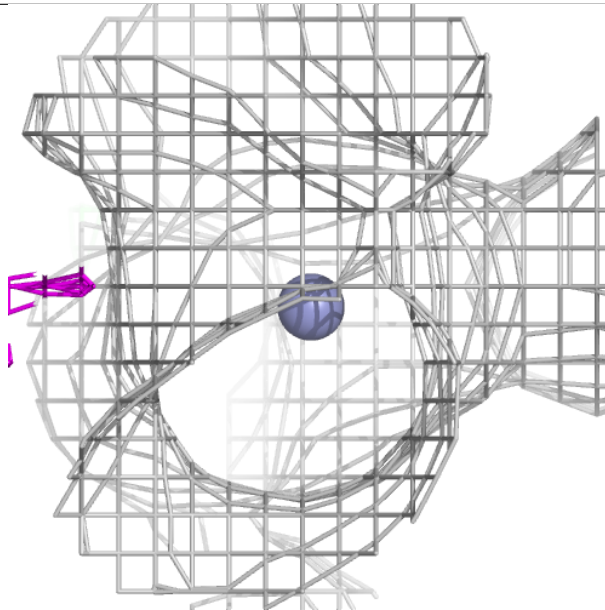
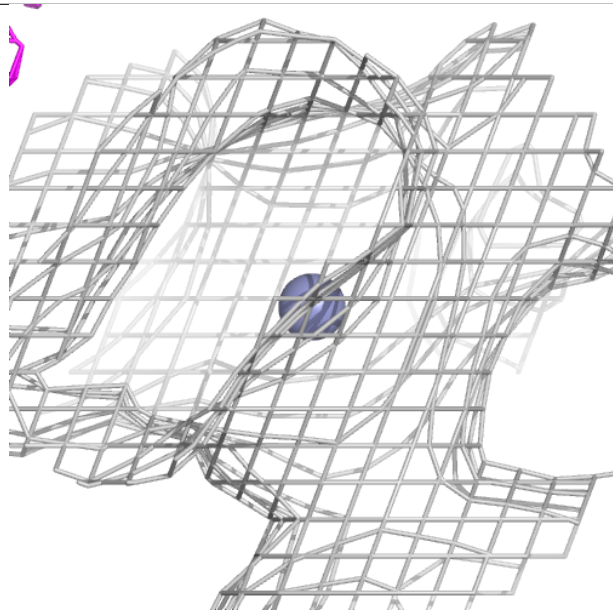
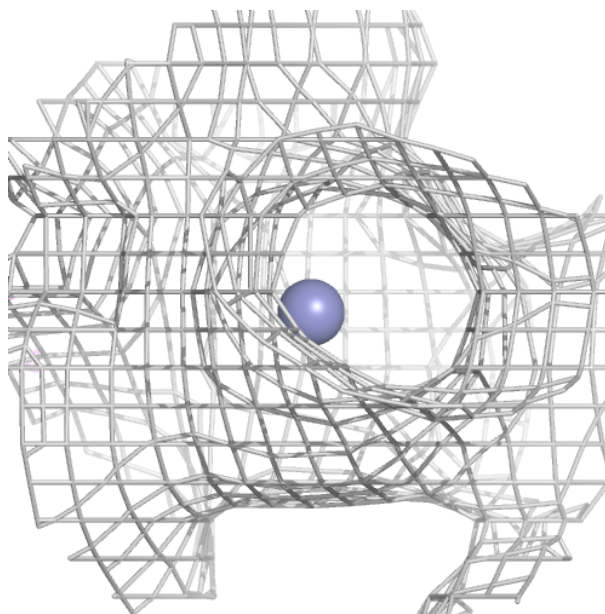
Electron density around ZN F 401:

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



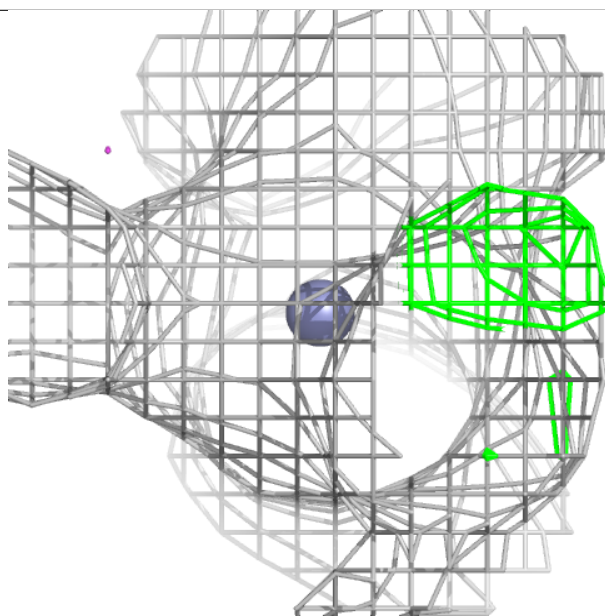
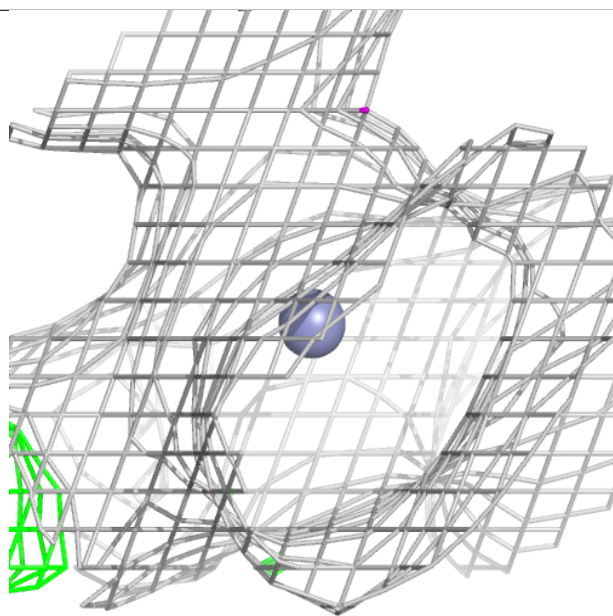
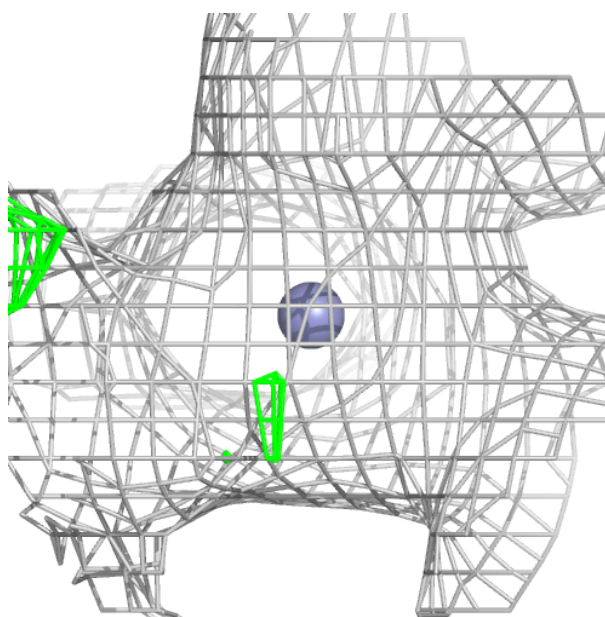
Electron density around ZN E 401:

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



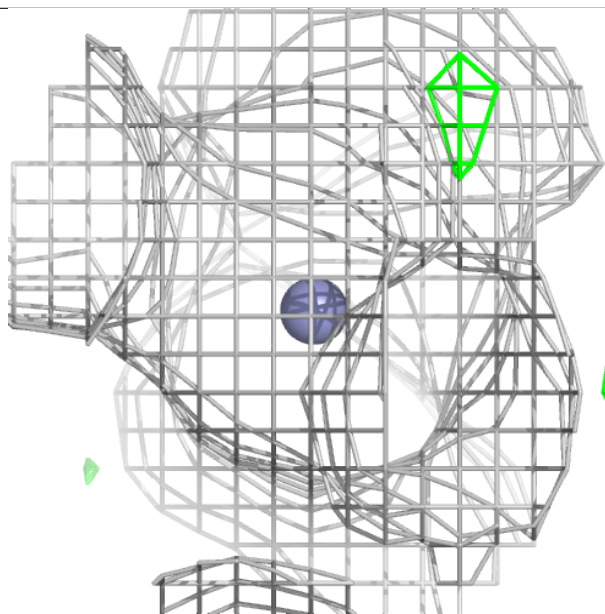
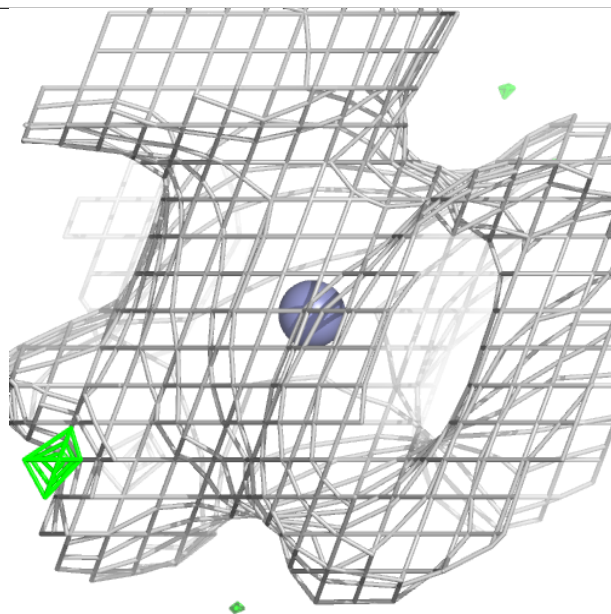
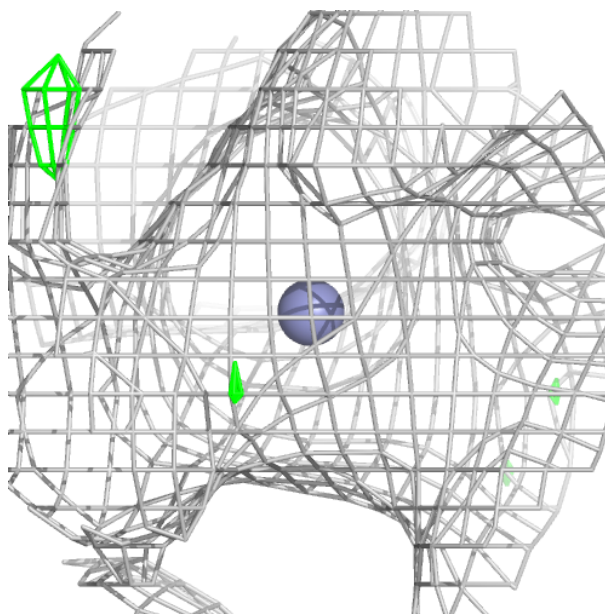
Electron density around ZN D 401:

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



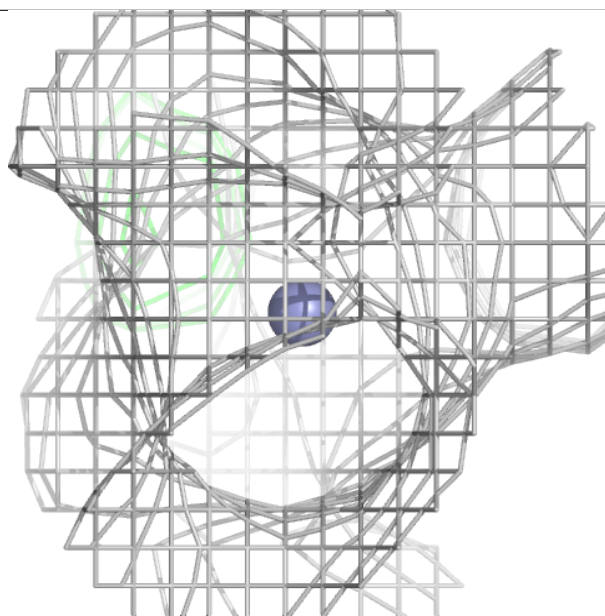
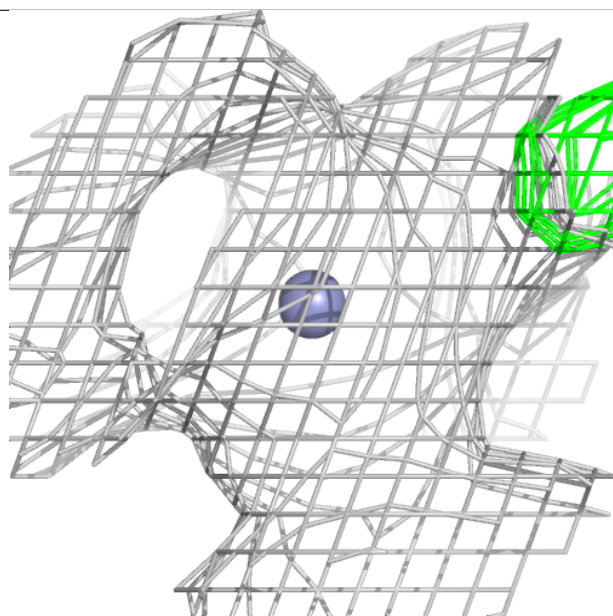
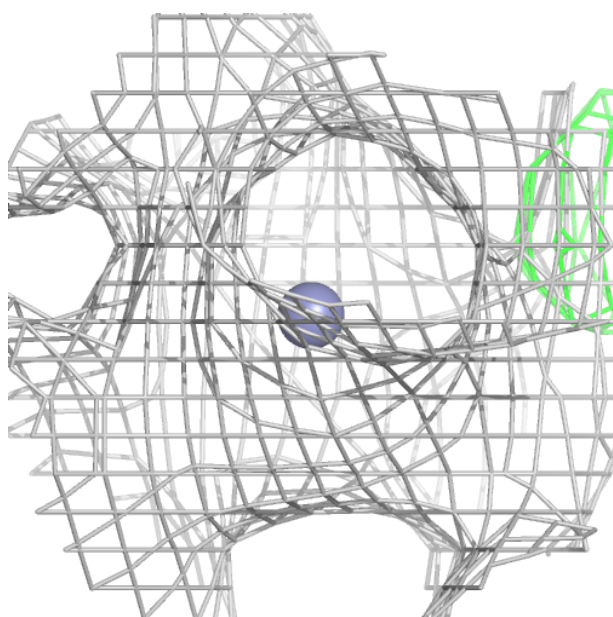
Electron density around ZN A 401:

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



Electron density around ZN H 401:

$2mF_o-DF_c$ (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.