



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 07:45 PM JST

PDB ID : 6KAN
Title : Crystal structure of FKRP in complex with Ba ion
Authors : Kuwabara, N.
Deposited on : 2019-06-23
Resolution : 2.25 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

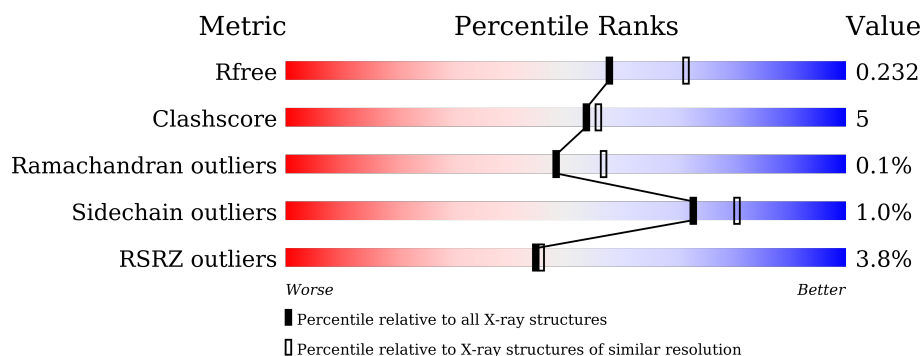
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	455	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	455	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	455	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	455	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14132 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 Fukutin-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3410	2188	603	610	9			
1	B	444	Total	C	N	O	S	0	0	0
			3420	2194	601	616	9			
1	C	441	Total	C	N	O	S	0	0	0
			3400	2184	598	609	9			
1	D	430	Total	C	N	O	S	0	0	0
			3311	2123	582	597	9			

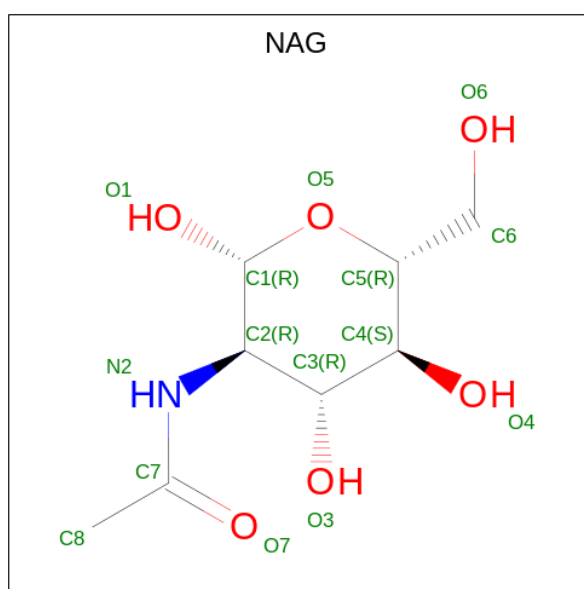
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLY	-	expression tag	UNP Q9H9S5
A	42	GLY	-	expression tag	UNP Q9H9S5
A	43	ARG	-	expression tag	UNP Q9H9S5
A	44	PRO	-	expression tag	UNP Q9H9S5
B	41	GLY	-	expression tag	UNP Q9H9S5
B	42	GLY	-	expression tag	UNP Q9H9S5
B	43	ARG	-	expression tag	UNP Q9H9S5
B	44	PRO	-	expression tag	UNP Q9H9S5
C	41	GLY	-	expression tag	UNP Q9H9S5
C	42	GLY	-	expression tag	UNP Q9H9S5
C	43	ARG	-	expression tag	UNP Q9H9S5
C	44	PRO	-	expression tag	UNP Q9H9S5
D	41	GLY	-	expression tag	UNP Q9H9S5
D	42	GLY	-	expression tag	UNP Q9H9S5
D	43	ARG	-	expression tag	UNP Q9H9S5
D	44	PRO	-	expression tag	UNP Q9H9S5

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BARIUM ION (three-letter code: BA) (formula: Ba) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ba 1	0	0
4	B	2	Total 2	Ba 2	0	0
4	C	1	Total 1	Ba 1	0	0
4	D	1	Total 1	Ba 1	0	0

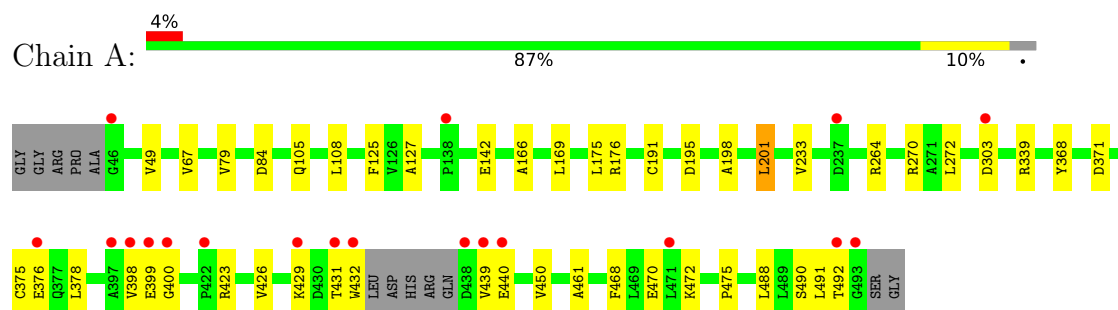
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total 137	O 137	0	0
5	B	103	Total 103	O 103	0	0
5	C	118	Total 118	O 118	0	0
5	D	126	Total 126	O 126	0	0

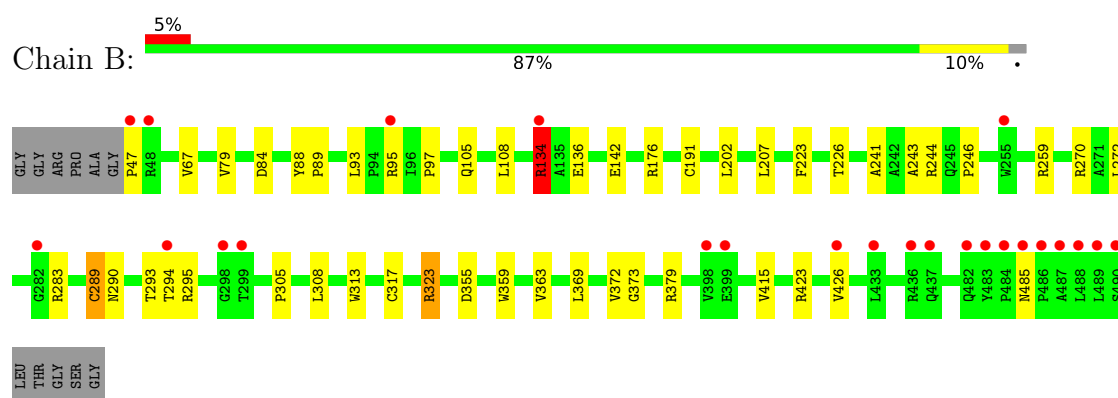
3 Residue-property plots [i](#)

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.

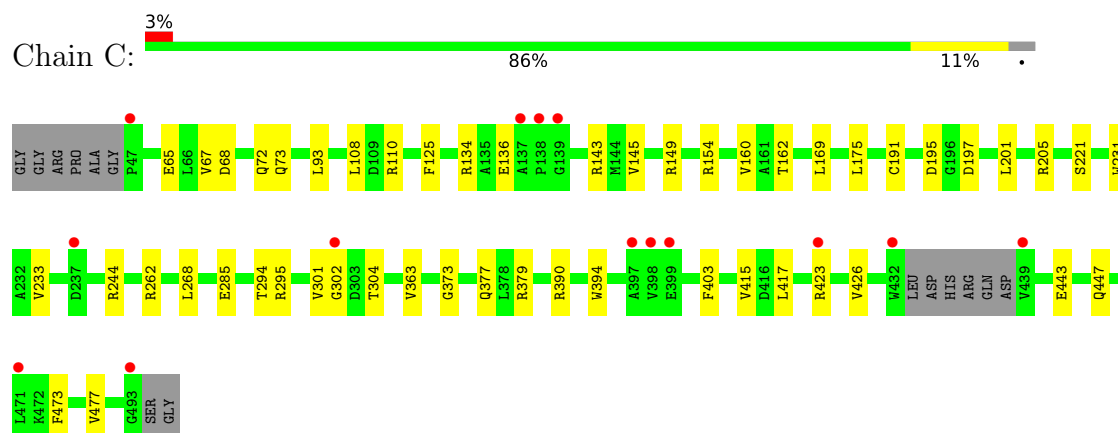
- Molecule 1: Fukutin-related protein



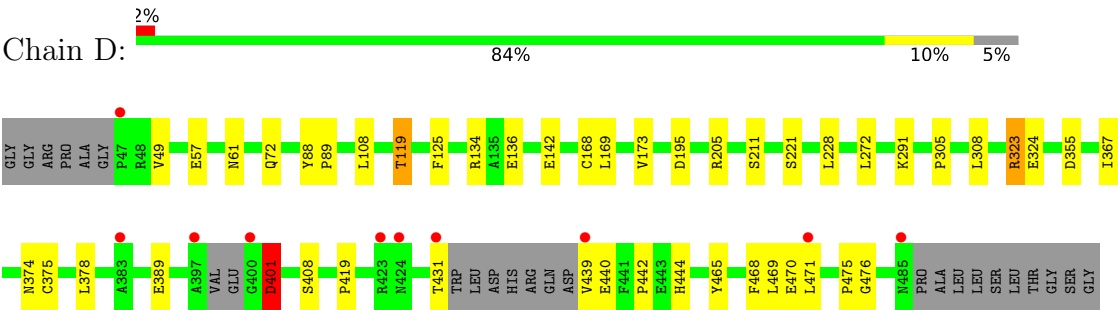
- Molecule 1: Fukutin-related protein



- Molecule 1: Fukutin-related protein



● Molecule 1: Fukutin-related protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.07Å 119.05Å 257.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.25 48.92 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.92-2.25) 99.8 (48.92-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.196 , 0.232 0.196 , 0.232	Depositor DCC
R_{free} test set	5718 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14132	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 23.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6532e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BA, 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	0.43	0/3504	0.61	1/4802 (0.0%)
1	B	0.42	1/3516 (0.0%)	0.65	4/4820 (0.1%)
1	C	0.42	0/3494	0.58	0/4787
1	D	0.45	1/3401 (0.0%)	0.64	2/4659 (0.0%)
All	All	0.43	2/13915 (0.0%)	0.62	7/19068 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	CYS	CB-SG	-6.30	1.71	1.82
1	D	168	CYS	CB-SG	-5.89	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	323	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	B	134	ARG	NE-CZ-NH1	-9.51	115.54	120.30
1	B	323	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	323	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	D	323	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	B	134	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	264	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	401	ASP	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	3410	0	3336	31	0
1	B	3420	0	3329	36	0
1	C	3400	0	3332	38	0
1	D	3311	0	3222	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	26	5	0
3	D	28	0	26	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	137	0	0	2	0
5	B	103	0	0	1	0
5	C	118	0	0	4	0
5	D	126	0	0	3	0
All	All	14132	0	13310	128	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 5.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:HH22	1:B:244:ARG:NE	1.44	1.13
1:B:134:ARG:NH2	1:B:244:ARG:NE	2.01	1.08
1:B:134:ARG:HH22	1:B:244:ARG:CD	1.75	1.00
1:C:205:ARG:HE	3:C:503:NAG:H81	1.39	0.85
1:C:302:GLY:HA3	1:C:304:THR:N	1.96	0.80
1:B:134:ARG:NH2	1:B:244:ARG:HE	1.78	0.78
1:A:339:ARG:NH1	1:A:371:ASP:OD2	2.19	0.75
1:B:134:ARG:HH22	1:B:244:ARG:HE	1.32	0.73
1:A:169:LEU:HD11	1:A:195:ASP:HB2	1.70	0.72
1:D:470:GLU:OE2	1:D:476:GLY:N	2.20	0.70
1:C:302:GLY:HA3	1:C:304:THR:H	1.53	0.69
1:C:443:GLU:OE2	1:C:447:GLN:NE2	2.26	0.69
1:D:205:ARG:HA	3:D:503:NAG:H83	1.75	0.69
1:C:134:ARG:HD3	1:C:136:GLU:OE1	1.92	0.68
1:A:400:GLY:HA2	1:A:431:THR:HG21	1.75	0.66
1:B:47:PRO:HG2	1:B:142:GLU:HG3	1.78	0.66
1:B:134:ARG:NH2	1:B:244:ARG:CG	2.59	0.66
1:A:142:GLU:N	1:A:142:GLU:OE2	2.31	0.64
1:A:488:LEU:O	1:A:492:THR:HG22	1.98	0.64
1:B:134:ARG:HH22	1:B:244:ARG:CG	2.11	0.64
1:D:401:ASP:OD2	1:D:431:THR:HB	1.97	0.63
1:B:134:ARG:NH2	1:B:244:ARG:HG2	2.14	0.62
3:C:502:NAG:O7	5:C:601:HOH:O	2.16	0.61
1:C:169:LEU:HD11	1:C:195:ASP:HB2	1.83	0.61
1:A:108:LEU:HD21	1:B:272:LEU:HD13	1.83	0.61
1:A:270:ARG:NH1	5:A:601:HOH:O	2.35	0.60
1:D:389:GLU:H	1:D:389:GLU:CD	2.04	0.60
1:C:110:ARG:NH1	5:C:602:HOH:O	2.34	0.59
1:C:73:GLN:NE2	1:C:136:GLU:O	2.35	0.58
1:B:294:THR:HG22	1:B:295:ARG:O	2.04	0.58
1:A:470:GLU:OE2	1:A:475:PRO:HA	2.04	0.57
1:A:468:PHE:CZ	1:A:472:LYS:HE3	2.40	0.57
1:A:272:LEU:HD13	1:B:108:LEU:HD21	1.85	0.57
1:D:324:GLU:HG3	5:D:617:HOH:O	2.04	0.56
1:C:160:VAL:HG23	1:C:162:THR:HG23	1.88	0.56
1:B:134:ARG:HD2	1:B:136:GLU:HB2	1.87	0.56
1:C:373:GLY:O	1:C:379:ARG:HD3	2.07	0.54
1:A:376:GLU:OE2	1:A:376:GLU:N	2.32	0.54
1:C:301:VAL:HG21	1:D:89:PRO:HB3	1.88	0.54
1:A:176:ARG:HD3	5:A:655:HOH:O	2.07	0.54
1:D:142:GLU:OE2	1:D:142:GLU:N	2.28	0.54
1:D:173:VAL:HB	1:D:228:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD21	1:D:272:LEU:HD13	1.89	0.53
1:B:423:ARG:HB3	1:B:426:VAL:HG13	1.91	0.53
1:A:423:ARG:HH22	1:A:426:VAL:CG2	2.21	0.53
1:D:291:LYS:HD2	1:D:408:SER:HB3	1.91	0.52
1:C:205:ARG:NE	3:C:503:NAG:H81	2.18	0.52
1:A:429:LYS:O	1:A:432:TRP:NE1	2.43	0.52
1:C:302:GLY:CA	1:C:304:THR:H	2.23	0.51
1:C:145:VAL:O	1:C:149:ARG:HG3	2.11	0.51
1:B:97:PRO:HB2	1:D:119:THR:HG23	1.93	0.51
1:A:423:ARG:HH22	1:A:426:VAL:HG22	1.76	0.50
1:A:67:VAL:HG22	1:A:79:VAL:HG11	1.93	0.49
1:D:468:PHE:O	1:D:471:LEU:HG	2.11	0.49
1:D:323:ARG:NH2	5:D:605:HOH:O	2.41	0.49
1:B:93:LEU:O	1:B:95:ARG:HD2	2.13	0.49
1:D:375:CYS:SG	1:D:378:LEU:HD12	2.52	0.49
1:C:294:THR:HG22	1:C:295:ARG:O	2.11	0.49
1:B:323:ARG:HD3	1:B:355:ASP:OD1	2.13	0.49
1:C:110:ARG:O	1:D:211:SER:HB2	2.12	0.48
1:D:169:LEU:HD11	1:D:195:ASP:HB2	1.94	0.48
1:C:423:ARG:O	1:C:426:VAL:HG12	2.13	0.48
1:D:442:PRO:HB2	1:D:444:HIS:CD2	2.49	0.48
1:B:88:TYR:HA	1:B:89:PRO:C	2.34	0.48
1:B:176:ARG:HD3	1:B:313:TRP:CD2	2.49	0.48
1:C:65:GLU:OE2	1:C:244:ARG:N	2.42	0.48
1:A:432:TRP:HH2	1:A:440:GLU:HB3	1.78	0.47
1:B:202:LEU:HD11	1:B:207:LEU:HB2	1.95	0.47
1:B:243:ALA:HB3	1:B:246:PRO:HA	1.95	0.47
1:D:134:ARG:HE	1:D:136:GLU:HG2	1.79	0.47
1:C:134:ARG:HH11	1:C:136:GLU:HG3	1.79	0.47
1:C:175:LEU:HD21	1:D:108:LEU:HD12	1.96	0.47
1:C:473:PHE:HB2	1:C:477:VAL:HG11	1.97	0.47
1:A:84:ASP:O	1:A:105:GLN:HB3	2.15	0.47
1:B:308:LEU:HD11	1:B:359:TRP:HB2	1.97	0.47
1:C:377:GLN:HB3	1:C:394:TRP:CD2	2.50	0.46
1:C:125:PHE:HB3	1:C:201:LEU:HD11	1.97	0.46
1:C:390:ARG:NH2	5:C:610:HOH:O	2.48	0.46
1:D:323:ARG:HD3	1:D:355:ASP:OD1	2.15	0.46
1:B:290:ASN:OD1	1:B:293:THR:HG23	2.16	0.46
1:B:289:CYS:HB2	1:B:317:CYS:HB2	1.98	0.46
1:C:154:ARG:HD3	1:C:231:TRP:CD2	2.50	0.46
1:A:491:LEU:HD12	3:C:503:NAG:O6	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:502:NAG:H2	5:D:652:HOH:O	2.16	0.45
1:C:221:SER:HB2	1:C:268:LEU:HD21	1.97	0.45
1:B:305:PRO:HD2	1:B:308:LEU:HD22	1.98	0.45
1:A:339:ARG:NH2	1:A:368:TYR:CG	2.84	0.45
1:D:88:TYR:HA	1:D:89:PRO:C	2.36	0.45
1:A:398:VAL:HG23	1:A:399:GLU:H	1.82	0.45
1:B:373:GLY:O	1:B:379:ARG:HD3	2.17	0.45
1:A:398:VAL:HG23	1:A:399:GLU:N	2.32	0.44
1:C:68:ASP:O	1:C:72:GLN:HG3	2.18	0.44
1:C:205:ARG:HH21	3:C:503:NAG:C8	2.31	0.44
1:C:262:ARG:NH2	1:C:285:GLU:OE2	2.50	0.44
1:D:367:ILE:O	1:D:419:PRO:HA	2.17	0.44
1:B:223:PHE:HA	1:B:226:THR:OG1	2.18	0.44
1:A:175:LEU:HD21	1:B:108:LEU:HD12	2.00	0.44
1:A:432:TRP:CH2	1:A:440:GLU:HB3	2.53	0.44
1:A:166:ALA:HB2	1:A:198:ALA:HB2	2.00	0.44
1:A:49:VAL:HG22	1:A:125:PHE:HB2	2.00	0.44
1:C:154:ARG:HD2	5:C:635:HOH:O	2.18	0.44
1:B:363:VAL:HB	1:B:415:VAL:HG22	1.99	0.43
1:C:363:VAL:HB	1:C:415:VAL:HG22	2.00	0.43
1:D:49:VAL:HG22	1:D:125:PHE:HB2	2.01	0.43
1:B:369:LEU:O	1:B:372:VAL:HG13	2.18	0.43
1:A:127:ALA:HB2	1:A:201:LEU:HD12	1.99	0.43
1:B:134:ARG:HG3	1:B:241:ALA:HB3	2.00	0.43
1:D:470:GLU:OE2	1:D:475:PRO:HA	2.18	0.43
1:A:375:CYS:HB3	1:A:378:LEU:HB2	2.01	0.42
1:B:270:ARG:HD3	5:B:602:HOH:O	2.18	0.42
1:D:439:VAL:HG22	1:D:440:GLU:H	1.84	0.42
1:A:423:ARG:NH2	1:A:426:VAL:HG22	2.34	0.42
1:C:191:CYS:HB2	1:C:233:VAL:HG13	2.02	0.42
1:C:302:GLY:CA	1:C:304:THR:N	2.78	0.42
1:C:67:VAL:HG21	1:C:93:LEU:HD22	2.02	0.42
1:D:57:GLU:O	1:D:61:ASN:HB3	2.20	0.42
1:D:305:PRO:HD2	1:D:308:LEU:HD12	2.02	0.42
1:B:134:ARG:NH2	1:B:244:ARG:CZ	2.79	0.42
1:A:450:VAL:HG23	1:A:461:ALA:HB3	2.01	0.41
1:C:160:VAL:HG22	1:C:197:ASP:CB	2.50	0.41
1:D:465:TYR:O	1:D:469:LEU:N	2.54	0.41
1:B:67:VAL:HG22	1:B:79:VAL:HG11	2.02	0.41
1:A:191:CYS:HB2	1:A:233:VAL:HG13	2.03	0.41
1:B:84:ASP:O	1:B:105:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:NH2	1:B:244:ARG:CD	2.55	0.40
1:C:403:PHE:HB2	1:C:417:LEU:HB2	2.02	0.40
1:C:390:ARG:HE	1:C:390:ARG:HB3	1.67	0.40
1:D:468:PHE:HA	1:D:471:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/455 (96%)	430 (98%)	7 (2%)	2 (0%)	25	25
1	B	442/455 (97%)	430 (97%)	12 (3%)	0	100	100
1	C	437/455 (96%)	426 (98%)	11 (2%)	0	100	100
1	D	424/455 (93%)	414 (98%)	10 (2%)	0	100	100
All	All	1742/1820 (96%)	1700 (98%)	40 (2%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	VAL
1	A	303	ASP

5.3.2 Protein sidechains [i](#)

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	341/357 (96%)	339 (99%)	2 (1%)	84	89
1	B	342/357 (96%)	337 (98%)	5 (2%)	60	70
1	C	341/357 (96%)	340 (100%)	1 (0%)	91	94
1	D	331/357 (93%)	326 (98%)	5 (2%)	60	70
All	All	1355/1428 (95%)	1342 (99%)	13 (1%)	73	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LEU
1	A	490	SER
1	B	134	ARG
1	B	191	CYS
1	B	259	ARG
1	B	283	ARG
1	B	485	ASN
1	C	143	ARG
1	D	72	GLN
1	D	119	THR
1	D	221	SER
1	D	374	ASN
1	D	401	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	485	ASN
1	C	444	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	502	1	14,14,15	0.67	0	17,19,21	0.53	0
3	NAG	C	502	1	14,14,15	2.24	3 (21%)	17,19,21	1.78	5 (29%)
3	NAG	D	503	1	14,14,15	0.30	0	17,19,21	0.79	0
3	NAG	B	502	1	14,14,15	0.42	0	17,19,21	0.37	0
3	NAG	A	503	1	14,14,15	1.29	1 (7%)	17,19,21	1.35	1 (5%)
3	NAG	C	503	1	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
3	NAG	D	502	1	14,14,15	1.16	2 (14%)	17,19,21	2.90	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	C	502	1	-	2/6/23/26	0/1/1/1
3	NAG	D	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	2/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	C	503	1	-	2/6/23/26	0/1/1/1
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	NAG	O5-C1	6.85	1.54	1.43
3	A	503	NAG	O5-C1	4.63	1.51	1.43
3	C	502	NAG	C1-C2	3.00	1.56	1.52
3	D	502	NAG	C8-C7	-2.55	1.45	1.50
3	C	502	NAG	C4-C5	-2.31	1.48	1.53
3	D	502	NAG	C1-C2	2.07	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAG	C1-O5-C5	8.93	124.30	112.19
3	D	502	NAG	C3-C4-C5	-5.54	100.36	110.24
3	A	503	NAG	C1-O5-C5	4.64	118.47	112.19
3	C	502	NAG	O3-C3-C4	-4.10	100.87	110.35
3	D	502	NAG	O6-C6-C5	3.68	123.91	111.29
3	D	502	NAG	O3-C3-C2	-3.58	102.06	109.47
3	C	502	NAG	C6-C5-C4	-2.95	106.10	113.00
3	C	502	NAG	O6-C6-C5	-2.75	101.87	111.29
3	C	503	NAG	C1-O5-C5	2.32	115.33	112.19
3	C	502	NAG	C4-C3-C2	-2.08	107.97	111.02
3	C	502	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	NAG	O5-C5-C6-O6
3	C	503	NAG	O5-C5-C6-O6
3	C	503	NAG	C4-C5-C6-O6
3	C	502	NAG	C4-C5-C6-O6
3	D	503	NAG	C8-C7-N2-C2
3	D	503	NAG	O7-C7-N2-C2
3	B	502	NAG	C4-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NAG	1	0
3	D	503	NAG	1	0
3	C	503	NAG	4	0
3	D	502	NAG	1	0

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	443/455 (97%)	0.05	19 (4%)	40 40	32, 52, 92, 125	0
1	B	444/455 (97%)	0.11	24 (5%)	32 32	33, 55, 92, 114	0
1	C	441/455 (96%)	-0.04	14 (3%)	50 51	30, 53, 82, 103	0
1	D	430/455 (94%)	0.06	10 (2%)	61 61	32, 54, 93, 124	0
All	All	1758/1820 (96%)	0.04	67 (3%)	44 45	30, 54, 91, 125	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	PRO	5.6
1	A	398	VAL	5.6
1	D	397	ALA	5.3
1	B	398	VAL	5.3
1	D	439	VAL	5.2
1	A	438	ASP	4.8
1	B	47	PRO	4.4
1	C	399	GLU	3.9
1	B	488	LEU	3.8
1	D	485	ASN	3.7
1	A	493	GLY	3.7
1	D	423	ARG	3.6
1	A	439	VAL	3.5
1	B	437	GLN	3.5
1	C	398	VAL	3.5
1	D	431	THR	3.4
1	B	487	ALA	3.4
1	B	489	LEU	3.4
1	B	426	VAL	3.3
1	D	471	LEU	3.3
1	C	47	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	399	GLU	3.3
1	B	490	SER	3.2
1	A	432	TRP	3.1
1	C	439	VAL	3.0
1	C	302	GLY	3.0
1	B	399	GLU	2.9
1	B	485	ASN	2.9
1	B	433	LEU	2.8
1	A	400	GLY	2.7
1	B	299	THR	2.7
1	C	137	ALA	2.6
1	D	400	GLY	2.6
1	C	432	TRP	2.6
1	B	486	PRO	2.6
1	A	492	THR	2.5
1	A	376	GLU	2.5
1	B	282	GLY	2.5
1	B	298	GLY	2.5
1	A	138	PRO	2.5
1	C	138	PRO	2.5
1	A	397	ALA	2.5
1	C	423	ARG	2.4
1	A	303	ASP	2.3
1	A	471	LEU	2.3
1	A	431	THR	2.3
1	B	484	PRO	2.3
1	B	95	ARG	2.3
1	A	46	GLY	2.3
1	D	424	ASN	2.2
1	C	471	LEU	2.2
1	A	422	PRO	2.2
1	B	48	ARG	2.2
1	C	397	ALA	2.2
1	C	139	GLY	2.2
1	C	493	GLY	2.2
1	D	383	ALA	2.2
1	B	436	ARG	2.1
1	B	482	GLN	2.1
1	A	237	ASP	2.1
1	A	429	LYS	2.1
1	B	483	TYR	2.1
1	B	255	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	237	ASP	2.0
1	A	440	GLU	2.0
1	B	134	ARG	2.0
1	B	294	THR	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 monosaccharides 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.

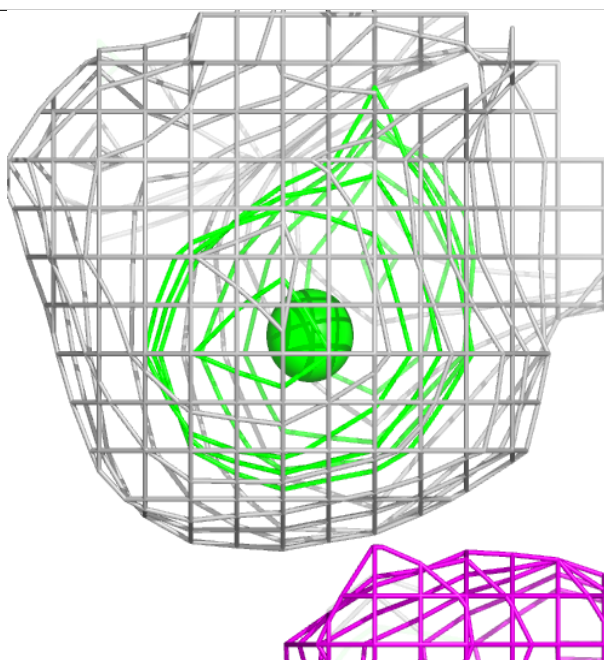
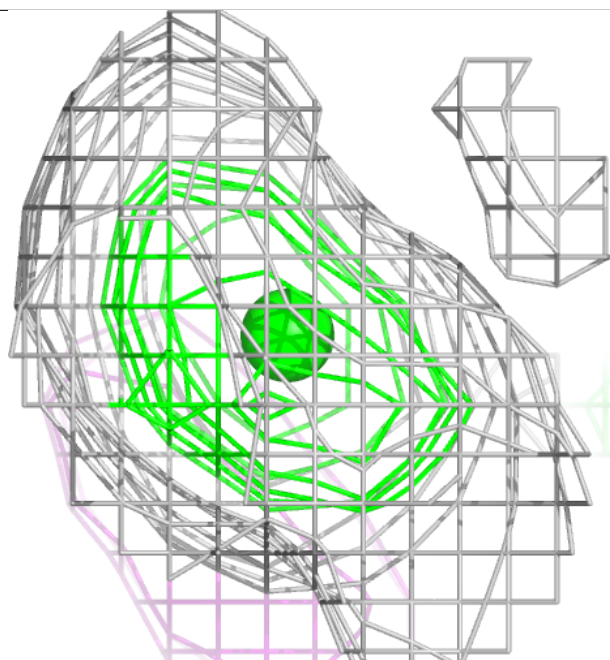
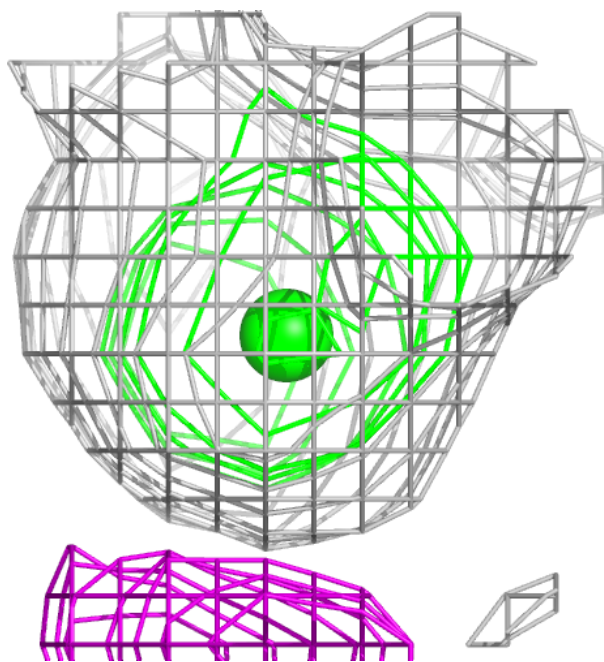
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BA	A	504	1/1	0.16	0.24	277,277,277,277	0
4	BA	B	504	1/1	0.46	0.20	313,313,313,313	0
4	BA	C	504	1/1	0.48	0.19	245,245,245,245	0
4	BA	B	503	1/1	0.49	0.23	258,258,258,258	0
3	NAG	D	503	14/15	0.66	0.17	70,77,85,86	0
3	NAG	D	502	14/15	0.68	0.16	84,89,96,96	0
3	NAG	A	503	14/15	0.76	0.15	65,76,81,82	0
3	NAG	C	503	14/15	0.80	0.13	61,66,72,74	0
3	NAG	B	502	14/15	0.81	0.12	67,77,82,85	0
4	BA	D	504	1/1	0.83	0.11	184,184,184,184	0
3	NAG	C	502	14/15	0.90	0.12	53,73,87,87	0
3	NAG	A	502	14/15	0.91	0.10	48,58,66,69	0
2	ZN	B	501	1/1	0.99	0.03	46,46,46,46	0
2	ZN	C	501	1/1	0.99	0.05	39,39,39,39	0
2	ZN	D	501	1/1	0.99	0.04	45,45,45,45	0
2	ZN	A	501	1/1	1.00	0.03	40,40,40,40	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.

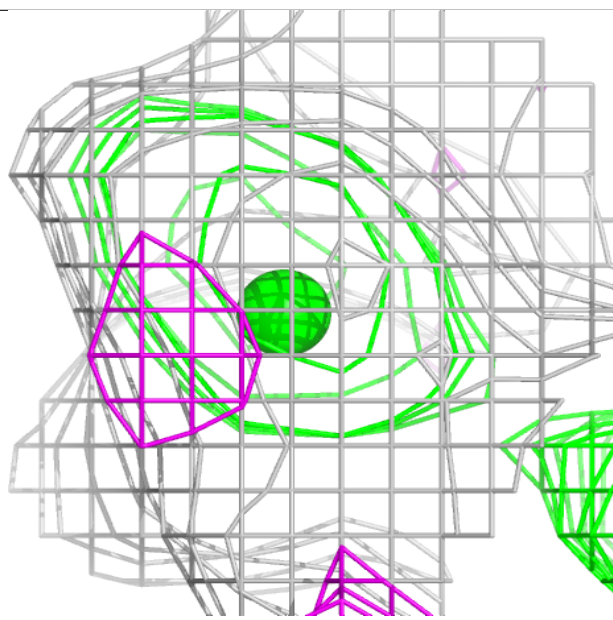
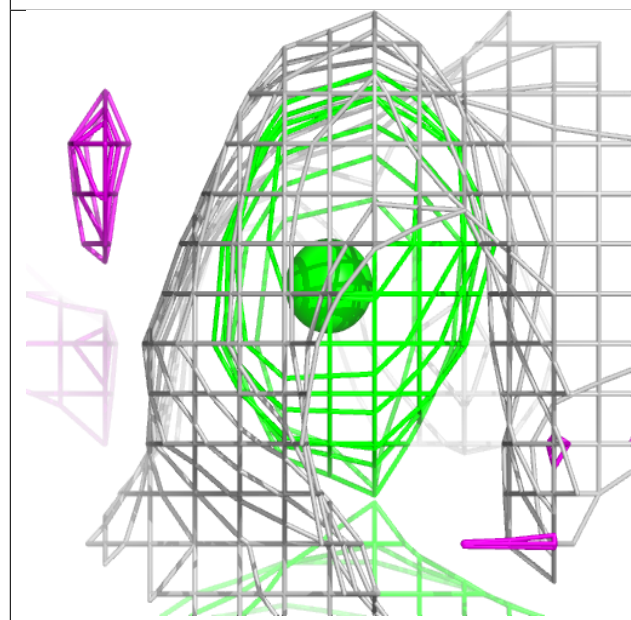
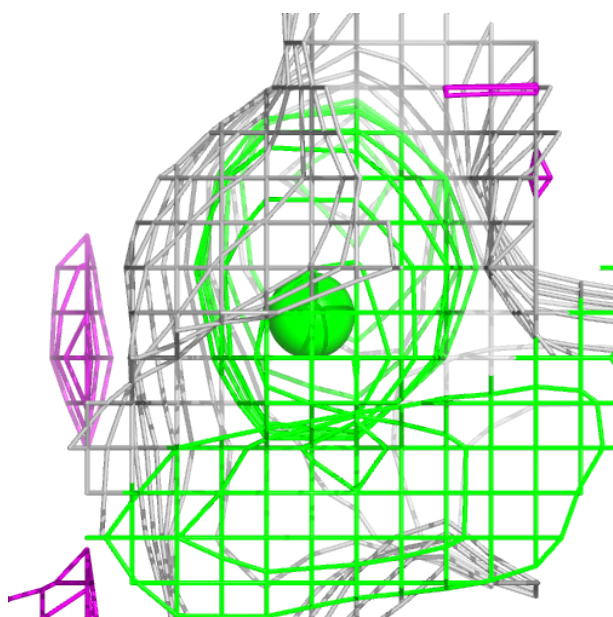
Electron density around BA A 504:

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



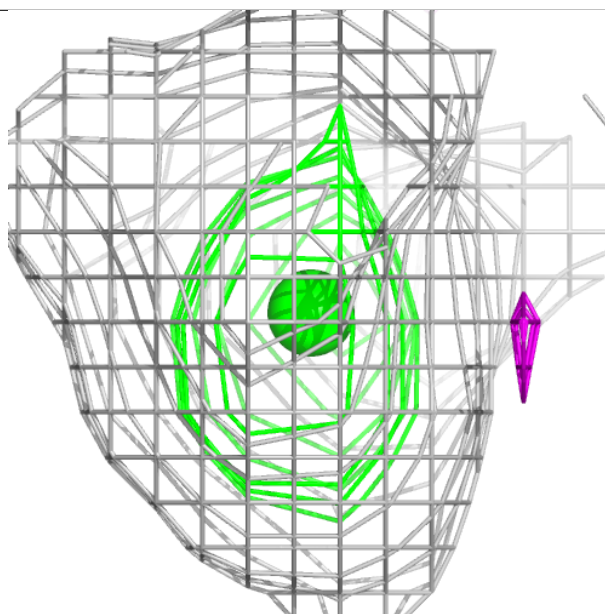
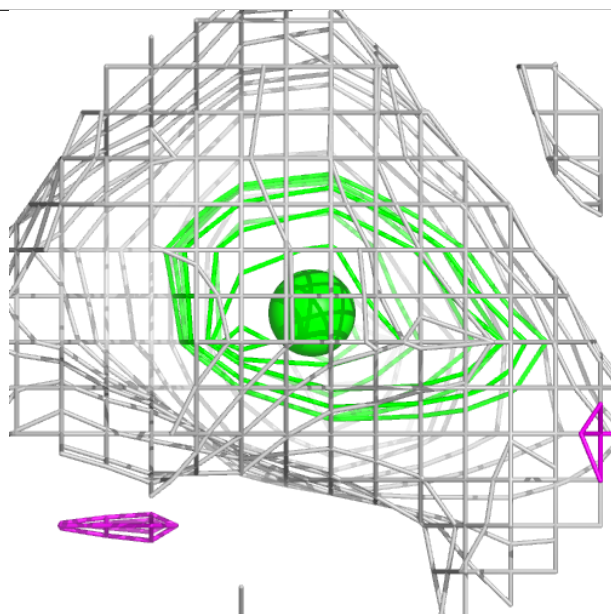
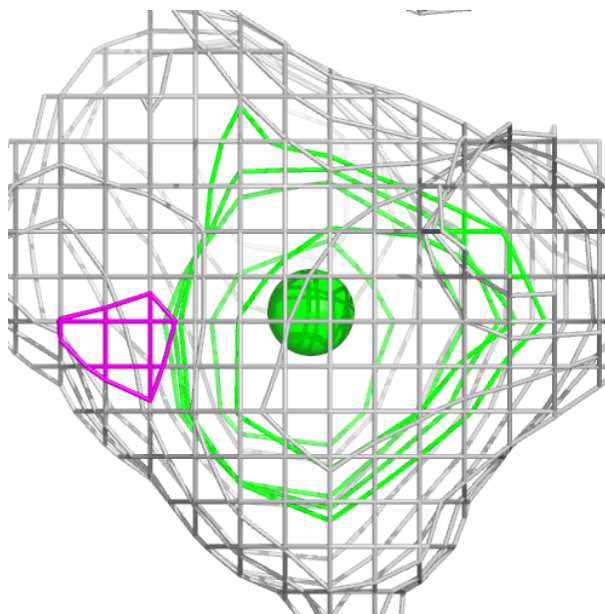
Electron density around BA B 504:

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and green (positive)



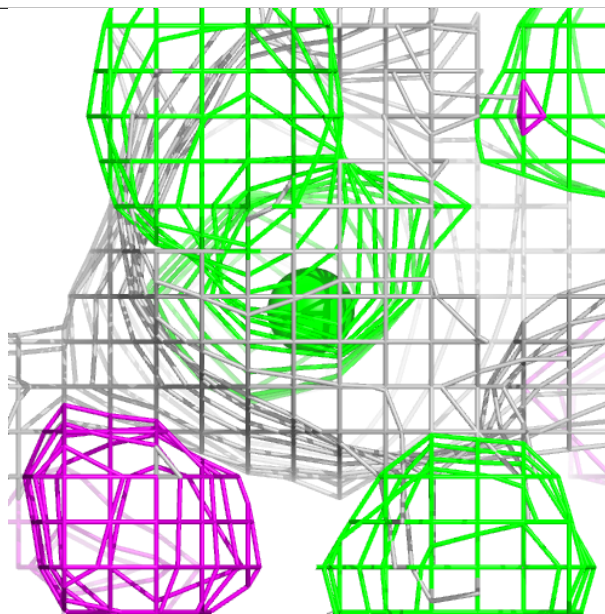
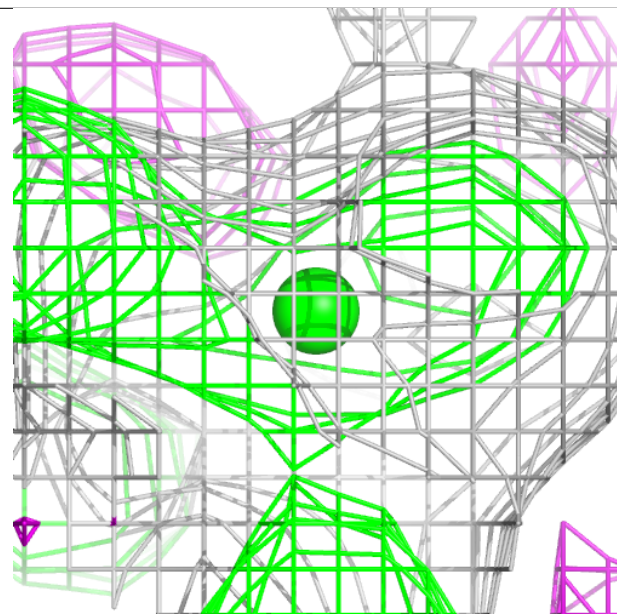
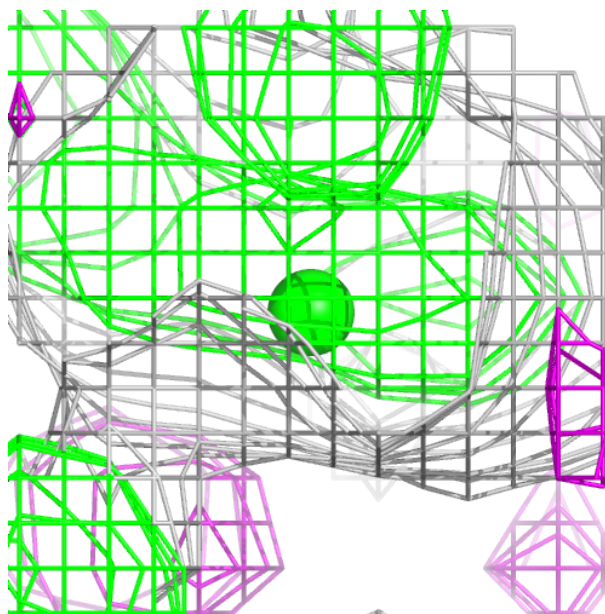
Electron density around BA C 504:

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



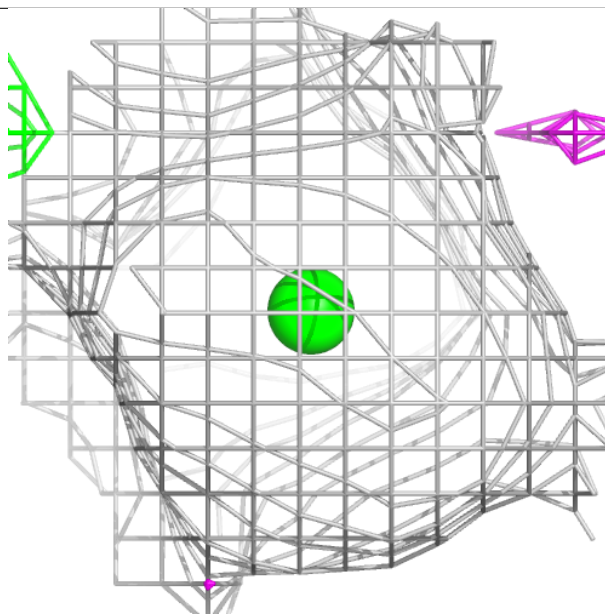
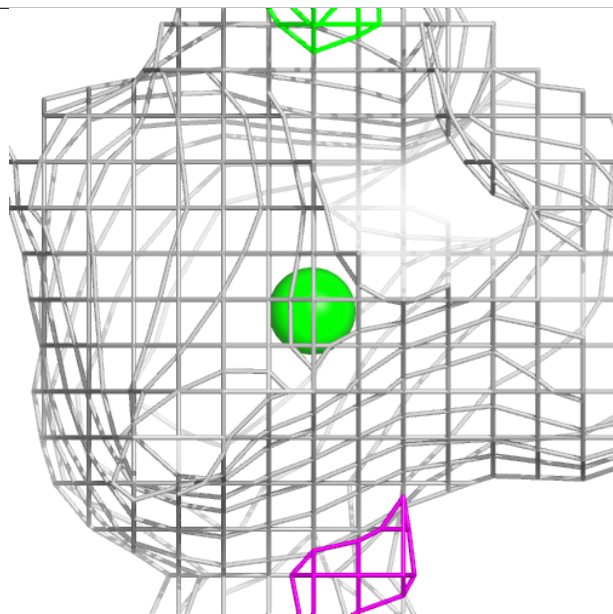
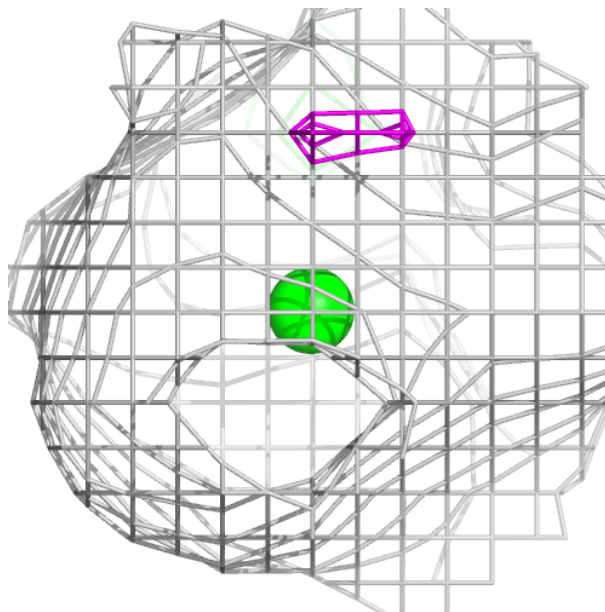
Electron density around BA B 503:

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and green (positive)



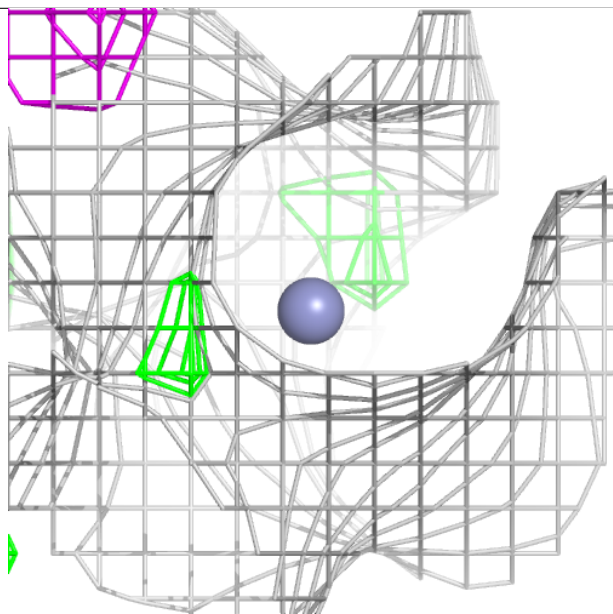
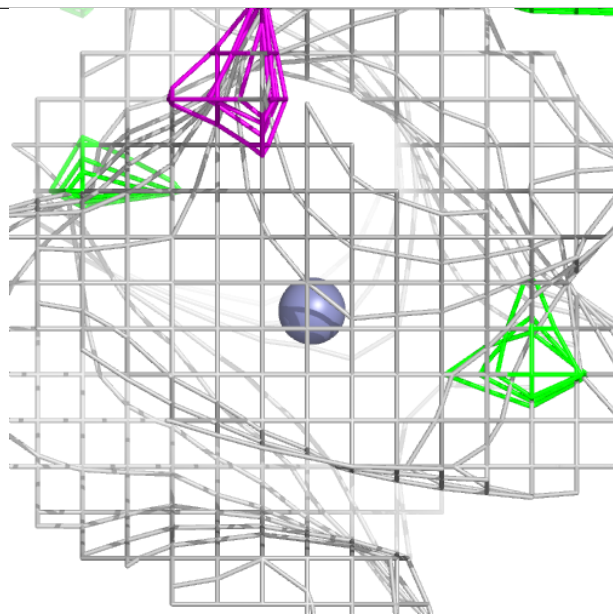
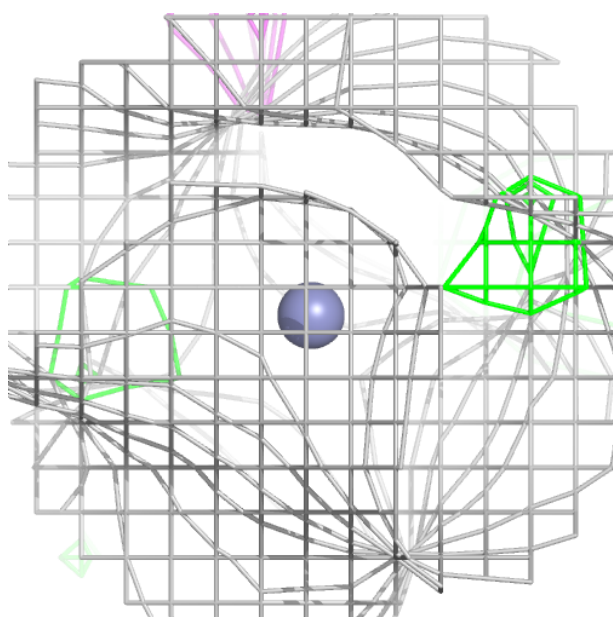
Electron density around BA D 504:

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



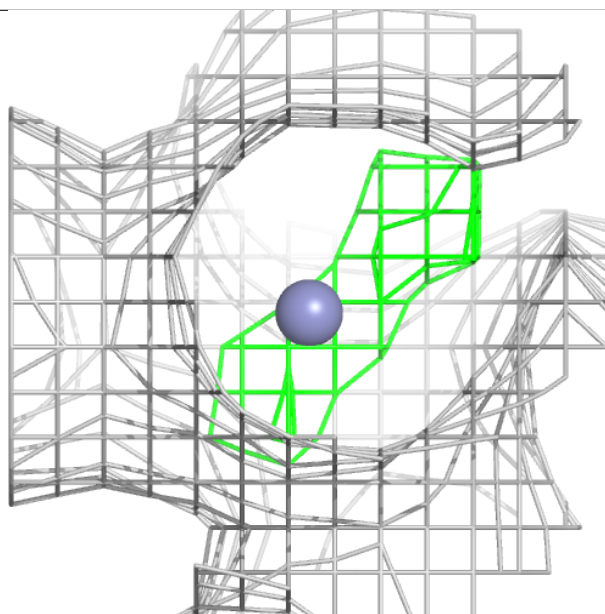
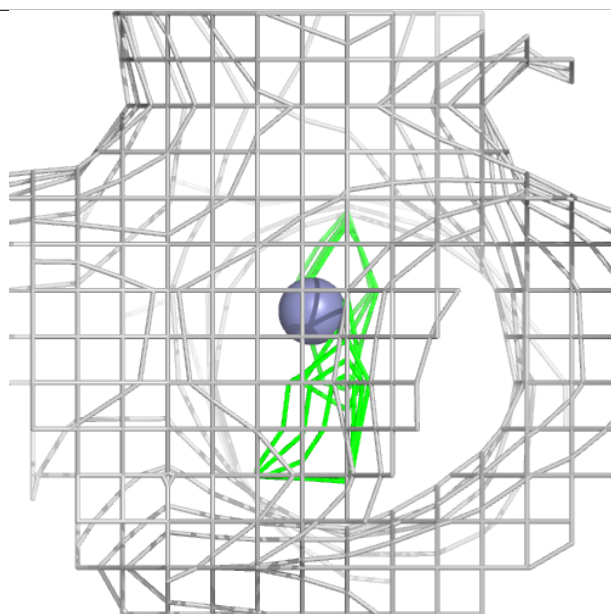
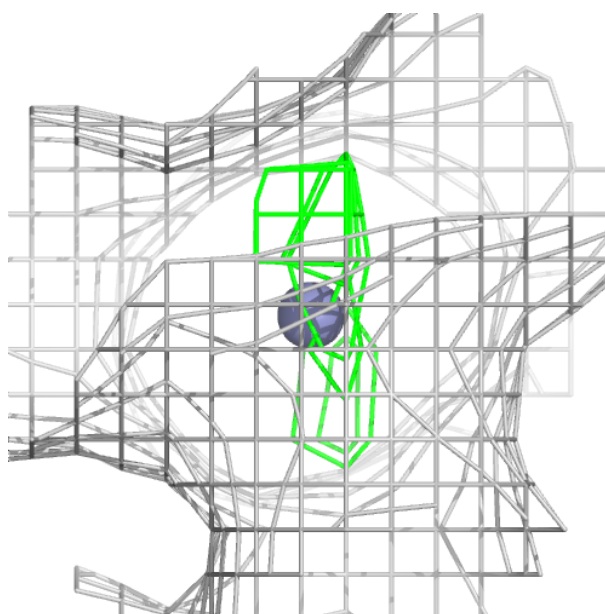
Electron density around ZN B 501:

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



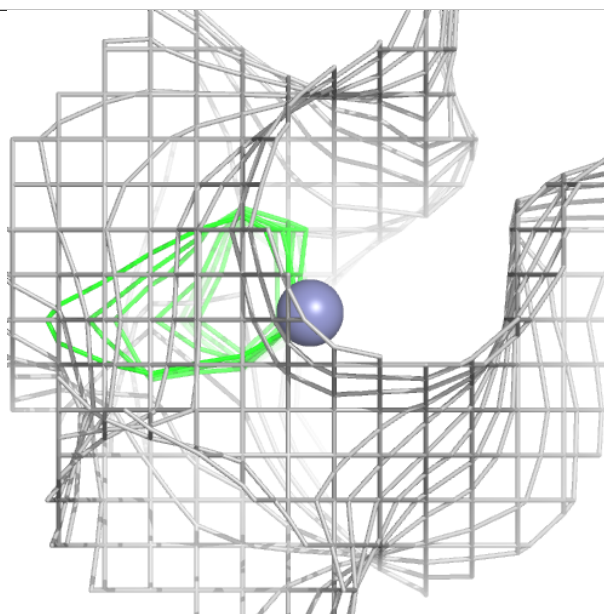
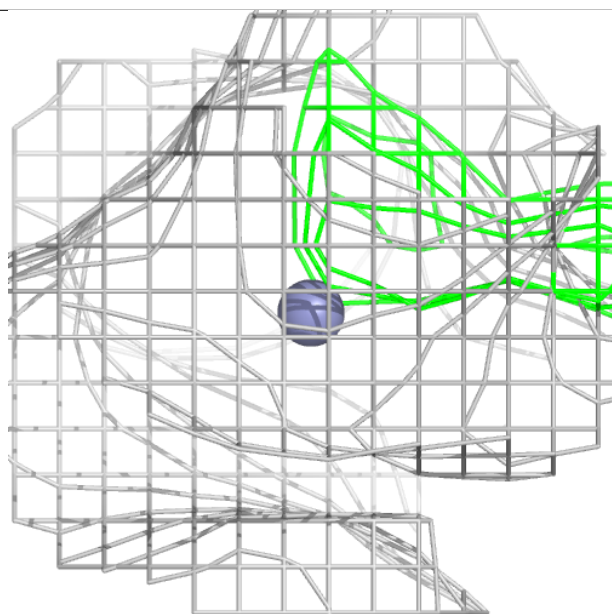
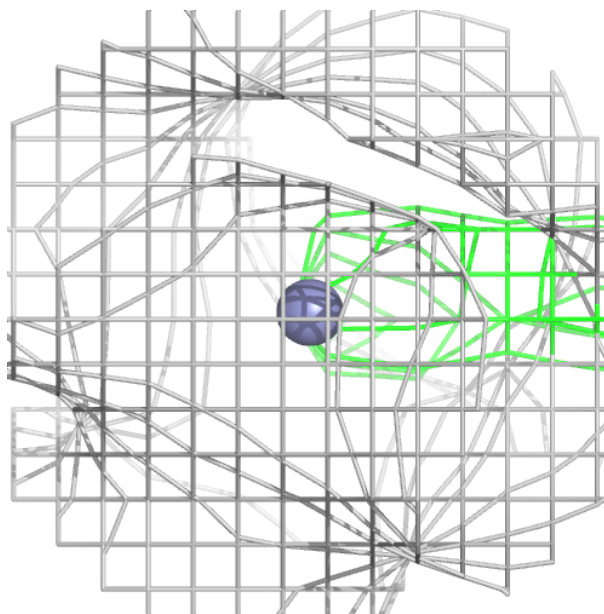
Electron density around ZN C 501:

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



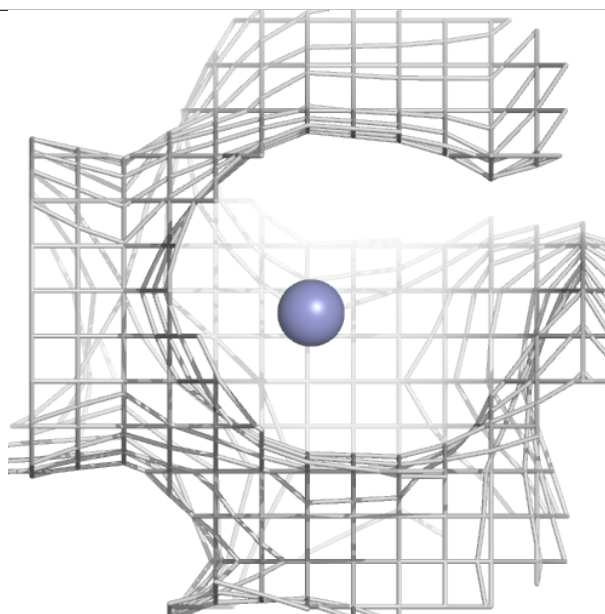
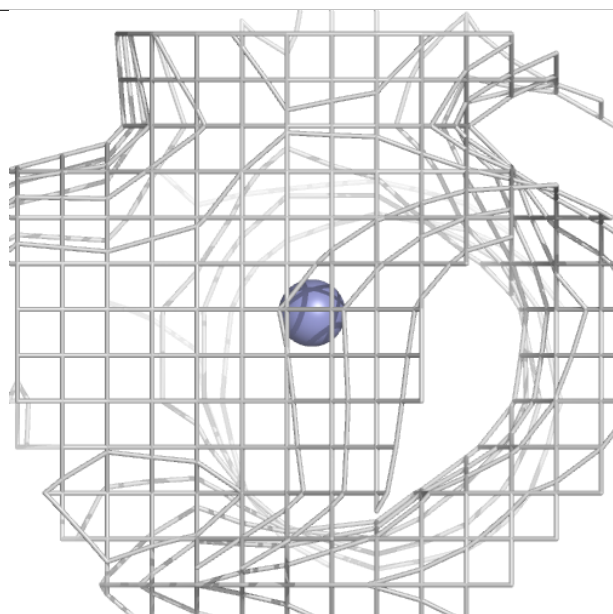
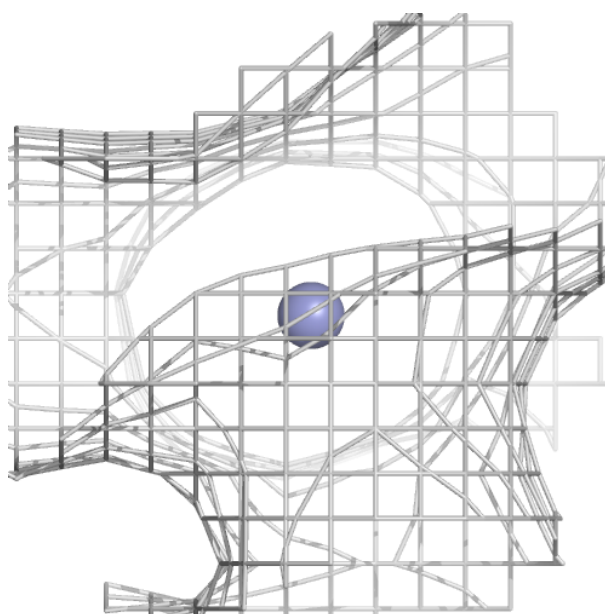
Electron density around ZN D 501:

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



Electron density around ZN A 501:

$2mF_o-DF_c$ (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.