



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:41 PM UTC

PDB ID : 8HWN / pdb_00008hwn
Title : aldo-keto reductase DepB
Authors : Chen, M.; Yang, H.; Lu, F.
Deposited on : 2022-12-31
Resolution : 2.70 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

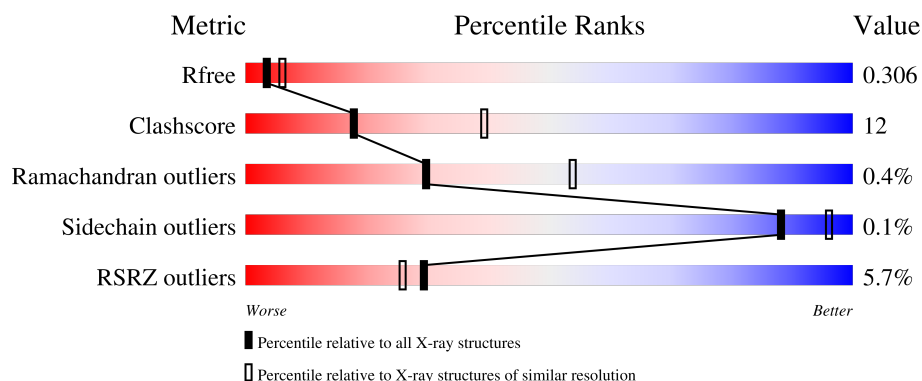
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	343	
1	B	343	
1	C	343	
1	D	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	404	-	-	X	-
3	CL	A	405	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9573 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 DepB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	324	Total	C	N	O	S	0	1	0
			2474	1554	446	462	12			
1	A	304	Total	C	N	O	S	0	0	0
			2326	1466	418	431	11			
1	C	302	Total	C	N	O	S	9	1	0
			2338	1471	419	437	11			
1	D	303	Total	C	N	O	S	0	0	0
			2334	1469	417	437	11			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Na	0	0
			3	3		
2	A	2	Total	Na	0	0
			2	2		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	3	Total	Cl	0	0
			3	3		

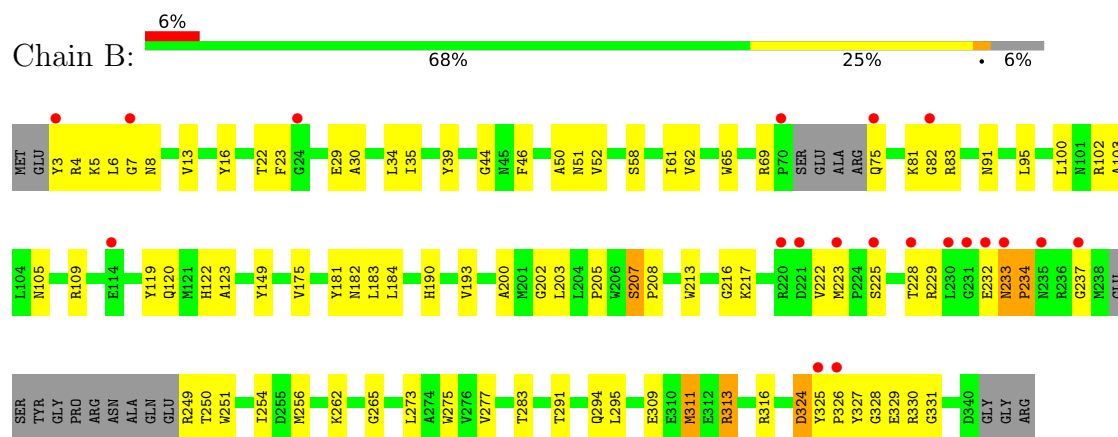
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	24	Total 24	O 24	0	0
4	A	18	Total 18	O 18	0	0
4	C	24	Total 24	O 24	0	0
4	D	22	Total 22	O 22	0	0

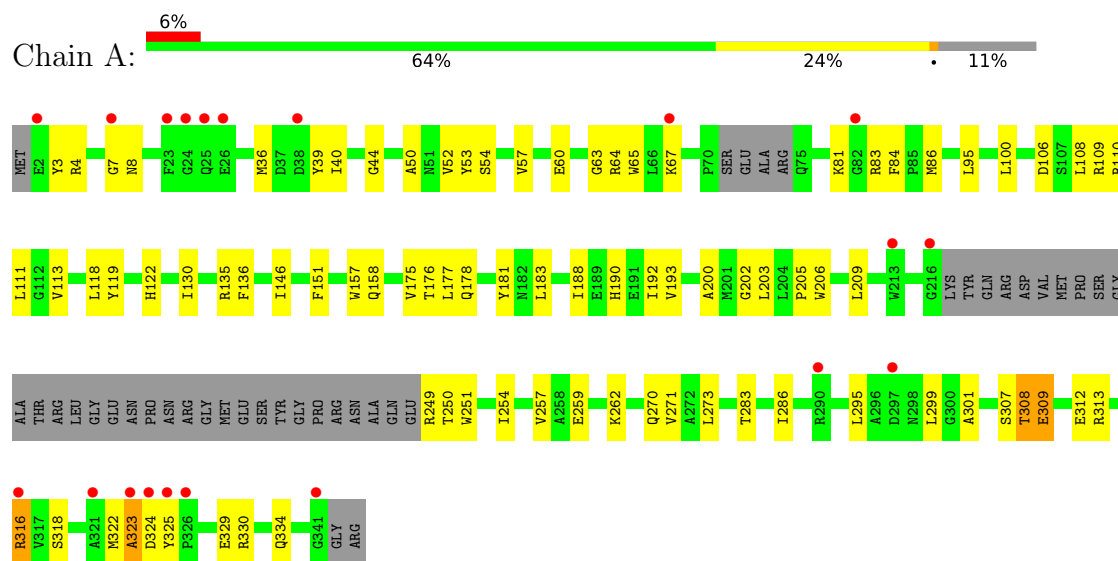
3 Residue-property plots [i](#)

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: DepB

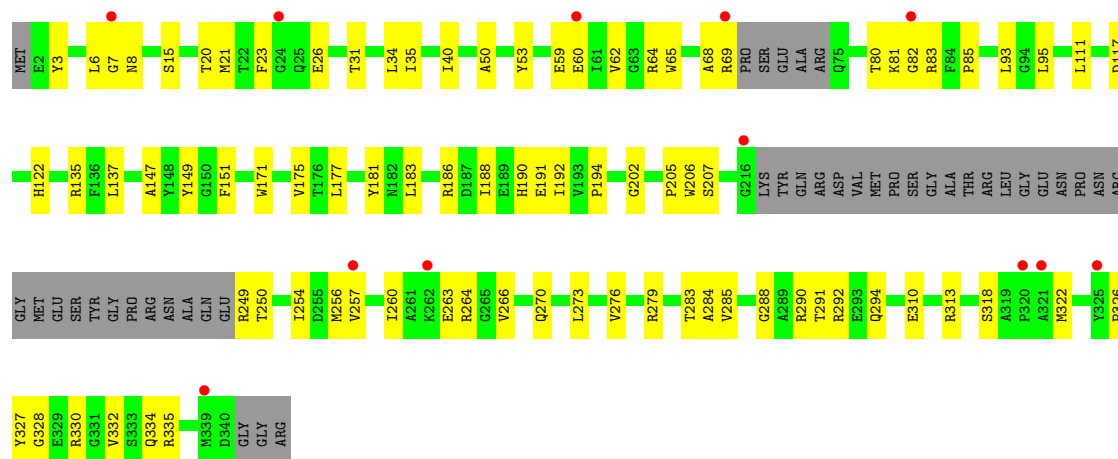


• Molecule 1: DepB

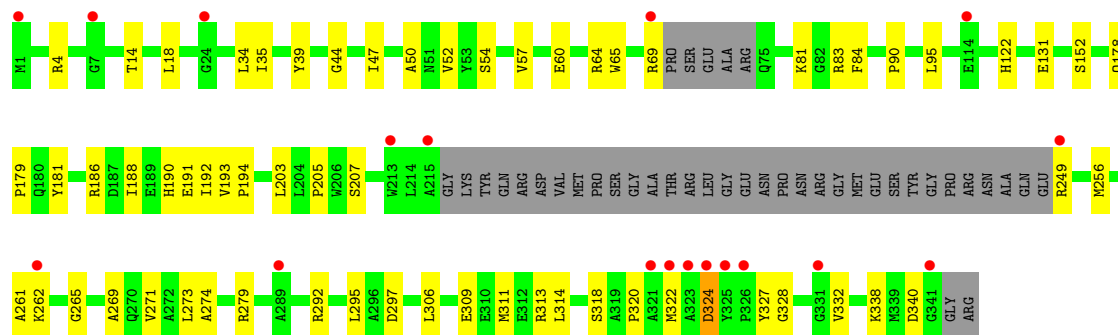


• Molecule 1: DepB





● Molecule 1: DepB



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	83.20Å 98.29Å 174.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.70 47.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.72-2.70) 99.9 (47.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.235 , 0.306 0.237 , 0.306	Depositor DCC
R_{free} test set	2000 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9573	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 47.93 % 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 9.2561e-05. 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: CL, NA

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	0.47	0/2373	0.81	12/3228 (0.4%)
1	B	0.60	3/2521 (0.1%)	0.75	5/3424 (0.1%)
1	C	0.42	0/2382	0.66	0/3236
1	D	0.43	1/2379 (0.0%)	0.62	0/3234
All	All	0.49	4/9655 (0.0%)	0.72	17/13122 (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
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	SER	C-O	-11.89	1.18	1.23
1	B	313	ARG	CZ-NH1	7.20	1.42	1.32
1	B	313	ARG	CD-NE	6.94	1.55	1.46
1	D	207	SER	C-O	6.03	1.31	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ARG	NE-CZ-NH1	-11.11	110.39	121.50
1	A	316	ARG	NH1-CZ-NH2	9.61	131.79	119.30
1	A	316	ARG	CB-CG-CD	-8.29	92.24	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ARG	CG-CD-NE	-7.87	94.70	112.00
1	A	309	GLU	CB-CG-CD	7.53	125.40	112.60
1	A	324	ASP	CA-C-N	-6.89	105.00	121.80
1	A	324	ASP	C-N-CA	-6.89	105.00	121.80
1	A	309	GLU	CA-CB-CG	-6.29	101.52	114.10
1	A	316	ARG	CA-CB-CG	6.03	126.16	114.10
1	B	234	PRO	N-CA-CB	5.66	109.20	103.25
1	B	313	ARG	CG-CD-NE	-5.46	99.99	112.00
1	A	324	ASP	N-CA-C	5.42	122.34	110.80
1	A	323	ALA	CA-C-N	5.29	131.65	121.54
1	A	323	ALA	C-N-CA	5.29	131.65	121.54
1	B	311	MET	CA-CB-CG	-5.24	103.62	114.10
1	B	233	ASN	CA-C-N	5.16	126.29	119.84
1	B	233	ASN	C-N-CA	5.16	126.29	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ALA	Peptide
1	D	324	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	2326	0	2294	68	0
1	B	2474	0	2418	62	0
1	C	2338	0	2304	59	0
1	D	2334	0	2303	42	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	5	0
3	B	3	0	0	1	0
4	A	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	2	0
4	C	24	0	0	0	0
4	D	22	0	0	3	0
All	All	9573	0	9319	231	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 12.

All (231) 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:63:GLY:O	1:A:67:LYS:HE2	1.59	1.02
1:D:34:LEU:HB3	1:D:292:ARG:HE	1.24	1.00
1:A:313:ARG:HA	1:A:316:ARG:CZ	2.01	0.90
3:A:405:CL:CL	4:A:518:HOH:O	2.28	0.89
1:A:63:GLY:O	1:A:67:LYS:CE	2.23	0.87
1:B:275:TRP:CD1	1:B:311:MET:HE3	2.14	0.82
1:A:151:PHE:HB2	1:A:177:LEU:HD12	1.62	0.81
1:D:297:ASP:OD2	4:D:501:HOH:O	1.99	0.79
1:B:91:ASN:O	1:B:102:ARG:NH2	2.17	0.78
1:C:6:LEU:HD12	1:C:7:GLY:O	1.84	0.78
1:A:249:ARG:HH11	1:A:251:TRP:HD1	1.32	0.77
1:C:326:PRO:O	1:C:335:ARG:NH2	2.17	0.77
1:C:249:ARG:HD3	1:C:250:THR:H	1.51	0.75
1:D:181:TYR:HB3	1:D:205:PRO:HB3	1.69	0.74
1:C:186:ARG:NH1	1:C:318:SER:O	2.21	0.74
1:A:313:ARG:HA	1:A:316:ARG:NH1	2.03	0.73
1:A:109:ARG:NH2	4:A:502:HOH:O	2.20	0.73
1:C:181:TYR:HB3	1:C:205:PRO:HB3	1.69	0.73
1:A:135:ARG:HD3	3:A:404:CL:CL	2.26	0.72
1:B:8:ASN:ND2	1:B:200:ALA:O	2.22	0.71
1:A:175:VAL:HG23	1:A:176:THR:HB	1.73	0.70
1:B:182:ASN:ND2	1:B:207:SER:O	2.26	0.69
1:A:249:ARG:NH1	1:A:251:TRP:HD1	1.91	0.68
1:D:152:SER:HB2	1:D:178:GLN:HB3	1.74	0.68
1:B:29:GLU:HG3	1:B:61:ILE:HG12	1.76	0.67
1:B:265:GLY:O	4:B:501:HOH:O	2.13	0.67
1:A:50:ALA:HB2	1:A:81:LYS:HD2	1.77	0.67
1:A:7:GLY:HA3	3:A:405:CL:CL	2.32	0.66
1:B:83:ARG:HB2	1:B:95:LEU:HD21	1.76	0.66
1:B:250:THR:HG22	1:B:254:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:HA	1:B:309:GLU:OE1	1.96	0.65
1:A:63:GLY:O	1:A:67:LYS:NZ	2.29	0.64
1:A:307:SER:C	1:A:309:GLU:H	2.05	0.64
1:B:232:GLU:N	4:B:504:HOH:O	2.31	0.64
1:A:181:TYR:HB3	1:A:205:PRO:HB3	1.79	0.63
1:B:324:ASP:OD2	1:B:330:ARG:NH2	2.28	0.63
1:A:135:ARG:NH1	3:A:404:CL:CL	2.61	0.63
1:A:202:GLY:HA3	1:A:283:THR:CG2	2.29	0.63
1:B:30:ALA:O	1:B:34:LEU:HG	1.98	0.63
1:D:4:ARG:HG3	1:D:4:ARG:HH11	1.63	0.63
1:B:181:TYR:HB3	1:B:205:PRO:HB3	1.81	0.63
1:D:60:GLU:O	1:D:64:ARG:HG2	1.99	0.62
1:C:264:ARG:HD2	1:C:310:GLU:OE2	1.99	0.62
1:D:50:ALA:HB2	1:D:81:LYS:HD2	1.82	0.61
1:B:16:TYR:HE2	1:B:273:LEU:HG	1.65	0.61
1:A:106:ASP:HB3	1:A:110:ARG:NH1	2.16	0.60
1:B:6:LEU:H	1:B:6:LEU:HD23	1.66	0.60
1:A:313:ARG:HA	1:A:316:ARG:NH2	2.16	0.60
1:D:52:VAL:HG11	1:D:84:PHE:HB2	1.82	0.60
1:A:209:LEU:HD21	1:A:273:LEU:HG	1.83	0.59
1:C:31:THR:O	1:C:35:ILE:HG13	2.03	0.59
1:B:58:SER:O	1:B:62:VAL:HG23	2.02	0.59
1:A:308:THR:O	1:A:312:GLU:HG3	2.03	0.58
1:D:188:ILE:HG22	1:D:192:ILE:HD12	1.85	0.58
1:B:222:VAL:HG23	1:B:225:SER:HB2	1.86	0.58
1:D:338:LYS:HB3	1:D:340:ASP:OD1	2.03	0.58
1:A:330:ARG:NH2	1:A:334:GLN:OE1	2.37	0.58
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.19	0.58
1:B:35:ILE:HG23	1:B:295:LEU:HD22	1.86	0.57
1:A:249:ARG:NH1	1:A:251:TRP:CD1	2.72	0.57
1:C:59:GLU:OE2	1:C:80:THR:OG1	2.15	0.57
1:C:82:GLY:O	1:C:122:HIS:HB2	2.05	0.57
1:C:330:ARG:HG2	1:C:334:GLN:NE2	2.20	0.57
1:A:7:GLY:O	1:A:175:VAL:HB	2.05	0.57
1:A:193:VAL:HG22	1:A:203:LEU:HD11	1.86	0.57
1:B:7:GLY:HA3	3:B:404:CL:CL	2.41	0.57
1:D:35:ILE:HG23	1:D:295:LEU:HD22	1.86	0.56
1:A:60:GLU:O	1:A:64:ARG:HG2	2.05	0.56
1:A:83:ARG:HB3	1:A:122:HIS:CB	2.36	0.56
1:C:205:PRO:HD2	1:C:284:ALA:O	2.05	0.55
1:D:309:GLU:O	1:D:313:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:O	1:A:254:ILE:HG12	2.06	0.55
1:C:26:GLU:OE2	1:C:290:ARG:HD3	2.07	0.55
1:C:20:THR:HG22	1:C:23:PHE:CE2	2.42	0.54
1:A:295:LEU:O	1:A:299:LEU:HG	2.07	0.54
1:A:307:SER:C	1:A:309:GLU:N	2.65	0.54
1:D:261:ALA:HA	1:D:271:VAL:HG21	1.89	0.53
1:A:307:SER:O	1:A:309:GLU:N	2.41	0.53
1:C:291:THR:OG1	1:C:294:GLN:HG3	2.09	0.53
1:B:65:TRP:CH2	1:B:69:ARG:HD2	2.43	0.53
1:C:83:ARG:HB2	1:C:95:LEU:HD21	1.91	0.53
1:D:54:SER:O	1:D:57:VAL:HG23	2.08	0.53
1:B:16:TYR:CZ	1:B:277:VAL:HG21	2.44	0.53
1:B:105:ASN:O	1:B:109:ARG:HG3	2.09	0.53
1:A:52:VAL:HG11	1:A:84:PHE:HB2	1.90	0.53
1:B:7:GLY:O	1:B:175:VAL:HB	2.09	0.53
1:D:18:LEU:HB3	1:D:47:ILE:HG12	1.91	0.52
1:C:151:PHE:HB2	1:C:177:LEU:HD13	1.91	0.52
1:B:82:GLY:O	1:B:122:HIS:HB2	2.09	0.52
1:B:69:ARG:HH22	1:B:75:GLN:HA	1.74	0.52
1:A:39:TYR:CZ	1:A:44:GLY:HA3	2.45	0.52
1:B:182:ASN:HB3	1:B:208:PRO:HA	1.91	0.52
1:A:190:HIS:CE1	1:A:322:MET:HG3	2.45	0.52
1:C:83:ARG:HB2	1:C:95:LEU:CD2	2.40	0.52
1:D:322:MET:HB3	1:D:324:ASP:OD2	2.10	0.51
1:A:206:TRP:HB3	1:A:286:ILE:HD12	1.92	0.51
1:D:328:GLY:O	1:D:332:VAL:HG13	2.11	0.51
1:A:329:GLU:HG3	1:A:330:ARG:N	2.26	0.51
1:C:8:ASN:HB3	1:C:175:VAL:HA	1.91	0.51
1:C:68:ALA:O	1:C:69:ARG:HB2	2.09	0.51
1:A:54:SER:O	1:A:57:VAL:HG12	2.11	0.51
1:B:249:ARG:HH11	1:B:251:TRP:CD1	2.29	0.51
1:D:65:TRP:CZ2	1:D:69:ARG:HD2	2.46	0.51
1:B:3:TYR:CD2	1:B:5:LYS:HE2	2.46	0.50
1:C:183:LEU:O	1:C:318:SER:HB2	2.11	0.50
1:B:39:TYR:CZ	1:B:44:GLY:HA3	2.46	0.50
1:A:188:ILE:HG22	1:A:192:ILE:HG13	1.93	0.50
1:A:181:TYR:CD1	1:A:188:ILE:HD11	2.47	0.50
1:D:34:LEU:HD23	1:D:292:ARG:NE	2.27	0.50
1:C:188:ILE:HG22	1:C:192:ILE:HD12	1.93	0.50
1:A:190:HIS:CD2	1:A:322:MET:HE3	2.47	0.50
1:C:249:ARG:HD3	1:C:250:THR:N	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD23	1:A:113:VAL:HG23	1.94	0.50
1:B:83:ARG:HG2	1:B:123:ALA:H	1.76	0.49
1:C:151:PHE:O	1:C:177:LEU:HA	2.12	0.49
1:C:250:THR:O	1:C:254:ILE:HG12	2.12	0.49
1:C:256:MET:HE2	1:C:313:ARG:NH2	2.28	0.49
1:C:206:TRP:CE3	1:C:207:SER:HB2	2.48	0.49
1:B:119:TYR:O	1:B:149:TYR:HA	2.13	0.49
1:B:184:LEU:HB3	1:B:237:GLY:O	2.13	0.48
1:D:190:HIS:HB3	1:D:327:TYR:CD1	2.48	0.48
1:C:85:PRO:HG3	1:C:93:LEU:HD13	1.95	0.48
1:C:256:MET:HE2	1:C:313:ARG:HH21	1.79	0.48
1:C:288:GLY:O	1:C:290:ARG:NH1	2.47	0.48
1:B:325:TYR:HB3	1:B:326:PRO:HD3	1.96	0.48
1:A:36:MET:O	1:A:40:ILE:HG12	2.13	0.48
1:A:7:GLY:CA	3:A:405:CL:CL	2.99	0.48
1:A:4:ARG:HD3	1:D:90:PRO:HB3	1.95	0.47
1:C:276:VAL:HG23	1:C:285:VAL:HG21	1.96	0.47
1:B:51:ASN:OD1	1:B:52:VAL:N	2.48	0.47
1:A:67:LYS:NZ	1:A:111:LEU:O	2.38	0.47
1:C:183:LEU:HD13	1:C:257:VAL:CG2	2.45	0.47
1:C:266:VAL:HG22	1:C:270:GLN:OE1	2.14	0.47
1:A:249:ARG:HH11	1:A:251:TRP:CD1	2.21	0.47
1:D:249:ARG:N	4:D:504:HOH:O	2.48	0.47
1:B:202:GLY:HA3	1:B:283:THR:CG2	2.45	0.47
1:B:213:TRP:NE1	1:B:228:THR:O	2.48	0.47
1:C:181:TYR:CD1	1:C:188:ILE:HD11	2.50	0.47
1:C:34:LEU:HD13	1:C:292:ARG:NH1	2.30	0.46
1:C:191:GLU:C	1:C:194:PRO:HD2	2.40	0.46
1:C:190:HIS:NE2	1:C:322:MET:HG3	2.31	0.46
1:B:50:ALA:HB2	1:B:81:LYS:HD2	1.97	0.46
1:A:118:LEU:HD21	1:A:176:THR:HG21	1.97	0.46
1:B:190:HIS:CD2	1:B:327:TYR:HB3	2.51	0.46
1:C:50:ALA:HB2	1:C:81:LYS:HD2	1.98	0.46
1:A:259:GLU:HA	1:A:262:LYS:HE2	1.97	0.45
1:A:119:TYR:HB2	1:A:146:ILE:HD12	1.98	0.45
1:D:179:PRO:HG3	1:D:203:LEU:HD22	1.98	0.45
1:A:151:PHE:O	1:A:177:LEU:HA	2.16	0.45
1:B:4:ARG:HG3	1:B:4:ARG:HH11	1.81	0.45
1:C:273:LEU:HA	1:C:273:LEU:HD12	1.57	0.45
1:A:83:ARG:HD3	1:A:95:LEU:HG	1.99	0.45
1:B:83:ARG:HG2	1:B:123:ALA:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:HB3	1:D:122:HIS:CB	2.47	0.44
1:C:3:TYR:O	1:C:15:SER:N	2.50	0.44
1:B:29:GLU:HG3	1:B:61:ILE:HG23	1.99	0.44
1:A:178:GLN:HG2	1:A:206:TRP:HD1	1.81	0.44
1:B:313:ARG:HA	1:B:316:ARG:HH12	1.83	0.44
1:D:4:ARG:HG3	1:D:4:ARG:NH1	2.31	0.44
1:A:100:LEU:HB3	1:A:136:PHE:CE2	2.52	0.44
1:C:190:HIS:CD2	1:C:327:TYR:HB3	2.53	0.44
1:D:83:ARG:HB2	1:D:95:LEU:HD21	2.00	0.44
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.82	0.44
1:B:100:LEU:HA	1:B:103:ALA:HB3	2.00	0.44
1:C:330:ARG:HG2	1:C:334:GLN:HE21	1.82	0.44
1:B:262:LYS:HE3	1:B:262:LYS:O	2.17	0.43
1:D:193:VAL:HG22	1:D:203:LEU:HD11	1.99	0.43
1:A:257:VAL:HG13	1:A:271:VAL:HG12	2.00	0.43
1:D:52:VAL:HG11	1:D:84:PHE:CB	2.48	0.43
1:D:186:ARG:HB2	1:D:320:PRO:HG3	2.00	0.43
1:D:314:LEU:O	1:D:318:SER:HB3	2.17	0.43
1:C:202:GLY:HA3	1:C:283:THR:CG2	2.47	0.43
1:C:328:GLY:O	1:C:332:VAL:HG23	2.19	0.43
1:C:135:ARG:HB2	1:C:171:TRP:CH2	2.53	0.43
1:D:273:LEU:HD12	1:D:273:LEU:HA	1.78	0.43
1:B:316:ARG:HB3	1:B:316:ARG:NH1	2.33	0.43
1:C:53:TYR:HD1	1:C:53:TYR:HA	1.63	0.43
1:C:62:VAL:HG23	1:C:111:LEU:HD23	2.00	0.43
1:A:86:MET:HE2	1:A:110:ARG:HH22	1.84	0.43
1:B:81:LYS:HG2	1:B:120:GLN:HB2	2.00	0.43
1:C:60:GLU:HG3	1:C:64:ARG:CZ	2.49	0.43
1:C:188:ILE:HG22	1:C:192:ILE:CD1	2.48	0.43
1:B:256:MET:HE3	1:B:256:MET:HB2	1.77	0.43
1:C:260:ILE:HA	1:C:263:GLU:HG2	2.00	0.43
1:C:21:MET:HA	1:C:53:TYR:CD2	2.54	0.43
1:B:216:GLY:O	1:B:217:LYS:HB3	2.20	0.42
1:B:325:TYR:O	1:B:331:GLY:HA3	2.18	0.42
1:C:40:ILE:HG13	1:C:65:TRP:CH2	2.54	0.42
1:B:13:VAL:HG21	1:B:46:PHE:CD2	2.54	0.42
1:A:3:TYR:C	1:A:3:TYR:CD2	2.97	0.42
1:A:270:GLN:HA	1:A:301:ALA:HB2	2.00	0.42
1:B:183:LEU:HG	1:B:275:TRP:CE3	2.55	0.42
1:A:183:LEU:O	1:A:318:SER:HB2	2.19	0.42
1:B:291:THR:HG1	1:B:294:GLN:H	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:MET:HE2	1:D:313:ARG:HB2	2.01	0.42
1:D:262:LYS:HD3	1:D:265:GLY:HA2	2.01	0.42
1:A:57:VAL:HA	1:A:60:GLU:HG2	2.01	0.42
1:D:191:GLU:C	1:D:194:PRO:HD2	2.45	0.42
1:A:40:ILE:HD11	1:A:65:TRP:HH2	1.84	0.42
1:C:82:GLY:O	1:C:83:ARG:HB3	2.19	0.42
1:D:14:THR:HG21	1:D:44:GLY:HA2	2.01	0.42
1:C:334:GLN:H	1:C:334:GLN:HG2	1.77	0.42
1:A:312:GLU:O	1:A:316:ARG:NH1	2.53	0.42
1:D:279:ARG:HD2	1:D:279:ARG:HA	1.81	0.42
1:D:322:MET:HB3	1:D:322:MET:HE2	1.60	0.42
1:B:22:THR:HG23	1:B:23:PHE:HD1	1.85	0.41
1:B:193:VAL:HG22	1:B:203:LEU:HD11	2.01	0.41
1:A:178:GLN:HE21	1:A:206:TRP:CD1	2.38	0.41
1:D:39:TYR:CZ	1:D:44:GLY:HA3	2.54	0.41
1:A:8:ASN:HB2	1:A:200:ALA:O	2.20	0.41
1:C:137:LEU:HD13	1:C:149:TYR:CD2	2.55	0.41
1:A:50:ALA:HB3	1:A:53:TYR:CG	2.56	0.41
1:D:274:ALA:HB3	1:D:306:LEU:HD13	2.02	0.41
1:B:223:MET:HE1	1:B:250:THR:HG21	2.02	0.41
1:A:83:ARG:HB3	1:A:122:HIS:HB3	2.03	0.41
1:C:40:ILE:HG13	1:C:65:TRP:HH2	1.85	0.41
1:B:3:TYR:CE2	1:B:5:LYS:HE2	2.55	0.41
1:B:8:ASN:OD1	1:B:8:ASN:O	2.39	0.41
1:A:157:TRP:CE2	1:A:158:GLN:HG3	2.56	0.41
1:C:279:ARG:HA	1:C:279:ARG:HD2	1.88	0.41
1:D:131:GLU:H	1:D:131:GLU:CD	2.29	0.41
1:B:328:GLY:O	1:B:329:GLU:C	2.64	0.41
1:C:322:MET:HE2	1:C:327:TYR:HB2	2.03	0.41
1:D:306:LEU:HB2	1:D:311:MET:CE	2.51	0.41
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.95	0.40
1:C:151:PHE:HB2	1:C:177:LEU:CD1	2.51	0.40
1:B:249:ARG:HH11	1:B:251:TRP:HD1	1.68	0.40
1:C:117:ASP:O	1:C:147:ALA:HB3	2.21	0.40
1:D:269:ALA:HB3	4:D:501:HOH:O	2.20	0.40
1:B:217:LYS:HB3	1:B:217:LYS:HE3	1.68	0.40
1:A:130:ILE:HD12	1:A:130:ILE:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/343 (87%)	283 (95%)	13 (4%)	2 (1%)	18	41
1	B	318/343 (93%)	292 (92%)	23 (7%)	3 (1%)	14	35
1	C	297/343 (87%)	283 (95%)	14 (5%)	0	100	100
1	D	297/343 (87%)	282 (95%)	15 (5%)	0	100	100
All	All	1210/1372 (88%)	1140 (94%)	65 (5%)	5 (0%)	30	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	PRO
1	A	308	THR
1	B	233	ASN
1	B	229	ARG
1	A	325	TYR

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	236/271 (87%)	236 (100%)	0	100	100
1	B	249/271 (92%)	248 (100%)	1 (0%)	84	93
1	C	239/271 (88%)	239 (100%)	0	100	100
1	D	239/271 (88%)	239 (100%)	0	100	100
All	All	963/1084 (89%)	962 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	324	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	75	GLN
1	B	336	HIS
1	A	190	HIS
1	C	120	GLN
1	C	169	ASN
1	C	180	GLN
1	C	197	GLN
1	C	334	GLN
1	C	336	HIS
1	D	169	ASN
1	D	197	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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	304/343 (88%)	0.44	20 (6%) 24 21	27, 52, 76, 95	0
1	B	324/343 (94%)	0.45	20 (6%) 26 23	27, 51, 77, 92	1 (0%)
1	C	302/343 (88%)	0.38	12 (3%) 42 38	28, 52, 74, 90	1 (0%)
1	D	303/343 (88%)	0.45	18 (5%) 28 25	30, 54, 80, 101	0
All	All	1233/1372 (89%)	0.43	70 (5%) 29 26	27, 52, 77, 101	2 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	323	ALA	6.2
1	D	321	ALA	4.8
1	C	257	VAL	4.5
1	A	82	GLY	4.4
1	A	2	GLU	4.3
1	A	323	ALA	4.2
1	A	24	GLY	4.1
1	B	82	GLY	3.6
1	B	231	GLY	3.6
1	D	215	ALA	3.6
1	B	220	ARG	3.5
1	A	321	ALA	3.5
1	C	216	GLY	3.5
1	B	235	ASN	3.5
1	C	321	ALA	3.4
1	A	26	GLU	3.4
1	A	341	GLY	3.4
1	B	24	GLY	3.3
1	C	7	GLY	3.3
1	B	228	THR	3.3
1	A	324	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	230	LEU	3.2
1	A	7	GLY	3.2
1	D	324	ASP	3.2
1	D	7	GLY	3.1
1	B	7	GLY	3.1
1	D	24	GLY	3.1
1	C	24	GLY	3.0
1	D	322	MET	3.0
1	D	331	GLY	3.0
1	B	3	TYR	2.9
1	B	326	PRO	2.9
1	B	325	TYR	2.8
1	A	67	LYS	2.8
1	A	213	TRP	2.8
1	A	25	GLN	2.7
1	D	325	TYR	2.6
1	B	237	GLY	2.6
1	B	223	MET	2.6
1	A	316	ARG	2.5
1	B	233	ASN	2.5
1	B	225	SER	2.5
1	A	216	GLY	2.4
1	C	262	LYS	2.4
1	D	262	LYS	2.4
1	D	114	GLU	2.3
1	D	1	MET	2.3
1	D	326	PRO	2.3
1	D	289	ALA	2.3
1	A	325	TYR	2.3
1	C	60	GLU	2.3
1	C	69	ARG	2.3
1	D	249	ARG	2.2
1	B	221	ASP	2.2
1	A	326	PRO	2.2
1	B	75	GLN	2.2
1	C	82	GLY	2.2
1	A	290	ARG	2.1
1	B	70	PRO	2.1
1	D	69	ARG	2.1
1	C	339	MET	2.1
1	B	114	GLU	2.1
1	C	320	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	325	TYR	2.1
1	D	341	GLY	2.1
1	A	23	PHE	2.1
1	D	213	TRP	2.1
1	B	232	GLU	2.0
1	A	38	ASP	2.0
1	A	297	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

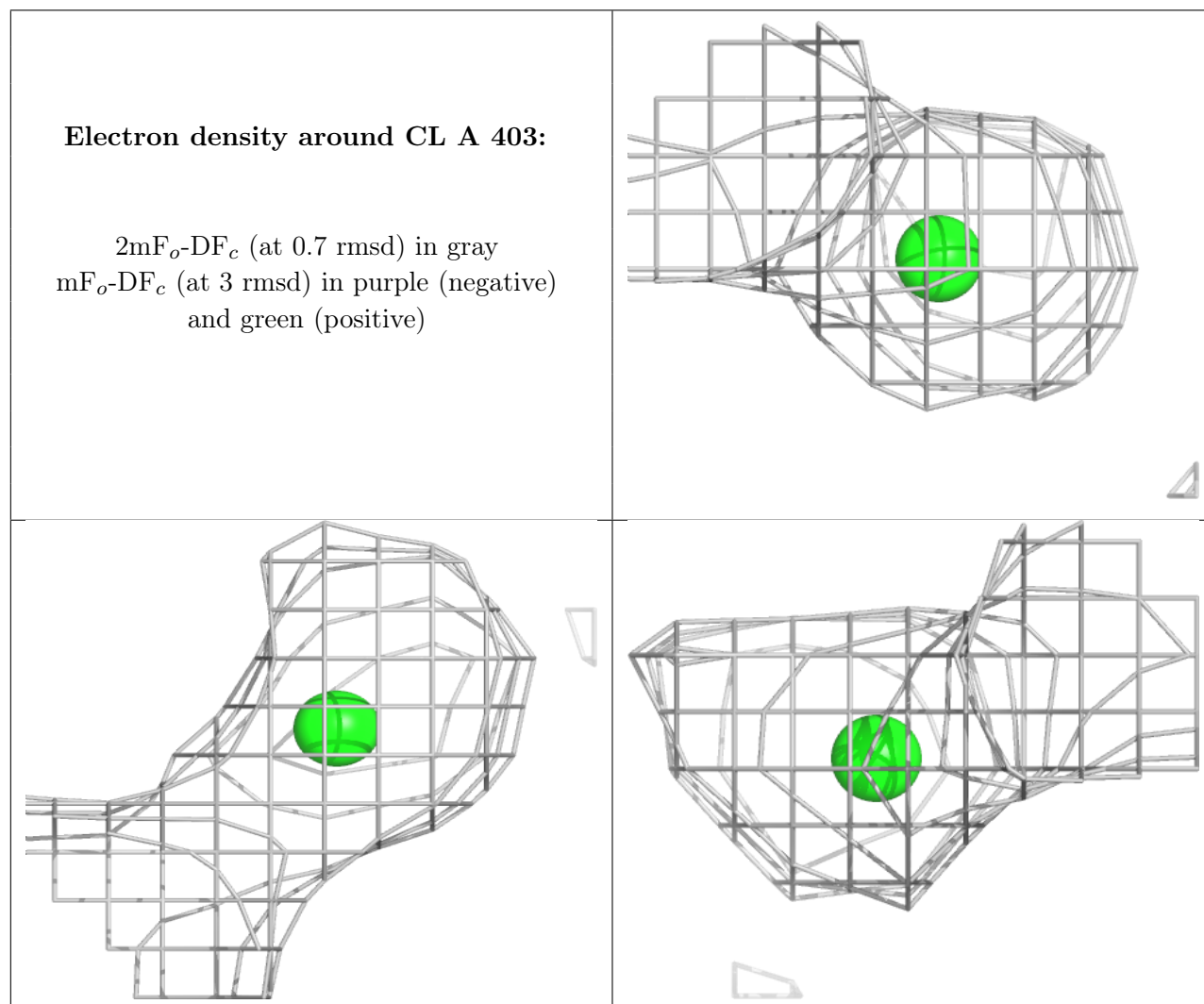
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	A	403	1/1	0.75	0.15	74,74,74,74	0
3	CL	A	405	1/1	0.86	0.14	71,71,71,71	0
3	CL	B	406	1/1	0.90	0.06	73,73,73,73	0
2	NA	A	402	1/1	0.90	0.25	57,57,57,57	0
3	CL	B	404	1/1	0.90	0.27	62,62,62,62	0
3	CL	B	405	1/1	0.91	0.10	68,68,68,68	0
2	NA	B	401	1/1	0.93	0.12	31,31,31,31	0
3	CL	A	404	1/1	0.93	0.11	53,53,53,53	0
2	NA	B	402	1/1	0.93	0.07	34,34,34,34	0
2	NA	A	401	1/1	0.94	0.07	42,42,42,42	0
2	NA	B	403	1/1	0.97	0.07	32,32,32,32	0
2	NA	C	401	1/1	0.97	0.06	45,45,45,45	0
2	NA	D	401	1/1	0.97	0.06	43,43,43,43	0

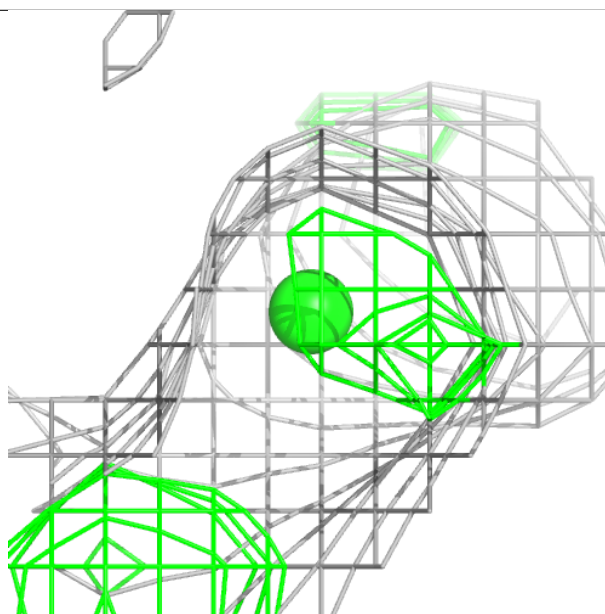
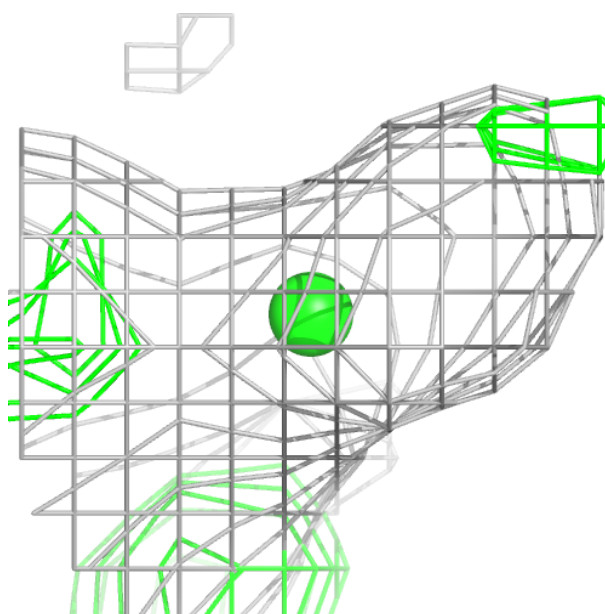
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



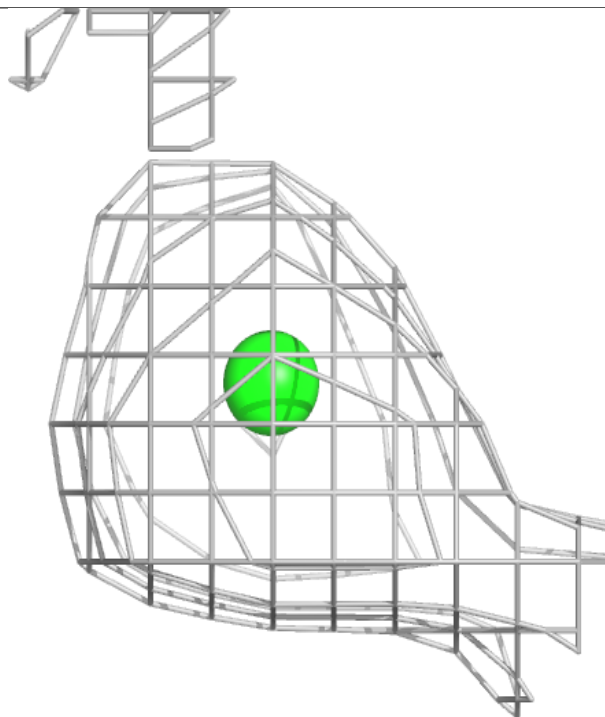
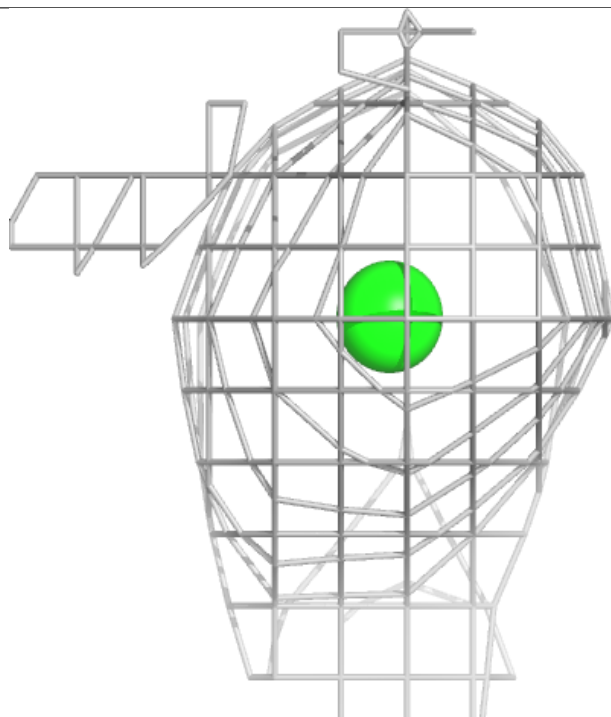
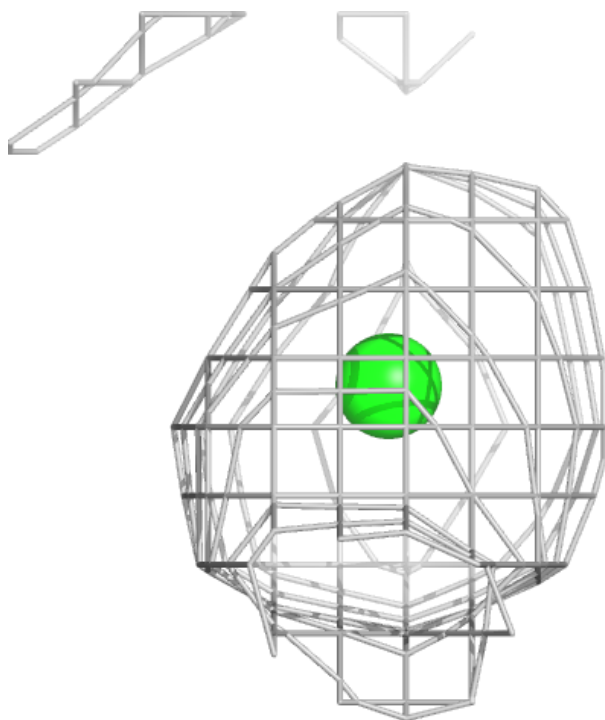
Electron density around CL A 405:

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



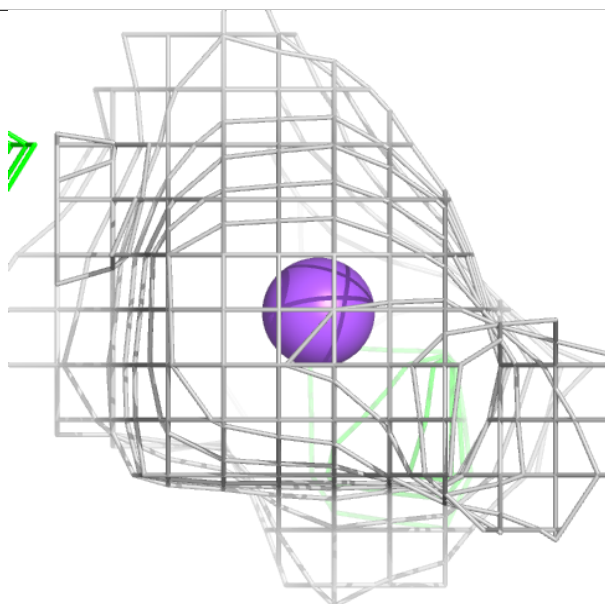
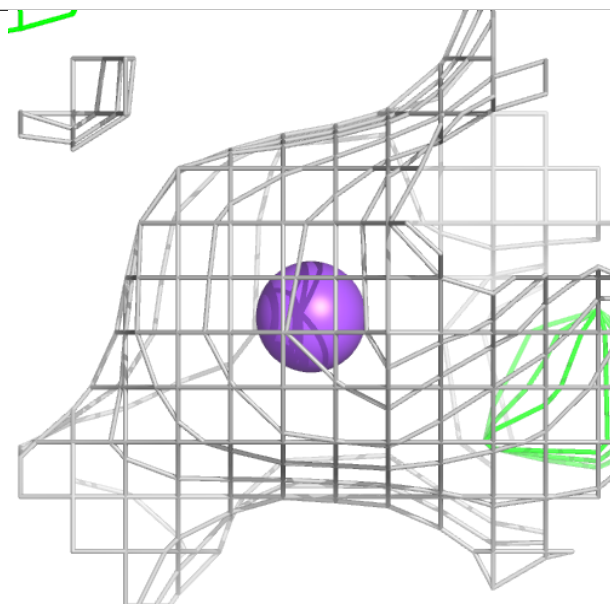
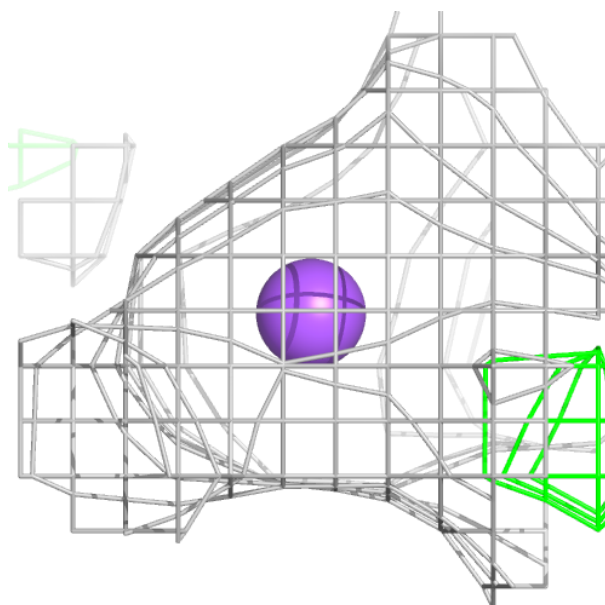
Electron density around CL B 406:

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



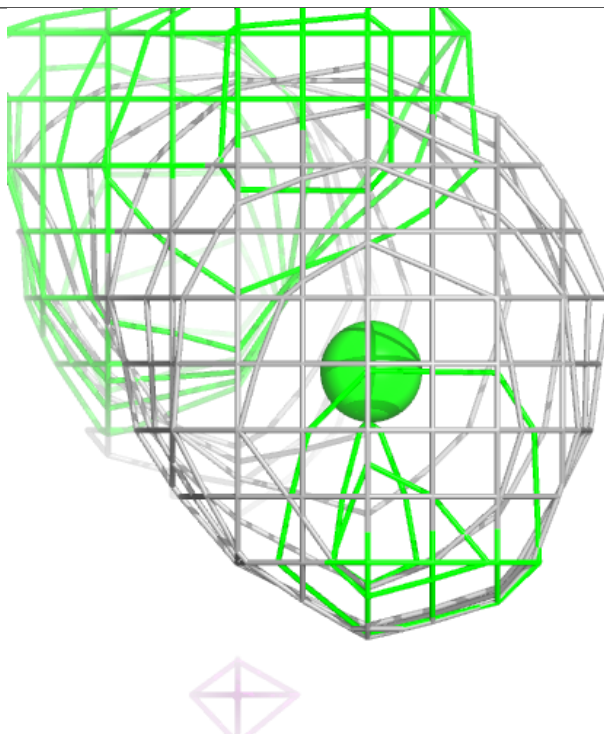
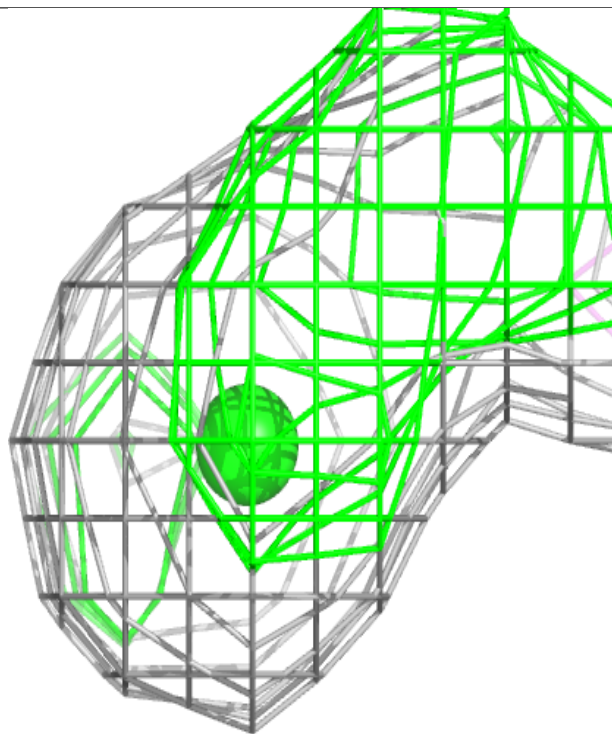
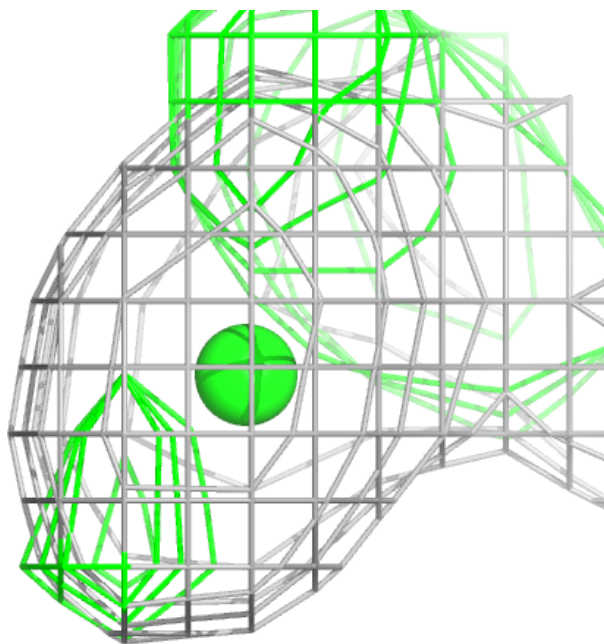
Electron density around NA A 402:

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



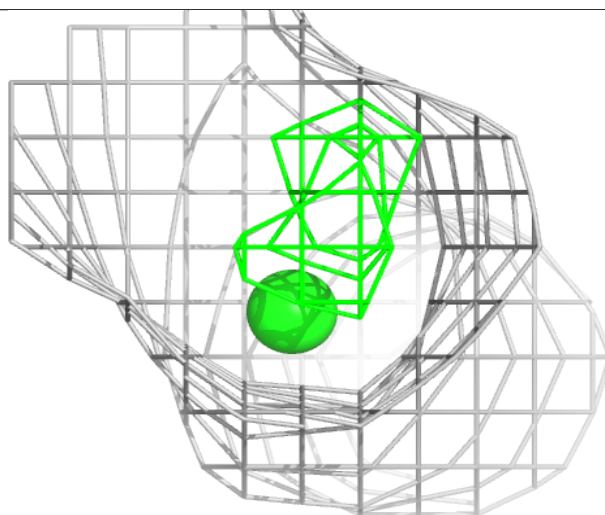
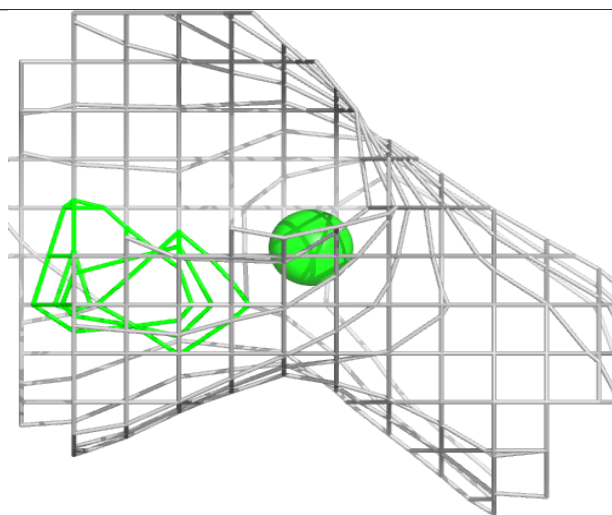
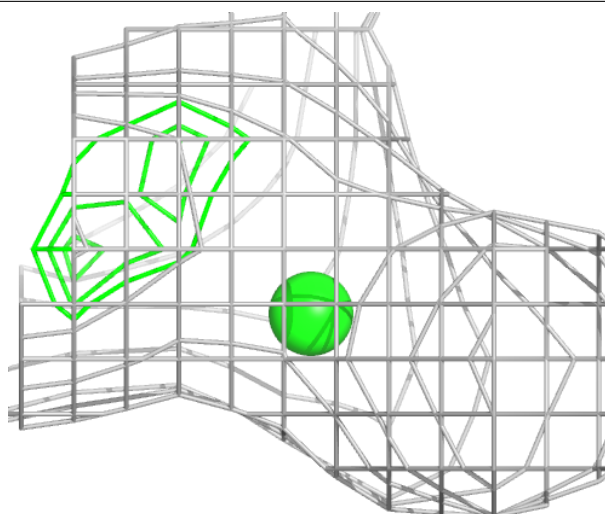
Electron density around CL B 404:

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



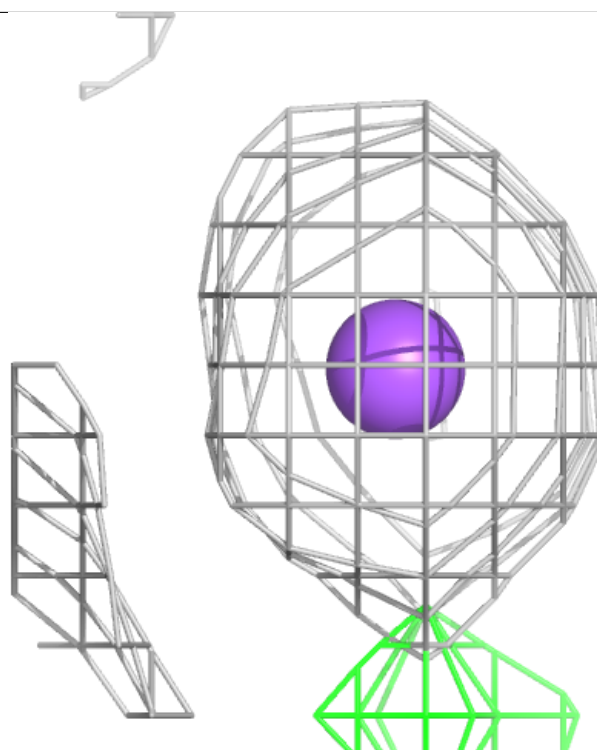
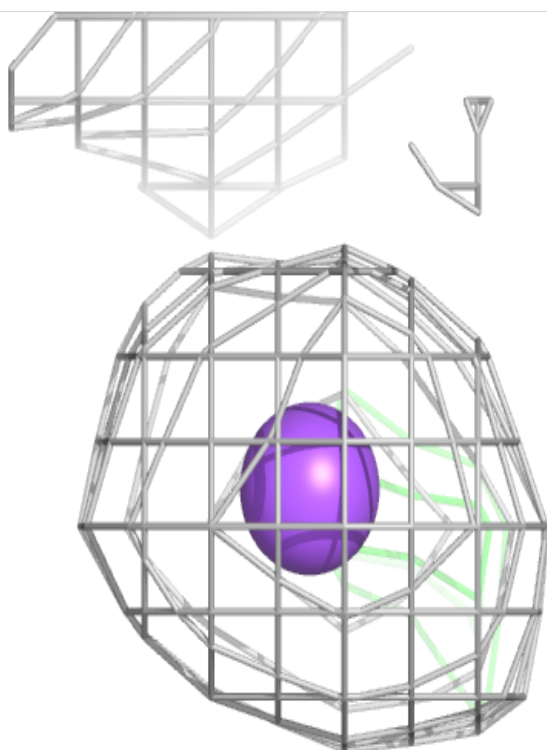
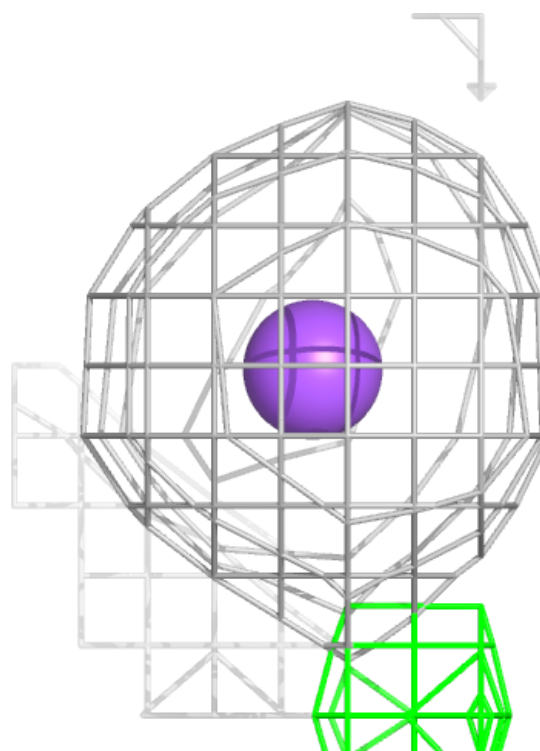
Electron density around CL B 405:

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



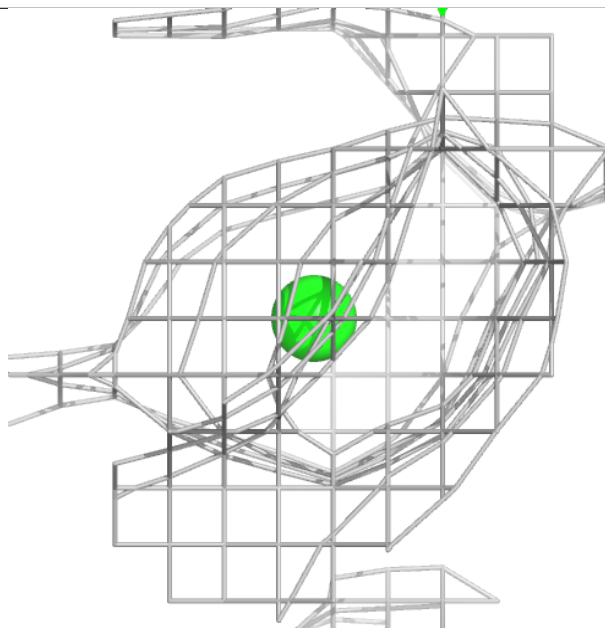
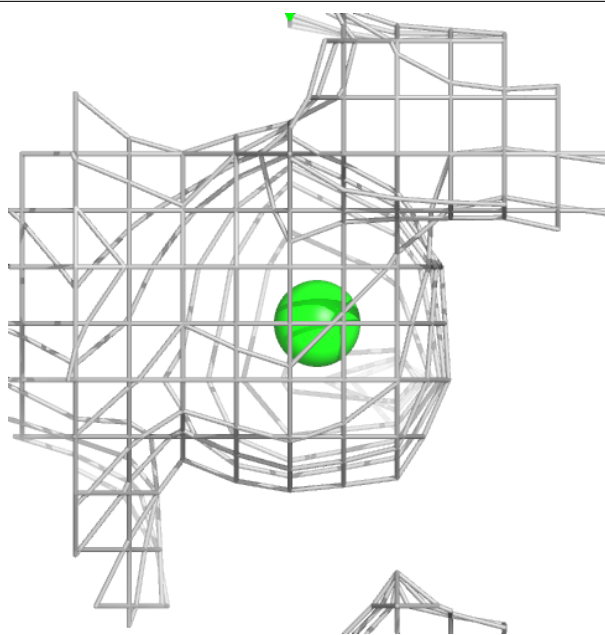
Electron density around NA B 401:

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



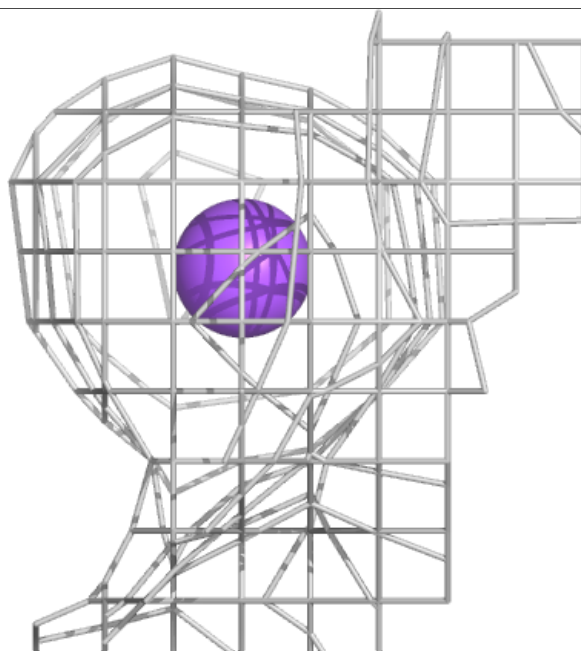
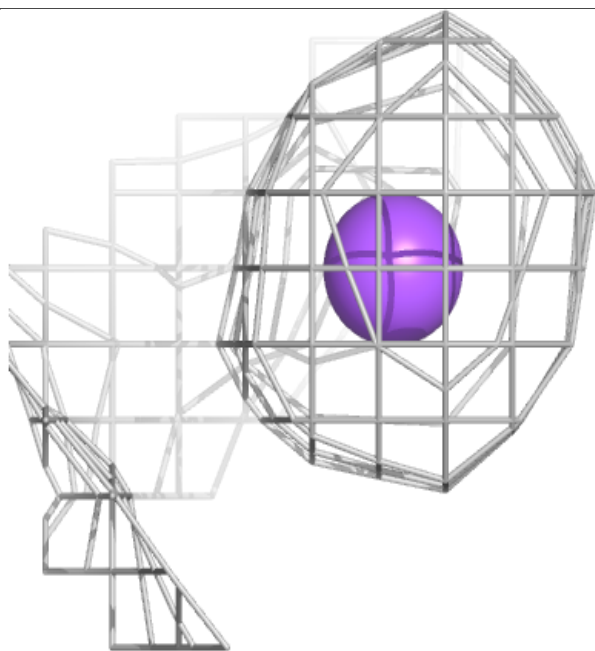
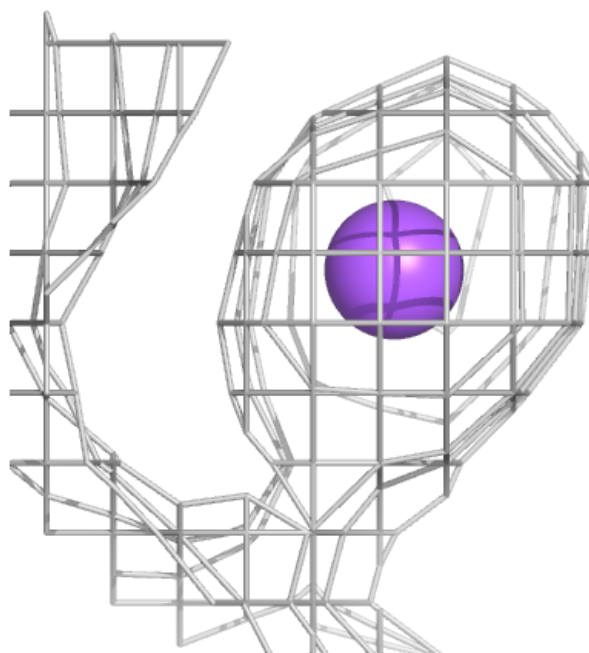
Electron density around CL A 404:

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



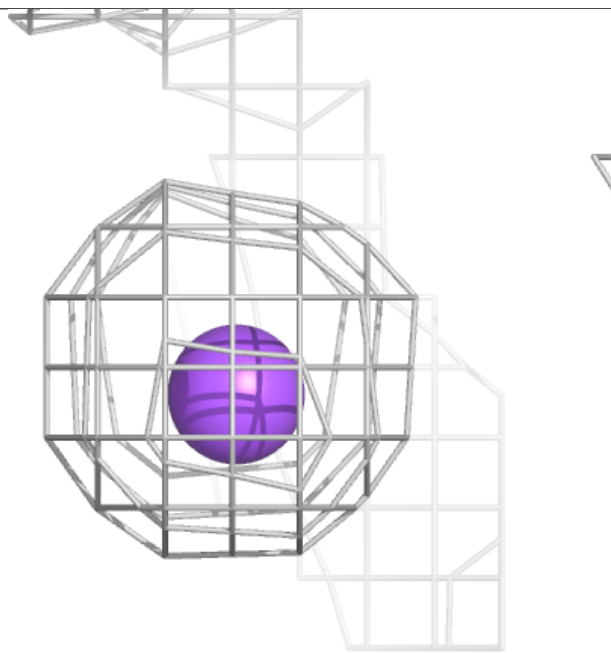
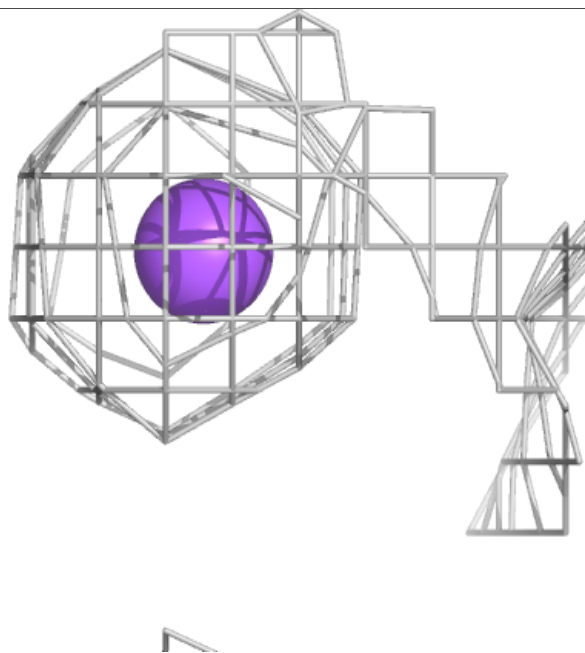
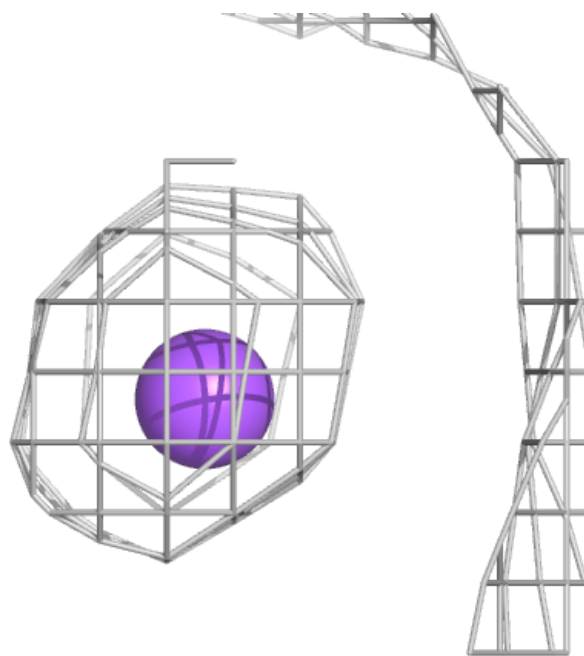
Electron density around NA B 402:

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



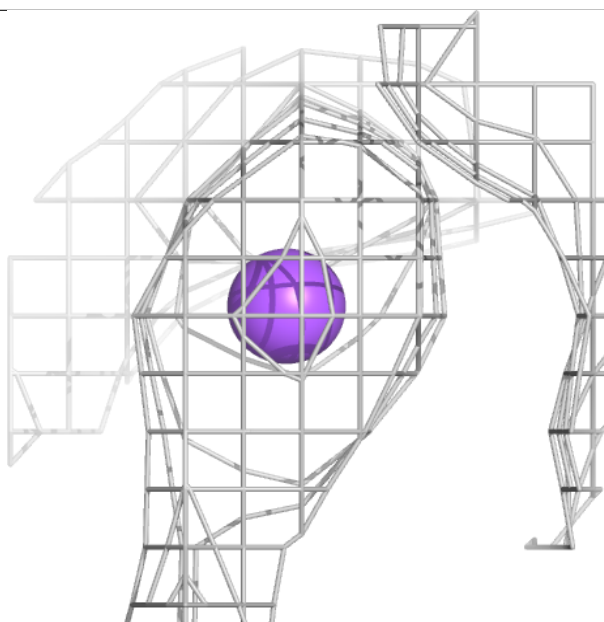
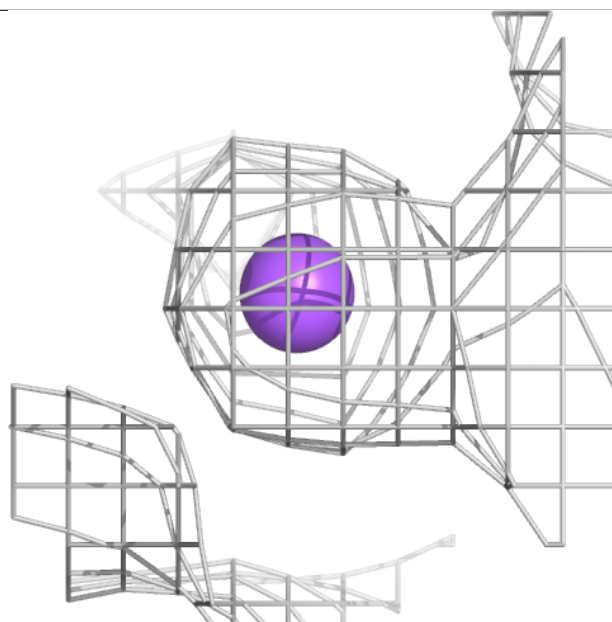
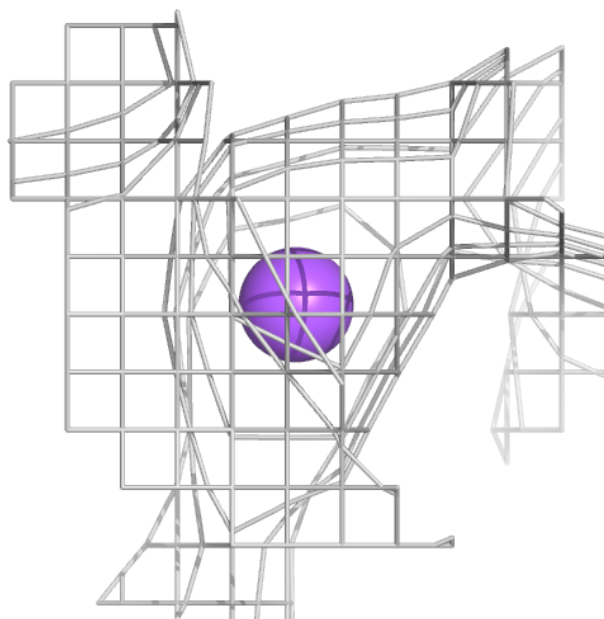
Electron density around NA A 401:

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



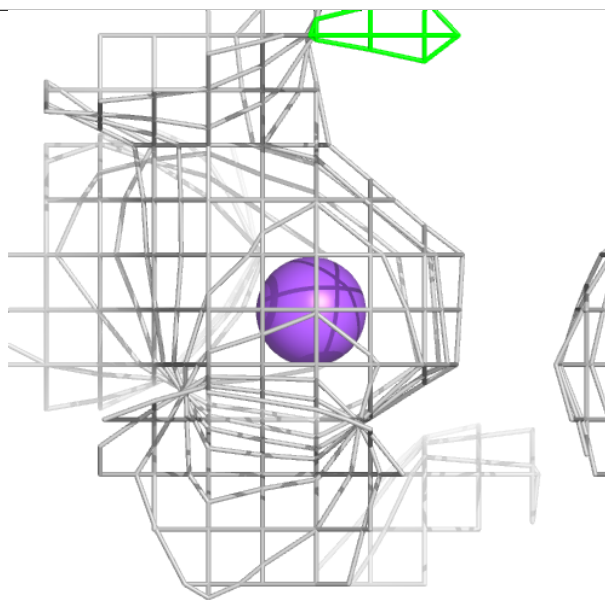
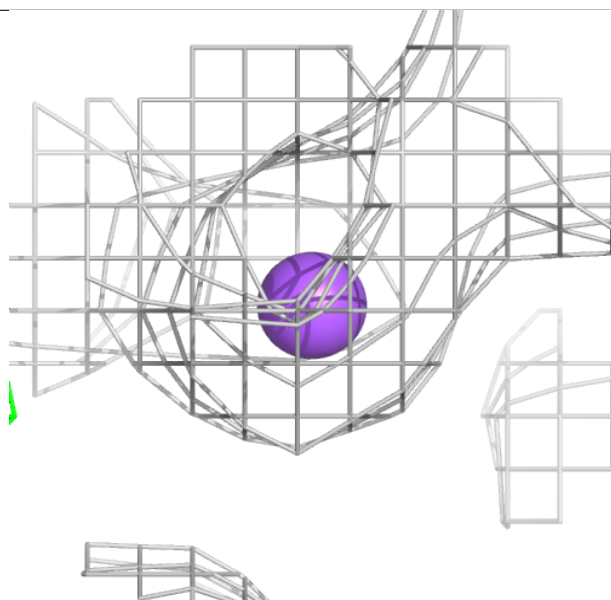
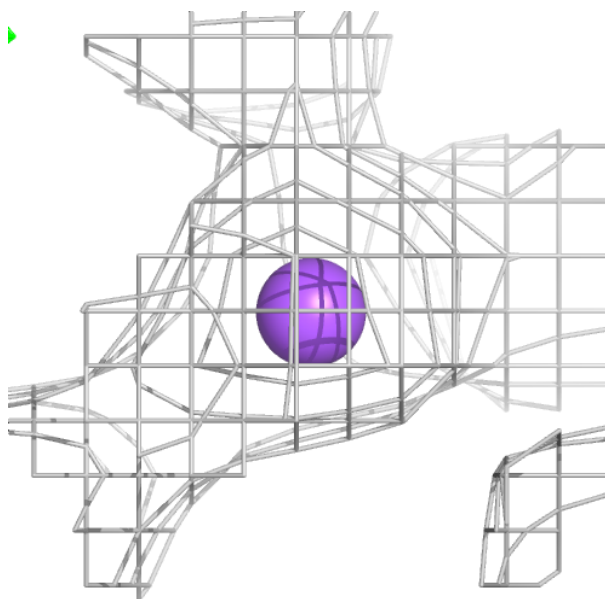
Electron density around NA B 403:

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



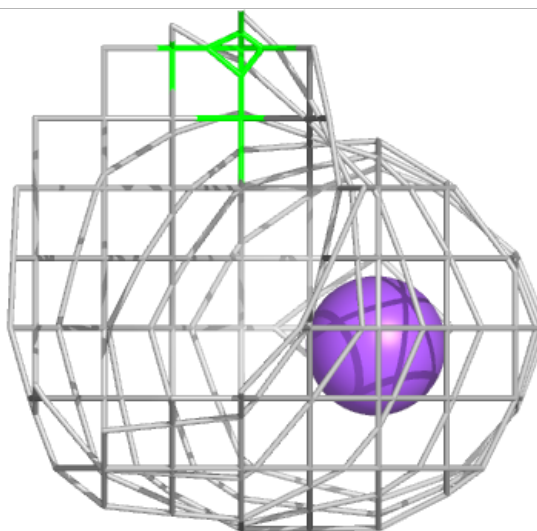
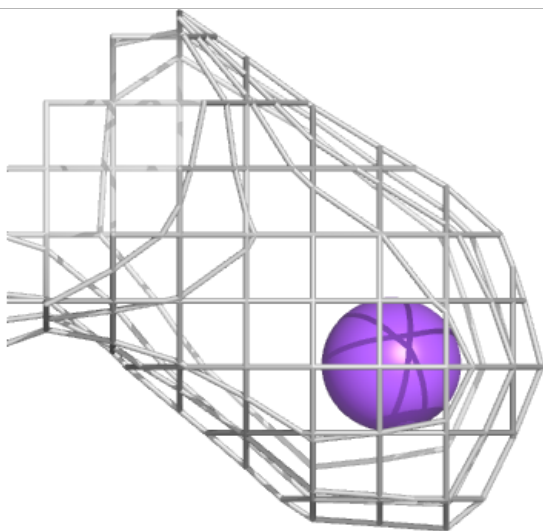
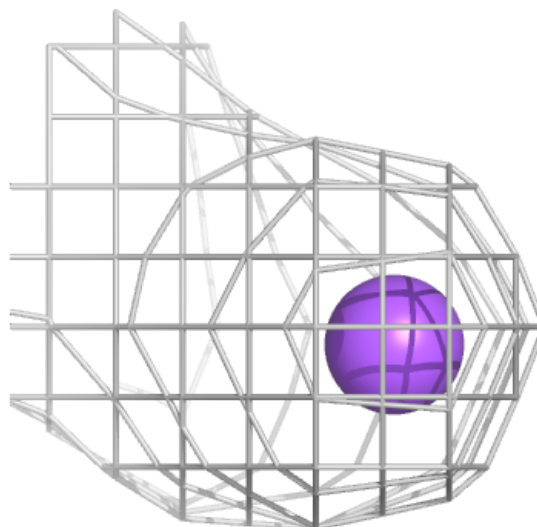
Electron density around NA C 401:

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



Electron density around NA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.