



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:41 AM UTC

PDB ID : 8D94 / pdb_00008d94
Title : SAMHD1-DNA complex
Authors : Hollis, T.J.; Batalis, S.M.
Deposited on : 2022-06-09
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

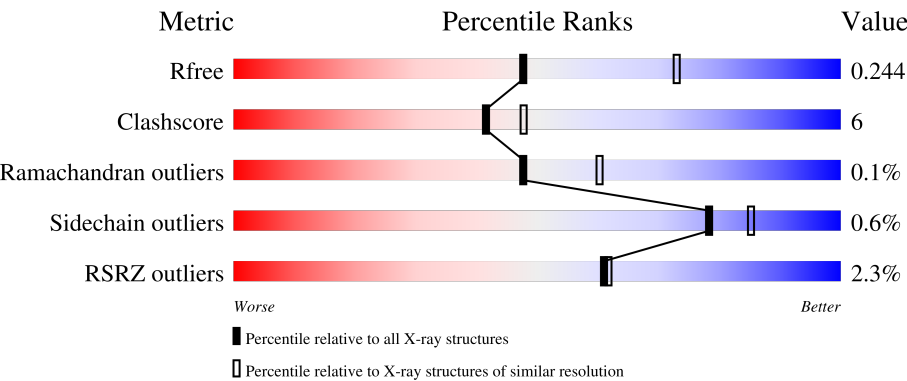
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.44 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.



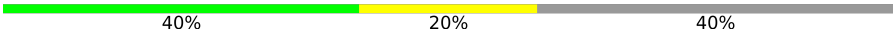
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	626	2% 60% 11% 29%
1	B	626	% 60% 9% 31%
1	C	626	% 62% 10% 27%
1	D	626	% 56% 12% 31%
2	F	5	40% 60% 40%

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Mol	Chain	Length	Quality of chain
2	G	5	 40% 20% 40%
2	H	5	 40% 60%
2	I	5	 20% 40% 40%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14917 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3616	2319	624	654	19			
1	B	434	Total	C	N	O	S	0	0	0
			3521	2258	611	633	19			
1	C	455	Total	C	N	O	S	0	0	0
			3668	2348	631	669	20			
1	D	431	Total	C	N	O	S	0	0	0
			3484	2234	606	625	19			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	P	0	0	0
			62	30	9	20	3			
2	G	3	Total	C	N	O	P	0	0	0
			62	30	9	20	3			
2	H	2	Total	C	N	O	P	0	0	0
			42	20	7	13	2			
2	I	3	Total	C	N	O	P	0	0	0
			62	30	9	20	3			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

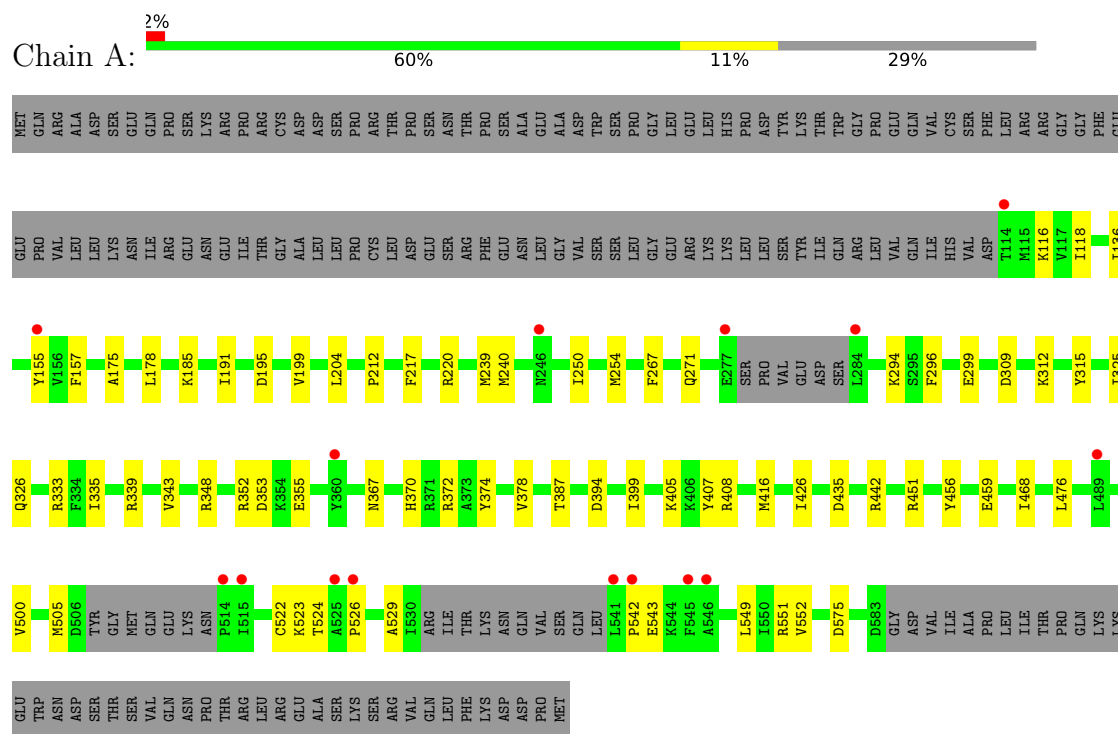
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	111	Total O 111 111	0	0
5	B	80	Total O 80 80	0	0
5	C	117	Total O 117 117	0	0
5	D	82	Total O 82 82	0	0
5	F	1	Total O 1 1	0	0
5	G	1	Total O 1 1	0	0

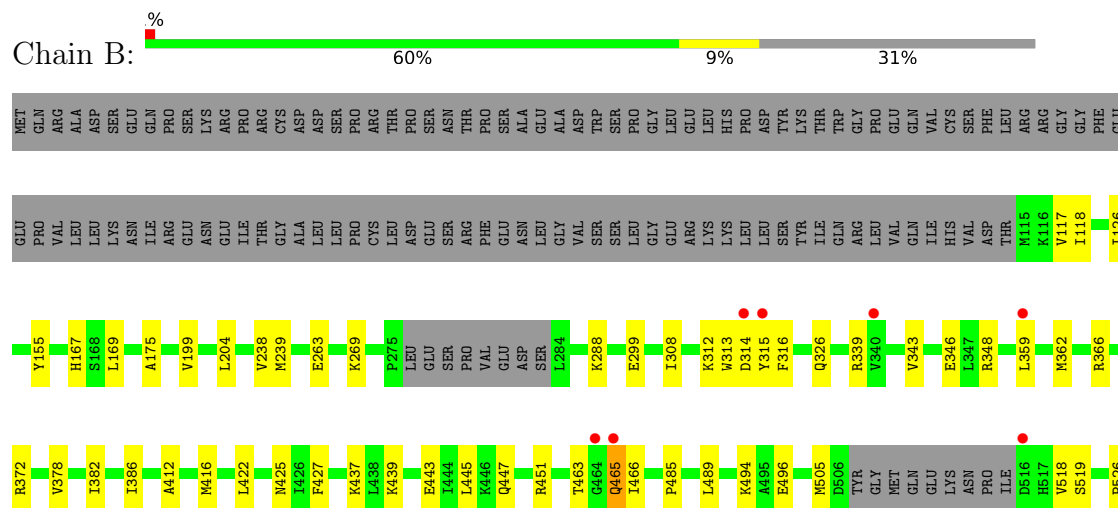
3 Residue-property plots

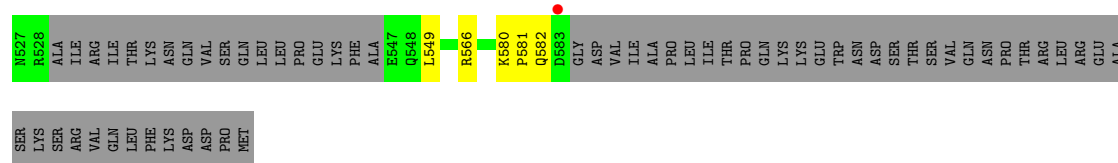
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

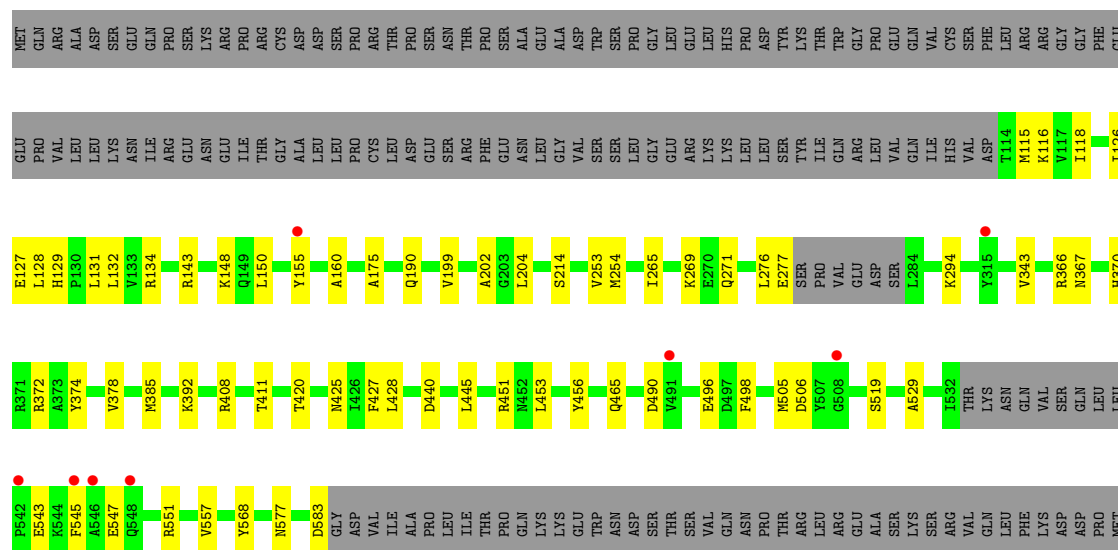


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

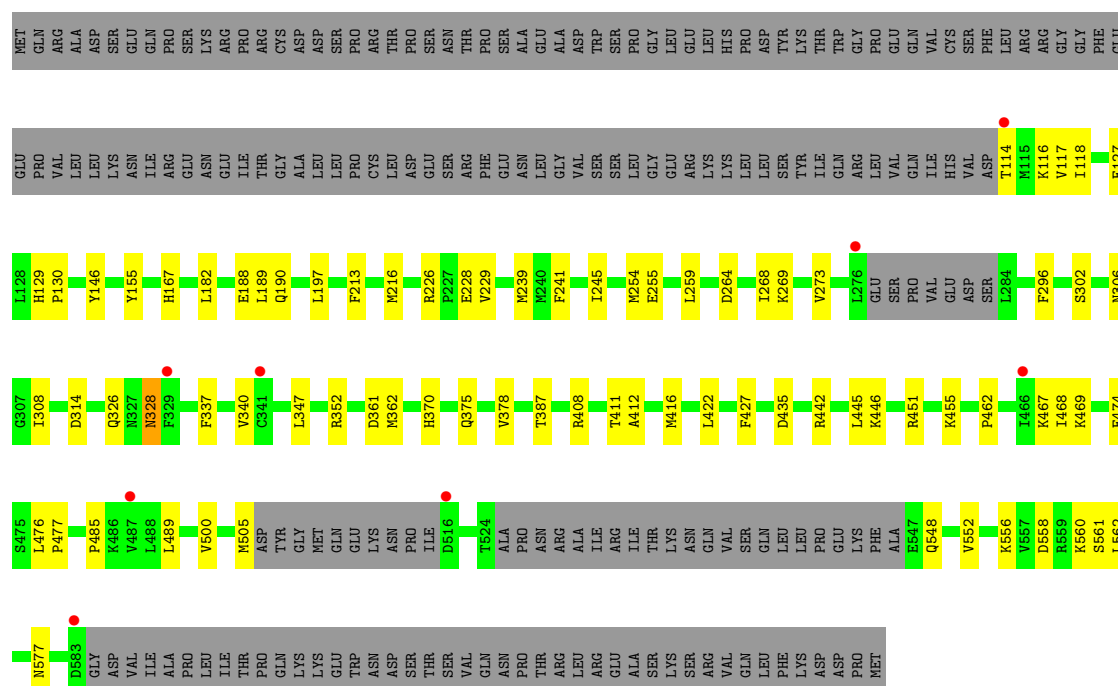




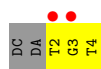
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 2: DNA (5'-D(P*TP*GP*T)-3')



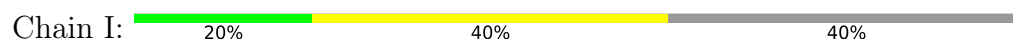
- Molecule 2: DNA (5'-D(P*TP*GP*T)-3')



- Molecule 2: DNA (5'-D(P*TP*GP*T)-3')



- Molecule 2: DNA (5'-D(P*TP*GP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.12Å 179.94Å 79.79Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	38.98 – 2.44 38.98 – 2.44	Depositor EDS
% Data completeness (in resolution range)	87.5 (38.98-2.44) 87.5 (38.98-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.243 0.190 , 0.244	Depositor DCC
R_{free} test set	1981 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	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	0.94	EDS
Total number of atoms	14917	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE

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	0.11	0/3702	0.28	0/5002
1	B	0.09	0/3604	0.26	0/4865
1	C	0.08	0/3756	0.25	0/5078
1	D	0.10	0/3566	0.27	0/4817
2	F	0.22	0/68	0.51	0/103
2	G	0.22	0/68	0.52	0/103
2	H	0.15	0/46	0.36	0/69
2	I	0.16	0/68	0.45	0/103
All	All	0.10	0/14878	0.27	0/20140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3616	0	3540	49	0
1	B	3521	0	3461	39	0
1	C	3668	0	3564	44	0
1	D	3484	0	3410	54	0
2	F	62	0	36	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	62	0	36	4	0
2	H	42	0	24	6	0
2	I	62	0	36	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	111	0	0	5	0
5	B	80	0	0	1	0
5	C	117	0	0	3	0
5	D	82	0	0	7	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
All	All	14917	0	14107	184	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 6.

All (184) 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:238:VAL:HG13	1:B:269:LYS:HD3	1.68	0.76
1:B:117:VAL:HG13	2:H:4:DT:H5"	1.69	0.74
1:B:308:ILE:HG12	1:B:362:MET:HE1	1.70	0.74
1:A:239:MET:HE2	1:A:416:MET:HE3	1.74	0.69
1:A:378:VAL:HG11	2:F:3:DG:H5"	1.75	0.68
1:D:476:LEU:HD23	1:D:500:VAL:HG11	1.76	0.68
1:D:462:PRO:HG3	1:D:548:GLN:HE21	1.58	0.67
1:A:326:GLN:H	1:A:326:GLN:CD	2.04	0.65
1:C:269:LYS:NZ	5:C:804:HOH:O	2.31	0.64
1:A:372:ARG:HE	2:F:4:DT:H3	1.45	0.63
1:D:577:ASN:ND2	5:D:804:HOH:O	2.31	0.63
1:C:254:MET:HE1	1:C:265:ILE:HG13	1.81	0.62
1:C:583:ASP:OD1	1:C:583:ASP:N	2.33	0.62
1:B:359:LEU:HD11	1:B:518:VAL:HG21	1.83	0.61
1:A:372:ARG:NH1	5:A:801:HOH:O	2.15	0.61
1:C:199:VAL:HA	1:C:271:GLN:HE22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:O	1:B:451:ARG:NH2	2.34	0.60
1:C:465:GLN:NE2	5:C:807:HOH:O	2.35	0.59
1:D:216:MET:SD	1:D:387:THR:OG1	2.60	0.59
1:A:116:LYS:NZ	2:I:2:DT:O3'	2.36	0.59
2:H:3:DG:N2	2:H:3:DG:OP1	2.35	0.59
1:D:254:MET:HG2	1:D:259:LEU:HD12	1.86	0.58
1:B:505:MET:HE1	1:B:549:LEU:HD23	1.83	0.58
1:B:566:ARG:NH2	1:B:582:GLN:O	2.36	0.57
1:C:465:GLN:OE1	1:C:577:ASN:ND2	2.34	0.57
1:B:326:GLN:NE2	1:D:326:GLN:OE1	2.37	0.57
1:A:343:VAL:HG22	1:A:529:ALA:HB2	1.87	0.57
1:A:523:LYS:HE3	1:A:524:THR:HG22	1.87	0.57
1:A:220:ARG:HG2	1:A:387:THR:HG21	1.86	0.57
1:D:155:TYR:O	1:D:451:ARG:NH2	2.35	0.56
1:A:191:ILE:HD11	1:A:296:PHE:HE2	1.69	0.56
1:C:116:LYS:NZ	2:G:3:DG:OP1	2.26	0.56
1:C:451:ARG:HG2	2:H:3:DG:N2	2.20	0.56
1:D:146:TYR:OH	5:D:801:HOH:O	2.17	0.56
1:D:500:VAL:HG22	1:D:552:VAL:HG22	1.86	0.56
1:B:439:LYS:O	1:B:443:GLU:HG2	2.05	0.56
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.39	0.56
1:D:114:THR:HB	1:D:130:PRO:HG3	1.87	0.55
1:B:425:ASN:HB2	1:C:428:LEU:HD13	1.89	0.54
1:D:340:VAL:HG12	1:D:347:LEU:HD12	1.89	0.54
1:D:455:LYS:HG3	1:D:562:LEU:HD11	1.88	0.54
1:D:370:HIS:O	1:D:375:GLN:HG3	2.07	0.54
1:B:580:LYS:HD2	1:B:581:PRO:HD2	1.88	0.54
1:C:155:TYR:HB3	1:C:451:ARG:HH22	1.72	0.54
1:D:167:HIS:ND1	1:D:314:ASP:OD2	2.37	0.53
1:A:155:TYR:HB3	1:A:451:ARG:HH22	1.73	0.53
1:A:195:ASP:OD2	1:A:294:LYS:NZ	2.32	0.53
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.90	0.53
1:B:494:LYS:HD3	1:B:496:GLU:HB3	1.91	0.53
1:C:132:LEU:HD22	1:C:204:LEU:HD22	1.90	0.53
1:C:148:LYS:O	1:C:214:SER:OG	2.25	0.53
1:A:370:HIS:HA	1:A:374:TYR:HB2	1.91	0.52
1:D:412:ALA:HB3	1:D:422:LEU:HD22	1.91	0.52
1:D:239:MET:HE2	1:D:416:MET:HE3	1.91	0.52
1:A:240:MET:HE2	1:A:416:MET:SD	2.50	0.52
1:D:213:PHE:HB2	1:D:216:MET:HE3	1.92	0.51
1:D:446:LYS:NZ	5:D:810:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:O	1:A:408:ARG:HD2	2.10	0.51
1:A:405:LYS:HD2	1:A:407:TYR:CZ	2.46	0.51
1:D:378:VAL:HG11	2:I:3:DG:H5'	1.93	0.51
1:D:375:GLN:HE22	1:D:505:MET:HE2	1.76	0.51
1:C:385:MET:HE1	1:C:453:LEU:HA	1.93	0.51
1:B:485:PRO:HG2	1:B:489:LEU:HD11	1.93	0.50
1:A:543:GLU:N	1:A:543:GLU:OE1	2.44	0.50
1:D:468:ILE:H	1:D:548:GLN:HE22	1.58	0.50
1:D:306:ASN:HB2	1:D:308:ILE:HG22	1.92	0.50
1:A:468:ILE:HG21	1:A:476:LEU:HD11	1.94	0.50
1:A:459:GLU:HG3	1:A:551:ARG:HG2	1.93	0.49
1:B:299:GLU:OE1	1:B:348:ARG:HB2	2.13	0.49
1:C:129:HIS:HD2	1:C:131:LEU:H	1.61	0.49
1:C:366:ARG:NH1	1:C:545:PHE:HE1	2.11	0.49
1:B:378:VAL:HG21	2:G:3:DG:H5''	1.94	0.49
1:C:372:ARG:HE	2:H:4:DT:H3	1.60	0.49
1:A:185:LYS:NZ	5:A:809:HOH:O	2.33	0.48
1:C:370:HIS:HA	1:C:374:TYR:HB2	1.95	0.48
1:D:560:LYS:HD2	1:D:560:LYS:HA	1.66	0.48
1:A:155:TYR:HB3	1:A:451:ARG:NH2	2.29	0.48
1:C:129:HIS:CD2	1:C:131:LEU:H	2.32	0.48
1:C:392:LYS:HD3	1:C:440:ASP:HB3	1.95	0.48
1:C:115:MET:HE2	1:C:127:GLU:HB3	1.94	0.48
1:D:308:ILE:HD11	1:D:362:MET:HE1	1.96	0.48
1:C:276:LEU:HD12	1:C:277:GLU:HG3	1.94	0.48
1:B:494:LYS:HD3	1:B:496:GLU:H	1.79	0.48
1:D:189:LEU:C	1:D:190:GLN:HG2	2.39	0.48
1:D:264:ASP:O	1:D:268:ILE:HG12	2.14	0.48
1:B:372:ARG:NH2	1:D:361:ASP:OD2	2.41	0.47
1:A:372:ARG:NH2	5:A:801:HOH:O	2.47	0.47
1:D:558:ASP:OD2	1:D:561:SER:N	2.47	0.47
1:A:309:ASP:OD1	1:A:312:LYS:HG2	2.15	0.47
1:D:117:VAL:HG22	1:D:127:GLU:HG2	1.95	0.47
1:D:485:PRO:HG2	1:D:489:LEU:HD11	1.97	0.47
1:A:435:ASP:O	1:A:442:ARG:NH2	2.46	0.47
1:B:167:HIS:ND1	1:B:314:ASP:OD2	2.48	0.47
1:B:463:THR:C	1:B:465:GLN:H	2.23	0.47
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.96	0.47
1:B:288:LYS:HA	1:B:288:LYS:HD2	1.76	0.46
1:D:189:LEU:HD12	1:D:296:PHE:CZ	2.50	0.46
1:C:378:VAL:HG11	2:H:3:DG:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD12	1:C:160:ALA:HB1	1.96	0.46
1:C:506:ASP:N	1:C:506:ASP:OD1	2.46	0.46
1:C:190:GLN:O	1:C:294:LYS:NZ	2.49	0.46
1:B:118:ILE:HD13	2:H:3:DG:H2''	1.97	0.46
1:C:143:ARG:HD2	1:C:420:THR:HA	1.97	0.46
1:A:353:ASP:OD2	1:A:522:CYS:HA	2.15	0.46
1:D:116:LYS:HE3	2:F:3:DG:OP1	2.16	0.46
1:C:202:ALA:HB3	1:C:271:GLN:HE21	1.81	0.46
1:D:188:GLU:HG2	1:D:189:LEU:HD22	1.97	0.45
1:D:306:ASN:CB	1:D:308:ILE:HG22	2.46	0.45
1:D:302:SER:O	5:D:802:HOH:O	2.21	0.45
1:D:337:PHE:HD1	1:D:352:ARG:HB2	1.80	0.45
1:A:267:PHE:O	1:A:271:GLN:HG2	2.15	0.45
1:B:451:ARG:NH1	5:B:802:HOH:O	2.37	0.45
1:B:343:VAL:HG21	1:B:519:SER:HB2	1.99	0.45
1:B:326:GLN:NE2	1:D:328:ASN:HD22	2.15	0.45
1:C:115:MET:HE3	1:C:128:LEU:C	2.42	0.45
1:C:496:GLU:H	1:C:496:GLU:HG2	1.59	0.45
1:D:435:ASP:O	1:D:442:ARG:NH2	2.50	0.45
1:A:250:ILE:O	1:A:254:MET:HG3	2.17	0.44
1:A:333:ARG:HB3	1:A:355:GLU:OE1	2.18	0.44
1:A:500:VAL:HG22	1:A:552:VAL:HG22	1.99	0.44
1:A:505:MET:HE2	1:A:505:MET:HB3	1.76	0.44
1:D:118:ILE:HD11	2:F:3:DG:C8	2.52	0.44
2:F:2:DT:H2''	2:F:3:DG:O5'	2.15	0.44
1:B:412:ALA:HB3	1:B:422:LEU:HD22	1.98	0.44
1:D:556:LYS:HE2	1:D:561:SER:OG	2.17	0.44
1:A:575:ASP:OD1	1:A:575:ASP:N	2.50	0.44
1:C:343:VAL:HG22	1:C:529:ALA:HB2	2.00	0.44
1:A:178:LEU:HA	1:A:335:ILE:HG23	1.99	0.44
1:B:169:LEU:HD23	1:B:204:LEU:HD11	2.00	0.44
1:D:352:ARG:NH2	5:D:814:HOH:O	2.48	0.44
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.53	0.44
1:D:241:PHE:CZ	1:D:245:ILE:HD11	2.53	0.44
1:B:239:MET:HE2	1:B:416:MET:HE3	1.99	0.44
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.99	0.43
1:A:339:ARG:HD3	1:A:526:PRO:O	2.18	0.43
1:C:456:TYR:HE1	1:C:551:ARG:HD3	1.82	0.43
1:B:118:ILE:HB	1:B:126:ILE:HG13	2.00	0.43
1:C:498:PHE:HZ	1:C:568:TYR:HD1	1.67	0.43
1:A:326:GLN:CD	1:A:326:GLN:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:TYR:OH	1:A:459:GLU:HB2	2.18	0.43
1:C:505:MET:HG3	1:C:547:GLU:HA	1.99	0.43
1:D:255:GLU:OE1	5:D:803:HOH:O	2.21	0.43
1:D:408:ARG:H	1:D:411:THR:HG1	1.65	0.43
1:A:157:PHE:CE2	2:F:4:DT:H2''	2.54	0.42
1:A:367:ASN:ND2	1:A:543:GLU:HB3	2.34	0.42
1:C:199:VAL:HA	1:C:271:GLN:NE2	2.33	0.42
1:A:312:LYS:HD3	1:A:315:TYR:OH	2.20	0.42
1:A:118:ILE:HD11	2:I:3:DG:C8	2.55	0.42
1:A:399:ILE:HD11	1:A:426:ILE:HD11	2.01	0.42
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.55	0.42
1:C:427:PHE:CE2	1:C:445:LEU:HD22	2.54	0.42
1:B:316:PHE:CZ	1:B:366:ARG:HB2	2.55	0.42
1:A:367:ASN:HD21	1:A:543:GLU:HB3	1.85	0.42
1:B:427:PHE:CE2	1:B:445:LEU:HD22	2.55	0.42
1:C:490:ASP:OD1	1:C:490:ASP:N	2.42	0.42
1:D:155:TYR:HB3	1:D:451:ARG:NH2	2.34	0.42
1:A:136:ILE:HG13	1:A:204:LEU:HD21	2.02	0.41
1:C:155:TYR:O	1:C:451:ARG:NH2	2.53	0.41
1:C:366:ARG:NH1	5:C:824:HOH:O	2.53	0.41
1:B:313:TRP:HA	1:B:316:PHE:HB2	2.01	0.41
1:D:129:HIS:N	5:D:817:HOH:O	2.53	0.41
1:D:467:LYS:O	1:D:469:LYS:HE3	2.20	0.41
1:A:299:GLU:OE2	1:A:348:ARG:HG2	2.21	0.41
1:B:339:ARG:NH1	1:B:526:PRO:HB3	2.36	0.41
1:B:346:GLU:HB3	1:B:348:ARG:NH2	2.36	0.41
2:G:3:DG:H2'	2:G:3:DG:N3	2.35	0.41
1:B:443:GLU:O	1:B:447:GLN:HG2	2.20	0.41
1:D:182:LEU:HD22	1:D:340:VAL:HG23	2.02	0.41
1:D:226:ARG:CZ	1:D:229:VAL:HG21	2.51	0.41
1:D:228:GLU:OE2	1:D:228:GLU:N	2.31	0.41
1:A:312:LYS:NZ	5:A:819:HOH:O	2.53	0.41
1:B:451:ARG:HG2	2:G:3:DG:N2	2.35	0.41
1:D:427:PHE:CE2	1:D:445:LEU:HD22	2.56	0.41
1:A:254:MET:HG3	1:A:254:MET:H	1.74	0.41
1:C:408:ARG:H	1:C:411:THR:HG1	1.64	0.41
1:D:474:GLU:O	1:D:477:PRO:HD2	2.20	0.41
1:A:352:ARG:HB3	1:A:355:GLU:HG2	2.02	0.41
1:C:134:ARG:HG3	1:C:253:VAL:HG11	2.03	0.41
1:D:269:LYS:O	1:D:273:VAL:HG12	2.22	0.41
1:C:367:ASN:HB2	1:C:543:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH1	5:A:817:HOH:O	2.50	0.40
1:B:382:ILE:O	1:B:386:ILE:HG13	2.22	0.40
1:C:118:ILE:O	1:C:126:ILE:HG12	2.21	0.40
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.86	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	439/626 (70%)	426 (97%)	12 (3%)	1 (0%)	43	53
1	B	426/626 (68%)	414 (97%)	12 (3%)	0	100	100
1	C	449/626 (72%)	434 (97%)	15 (3%)	0	100	100
1	D	423/626 (68%)	414 (98%)	9 (2%)	0	100	100
All	All	1737/2504 (69%)	1688 (97%)	48 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	PRO

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	385/560 (69%)	383 (100%)	2 (0%)	81	87
1	B	376/560 (67%)	372 (99%)	4 (1%)	65	75
1	C	389/560 (70%)	387 (100%)	2 (0%)	81	87
1	D	370/560 (66%)	369 (100%)	1 (0%)	86	91
All	All	1520/2240 (68%)	1511 (99%)	9 (1%)	78	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ILE
1	A	549	LEU
1	B	263	GLU
1	B	437	LYS
1	B	465	GLN
1	B	466	ILE
1	C	519	SER
1	C	557	VAL
1	D	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	243	HIS
1	A	248	ASN
1	A	465	GLN
1	A	571	GLN
1	B	215	HIS
1	B	326	GLN
1	B	425	ASN
1	B	447	GLN
1	B	465	GLN
1	C	119	ASN
1	C	125	HIS
1	C	235	GLN
1	C	248	ASN
1	C	271	GLN
1	C	326	GLN
1	C	517	HIS
1	D	215	HIS

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Mol	Chain	Res	Type
1	D	248	ASN
1	D	327	ASN
1	D	375	GLN
1	D	452	ASN
1	D	548	GLN
1	D	567	GLN

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	447/626 (71%)	-0.01	15 (3%) 48 46	24, 41, 87, 114	0
1	B	434/626 (69%)	0.13	8 (1%) 67 68	27, 46, 93, 117	0
1	C	455/626 (72%)	0.03	8 (1%) 67 68	25, 45, 83, 109	0
1	D	431/626 (68%)	0.17	8 (1%) 66 67	28, 47, 89, 114	0
2	F	3/5 (60%)	2.04	2 (66%) 0 0	46, 46, 48, 50	3 (100%)
2	G	3/5 (60%)	1.11	0 100 100	37, 37, 41, 56	3 (100%)
2	H	2/5 (40%)	1.18	0 100 100	41, 41, 41, 43	2 (100%)
2	I	3/5 (60%)	1.44	0 100 100	36, 36, 46, 70	3 (100%)
All	All	1778/2524 (70%)	0.08	41 (2%) 61 62	24, 45, 88, 117	11 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	ILE	4.7
1	C	542	PRO	4.0
1	C	545	PHE	3.5
1	B	315	TYR	3.5
1	D	329	PHE	3.3
1	A	284	LEU	3.3
1	A	514	PRO	3.0
1	C	546	ALA	2.9
1	A	545	PHE	2.9
1	A	525	ALA	2.9
1	A	360	TYR	2.7
1	A	542	PRO	2.7
1	D	466	ILE	2.7
1	B	314	ASP	2.7
1	A	526	PRO	2.7
1	B	583	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	516	ASP	2.5
1	B	516	ASP	2.5
1	C	491	VAL	2.4
1	D	583	ASP	2.3
2	F	3	DG	2.3
1	A	114	THR	2.3
1	D	114	THR	2.3
1	A	277	GLU	2.3
1	A	246	ASN	2.2
1	A	546	ALA	2.2
1	C	508	GLY	2.2
1	D	341	CYS	2.2
1	B	465	GLN	2.2
1	C	548	GLN	2.2
1	A	155	TYR	2.2
1	A	541	LEU	2.1
1	B	464	GLY	2.1
1	B	359	LEU	2.1
1	B	340	VAL	2.1
1	C	155	TYR	2.1
2	F	2	DT	2.1
1	D	487	VAL	2.0
1	D	276	LEU	2.0
1	A	489	LEU	2.0
1	C	315	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

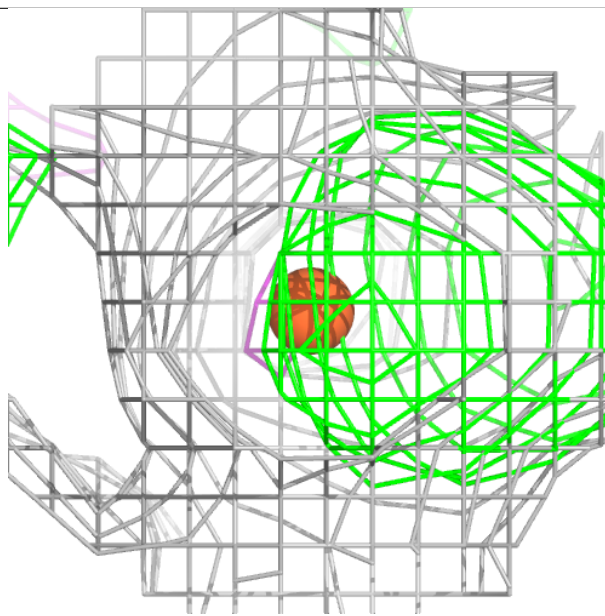
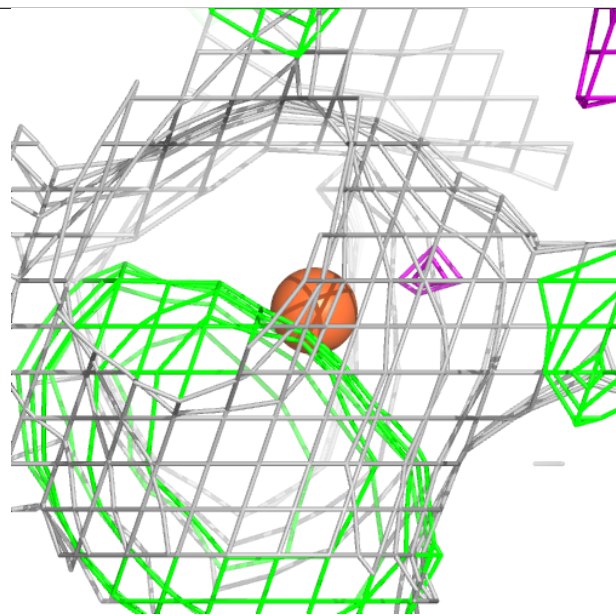
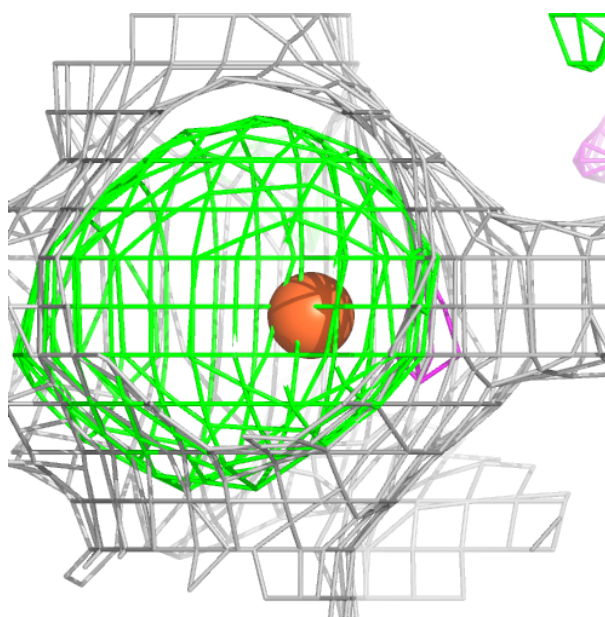
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	B	701	1/1	0.77	0.12	42,42,42,42	0
4	CA	D	702	1/1	0.85	0.11	80,80,80,80	0
4	CA	B	702	1/1	0.87	0.09	69,69,69,69	0
3	FE	C	701	1/1	0.88	0.10	42,42,42,42	0
4	CA	A	702	1/1	0.93	0.09	63,63,63,63	0
4	CA	C	702	1/1	0.96	0.04	56,56,56,56	0
3	FE	D	701	1/1	0.98	0.06	35,35,35,35	0
3	FE	A	701	1/1	0.99	0.06	33,33,33,33	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.

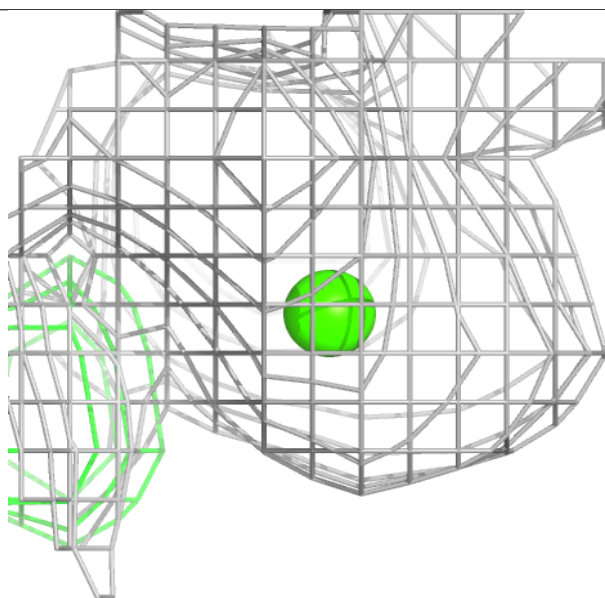
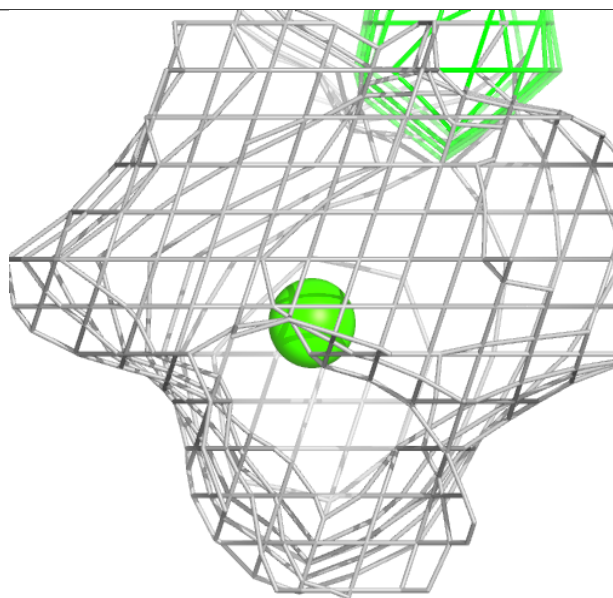
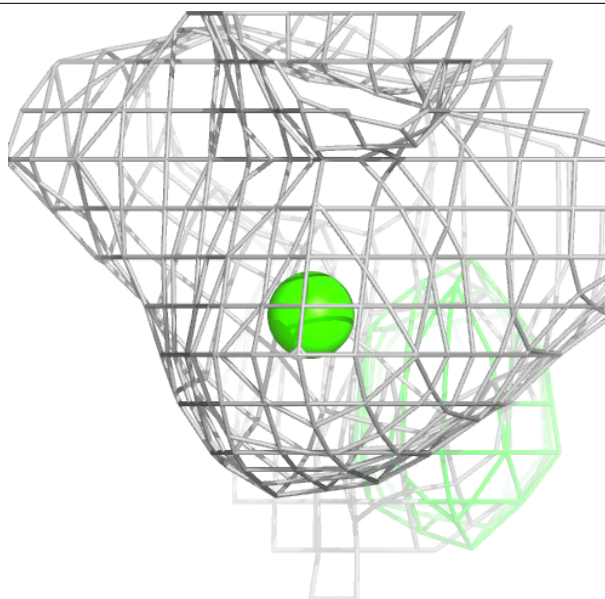
Electron density around FE B 701:

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



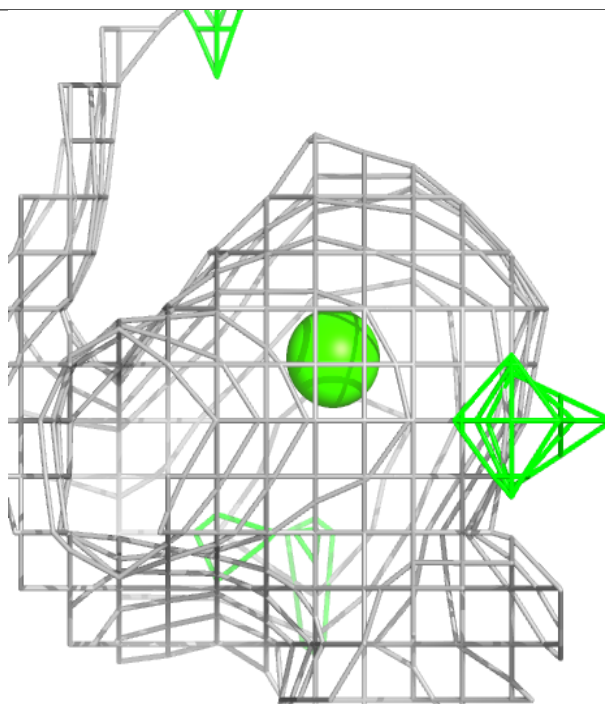
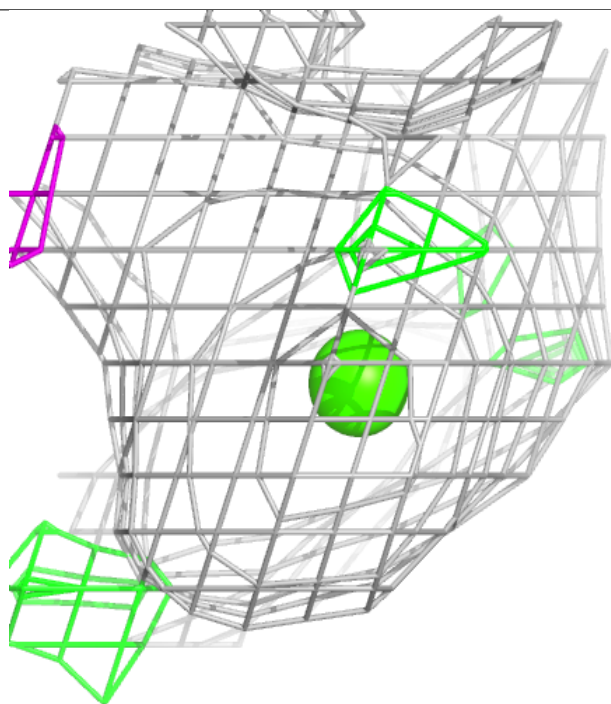
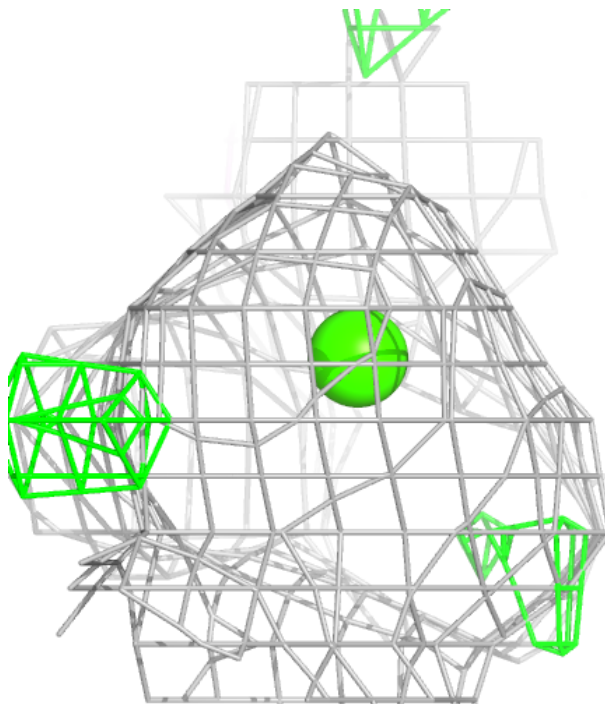
Electron density around CA D 702:

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



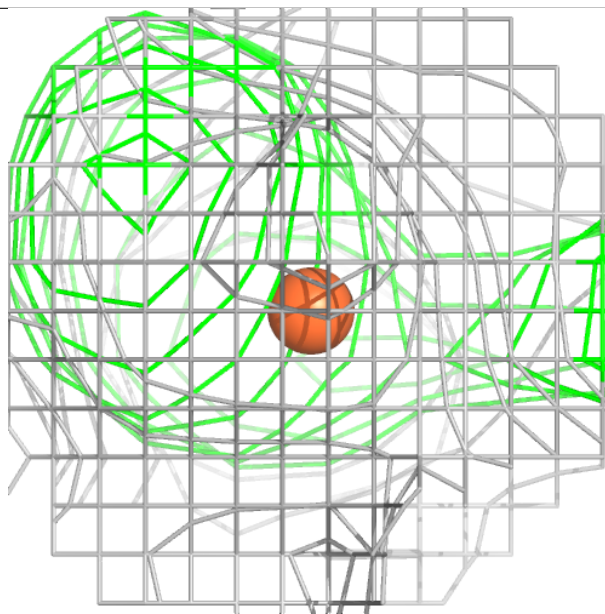
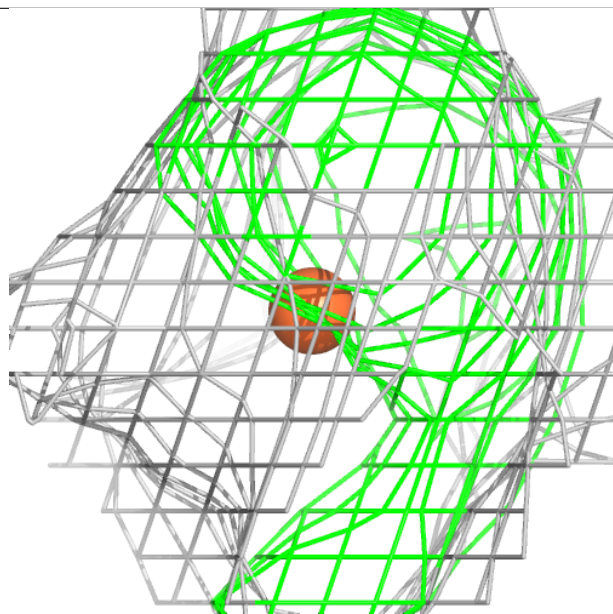
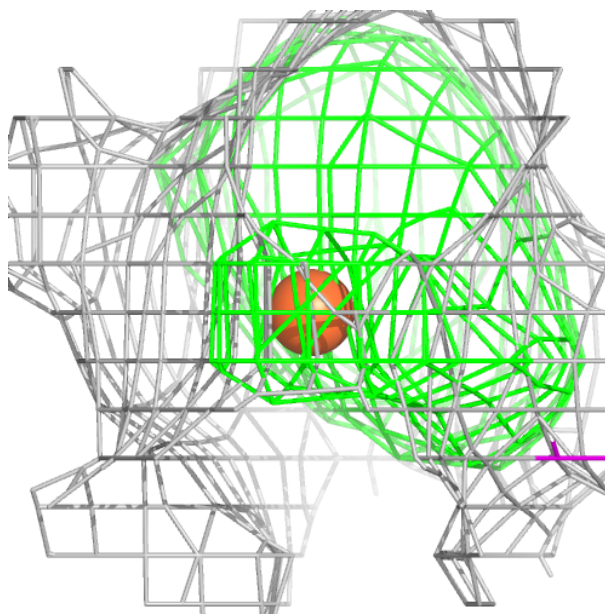
Electron density around CA B 702:

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



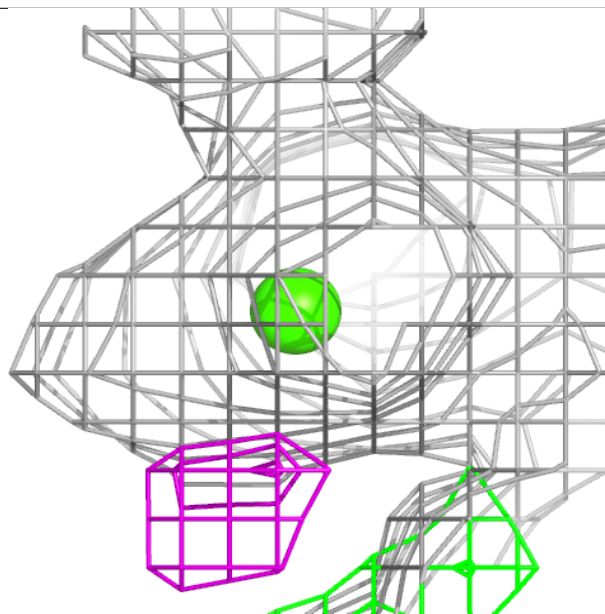
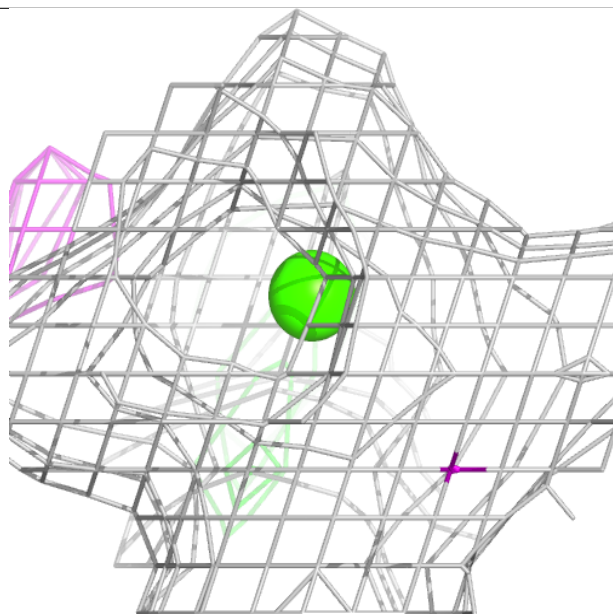
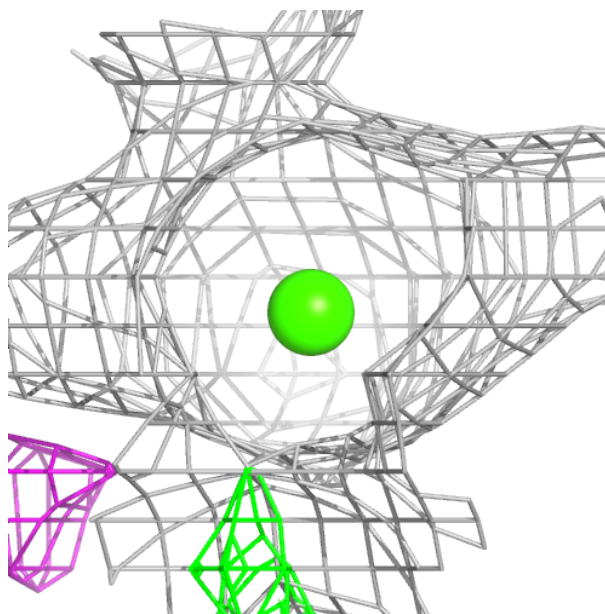
Electron density around FE C 701:

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



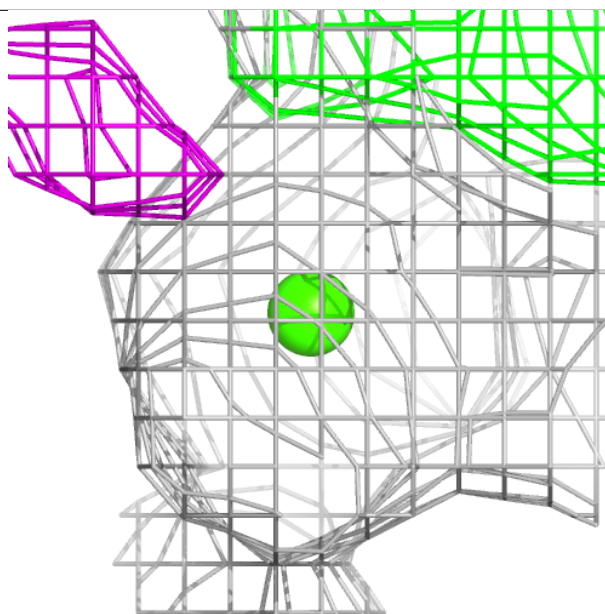
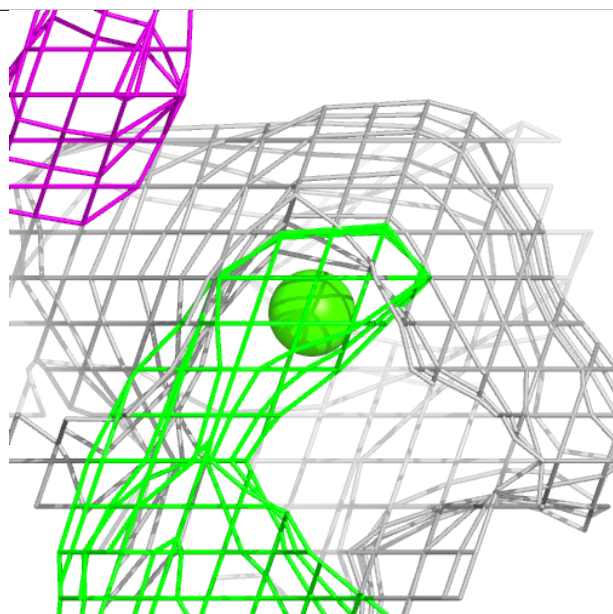
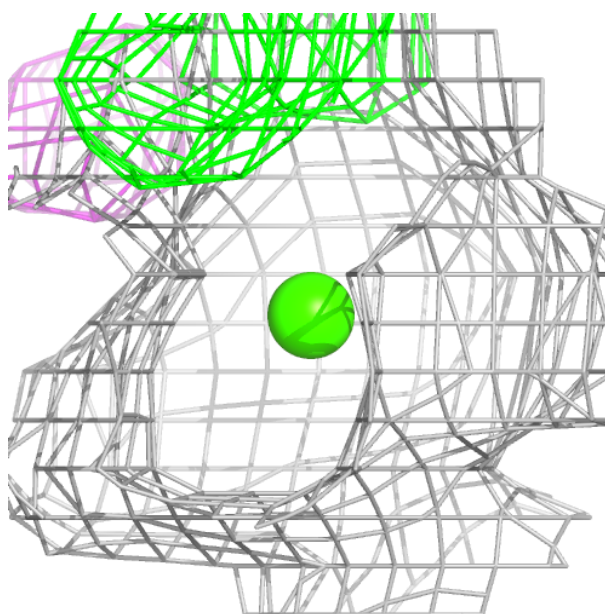
Electron density around CA A 702:

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



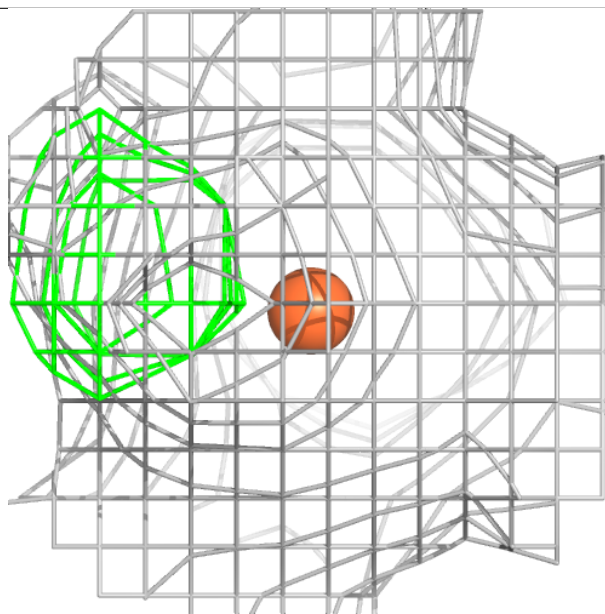
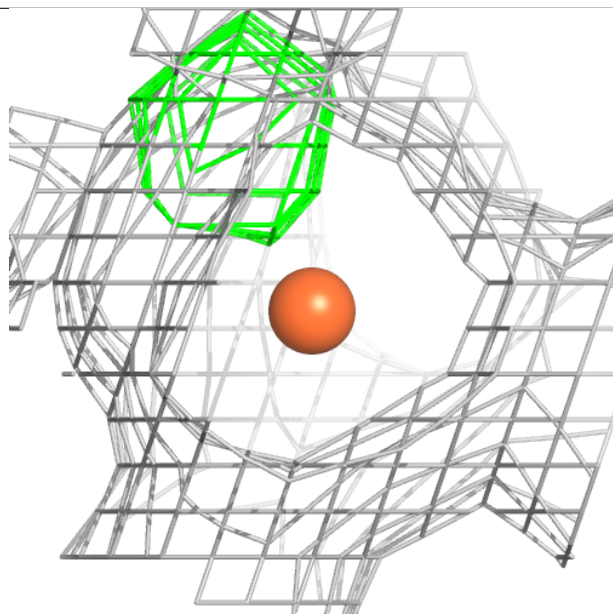
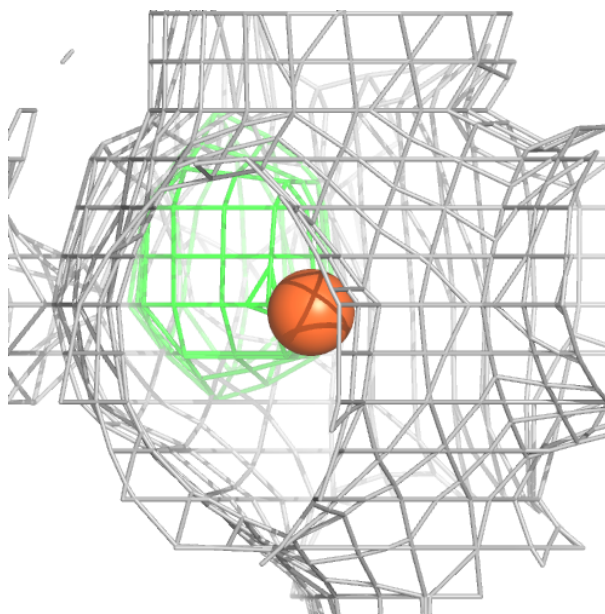
Electron density around CA C 702:

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



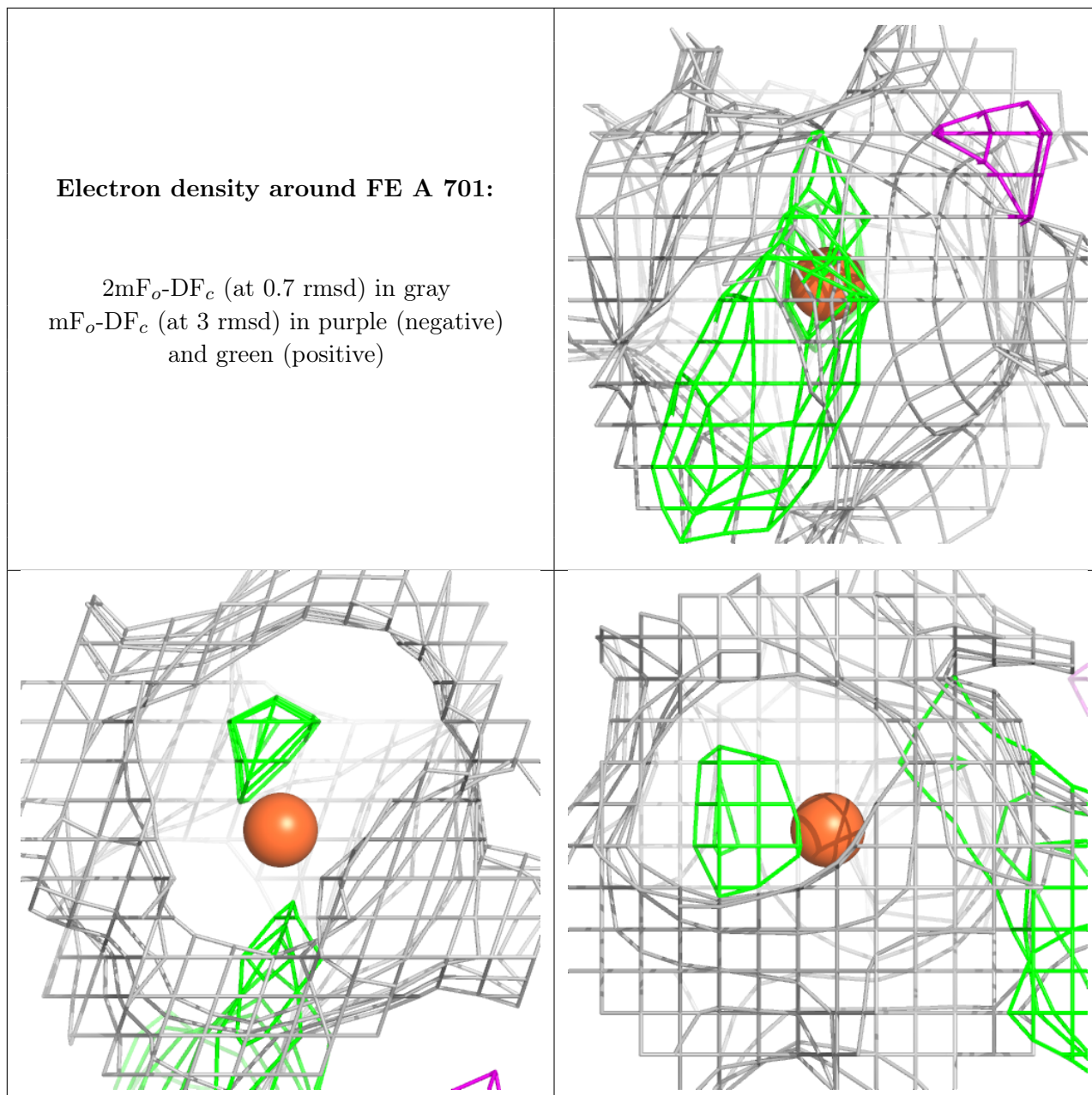
Electron density around FE D 701:

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



Electron density around FE A 701:

$2mF_o-DF_c$ (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.