



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2025 – 12:18 PM JST

PDB ID : 9JUS / pdb_00009jus
Title : Structure of villin bound to an actin trimer
Authors : Robinson, R.C.
Deposited on : 2024-10-08
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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

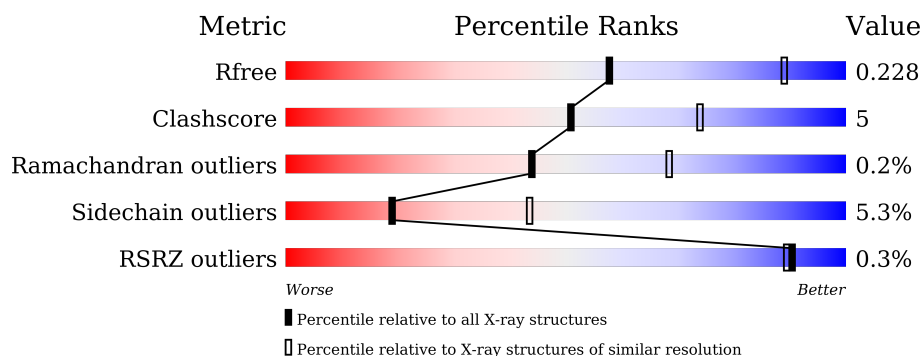
1 Overall quality at a glance

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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	F	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 17% .. </div> </div>
1	G	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 18% .. </div> </div>
1	P	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 16% .. </div> </div>
1	f	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% 13% .. </div> </div>
1	g	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 84% 11% .. </div> </div>
1	p	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 14% .. </div> </div>

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Mol	Chain	Length	Quality of chain
2	V	823	<div><div></div><div>82%</div><div>16%</div><div>..</div></div>
2	v	823	<div><div></div><div>82%</div><div>16%</div><div>..</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30576 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.

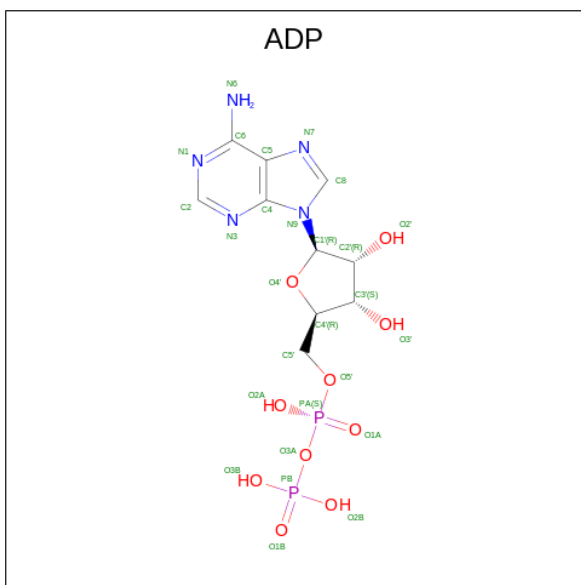
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	p	361	Total	C	N	O	S	0	1	0
			2831	1793	475	543	20			
1	f	372	Total	C	N	O	S	0	0	0
			2909	1842	490	556	21			
1	g	362	Total	C	N	O	S	0	1	0
			2847	1805	479	544	19			
1	P	363	Total	C	N	O	S	0	0	0
			2841	1797	475	549	20			
1	F	372	Total	C	N	O	S	0	0	0
			2909	1842	490	556	21			
1	G	361	Total	C	N	O	S	0	1	0
			2839	1801	478	541	19			

- Molecule 2 is a protein called villin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	v	815	Total	C	N	O	S	0	0	0
			6510	4107	1099	1274	30			
2	V	814	Total	C	N	O	S	0	3	0
			6515	4108	1102	1275	30			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	p	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	f	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	g	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	p	1	Total Mg 1 1	0	0
4	f	1	Total Mg 1 1	0	0
4	g	1	Total Mg 1 1	0	0
4	P	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		

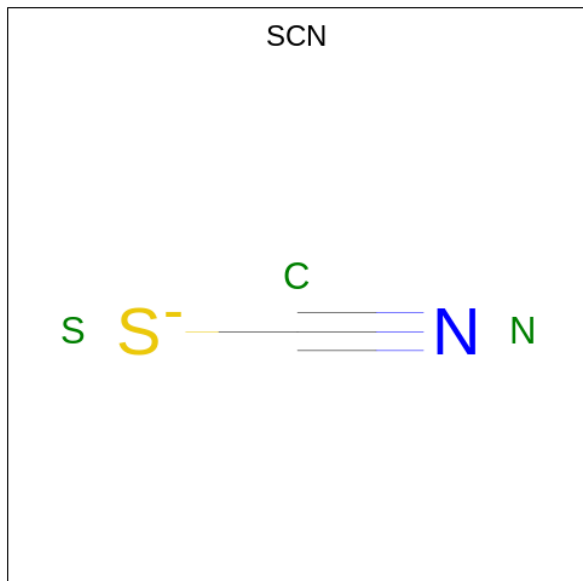
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	v	8	Total	Ca	0	0
			8	8		
5	V	8	Total	Ca	0	0
			8	8		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	v	1	Total	Cl	0	0
			1	1		

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	V	1	Total	C	N	S	0	0
			3	1	1	1		

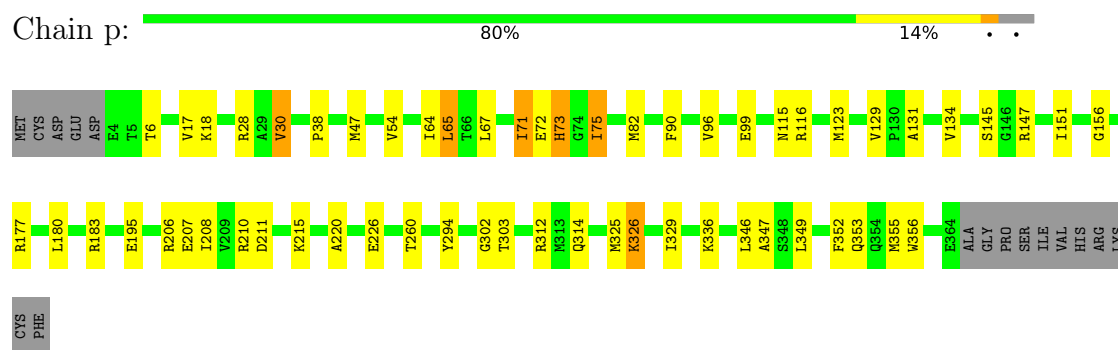
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	p	18	Total 18	O 18	0	0
8	f	32	Total 32	O 32	0	0
8	g	19	Total 19	O 19	0	0
8	v	39	Total 39	O 39	0	0
8	P	26	Total 26	O 26	0	0
8	F	11	Total 11	O 11	0	0
8	G	8	Total 8	O 8	0	0
8	V	34	Total 34	O 34	0	0

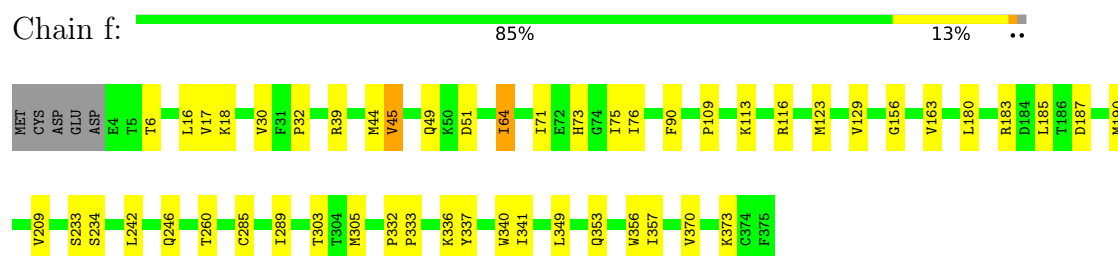
3 Residue-property plots [i](#)

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.

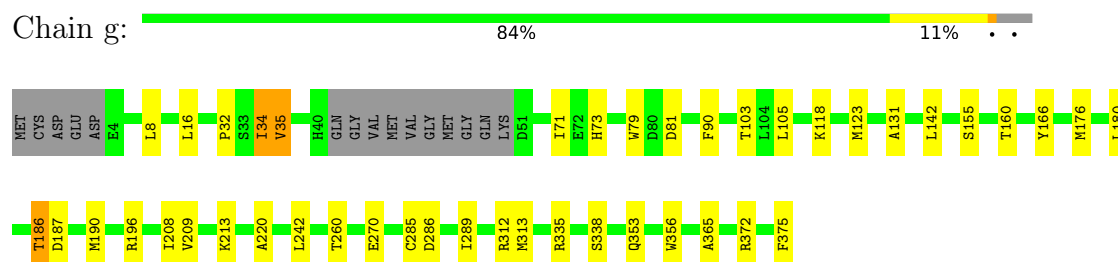
- Molecule 1: Actin, alpha skeletal muscle



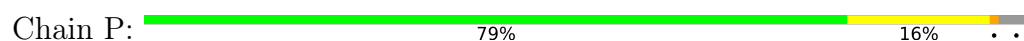
- Molecule 1: Actin, alpha skeletal muscle

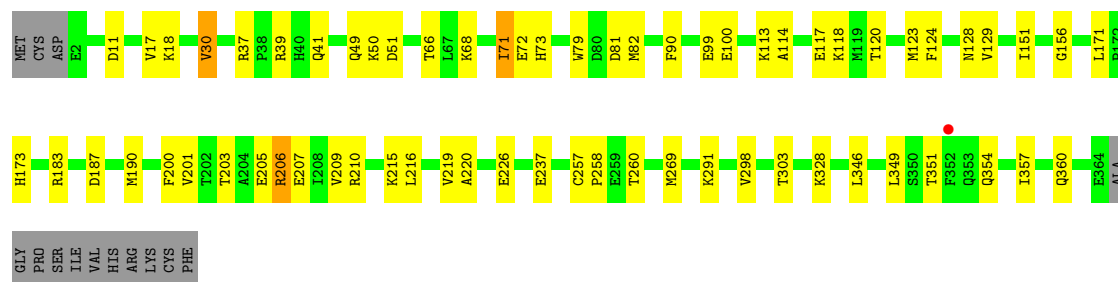


- Molecule 1: Actin, alpha skeletal muscle

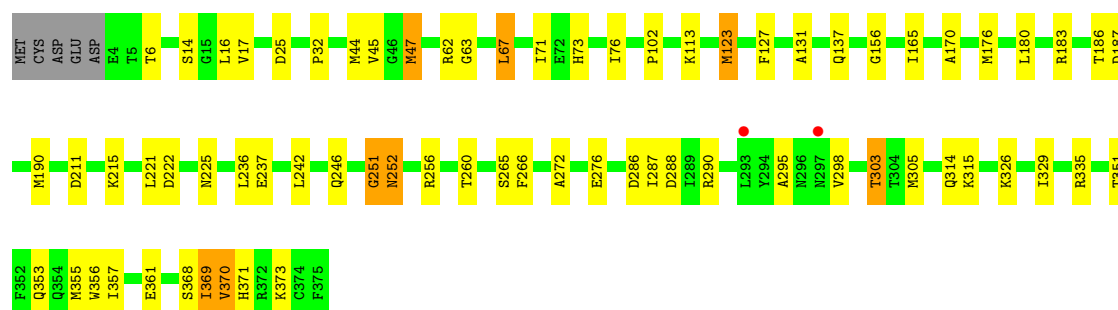
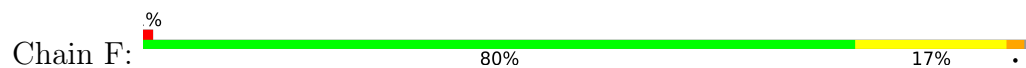


- Molecule 1: Actin, alpha skeletal muscle

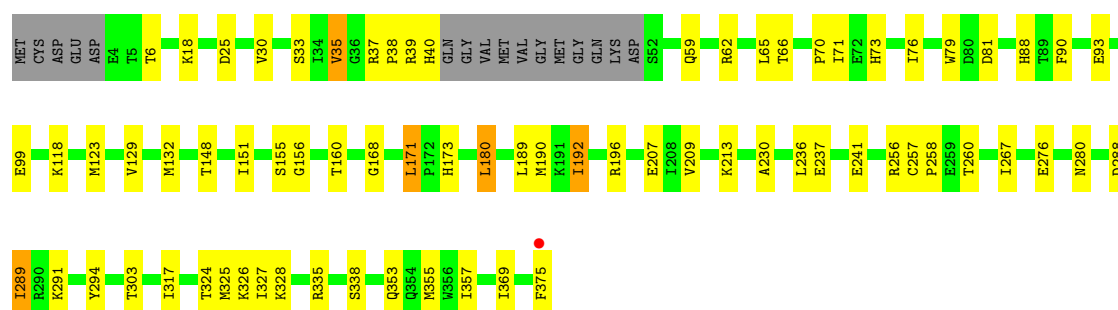
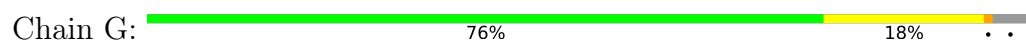




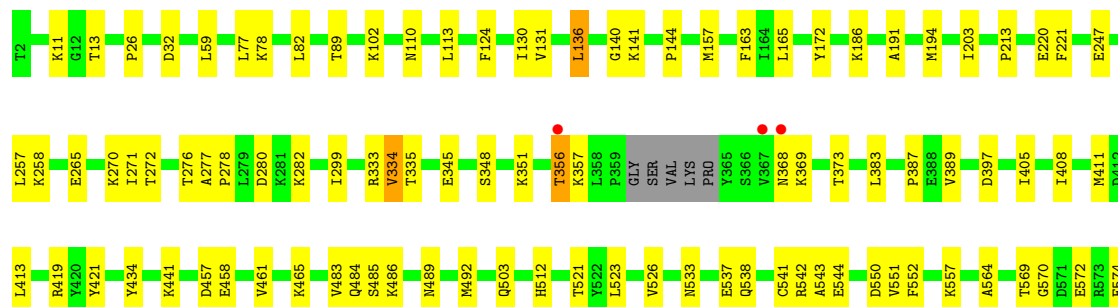
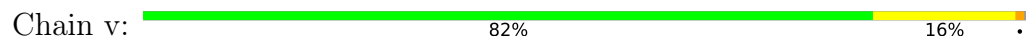
- Molecule 1: Actin, alpha skeletal muscle

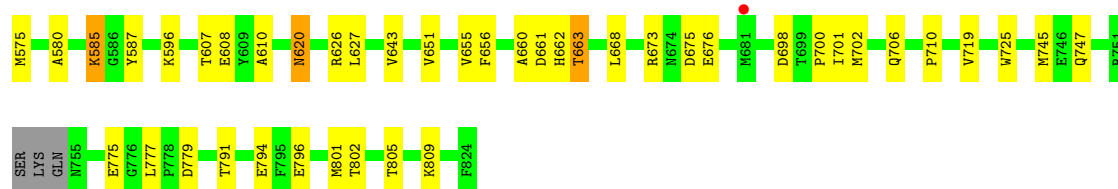


- Molecule 1: Actin, alpha skeletal muscle



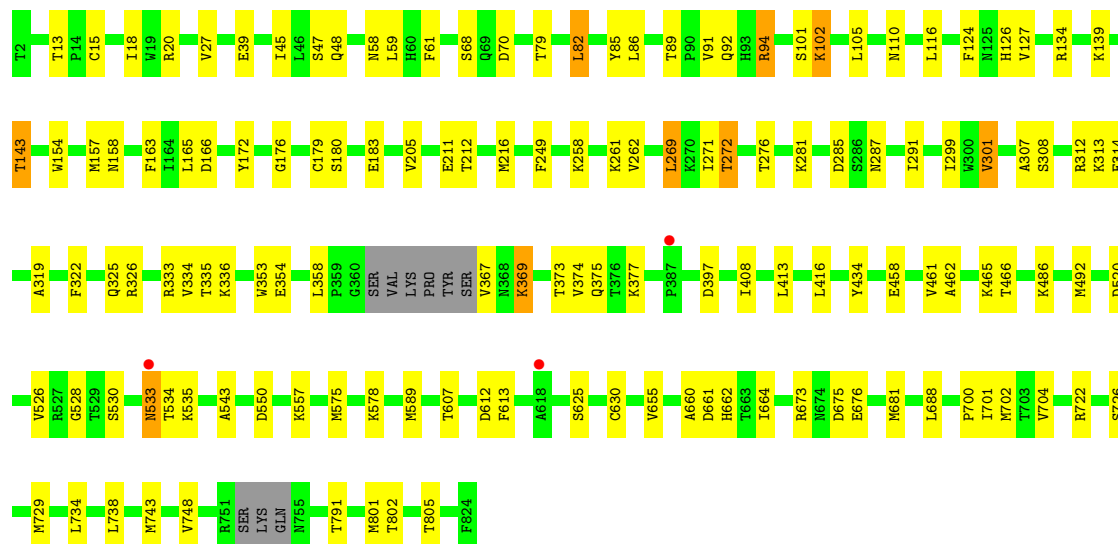
- Molecule 2: villin





• Molecule 2: villin

Chain V: 82% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.14Å 102.43Å 147.13Å 77.95° 72.59° 65.96°	Depositor
Resolution (Å)	29.90 – 2.70 29.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.90-2.70) 97.9 (29.90-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.196 , 0.226 0.197 , 0.228	Depositor DCC
R_{free} test set	6646 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30576	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, SCN, CL, HIC, ADP, MG

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	F	0.10	0/2959	0.26	0/4006
1	G	0.09	0/2892	0.26	0/3917
1	P	0.10	0/2888	0.27	0/3912
1	f	0.10	0/2959	0.28	0/4006
1	g	0.10	0/2900	0.27	0/3928
1	p	0.09	0/2882	0.27	0/3904
2	V	0.09	0/6662	0.27	0/8972
2	v	0.09	0/6652	0.26	0/8959
All	All	0.09	0/30794	0.27	0/41604

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	F	2909	0	2878	40	0
1	G	2839	0	2806	38	0
1	P	2841	0	2801	29	0
1	f	2909	0	2878	30	0
1	g	2847	0	2810	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	p	2831	0	2798	28	0
2	V	6515	0	6308	70	0
2	v	6510	0	6300	59	0
3	F	27	0	12	0	0
3	G	27	0	12	2	0
3	P	27	0	12	0	0
3	f	27	0	12	2	0
3	g	27	0	12	0	0
3	p	27	0	12	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	P	1	0	0	0	0
4	f	1	0	0	0	0
4	g	1	0	0	0	0
4	p	1	0	0	0	0
5	V	8	0	0	0	0
5	v	8	0	0	0	0
6	v	1	0	0	0	0
7	V	3	0	0	0	0
8	F	11	0	0	1	0
8	G	8	0	0	0	0
8	P	26	0	0	1	0
8	V	34	0	0	1	0
8	f	32	0	0	1	0
8	g	19	0	0	0	0
8	p	18	0	0	0	0
8	v	39	0	0	2	0
All	All	30576	0	29651	307	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 (307) 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)
2:v:801:MET:HE1	2:v:809:LYS:HE2	1.62	0.81
2:V:734:LEU:HB3	2:V:743:MET:HE1	1.68	0.74
1:P:190:MET:HG3	1:P:209:VAL:HG11	1.68	0.74
1:G:35:VAL:HG11	1:G:81:ASP:HB3	1.69	0.74
2:V:664:ILE:HB	2:V:701:ILE:HG22	1.73	0.71
2:v:503:GLN:H	2:v:538:GLN:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:71:ILE:HG12	1:p:82:MET:HE1	1.72	0.69
1:F:47:MET:HG3	1:G:148:THR:HG22	1.75	0.69
2:v:413:LEU:HG	2:v:465:LYS:HD3	1.75	0.68
2:v:551:VAL:HG12	2:v:564:ALA:HA	1.75	0.67
2:V:673:ARG:HB2	2:V:676:GLU:HG3	1.76	0.67
2:V:307:ALA:O	2:V:312:ARG:NH1	2.29	0.65
1:G:291:LYS:HG3	1:G:325:MET:HE1	1.78	0.65
2:V:543:ALA:HB3	2:V:607:THR:HG22	1.78	0.65
1:g:285:CYS:HB3	1:g:289:ILE:HD11	1.76	0.65
1:f:180:LEU:HD11	1:f:260:THR:HG22	1.79	0.64
1:f:49:GLN:HB2	2:v:357:LYS:HE2	1.80	0.64
2:V:59:LEU:HB2	2:V:92:GLN:HA	1.80	0.64
2:v:543:ALA:HB3	2:v:607:THR:HG22	1.78	0.63
3:f:401:ADP:O2B	8:f:501:HOH:O	2.15	0.63
2:v:136:LEU:HD13	2:v:194:MET:HE1	1.79	0.63
1:P:37:ARG:NH1	1:P:81:ASP:OD1	2.31	0.63
1:P:220:ALA:HB1	1:P:226:GLU:HG3	1.80	0.63
1:f:190:MET:HG2	1:f:209:VAL:HG21	1.80	0.63
1:F:361:GLU:HB3	1:F:369:ILE:HD13	1.82	0.62
2:V:630:CYS:HB2	2:V:655:VAL:HG23	1.81	0.62
1:G:335:ARG:HA	1:G:338:SER:HB2	1.80	0.62
1:P:156:GLY:O	1:P:303:THR:OG1	2.17	0.62
1:F:357:ILE:HD13	1:F:370:VAL:HA	1.82	0.62
2:v:383:LEU:O	2:v:626:ARG:NH2	2.30	0.61
1:G:90:PHE:HZ	1:G:123:MET:HE1	1.64	0.61
1:p:294:TYR:HB2	1:p:325:MET:HE2	1.81	0.61
1:G:88:HIS:NE2	1:G:93:GLU:OE1	2.34	0.61
2:V:397:ASP:OD2	2:V:434:TYR:OH	2.16	0.61
2:V:154:TRP:HA	2:V:157:MET:HE3	1.82	0.61
2:V:299:ILE:HB	2:V:334:VAL:HG12	1.83	0.60
1:g:190:MET:HG2	1:g:209:VAL:HG21	1.81	0.60
2:V:61:PHE:HB3	2:V:79:THR:HG21	1.84	0.59
1:p:220:ALA:HB1	1:p:226:GLU:HG3	1.84	0.59
1:g:35:VAL:HG11	1:g:81:ASP:HB3	1.85	0.59
2:v:655:VAL:HG12	2:v:668:LEU:HA	1.84	0.59
1:G:276:GLU:O	1:G:280:ASN:ND2	2.35	0.58
2:v:387:PRO:HD3	2:v:626:ARG:HH12	1.68	0.58
1:f:71:ILE:HG12	1:f:76:ILE:HG12	1.86	0.58
1:P:207:GLU:OE2	1:P:210:ARG:NH2	2.37	0.58
1:F:252:ASN:HD21	1:F:256:ARG:HD3	1.68	0.57
1:p:353:GLN:HA	1:p:356:TRP:HD1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:LEU:HD11	1:F:260:THR:HG22	1.85	0.57
2:v:165:LEU:HB3	2:v:172:TYR:HB2	1.85	0.57
1:g:186:THR:HG22	1:g:213:LYS:HZ3	1.69	0.57
2:V:262:VAL:HG22	2:V:271:ILE:HG22	1.85	0.57
2:V:526:VAL:HG13	2:V:575:MET:HE3	1.86	0.57
2:V:612:ASP:OD1	2:V:613:PHE:N	2.38	0.57
2:v:389:VAL:HG22	2:v:643:VAL:HG11	1.87	0.57
1:p:346:LEU:HD12	1:p:349:LEU:HD12	1.86	0.56
2:v:397:ASP:OD2	2:v:434:TYR:OH	2.18	0.56
1:F:113:LYS:HE3	1:F:371:HIS:CD2	2.41	0.56
1:G:230:ALA:HB2	1:G:236:LEU:HD12	1.88	0.56
1:F:187:ASP:HA	1:F:190:MET:HE2	1.88	0.56
1:F:44:MET:HE3	1:G:168:GLY:HA2	1.87	0.56
1:G:37:ARG:NH2	1:G:81:ASP:OD1	2.38	0.56
2:v:191:ALA:HB1	2:v:203:ILE:HD12	1.87	0.56
1:g:32:PRO:HB2	1:g:34:ILE:HG13	1.88	0.56
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.87	0.55
1:F:353:GLN:HA	1:F:356:TRP:CD1	2.42	0.55
1:f:45:VAL:HB	1:g:375:PHE:HZ	1.72	0.55
1:p:116:ARG:HD2	1:p:134:VAL:HG11	1.89	0.54
1:G:39:ARG:HG2	1:G:66:THR:OG1	2.07	0.54
1:g:208:ILE:HG21	1:g:242:LEU:HD23	1.89	0.54
2:V:59:LEU:HD12	2:V:92:GLN:HG2	1.89	0.54
2:v:580:ALA:HB1	2:v:587:TYR:HB3	1.90	0.54
2:V:492:MET:HE2	2:V:533[A]:ASN:HA	1.89	0.54
1:P:41:GLN:HG2	1:P:49:GLN:HG3	1.90	0.54
1:G:156:GLY:O	1:G:303:THR:OG1	2.25	0.54
1:f:90:PHE:HZ	1:f:123:MET:HE1	1.71	0.53
1:P:39:ARG:HG2	1:P:66:THR:HG23	1.89	0.53
2:v:526:VAL:HB	2:v:551:VAL:HG23	1.90	0.53
1:P:215:LYS:HB3	1:P:216:LEU:HD22	1.90	0.53
1:F:156:GLY:O	1:F:303:THR:OG1	2.25	0.53
1:g:187:ASP:HA	1:g:190:MET:HE2	1.90	0.53
2:V:325:GLN:HG3	2:V:326:ARG:HD2	1.90	0.53
1:g:131:ALA:HB1	1:g:356:TRP:HB3	1.89	0.53
2:V:134:ARG:HG2	2:V:166:ASP:HB3	1.89	0.53
2:V:738:LEU:HB2	2:V:743:MET:HE3	1.90	0.53
1:P:71:ILE:HG12	1:P:82:MET:HE1	1.91	0.53
1:G:190:MET:HG3	1:G:209:VAL:HG11	1.91	0.53
1:f:123:MET:HE3	1:f:129:VAL:HG11	1.91	0.52
2:v:663:THR:HG22	2:v:700:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:GLN:HG3	1:F:329:ILE:HD13	1.90	0.52
2:V:211:GLU:HA	2:V:216:MET:HE3	1.91	0.52
1:f:285:CYS:HB3	1:f:289:ILE:HD11	1.91	0.52
2:V:82:LEU:HA	2:V:85:TYR:HB3	1.92	0.52
1:P:17:VAL:O	1:P:30:VAL:HA	2.10	0.52
1:f:337:TYR:O	1:f:341:ILE:HG12	2.10	0.52
2:v:59:LEU:HD21	2:v:82:LEU:HD23	1.92	0.52
2:V:18:ILE:HG12	2:V:45:ILE:HG13	1.92	0.52
1:f:187:ASP:HA	1:f:190:MET:HE2	1.92	0.51
2:V:319:ALA:HA	2:V:322:PHE:HD2	1.76	0.51
2:v:220:GLU:N	2:v:220:GLU:OE2	2.44	0.51
1:P:123:MET:HE3	1:P:129:VAL:HG11	1.92	0.51
1:p:90:PHE:HZ	1:p:123:MET:HE1	1.76	0.51
1:G:35:VAL:HG12	1:G:70:PRO:HD3	1.92	0.51
1:F:222:ASP:OD2	1:F:225:ASN:ND2	2.44	0.51
1:p:352:PHE:CD1	1:p:355:MET:HB2	2.46	0.50
2:v:278:PRO:HB3	2:v:351:LYS:HG3	1.93	0.50
1:P:11:ASP:HB3	1:P:18:LYS:HB2	1.92	0.50
1:P:346:LEU:HD12	1:P:349:LEU:HD12	1.92	0.50
1:f:39:ARG:NH1	1:g:286:ASP:OD2	2.45	0.50
1:P:171:LEU:HB3	1:P:173:HIS:CE1	2.47	0.50
2:V:59:LEU:HD22	2:V:82:LEU:HD21	1.94	0.50
1:p:38:PRO:HB3	1:p:47:MET:HE3	1.94	0.49
1:F:63:GLY:HA3	1:G:289:ILE:HG22	1.94	0.49
1:F:165:ILE:HA	1:F:170:ALA:HA	1.94	0.49
1:G:71:ILE:HG12	1:G:76:ILE:HG12	1.93	0.49
2:V:802:THR:HG23	2:V:805:THR:H	1.77	0.49
1:f:233:SER:OG	1:f:234:SER:N	2.44	0.49
1:g:90:PHE:HZ	1:g:123:MET:HE1	1.78	0.49
1:F:260:THR:HG23	1:F:266:PHE:HB2	1.95	0.49
1:P:187:ASP:HA	1:P:190:MET:HE3	1.94	0.49
1:p:72:GLU:HG3	1:p:183:ARG:HH12	1.77	0.49
1:g:79:TRP:CE2	1:g:118:LYS:HG2	2.48	0.49
2:v:585:LYS:H	2:v:585:LYS:HD2	1.78	0.49
2:v:673:ARG:HB2	2:v:676:GLU:HG3	1.95	0.49
1:p:180:LEU:HD11	1:p:260:THR:HG22	1.94	0.49
1:G:18:LYS:NZ	3:G:401:ADP:O2A	2.37	0.48
2:V:492:MET:HE2	2:V:533[B]:ASN:HA	1.94	0.48
2:V:15:CYS:H	2:V:48:GLN:HB2	1.78	0.48
2:V:660:ALA:O	2:V:662:HIS:N	2.44	0.48
1:G:59:GLN:OE1	1:G:62:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:176:GLY:N	2:V:179:CYS:SG	2.86	0.48
1:p:314:GLN:HB2	1:p:329:ILE:HD13	1.95	0.48
1:g:16:LEU:HD23	1:g:32:PRO:HA	1.96	0.48
2:v:627:LEU:HD11	2:v:656:PHE:HB3	1.95	0.48
2:v:673:ARG:NH1	2:v:675:ASP:OD2	2.45	0.48
1:g:180:LEU:HD11	1:g:260:THR:HG22	1.96	0.48
2:V:530:SER:HB3	2:V:533[A]:ASN:HD21	1.78	0.48
2:v:526:VAL:HG13	2:v:575:MET:HE3	1.95	0.48
1:F:221:LEU:HD12	1:F:315:LYS:HD2	1.94	0.48
1:p:347:ALA:HA	1:p:352:PHE:CD2	2.49	0.47
1:g:8:LEU:HB2	1:g:103:THR:HG22	1.96	0.47
1:F:295:ALA:HB2	1:F:326:LYS:HG3	1.96	0.47
2:V:143:THR:O	2:V:143:THR:OG1	2.29	0.47
2:V:165:LEU:HB3	2:V:172:TYR:HB2	1.96	0.47
1:f:18:LYS:HG3	1:f:30:VAL:HG22	1.97	0.47
2:v:489:ASN:ND2	8:v:1006:HOH:O	2.46	0.47
2:V:258:LYS:HE2	2:V:276:THR:HG22	1.96	0.47
1:p:123:MET:HE3	1:p:129:VAL:HG11	1.96	0.47
1:F:287:ILE:HA	1:F:290:ARG:HD2	1.97	0.47
1:F:14:SER:HB3	1:F:183:ARG:HH11	1.79	0.47
1:G:123:MET:HE3	1:G:129:VAL:HG11	1.97	0.47
2:V:68:SER:OG	2:V:70:ASP:OD1	2.32	0.47
1:g:155:SER:HA	1:g:160:THR:HG22	1.96	0.47
2:v:408:ILE:HG21	2:v:458:GLU:HA	1.96	0.47
1:G:213:LYS:NZ	3:G:401:ADP:O2'	2.46	0.47
2:V:261:LYS:HB3	2:V:272:THR:HG23	1.97	0.47
2:V:530:SER:HB3	2:V:533[A]:ASN:ND2	2.29	0.47
1:f:44:MET:HE1	1:g:142:LEU:HD23	1.97	0.47
1:P:328:LYS:NZ	8:P:501:HOH:O	2.39	0.47
2:V:269:LEU:HD22	2:V:314:GLU:HG3	1.95	0.47
1:f:349:LEU:HD11	2:v:77:LEU:HD13	1.96	0.47
2:v:356:THR:HG22	2:v:357:LYS:H	1.80	0.47
2:v:526:VAL:O	2:v:550:ASP:HB3	2.15	0.47
2:V:462:ALA:O	2:V:466:THR:HG23	2.15	0.46
1:f:305:MET:HG3	1:f:336:LYS:HE3	1.96	0.46
2:V:578:LYS:O	8:V:1001:HOH:O	2.20	0.46
1:f:357:ILE:HG12	1:f:373:LYS:HG3	1.98	0.46
1:p:352:PHE:HD1	1:p:355:MET:HB2	1.80	0.46
1:p:302:GLY:HA2	1:p:336:LYS:HG2	1.98	0.46
1:F:71:ILE:HG12	1:F:76:ILE:HG12	1.96	0.46
1:f:90:PHE:CZ	1:f:123:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:340:TRP:HE3	1:f:341:ILE:HD13	1.81	0.46
1:P:349:LEU:HD21	2:V:461:VAL:HG22	1.98	0.46
1:F:45:VAL:HG21	1:G:355:MET:HE2	1.98	0.46
2:V:20:ARG:N	2:V:27:VAL:O	2.42	0.46
1:F:131:ALA:HB1	1:F:356:TRP:HB3	1.98	0.46
1:G:189:LEU:HD23	1:G:209:VAL:HG13	1.98	0.46
2:V:139:LYS:HD3	2:V:249:PHE:CG	2.51	0.45
2:V:291:ILE:HD13	2:V:319:ALA:HB2	1.98	0.45
2:V:681:MET:HB3	2:V:748:VAL:HG11	1.98	0.45
1:G:357:ILE:HD13	1:G:369:ILE:HG23	1.97	0.45
1:p:73:HIC:HB2	1:p:177:ARG:HH22	1.81	0.45
2:v:702:MET:HA	2:v:747:GLN:HA	1.99	0.45
1:f:18:LYS:NZ	3:f:401:ADP:O1B	2.49	0.45
1:p:131:ALA:HB1	1:p:356:TRP:HB3	1.99	0.45
2:V:700:PRO:HB2	2:V:702:MET:HE1	1.98	0.45
1:g:105:LEU:HD11	1:g:123:MET:HG3	1.99	0.45
1:G:171:LEU:HD12	1:G:173[A]:HIS:HE1	1.82	0.45
1:g:353:GLN:HA	1:g:356:TRP:CD1	2.51	0.45
1:F:237:GLU:HG2	1:F:251:GLY:HA3	1.99	0.45
1:f:16:LEU:HD23	1:f:32:PRO:HA	1.99	0.45
2:v:660:ALA:O	2:v:662:HIS:N	2.46	0.45
1:G:180:LEU:HD11	1:G:260:THR:HG22	1.99	0.45
2:v:557:LYS:HD2	2:v:557:LYS:HA	1.86	0.45
2:v:710:PRO:HG3	2:v:745:MET:SD	2.56	0.45
1:P:219:VAL:HG22	1:P:258:PRO:HB2	1.98	0.45
1:P:72:GLU:HG3	1:P:183:ARG:HH12	1.81	0.44
1:P:90:PHE:HZ	1:P:123:MET:HE1	1.81	0.44
2:V:533[B]:ASN:OD1	2:V:535:LYS:NZ	2.50	0.44
1:G:79:TRP:CE2	1:G:118:LYS:HG2	2.53	0.44
2:v:484:GLN:O	2:v:485:SER:OG	2.26	0.44
1:F:242:LEU:HD12	1:F:246:GLN:HB2	1.99	0.44
2:v:706:GLN:HE21	2:v:725:TRP:CD1	2.36	0.44
2:V:94:ARG:H	2:V:94:ARG:HG3	1.46	0.44
2:V:557:LYS:HE2	2:V:557:LYS:HB3	1.86	0.44
1:f:357:ILE:HD13	1:f:370:VAL:HA	1.99	0.44
2:v:387:PRO:HD3	2:v:626:ARG:NH1	2.31	0.44
1:G:132:MET:HE2	1:G:132:MET:HB2	1.91	0.44
1:p:75:ILE:HG23	1:p:115:ASN:ND2	2.33	0.44
1:F:272:ALA:HB1	1:F:276:GLU:HB2	1.98	0.44
2:v:276:THR:OG1	2:v:277:ALA:N	2.51	0.44
1:f:156:GLY:O	1:f:303:THR:OG1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:102:LYS:HE2	2:v:102:LYS:HB3	1.82	0.44
1:P:117:GLU:HA	1:P:120:THR:HG22	1.99	0.44
2:v:408:ILE:HD12	2:v:461:VAL:HG12	1.99	0.43
2:v:544:GLU:HG2	2:v:608:GLU:O	2.17	0.43
1:F:355:MET:HA	1:F:373:LYS:HE2	1.99	0.43
2:v:523:LEU:HD11	2:v:552:PHE:HB3	2.00	0.43
1:F:236:LEU:HD12	1:F:236:LEU:HA	1.83	0.43
1:G:18:LYS:HG3	1:G:30:VAL:HG22	1.99	0.43
2:V:101:SER:O	2:V:105:LEU:HG	2.19	0.43
1:p:28:ARG:HH11	1:p:28:ARG:HB3	1.83	0.43
2:V:353:TRP:CD1	2:V:354:GLU:H	2.36	0.43
1:f:353:GLN:HA	1:f:356:TRP:CD1	2.54	0.43
2:V:526:VAL:O	2:V:550:ASP:HB3	2.18	0.43
1:p:207:GLU:CD	1:p:210:ARG:HH12	2.26	0.43
1:f:113:LYS:HD2	1:f:113:LYS:N	2.33	0.43
2:v:408:ILE:HB	8:v:1021:HOH:O	2.19	0.43
2:V:408:ILE:HG21	2:V:458:GLU:HA	1.99	0.43
1:F:62:ARG:HB2	1:F:67:LEU:HD21	1.99	0.43
1:g:79:TRP:CD2	1:g:118:LYS:HG2	2.54	0.43
2:V:139:LYS:HB3	2:V:249:PHE:CE1	2.54	0.43
1:F:137:GLN:NE2	8:F:503:HOH:O	2.52	0.43
1:F:368:SER:HA	1:F:371:HIS:CD2	2.54	0.43
2:V:180:SER:HB3	2:V:183:GLU:CD	2.44	0.43
1:f:64:ILE:HG12	1:g:166:TYR:HD2	1.83	0.43
1:P:79:TRP:NE1	1:P:118:LYS:HE3	2.34	0.43
2:V:291:ILE:HG12	2:V:301:VAL:HG13	2.01	0.43
1:P:257:CYS:HB3	1:P:258:PRO:HD3	2.01	0.42
1:G:257:CYS:HB3	1:G:258:PRO:HD3	2.01	0.42
1:F:16:LEU:HD23	1:F:32:PRO:HA	2.01	0.42
2:V:102:LYS:HE3	2:V:102:LYS:HB3	1.85	0.42
2:v:299:ILE:O	2:v:334:VAL:HA	2.19	0.42
2:v:492:MET:HE2	2:v:533:ASN:HA	2.00	0.42
1:P:99:GLU:HG2	1:P:100:GLU:HG3	2.01	0.42
2:V:373:THR:C	2:V:375:GLN:H	2.27	0.42
1:F:44:MET:HB3	1:F:47:MET:HG2	2.02	0.42
2:V:413:LEU:HD11	2:V:465:LYS:HB3	2.01	0.42
2:v:157:MET:HA	2:v:163:PHE:CZ	2.54	0.42
2:v:537:GLU:HB2	2:v:719:VAL:HG11	2.01	0.42
2:v:802:THR:HG23	2:v:805:THR:H	1.84	0.42
1:G:326:LYS:HE3	1:G:326:LYS:HB2	1.90	0.42
1:g:365:ALA:HB1	1:g:372:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:39:GLU:HG3	2:V:116:LEU:O	2.19	0.42
2:V:369:LYS:HD3	2:V:369:LYS:HA	1.93	0.42
1:p:211:ASP:OD1	1:p:215:LYS:NZ	2.36	0.42
1:F:62:ARG:HE	1:G:288:ASP:CG	2.27	0.42
1:F:305:MET:HA	1:F:335:ARG:HH21	1.85	0.42
2:V:726:SER:HB3	2:V:734:LEU:HD11	2.02	0.42
2:v:620:ASN:OD1	2:v:620:ASN:N	2.53	0.42
1:P:269:MET:HE2	1:P:269:MET:HB3	1.98	0.42
1:G:180:LEU:HG	1:G:267:ILE:HD11	2.00	0.42
1:F:14:SER:HB3	1:F:183:ARG:NH1	2.35	0.41
1:p:156:GLY:O	1:p:303:THR:OG1	2.36	0.41
1:f:113:LYS:HD2	1:f:113:LYS:H	1.85	0.41
1:f:242:LEU:HD12	1:f:246:GLN:HB2	2.01	0.41
1:g:186:THR:HG22	1:g:213:LYS:NZ	2.35	0.41
2:v:405:ILE:HD12	2:v:421:TYR:CD2	2.55	0.41
1:G:38:PRO:HA	1:G:65:LEU:HD23	2.02	0.41
2:V:157:MET:HA	2:V:163:PHE:CZ	2.55	0.41
2:v:411:MET:SD	2:v:457:ASP:HB2	2.60	0.41
1:P:200:PHE:HD1	1:P:205:GLU:HB3	1.84	0.41
2:V:528:GLY:HA3	2:V:534:THR:HG22	2.02	0.41
1:p:325:MET:HE3	1:p:326:LYS:N	2.36	0.41
2:v:345:GLU:O	2:v:348:SER:OG	2.34	0.41
1:f:332:PRO:HA	1:f:333:PRO:HD3	1.95	0.41
2:V:47:SER:HB3	2:V:58:ASN:HB2	2.02	0.41
2:V:722:ARG:HD3	2:V:729:MET:O	2.20	0.41
1:p:64:ILE:HG13	1:p:65:LEU:HD13	2.03	0.41
1:p:336:LYS:HB3	1:p:336:LYS:HE2	1.87	0.41
2:v:140:GLY:HA3	2:v:144:PRO:HA	2.03	0.41
2:v:570:GLY:O	2:v:574:GLU:HG2	2.20	0.41
1:G:155:SER:HA	1:G:160:THR:HG22	2.03	0.41
2:V:530:SER:O	2:V:534:THR:HG23	2.20	0.41
1:p:145:SER:HB2	1:p:147:ARG:HH11	1.85	0.41
2:v:333:ARG:HD3	2:v:333:ARG:HA	1.82	0.41
1:F:25:ASP:OD2	2:V:126:HIS:HA	2.20	0.41
1:G:317:ILE:HG22	1:G:327:ILE:HG12	2.03	0.41
2:V:313:LYS:HE3	2:V:313:LYS:HB3	1.96	0.41
2:v:26:PRO:HG3	2:v:78:LYS:HG3	2.03	0.40
2:v:186:LYS:HA	2:v:186:LYS:HD2	1.95	0.40
2:v:213:PRO:HG3	2:v:221:PHE:CD1	2.56	0.40
1:F:186:THR:O	1:F:190:MET:HG3	2.21	0.40
1:F:113:LYS:HE2	1:F:113:LYS:HB3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:408:ILE:HD13	2:V:413:LEU:HD23	2.03	0.40
2:v:569:THR:OG1	2:v:572:GLU:HG3	2.21	0.40
1:G:192:ILE:HD11	1:G:256:ARG:HH21	1.87	0.40
1:p:17:VAL:O	1:p:30:VAL:HA	2.22	0.40
1:g:220:ALA:O	1:g:312:ARG:HG3	2.21	0.40
1:g:335:ARG:HA	1:g:338:SER:HB3	2.03	0.40
1:P:124:PHE:HZ	1:P:357:ILE:O	2.04	0.40
1:P:206:ARG:HA	1:P:209:VAL:HG12	2.04	0.40
1:G:294:TYR:HD2	1:G:325:MET:HE2	1.86	0.40
1:G:328:LYS:HA	1:G:328:LYS:HD2	1.86	0.40
1:f:109:PRO:HG2	1:f:163:VAL:HG21	2.02	0.40
1:P:114:ALA:HA	1:P:117:GLU:HG2	2.03	0.40
1:F:123:MET:HE2	1:F:127:PHE:HD2	1.87	0.40
2:V:557:LYS:H	2:V:557:LYS:HG2	1.64	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	F	369/377 (98%)	358 (97%)	10 (3%)	1 (0%)	37	61
1	G	357/377 (95%)	342 (96%)	15 (4%)	0	100	100
1	P	360/377 (96%)	347 (96%)	13 (4%)	0	100	100
1	f	369/377 (98%)	361 (98%)	8 (2%)	0	100	100
1	g	358/377 (95%)	350 (98%)	8 (2%)	0	100	100
1	p	359/377 (95%)	348 (97%)	10 (3%)	1 (0%)	37	61
2	V	811/823 (98%)	783 (96%)	26 (3%)	2 (0%)	44	68
2	v	809/823 (98%)	778 (96%)	29 (4%)	2 (0%)	44	68
All	All	3792/3908 (97%)	3667 (97%)	119 (3%)	6 (0%)	44	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	374	VAL
1	p	67	LEU
1	F	251	GLY
2	v	610	ALA
2	v	661	ASP
2	V	661	ASP

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	F	314/319 (98%)	297 (95%)	17 (5%)	18	42
1	G	307/319 (96%)	289 (94%)	18 (6%)	16	38
1	P	307/319 (96%)	289 (94%)	18 (6%)	16	38
1	f	314/319 (98%)	305 (97%)	9 (3%)	37	67
1	g	308/319 (97%)	300 (97%)	8 (3%)	41	70
1	p	306/319 (96%)	291 (95%)	15 (5%)	21	47
2	V	702/708 (99%)	662 (94%)	40 (6%)	17	40
2	v	701/708 (99%)	654 (93%)	47 (7%)	13	33
All	All	3259/3330 (98%)	3087 (95%)	172 (5%)	19	43

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	6	THR
1	p	18	LYS
1	p	30	VAL
1	p	54	VAL
1	p	65	LEU
1	p	71	ILE
1	p	75	ILE
1	p	96	VAL

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Mol	Chain	Res	Type
1	p	99	GLU
1	p	151	ILE
1	p	195	GLU
1	p	206	ARG
1	p	208	ILE
1	p	312	ARG
1	p	326	LYS
1	f	6	THR
1	f	17	VAL
1	f	45	VAL
1	f	51	ASP
1	f	64	ILE
1	f	75	ILE
1	f	116	ARG
1	f	183	ARG
1	f	185	LEU
1	g	34	ILE
1	g	35	VAL
1	g	71	ILE
1	g	176	MET
1	g	186	THR
1	g	196	ARG
1	g	270	GLU
1	g	313	MET
2	v	11	LYS
2	v	13	THR
2	v	32	ASP
2	v	89	THR
2	v	110	ASN
2	v	113	LEU
2	v	124	PHE
2	v	130	ILE
2	v	131	VAL
2	v	136	LEU
2	v	141	LYS
2	v	247	GLU
2	v	257	LEU
2	v	258	LYS
2	v	265	GLU
2	v	270	LYS
2	v	271	ILE
2	v	272	THR

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Mol	Chain	Res	Type
2	v	280	ASP
2	v	282	LYS
2	v	334	VAL
2	v	335	THR
2	v	356	THR
2	v	368	ASN
2	v	369	LYS
2	v	373	THR
2	v	419	ARG
2	v	441	LYS
2	v	483	VAL
2	v	486	LYS
2	v	512	HIS
2	v	521	THR
2	v	541	CYS
2	v	542	ARG
2	v	585	LYS
2	v	596	LYS
2	v	620	ASN
2	v	651	VAL
2	v	663	THR
2	v	698	ASP
2	v	701	ILE
2	v	775	GLU
2	v	777	LEU
2	v	779	ASP
2	v	791	THR
2	v	794	GLU
2	v	796	GLU
1	P	30	VAL
1	P	50	LYS
1	P	51	ASP
1	P	68	LYS
1	P	71	ILE
1	P	113	LYS
1	P	128	ASN
1	P	151	ILE
1	P	201	VAL
1	P	203	THR
1	P	206	ARG
1	P	237	GLU
1	P	260	THR

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Mol	Chain	Res	Type
1	P	291	LYS
1	P	298	VAL
1	P	351	THR
1	P	354	GLN
1	P	360	GLN
1	F	6	THR
1	F	17	VAL
1	F	47	MET
1	F	67	LEU
1	F	123	MET
1	F	176	MET
1	F	211	ASP
1	F	215	LYS
1	F	252	ASN
1	F	265	SER
1	F	286	ASP
1	F	288	ASP
1	F	298	VAL
1	F	303	THR
1	F	351	THR
1	F	369	ILE
1	F	370	VAL
1	G	6	THR
1	G	25	ASP
1	G	33	SER
1	G	35	VAL
1	G	40	HIS
1	G	99	GLU
1	G	151	ILE
1	G	171	LEU
1	G	180	LEU
1	G	192	ILE
1	G	196	ARG
1	G	207	GLU
1	G	237	GLU
1	G	241	GLU
1	G	289	ILE
1	G	324	THR
1	G	353	GLN
1	G	375	PHE
2	V	13	THR
2	V	82	LEU

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Mol	Chain	Res	Type
2	V	86	LEU
2	V	89	THR
2	V	91	VAL
2	V	94	ARG
2	V	102	LYS
2	V	110	ASN
2	V	124	PHE
2	V	127	VAL
2	V	143	THR
2	V	158	ASN
2	V	205	VAL
2	V	212	THR
2	V	269	LEU
2	V	272	THR
2	V	281	LYS
2	V	285	ASP
2	V	287	ASN
2	V	301	VAL
2	V	308	SER
2	V	333	ARG
2	V	335	THR
2	V	336	LYS
2	V	358	LEU
2	V	367	VAL
2	V	369	LYS
2	V	377	LYS
2	V	416	LEU
2	V	486	LYS
2	V	520	ASP
2	V	533[A]	ASN
2	V	533[B]	ASN
2	V	589	MET
2	V	625	SER
2	V	675	ASP
2	V	688	LEU
2	V	704	VAL
2	V	791	THR
2	V	801	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	59	GLN
1	p	314	GLN
1	f	92	ASN
1	f	263	GLN
1	g	297	ASN
2	v	368	ASN
2	v	503	GLN
1	F	111	ASN
1	F	225	ASN
1	F	297	ASN
1	G	111	ASN
1	G	297	ASN
1	G	360	GLN
2	V	25	GLN
2	V	93	HIS
2	V	142	HIS
2	V	175	ASN
2	V	325	GLN
2	V	331	GLN
2	V	742	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	HIC	g	73	1	8,11,12	1.70	2 (25%)	6,14,16	1.10	1 (16%)
1	HIC	F	73	1	8,11,12	1.67	2 (25%)	6,14,16	1.12	0
1	HIC	G	73	1	8,11,12	1.72	2 (25%)	6,14,16	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	p	73	1	8,11,12	1.68	2 (25%)	6,14,16	1.21	1 (16%)
1	HIC	P	73	1	8,11,12	1.68	2 (25%)	6,14,16	1.21	1 (16%)
1	HIC	f	73	1	8,11,12	1.67	2 (25%)	6,14,16	1.36	1 (16%)

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
1	HIC	g	73	1	-	1/5/6/8	0/1/1/1
1	HIC	F	73	1	-	1/5/6/8	0/1/1/1
1	HIC	G	73	1	-	1/5/6/8	0/1/1/1
1	HIC	p	73	1	-	1/5/6/8	0/1/1/1
1	HIC	P	73	1	-	2/5/6/8	0/1/1/1
1	HIC	f	73	1	-	2/5/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	HIC	CD2-CG	3.76	1.41	1.36
1	g	73	HIC	CD2-CG	3.69	1.41	1.36
1	p	73	HIC	CD2-CG	3.69	1.41	1.36
1	P	73	HIC	CD2-CG	3.68	1.41	1.36
1	f	73	HIC	CD2-CG	3.68	1.41	1.36
1	F	73	HIC	CD2-CG	3.67	1.41	1.36
1	f	73	HIC	CZ-NE2	-2.03	1.42	1.48
1	g	73	HIC	CZ-NE2	-2.03	1.42	1.48
1	F	73	HIC	CZ-NE2	-2.02	1.42	1.48
1	G	73	HIC	CZ-NE2	-2.02	1.42	1.48
1	P	73	HIC	CZ-NE2	-2.01	1.42	1.48
1	p	73	HIC	CZ-NE2	-2.00	1.42	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	73	HIC	CB-CA-C	-2.62	106.56	111.47
1	P	73	HIC	CB-CA-C	-2.26	107.23	111.47
1	p	73	HIC	CB-CA-C	-2.20	107.34	111.47
1	g	73	HIC	CB-CA-C	-2.01	107.70	111.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	g	73	HIC	CA-CB-CG-ND1
1	F	73	HIC	CA-CB-CG-ND1
1	G	73	HIC	CA-CB-CG-ND1
1	p	73	HIC	C-CA-CB-CG
1	f	73	HIC	C-CA-CB-CG
1	P	73	HIC	C-CA-CB-CG
1	f	73	HIC	CA-CB-CG-ND1
1	P	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	p	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 23 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	ADP	F	401	4	24,29,29	0.95	1 (4%)	29,45,45	1.33	3 (10%)
3	ADP	G	401	4	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
3	ADP	g	401	4	24,29,29	0.95	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	P	401	4	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)
7	SCN	V	909	-	1,2,2	0.86	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	p	401	4	24,29,29	0.96	1 (4%)	29,45,45	1.33	3 (10%)
3	ADP	f	401	4	24,29,29	0.96	1 (4%)	29,45,45	1.29	4 (13%)

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	ADP	F	401	4	-	7/12/32/32	0/3/3/3
3	ADP	G	401	4	-	3/12/32/32	0/3/3/3
3	ADP	g	401	4	-	0/12/32/32	0/3/3/3
3	ADP	P	401	4	-	4/12/32/32	0/3/3/3
3	ADP	p	401	4	-	6/12/32/32	0/3/3/3
3	ADP	f	401	4	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	401	ADP	C5-C4	2.58	1.47	1.40
3	F	401	ADP	C5-C4	2.50	1.47	1.40
3	G	401	ADP	C5-C4	2.49	1.47	1.40
3	P	401	ADP	C5-C4	2.48	1.47	1.40
3	g	401	ADP	C5-C4	2.48	1.47	1.40
3	p	401	ADP	C5-C4	2.45	1.47	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	401	ADP	N3-C2-N1	-3.28	123.56	128.68
3	p	401	ADP	N3-C2-N1	-3.20	123.67	128.68
3	F	401	ADP	N3-C2-N1	-3.18	123.70	128.68
3	G	401	ADP	N3-C2-N1	-3.17	123.72	128.68
3	g	401	ADP	N3-C2-N1	-3.14	123.77	128.68
3	G	401	ADP	C3'-C2'-C1'	3.12	105.68	100.98
3	f	401	ADP	N3-C2-N1	-3.07	123.88	128.68
3	F	401	ADP	C3'-C2'-C1'	2.98	105.47	100.98
3	G	401	ADP	PA-O3A-PB	-2.86	123.01	132.83
3	P	401	ADP	C4-C5-N7	-2.83	106.45	109.40
3	g	401	ADP	PA-O3A-PB	-2.79	123.25	132.83
3	p	401	ADP	C4-C5-N7	-2.78	106.50	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	401	ADP	PA-O3A-PB	-2.69	123.61	132.83
3	G	401	ADP	C4-C5-N7	-2.68	106.61	109.40
3	F	401	ADP	C4-C5-N7	-2.63	106.66	109.40
3	p	401	ADP	PA-O3A-PB	-2.60	123.90	132.83
3	g	401	ADP	C4-C5-N7	-2.59	106.70	109.40
3	f	401	ADP	C4-C5-N7	-2.49	106.80	109.40
3	P	401	ADP	C3'-C2'-C1'	2.48	104.70	100.98
3	f	401	ADP	C3'-C2'-C1'	2.40	104.58	100.98
3	f	401	ADP	PA-O3A-PB	-2.24	125.15	132.83
3	g	401	ADP	C3'-C2'-C1'	2.01	104.01	100.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	p	401	ADP	C5'-O5'-PA-O3A
3	p	401	ADP	O4'-C4'-C5'-O5'
3	p	401	ADP	C3'-C4'-C5'-O5'
3	P	401	ADP	C5'-O5'-PA-O1A
3	F	401	ADP	C5'-O5'-PA-O2A
3	G	401	ADP	C5'-O5'-PA-O2A
3	F	401	ADP	PA-O3A-PB-O1B
3	P	401	ADP	PA-O3A-PB-O3B
3	P	401	ADP	C5'-O5'-PA-O3A
3	F	401	ADP	C5'-O5'-PA-O3A
3	p	401	ADP	C5'-O5'-PA-O1A
3	p	401	ADP	C5'-O5'-PA-O2A
3	F	401	ADP	C5'-O5'-PA-O1A
3	p	401	ADP	PA-O3A-PB-O3B
3	F	401	ADP	PA-O3A-PB-O2B
3	F	401	ADP	PA-O3A-PB-O3B
3	G	401	ADP	C5'-O5'-PA-O3A
3	F	401	ADP	PB-O3A-PA-O1A
3	G	401	ADP	C5'-O5'-PA-O1A
3	P	401	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

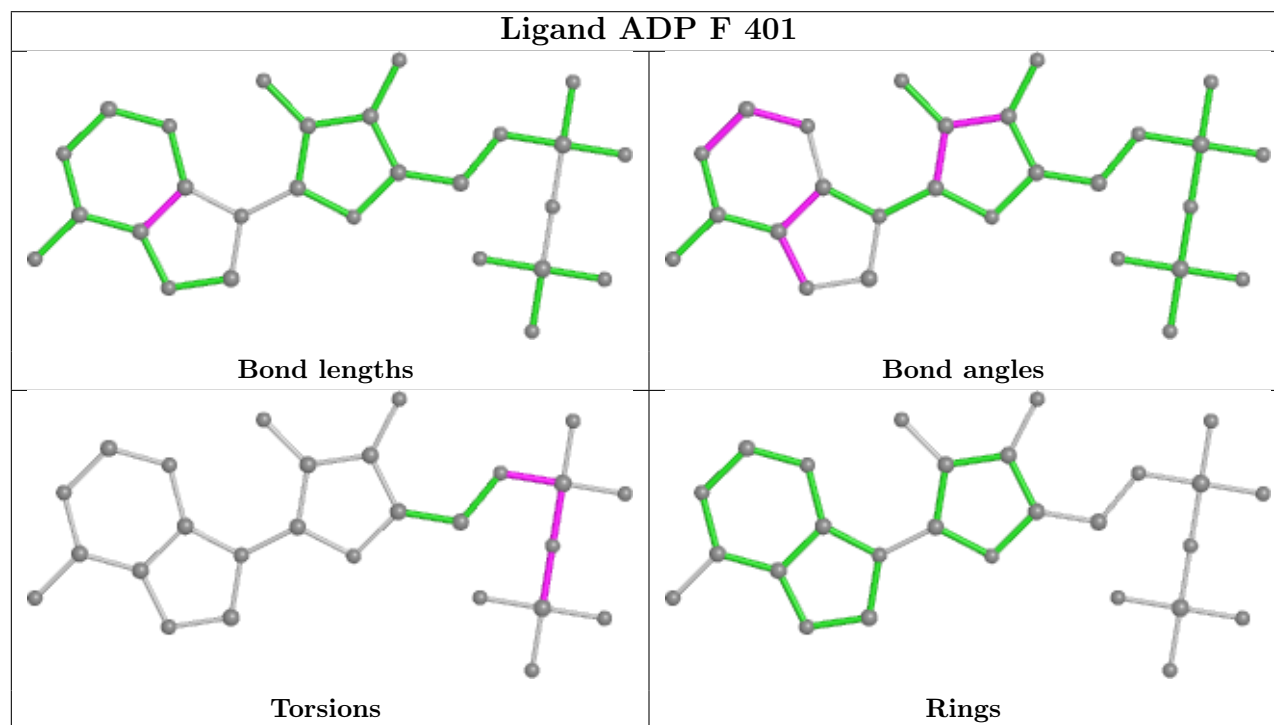
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	ADP	2	0

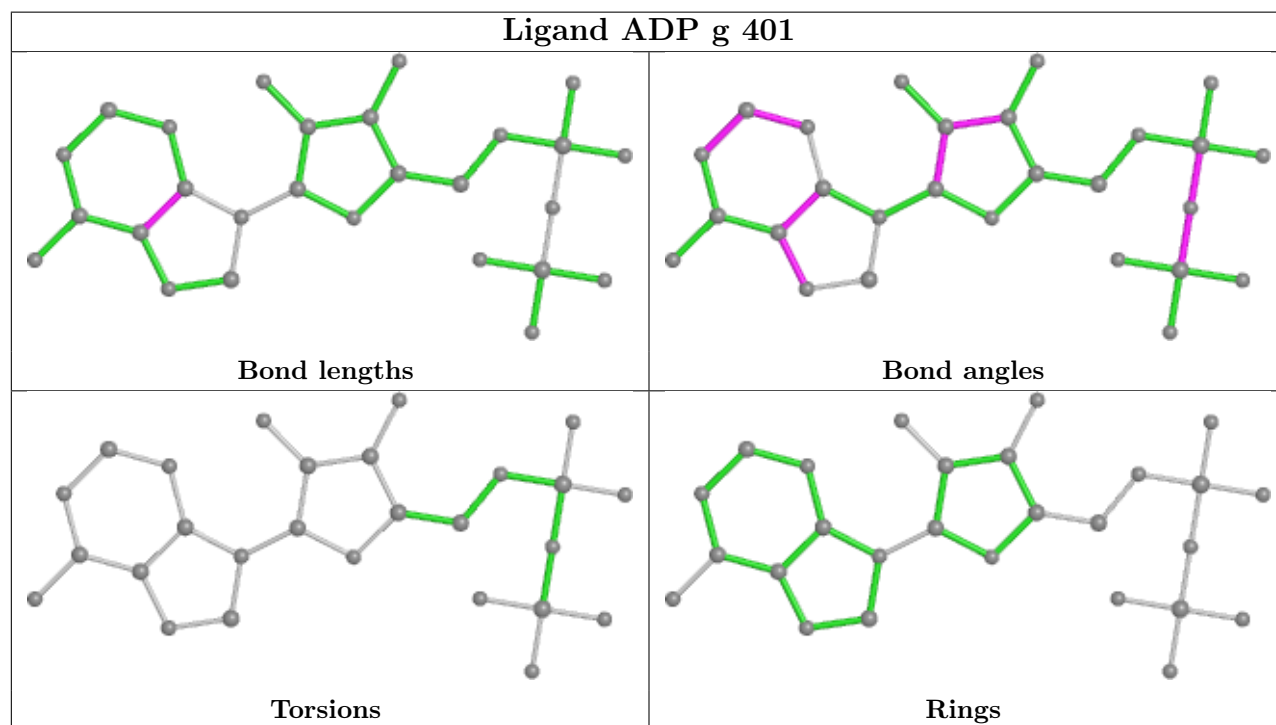
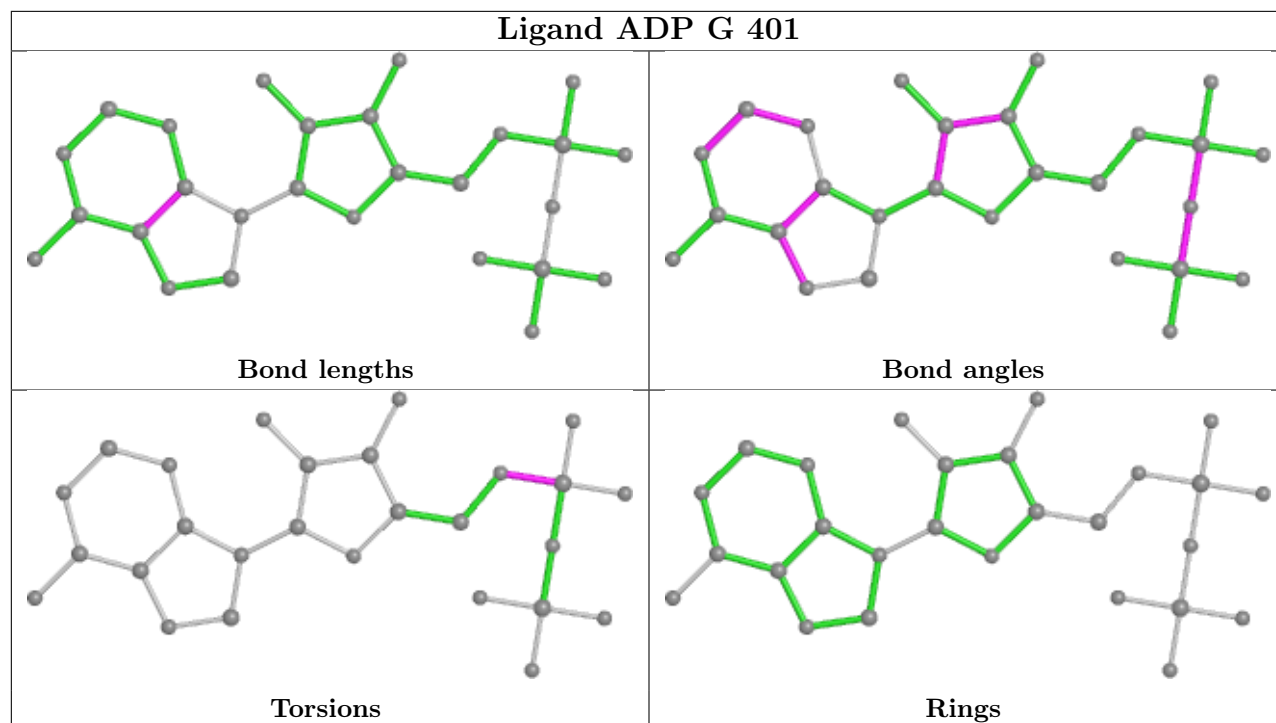
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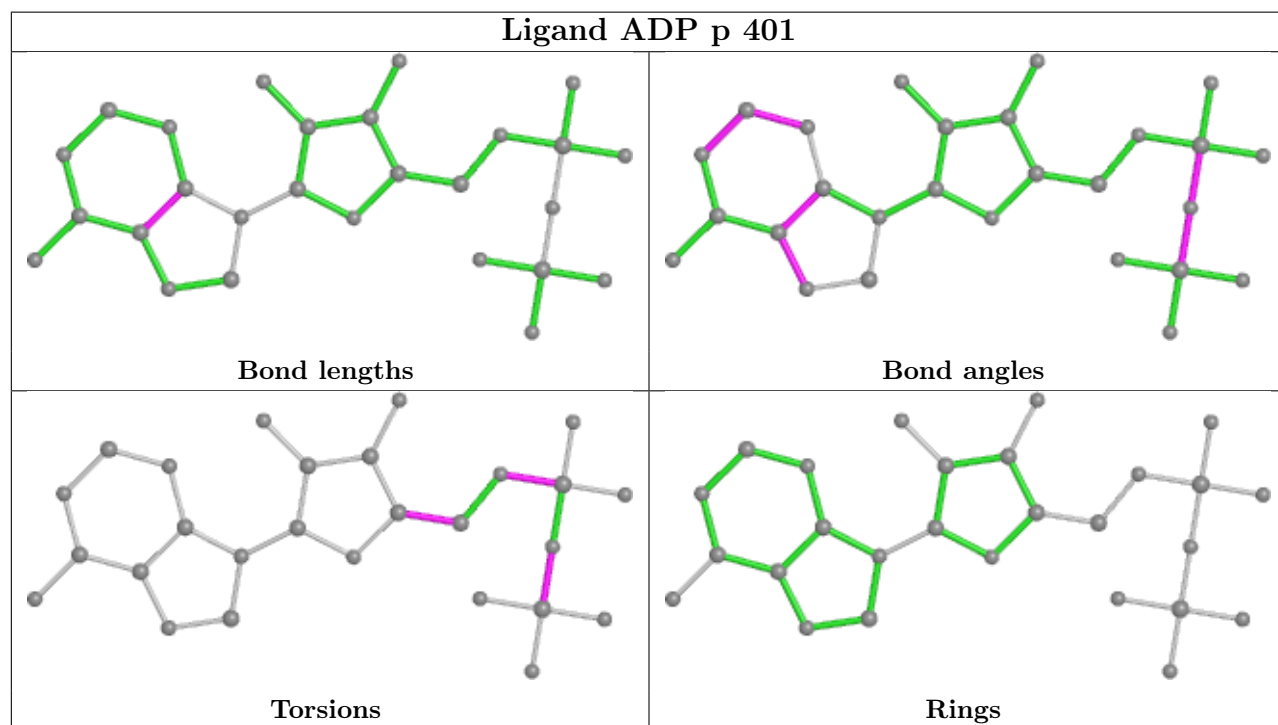
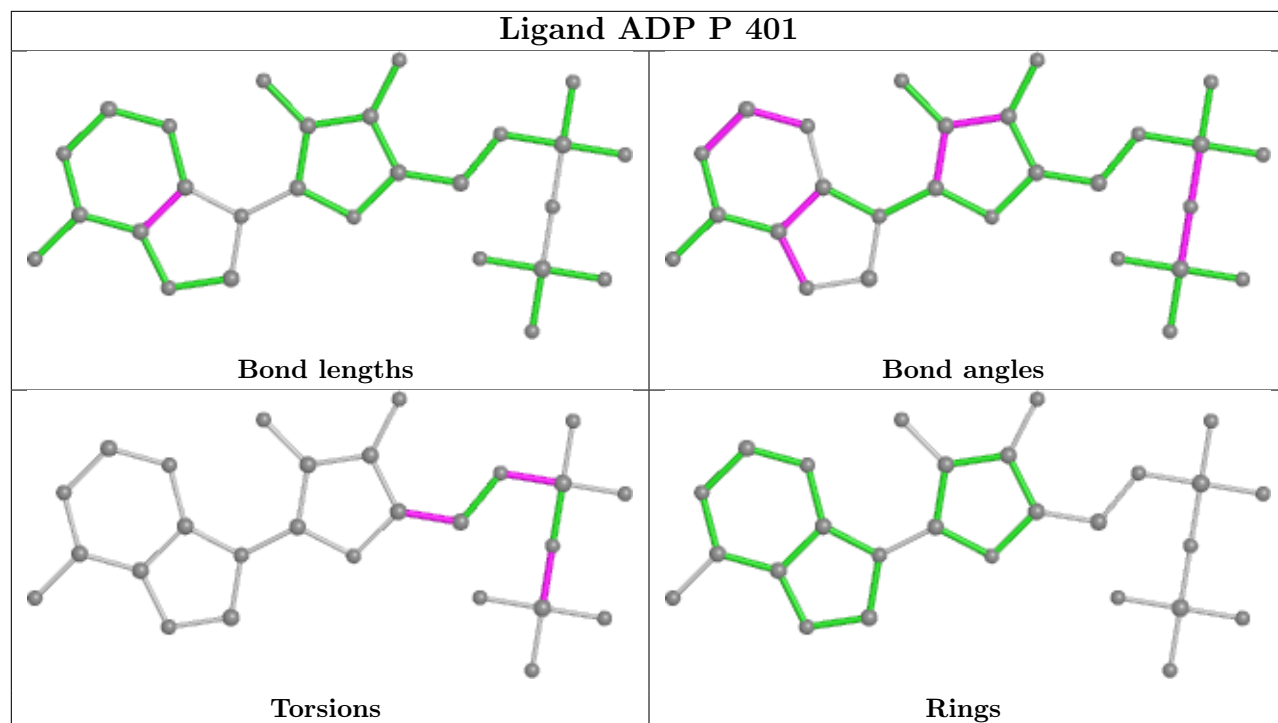
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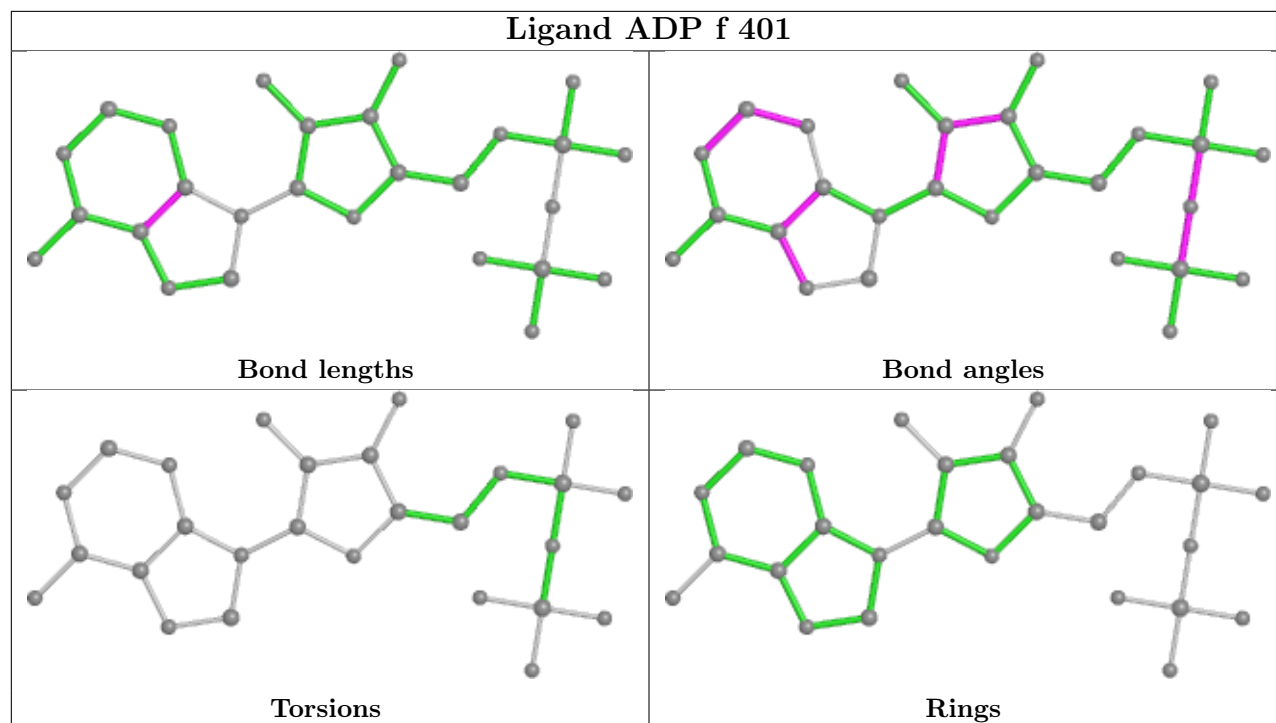
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	f	401	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	F	371/377 (98%)	-0.02	2 (0%) 87 86	78, 122, 177, 191	0
1	G	360/377 (95%)	-0.19	1 (0%) 90 89	60, 112, 169, 191	1 (0%)
1	P	362/377 (96%)	-0.42	1 (0%) 90 89	63, 91, 140, 166	0
1	f	371/377 (98%)	-0.56	0 100 100	55, 78, 119, 166	0
1	g	361/377 (95%)	-0.47	0 100 100	40, 83, 137, 180	1 (0%)
1	p	360/377 (95%)	-0.40	0 100 100	54, 90, 123, 161	1 (0%)
2	V	814/823 (98%)	-0.08	3 (0%) 89 88	61, 117, 175, 218	3 (0%)
2	v	815/823 (99%)	-0.20	4 (0%) 87 86	62, 108, 152, 183	0
All	All	3814/3908 (97%)	-0.26	11 (0%) 90 89	40, 102, 160, 218	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	v	681	MET	3.4
1	G	375	PHE	2.9
2	V	533[A]	ASN	2.7
2	v	367	VAL	2.7
1	F	293	LEU	2.5
2	v	356	THR	2.3
2	V	618	ALA	2.3
1	P	352	PHE	2.2
2	v	368	ASN	2.2
2	V	387	PRO	2.1
1	F	297	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	F	73	11/12	0.76	0.14	118,130,132,138	0
1	HIC	G	73	11/12	0.82	0.12	102,107,113,114	0
1	HIC	f	73	11/12	0.86	0.14	110,116,127,128	0
1	HIC	p	73	11/12	0.91	0.10	98,112,119,119	0
1	HIC	P	73	11/12	0.92	0.09	101,114,123,124	0
1	HIC	g	73	11/12	0.96	0.08	77,87,99,104	0

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
5	CA	V	901	1/1	0.91	0.07	117,117,117,117	0
7	SCN	V	909	3/3	0.91	0.24	109,109,110,112	0
3	ADP	F	401	27/27	0.93	0.07	84,90,106,108	0
5	CA	V	903	1/1	0.94	0.06	125,125,125,125	0
3	ADP	G	401	27/27	0.95	0.07	83,93,101,104	0
4	MG	f	402	1/1	0.96	0.05	68,68,68,68	0
6	CL	v	909	1/1	0.96	0.05	73,73,73,73	0
3	ADP	P	401	27/27	0.96	0.07	63,73,82,90	0
3	ADP	f	401	27/27	0.97	0.07	54,61,72,75	0
5	CA	V	902	1/1	0.97	0.06	134,134,134,134	0
3	ADP	g	401	27/27	0.97	0.06	59,68,78,79	0
5	CA	V	904	1/1	0.97	0.04	130,130,130,130	0
3	ADP	p	401	27/27	0.97	0.07	58,74,83,88	0
5	CA	v	904	1/1	0.97	0.06	117,117,117,117	0
5	CA	v	906	1/1	0.98	0.05	101,101,101,101	0
5	CA	v	907	1/1	0.98	0.04	104,104,104,104	0

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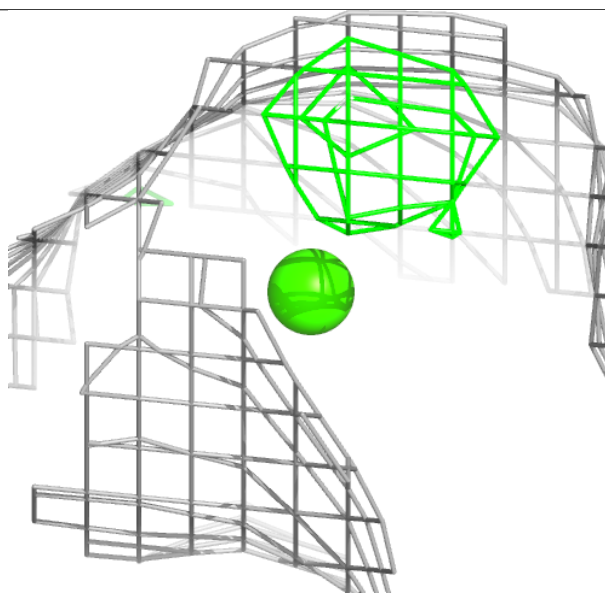
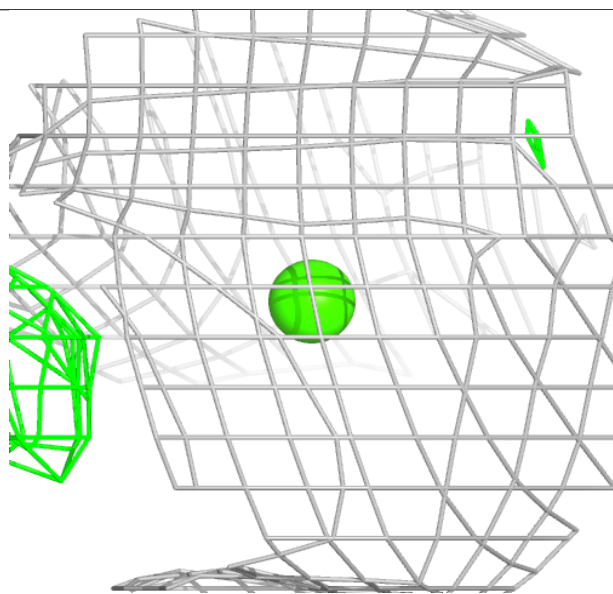
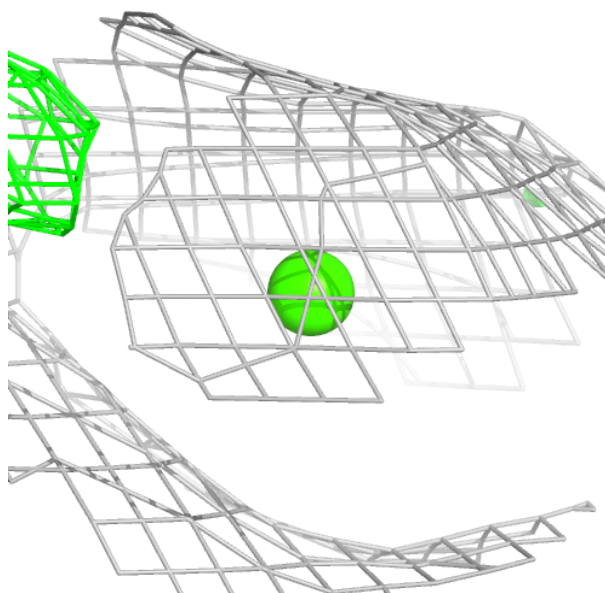
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	G	402	1/1	0.98	0.03	86,86,86,86	0
4	MG	F	402	1/1	0.98	0.04	86,86,86,86	0
4	MG	P	402	1/1	0.99	0.03	56,56,56,56	0
5	CA	v	901	1/1	0.99	0.02	69,69,69,69	0
5	CA	v	902	1/1	0.99	0.03	77,77,77,77	0
5	CA	V	905	1/1	0.99	0.04	68,68,68,68	0
5	CA	V	906	1/1	0.99	0.04	76,76,76,76	0
5	CA	V	907	1/1	0.99	0.03	83,83,83,83	0
5	CA	V	908	1/1	0.99	0.06	76,76,76,76	0
5	CA	v	908	1/1	0.99	0.04	86,86,86,86	0
5	CA	v	903	1/1	0.99	0.03	91,91,91,91	0
4	MG	p	402	1/1	1.00	0.02	64,64,64,64	0
5	CA	v	905	1/1	1.00	0.01	83,83,83,83	0
4	MG	g	402	1/1	1.00	0.04	69,69,69,69	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.

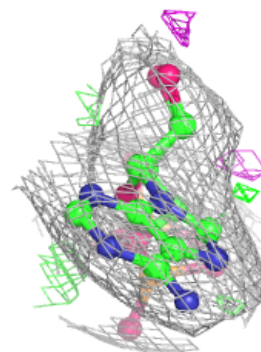
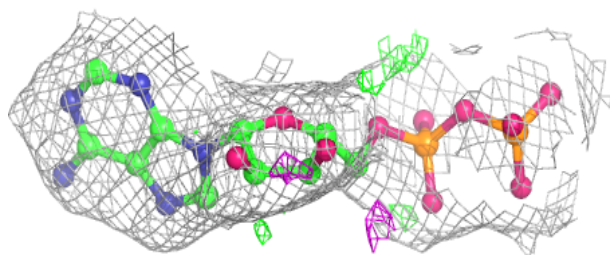
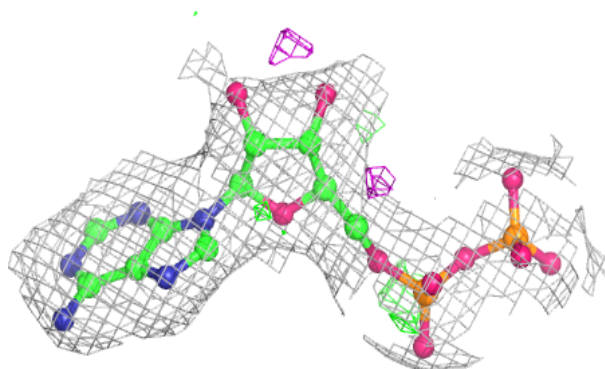
Electron density around CA V 901:

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



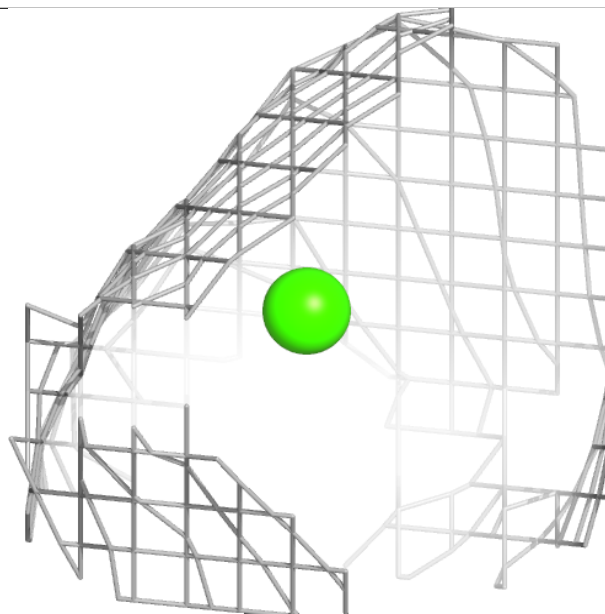
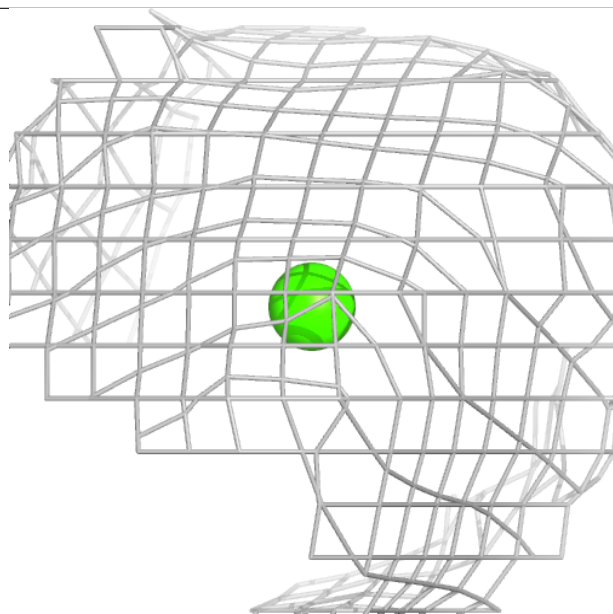
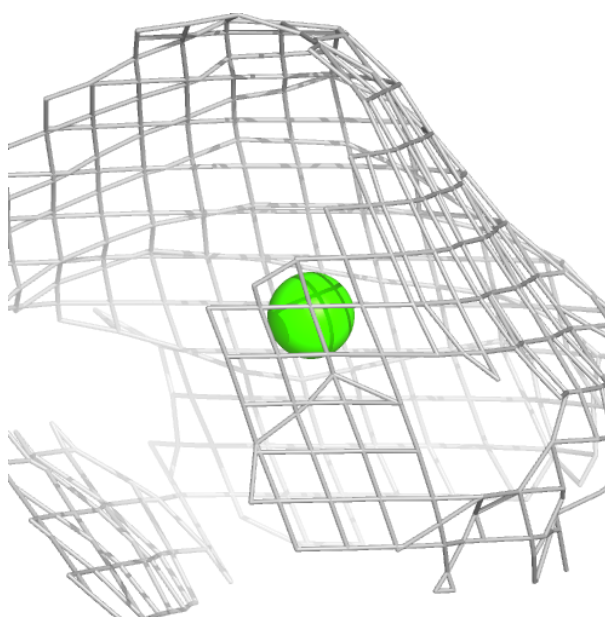
Electron density around ADP F 401:

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and green (positive)



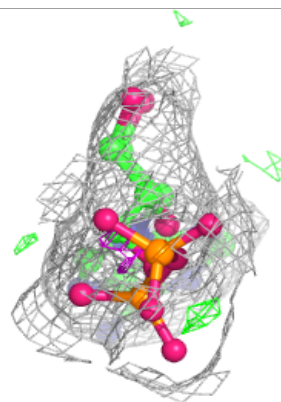
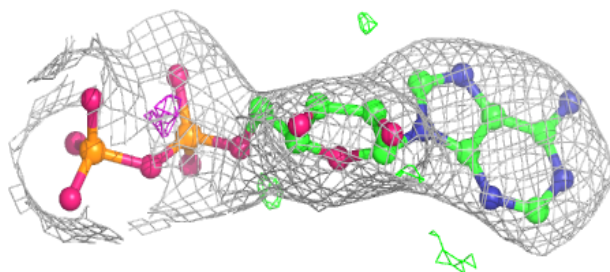
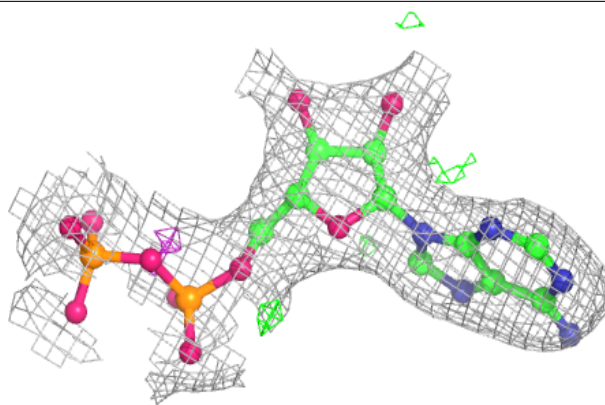
Electron density around CA V 903:

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and green (positive)



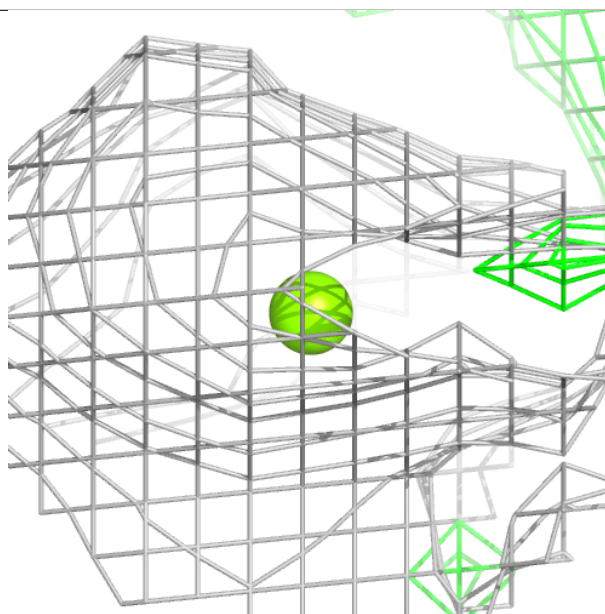
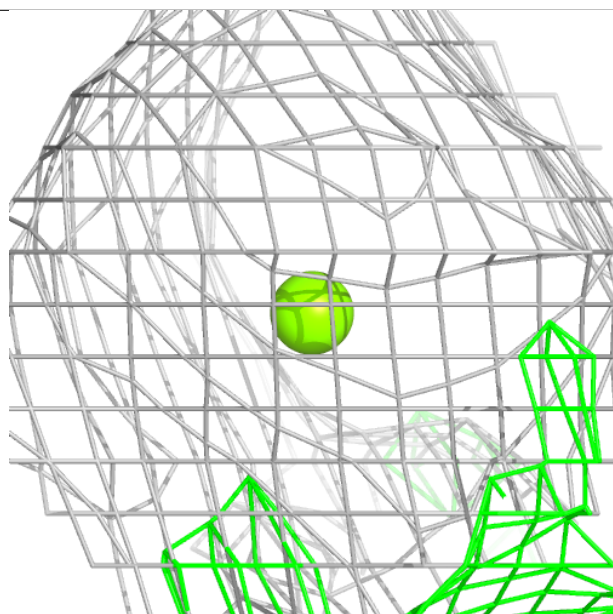
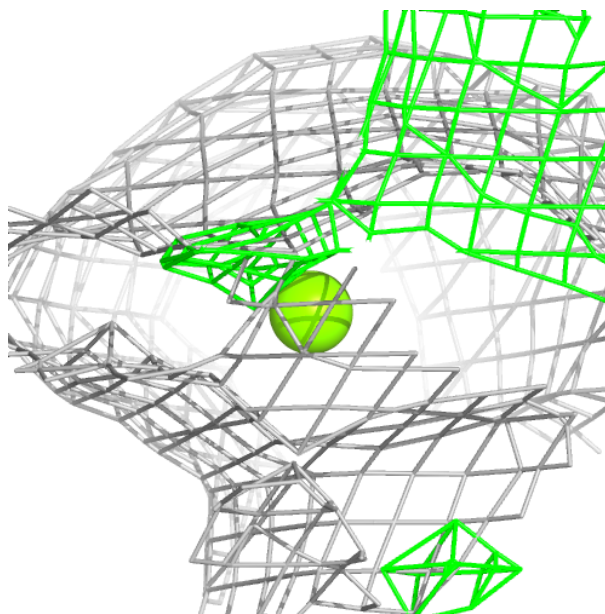
Electron density around ADP G 401:

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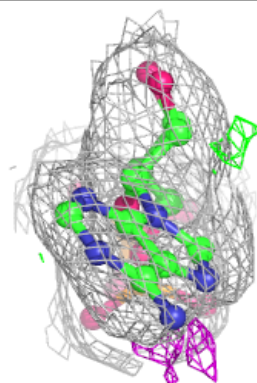
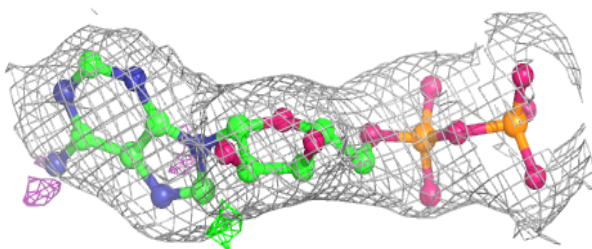
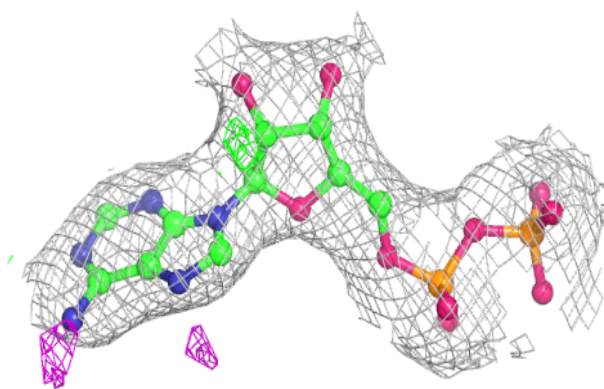
Electron density around MG f 402:

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and green (positive)

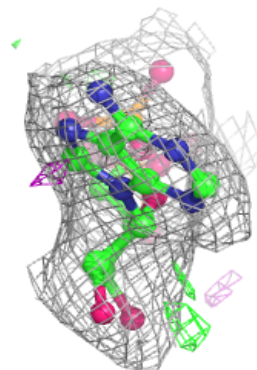
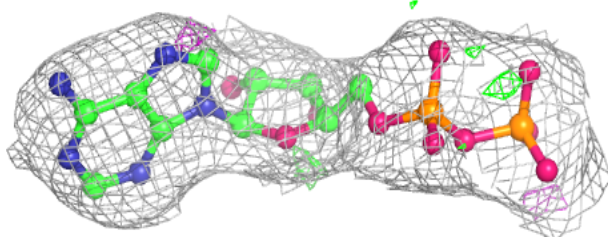
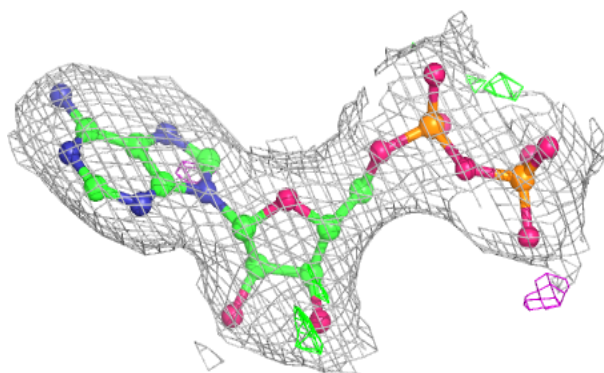


Electron density around ADP P 401:

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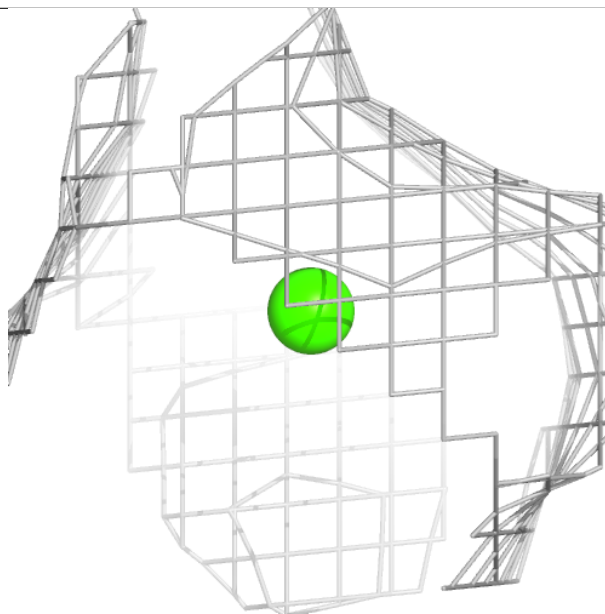
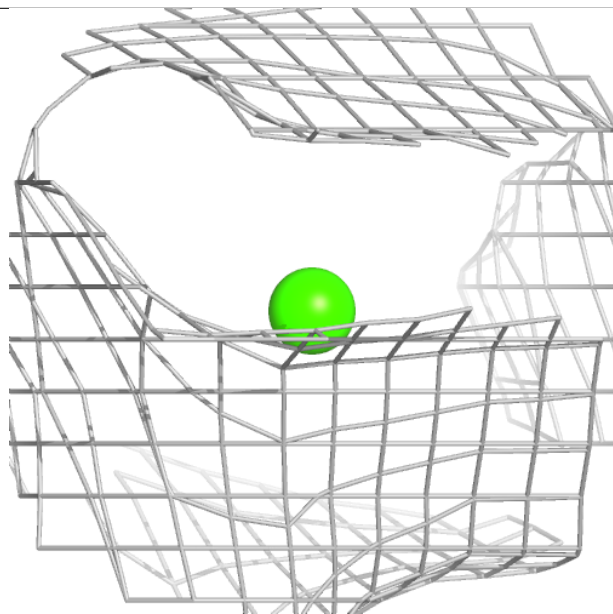
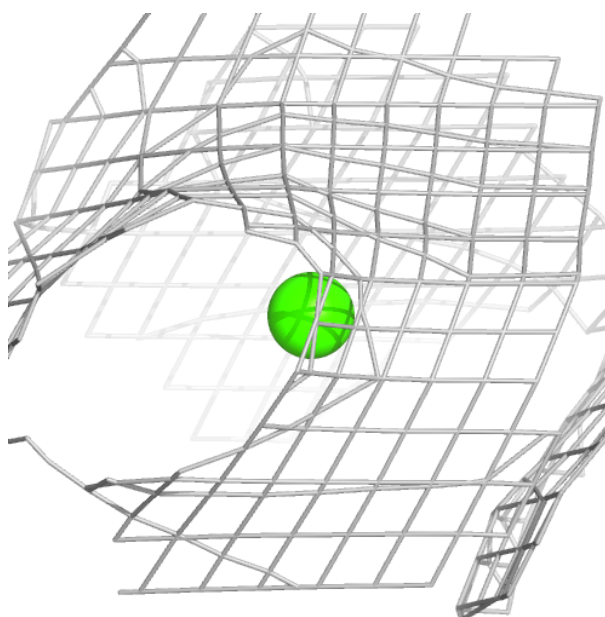
**Electron density around ADP f 401:**

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and green (positive)



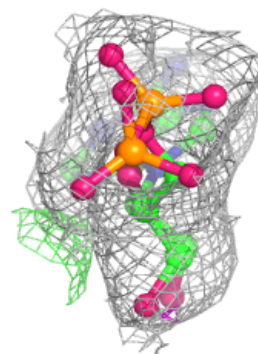
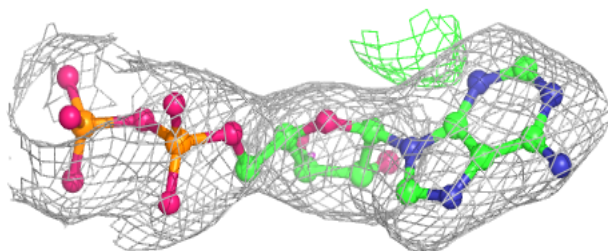
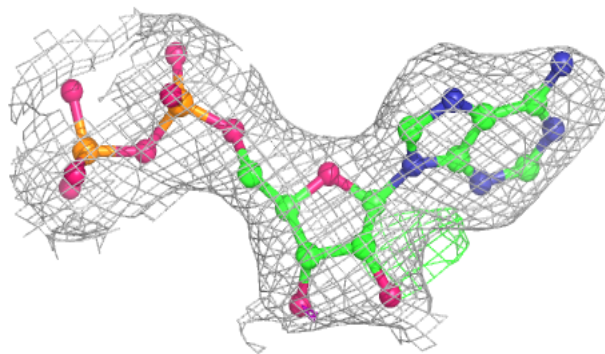
Electron density around CA V 902:

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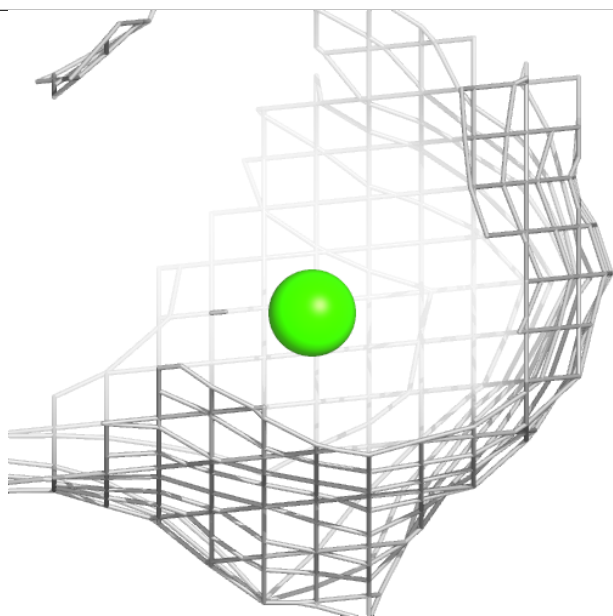
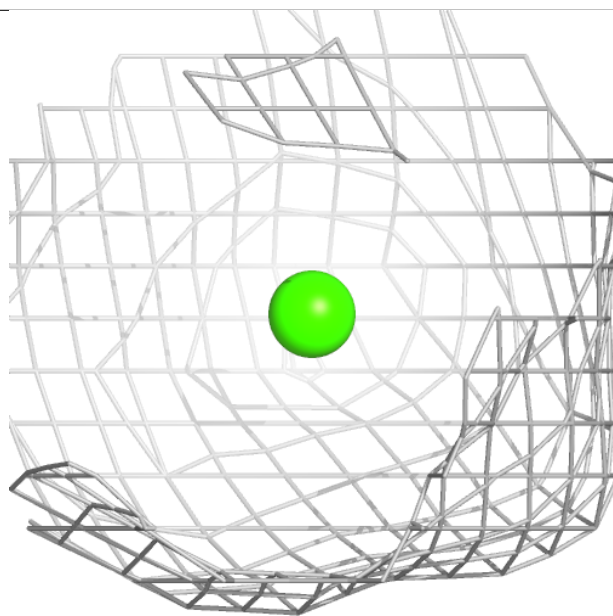
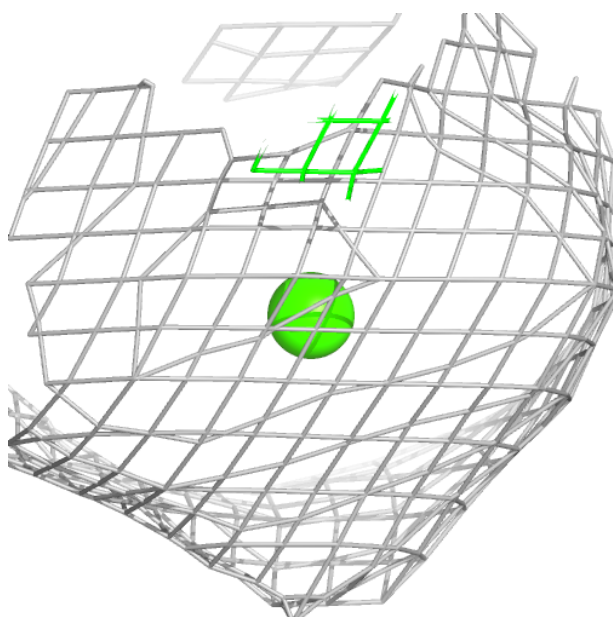
Electron density around ADP g 401:

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and green (positive)



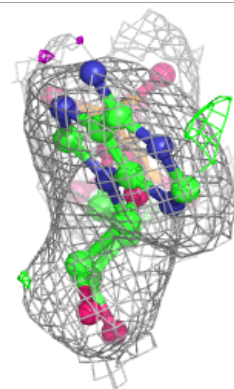
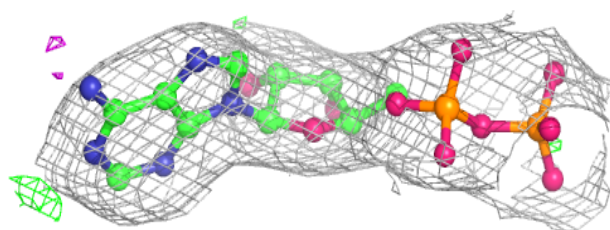
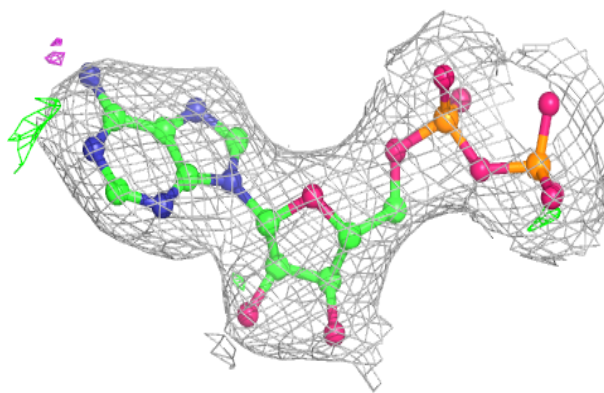
Electron density around CA V 904:

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and green (positive)



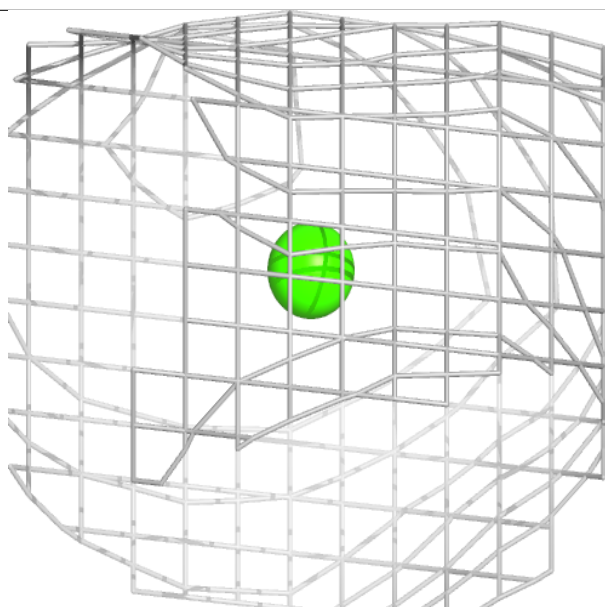
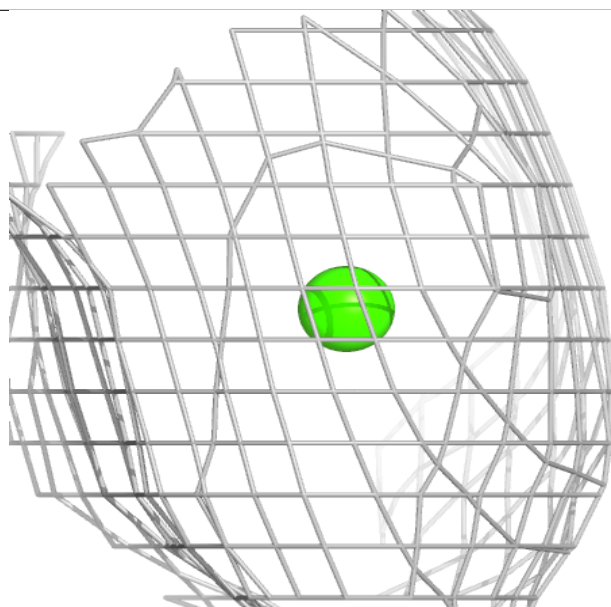
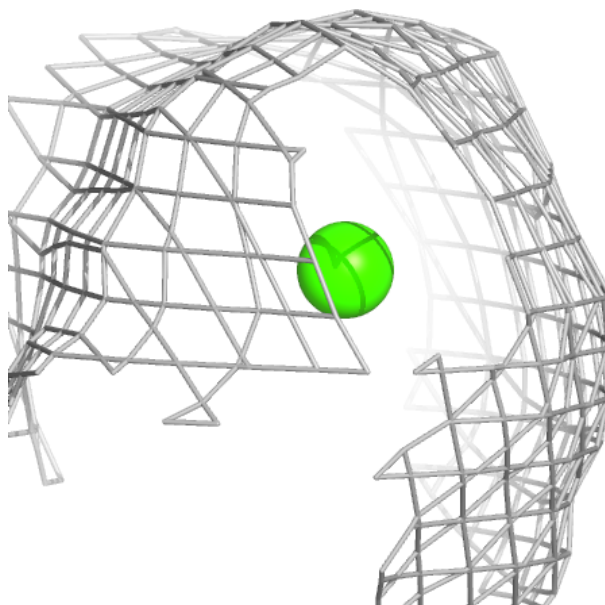
Electron density around ADP p 401:

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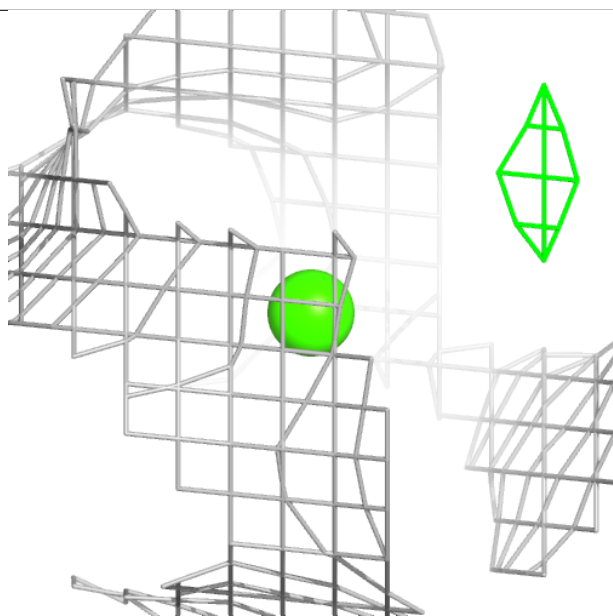
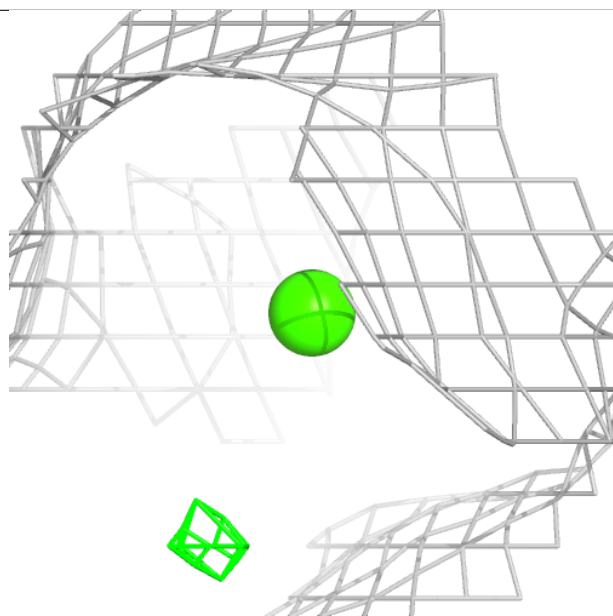
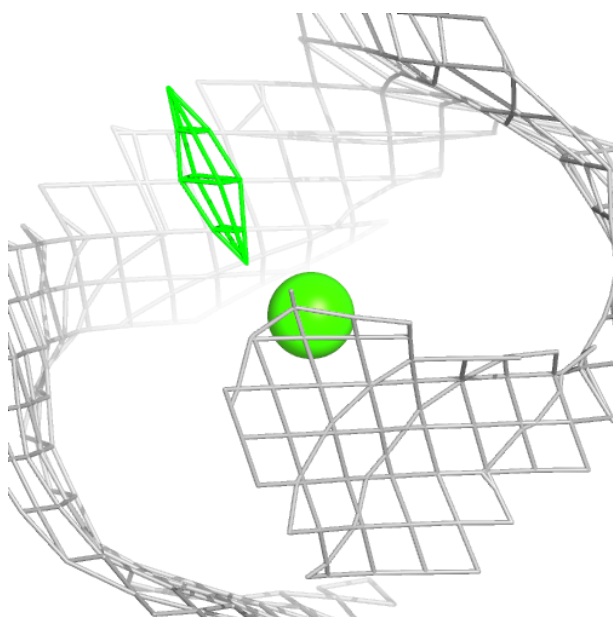
Electron density around CA v 904:

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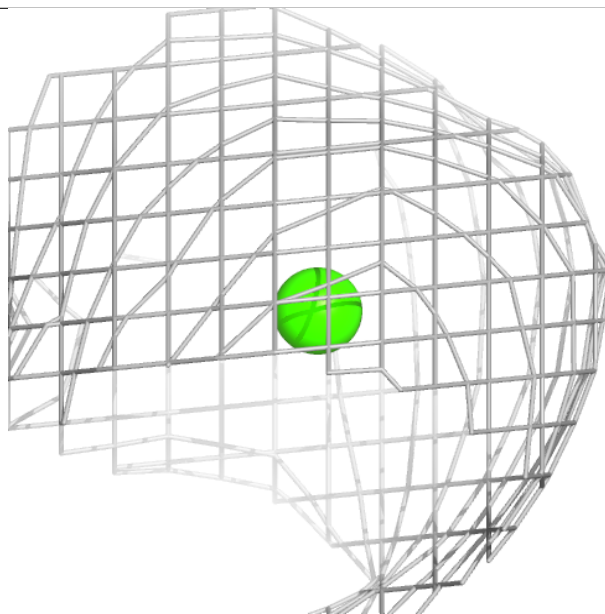
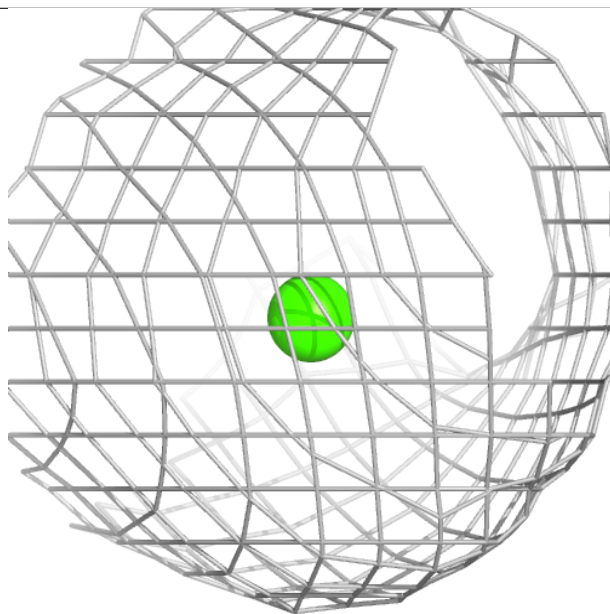
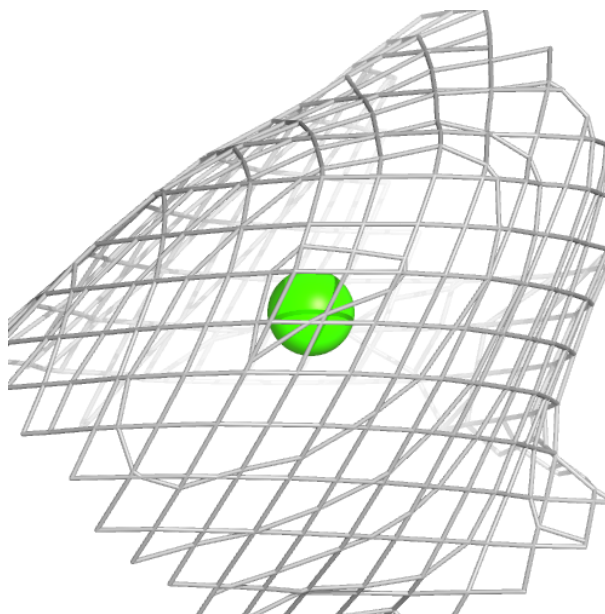
Electron density around CA v 906:

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and green (positive)



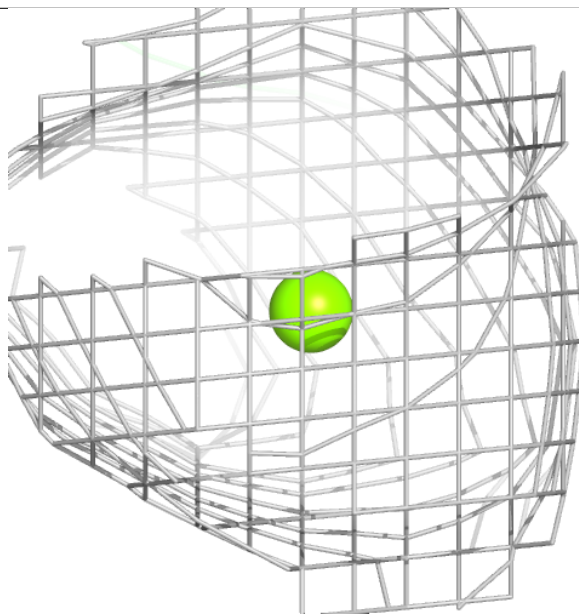
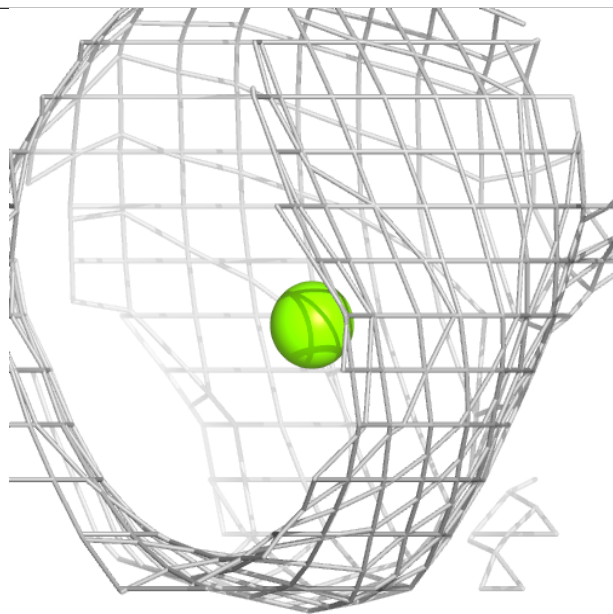
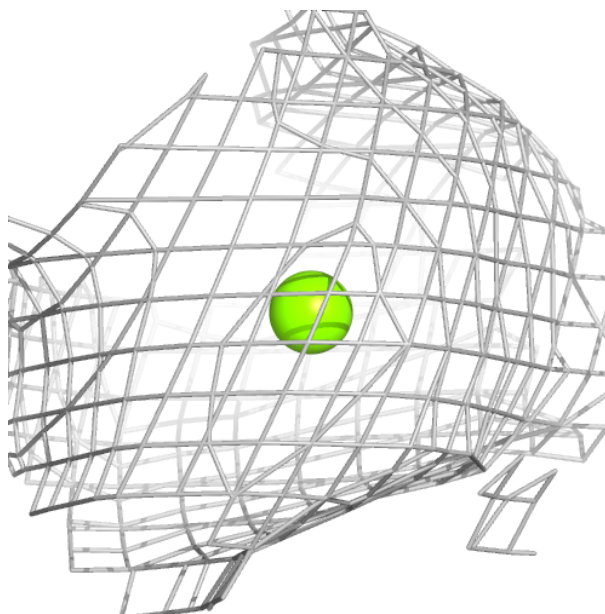
Electron density around CA v 907:

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and green (positive)



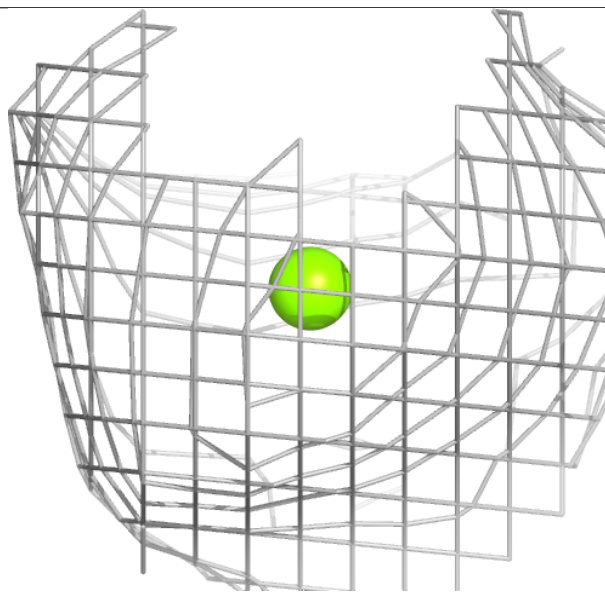
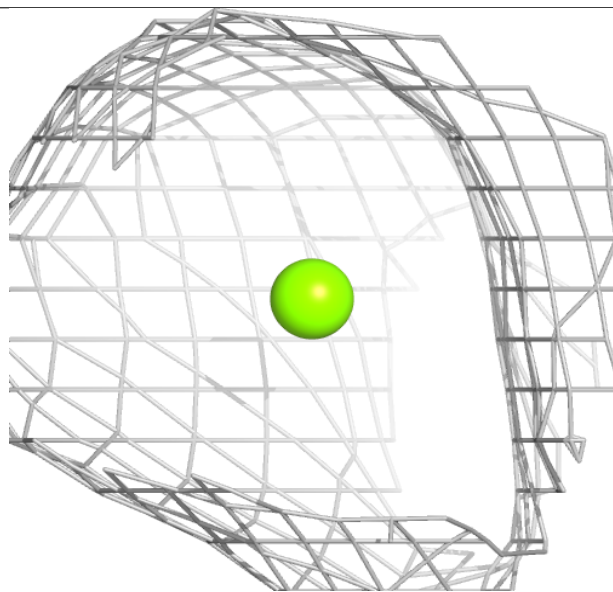
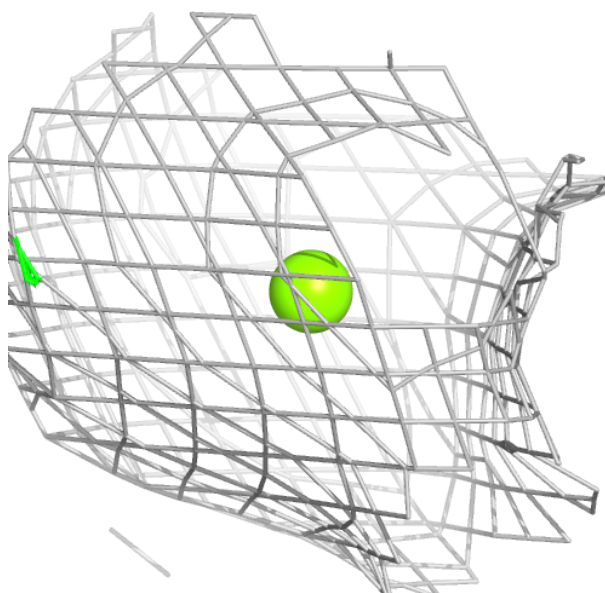
Electron density around MG G 402:

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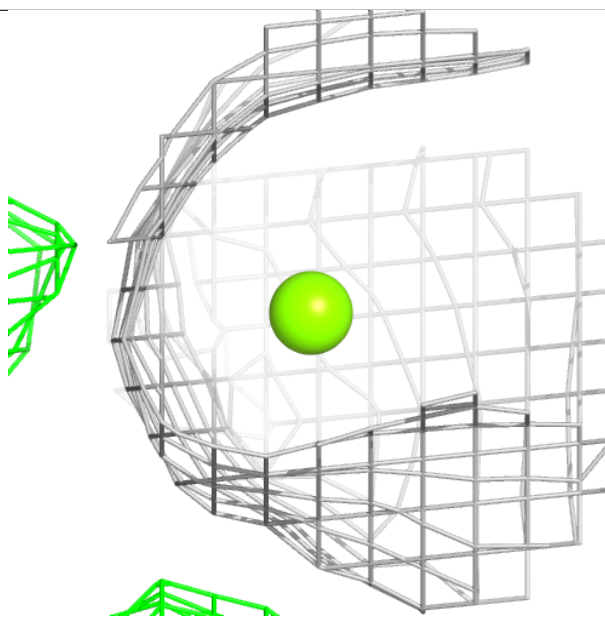
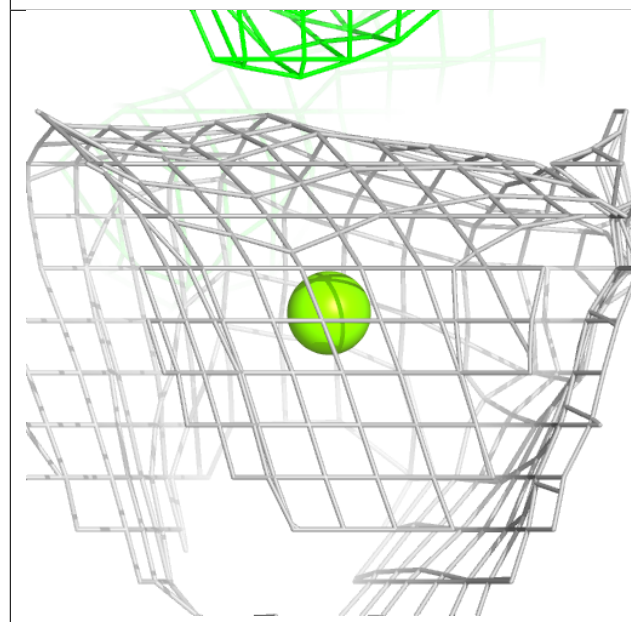
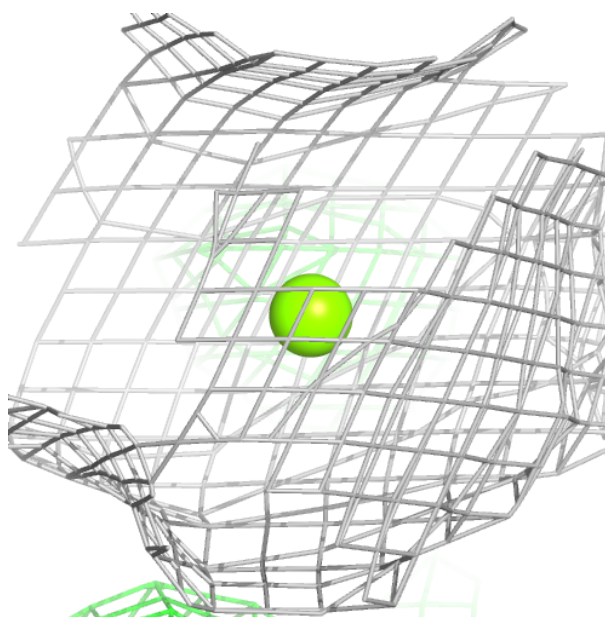
Electron density around MG F 402:

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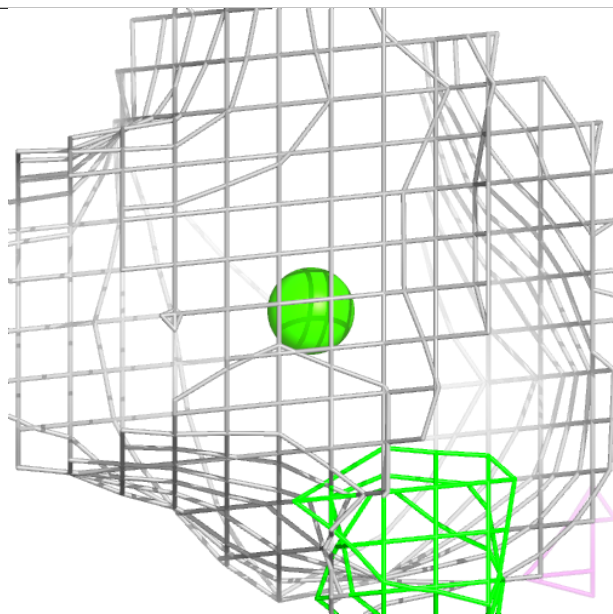
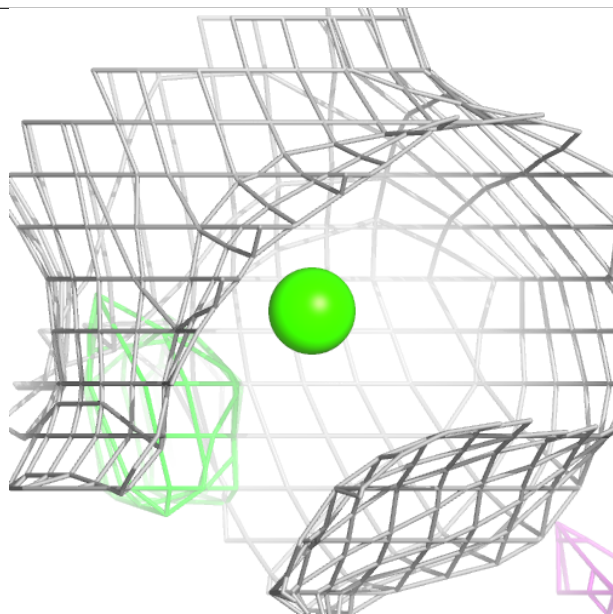
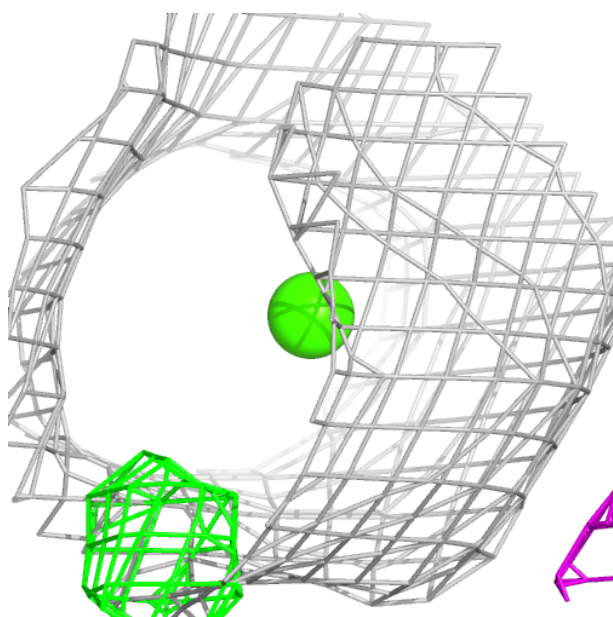
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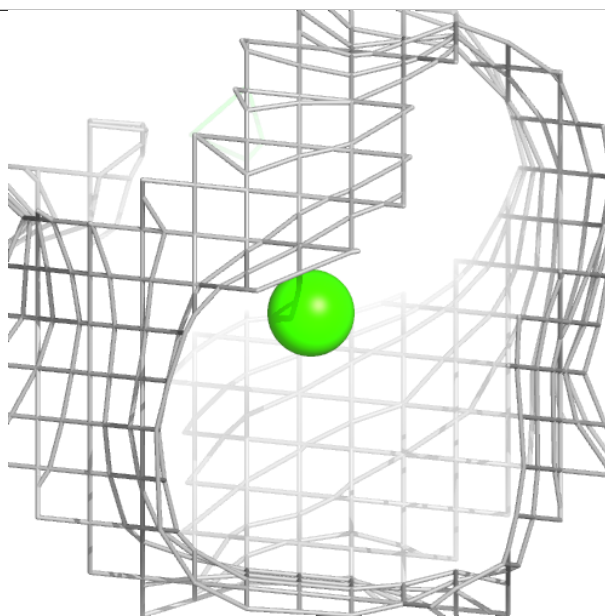
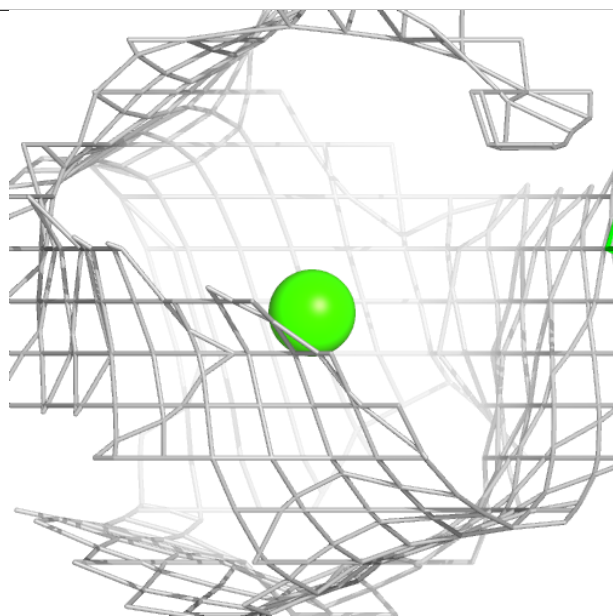
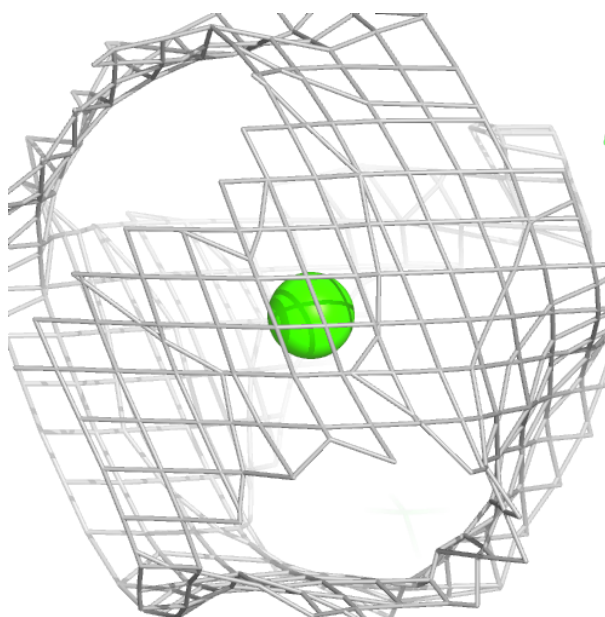
Electron density around CA v 901:

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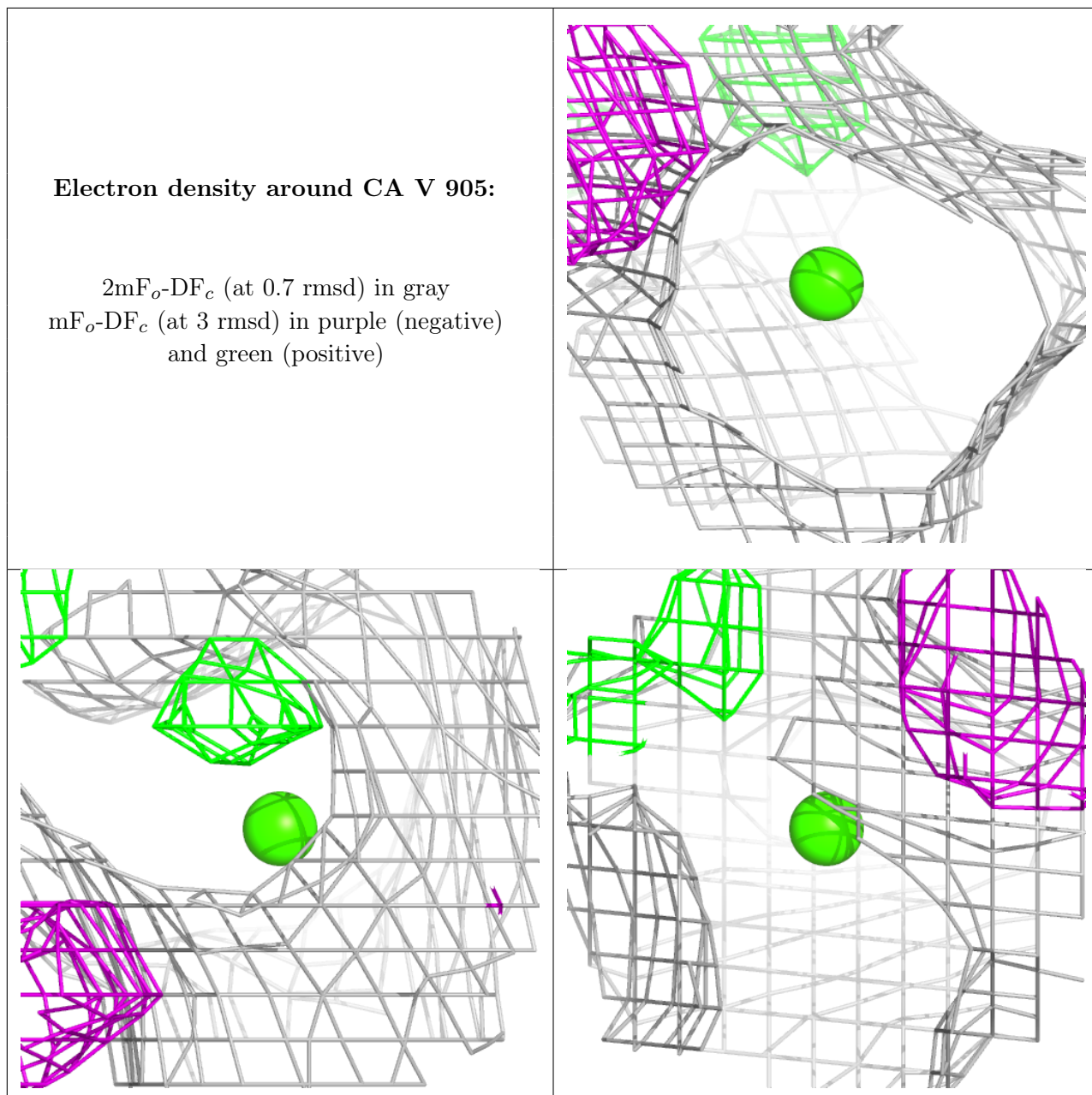
Electron density around CA v 902:

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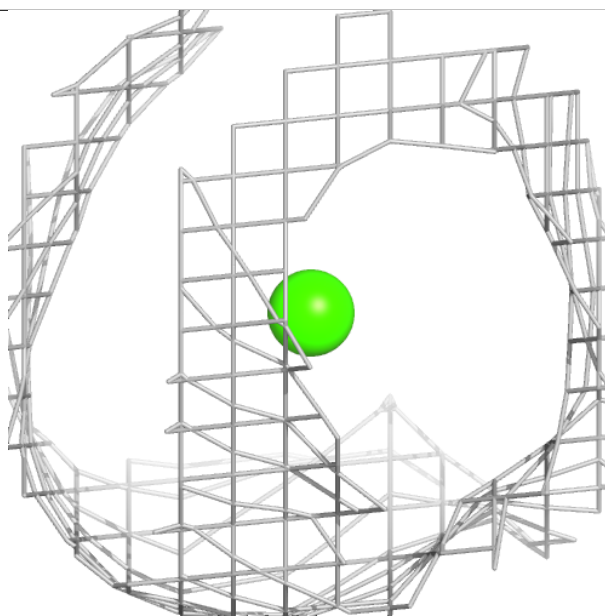
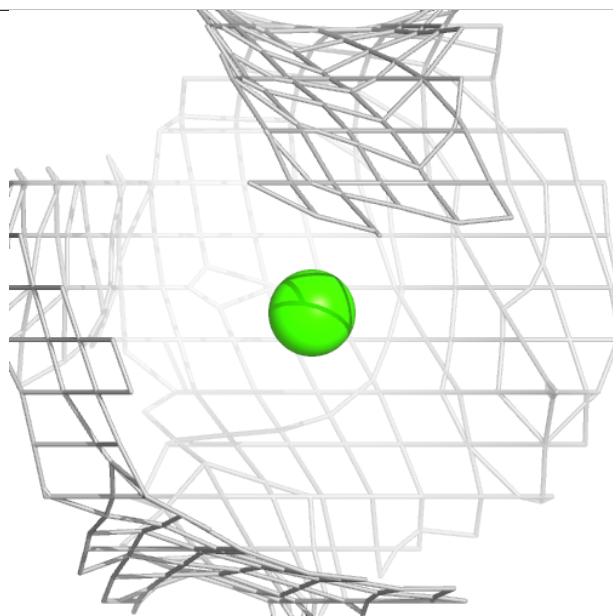
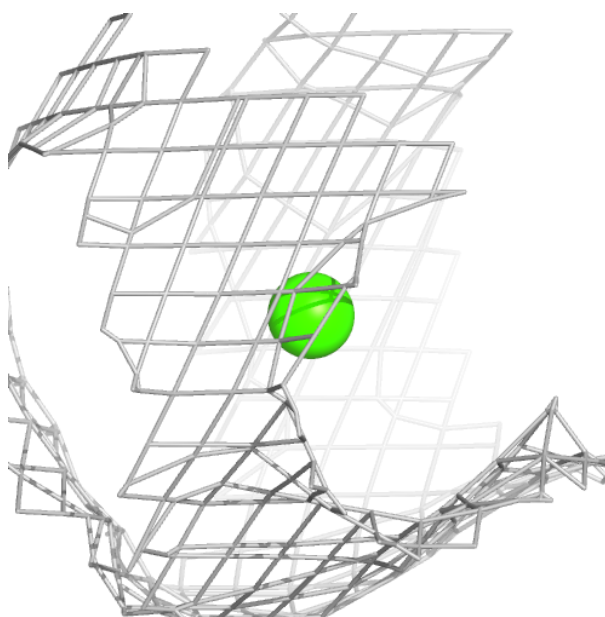
Electron density around CA V 905:

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and green (positive)



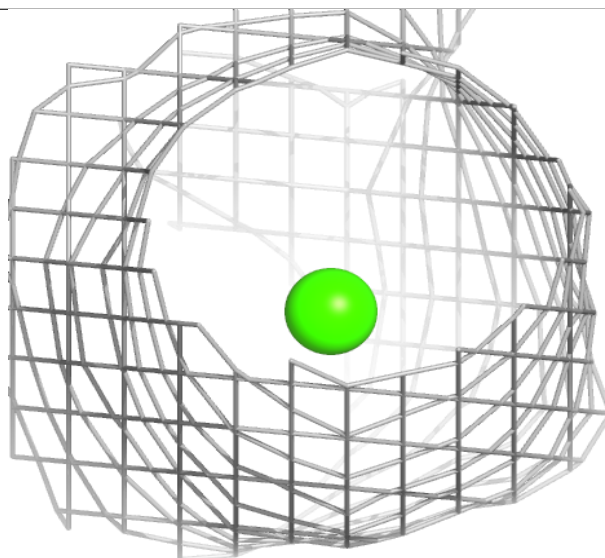
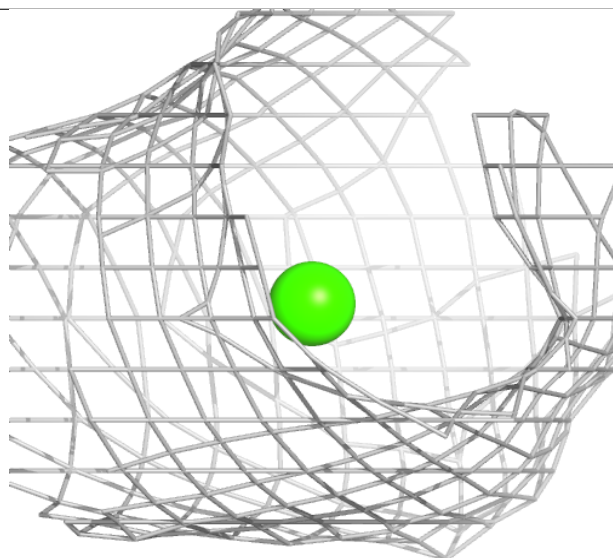
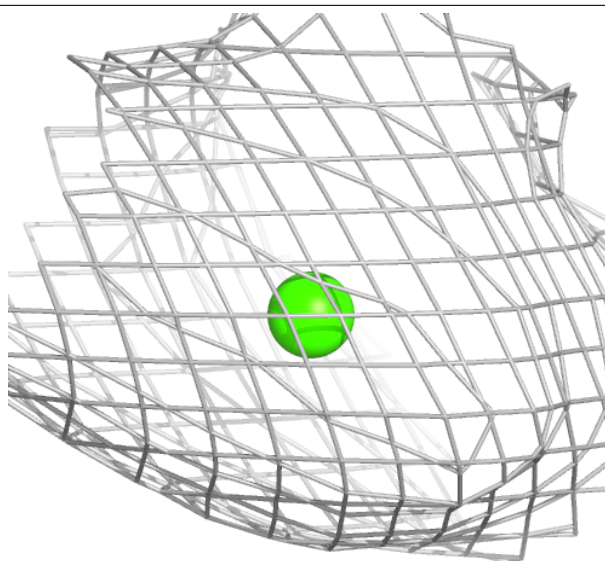
Electron density around CA V 906:

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and green (positive)



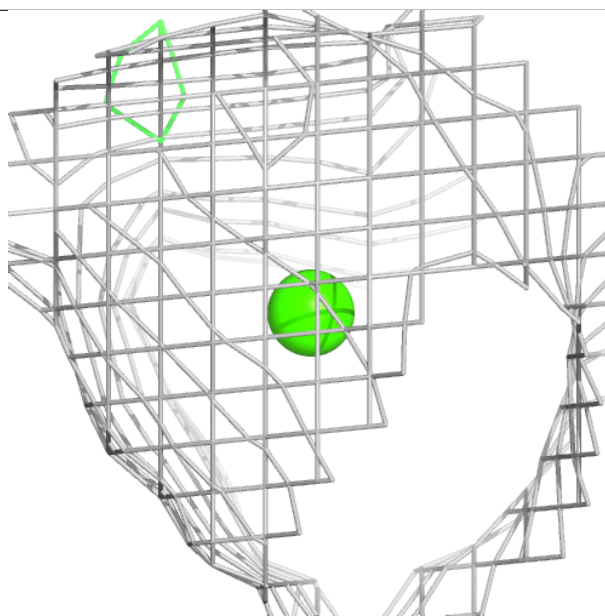
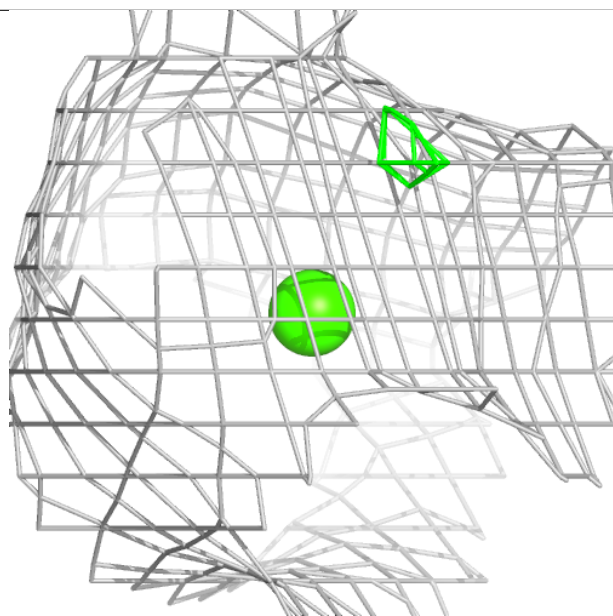
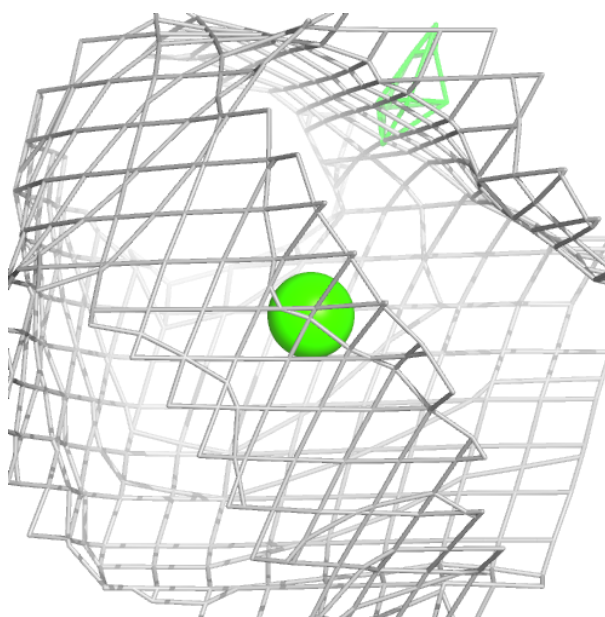
Electron density around CA V 907:

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



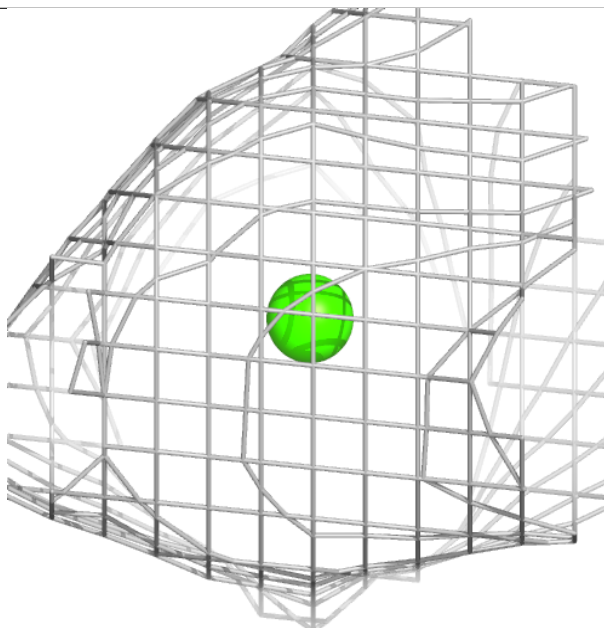
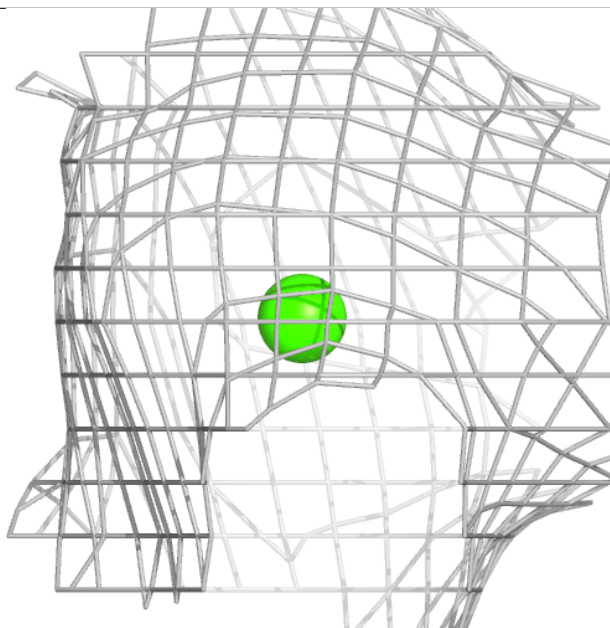
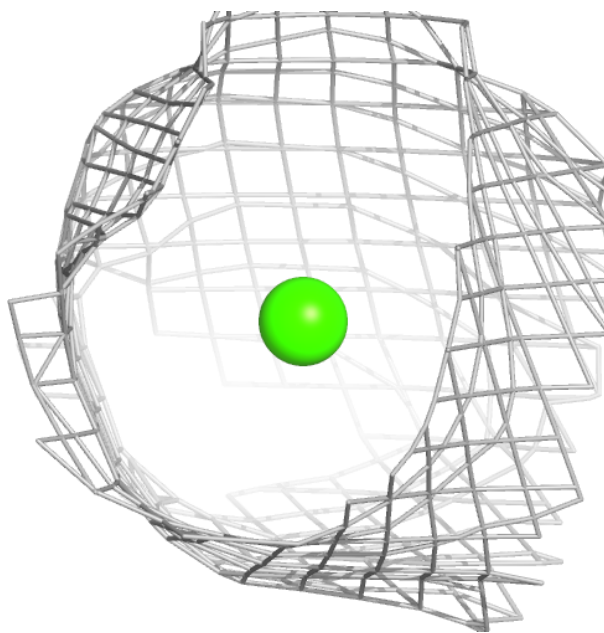
Electron density around CA V 908:

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



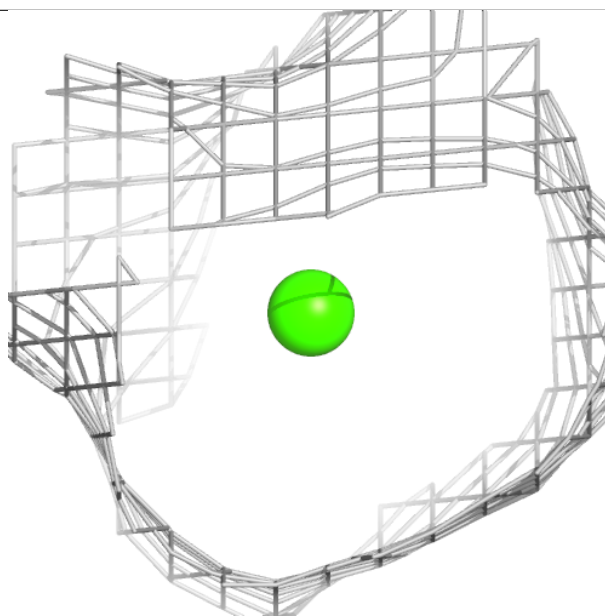
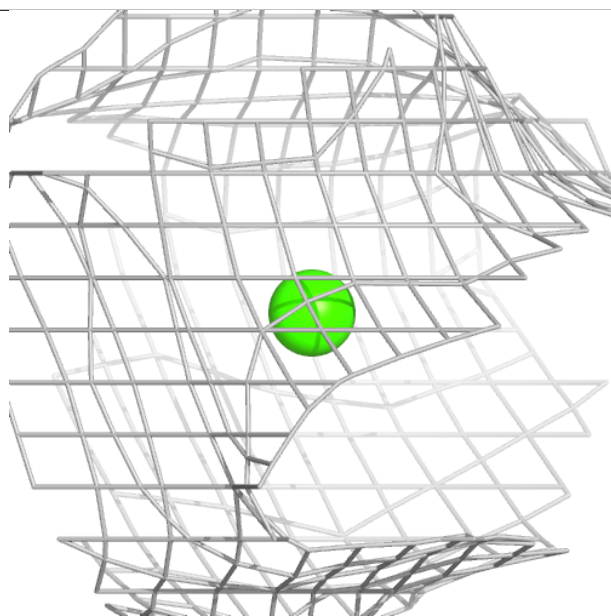
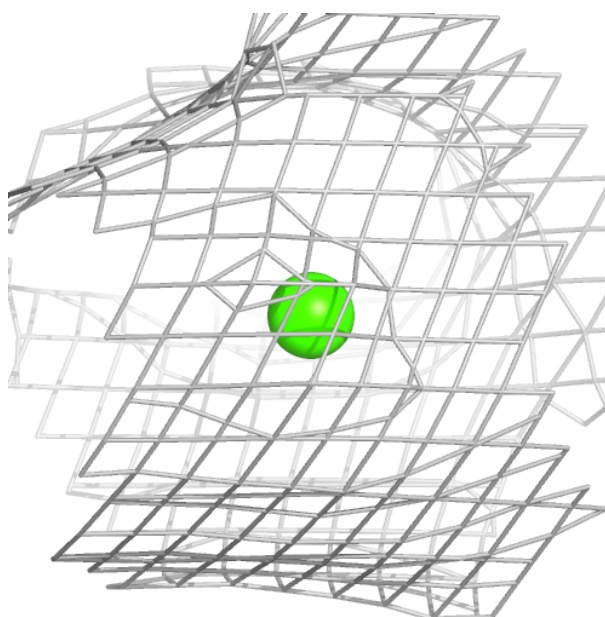
Electron density around CA v 908:

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



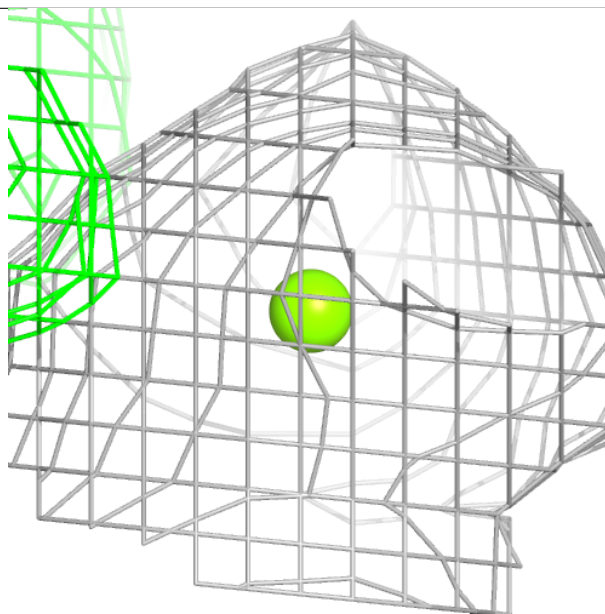
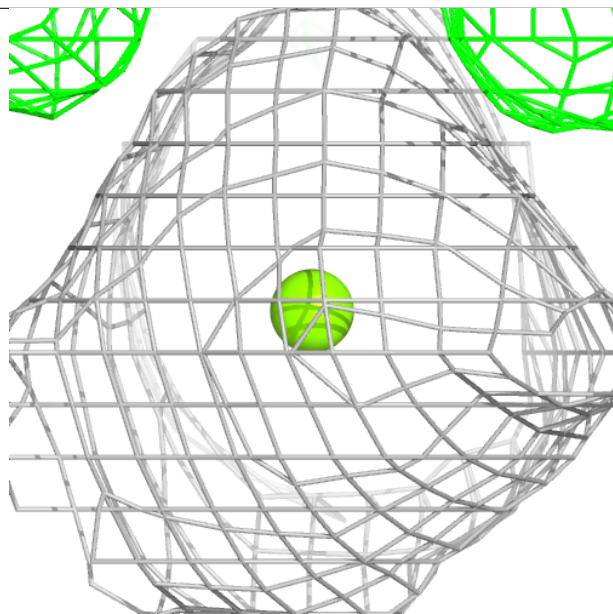
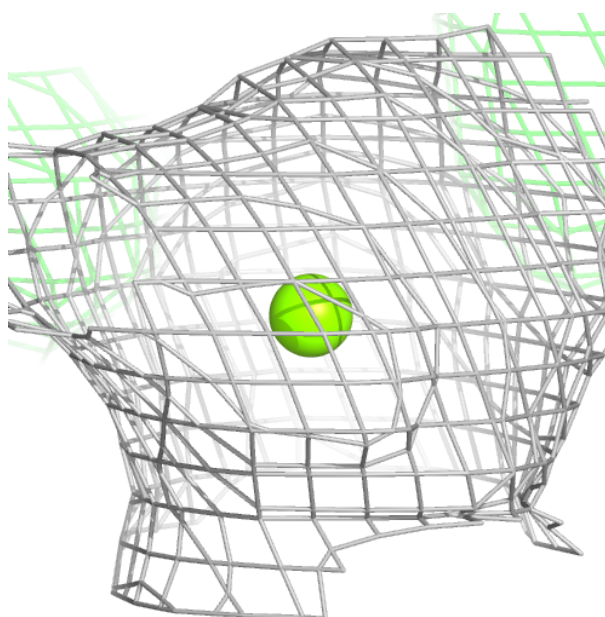
Electron density around CA v 903:

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



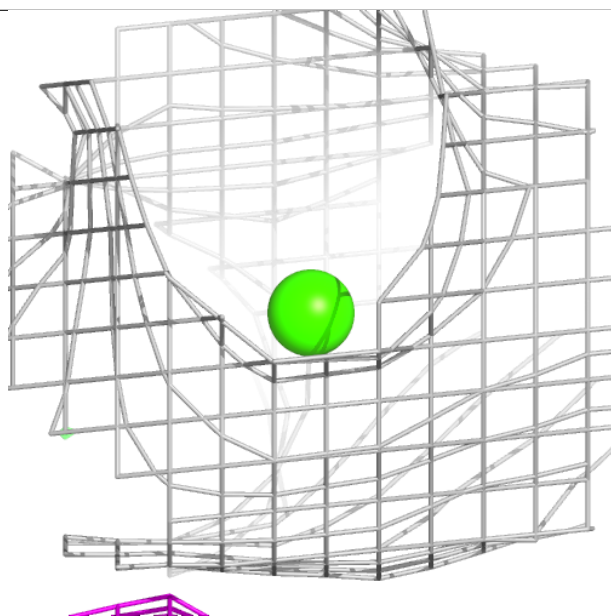
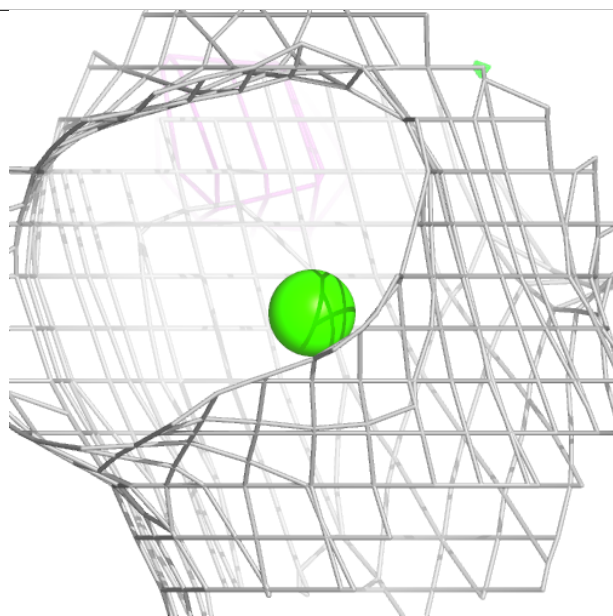
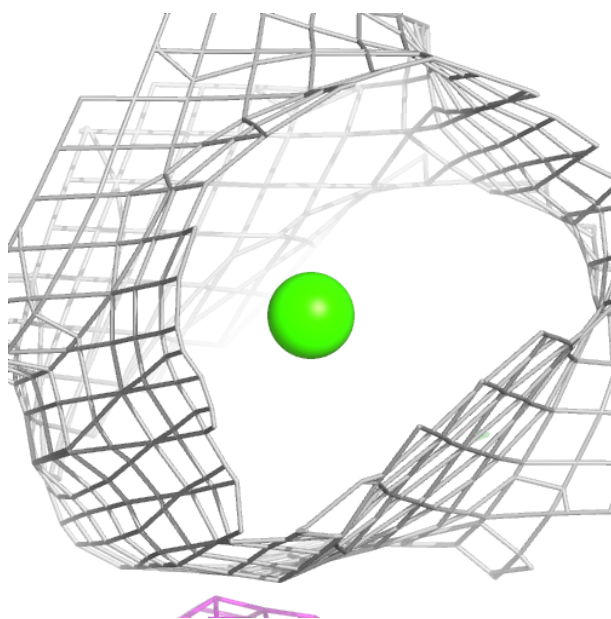
Electron density around MG p 402:

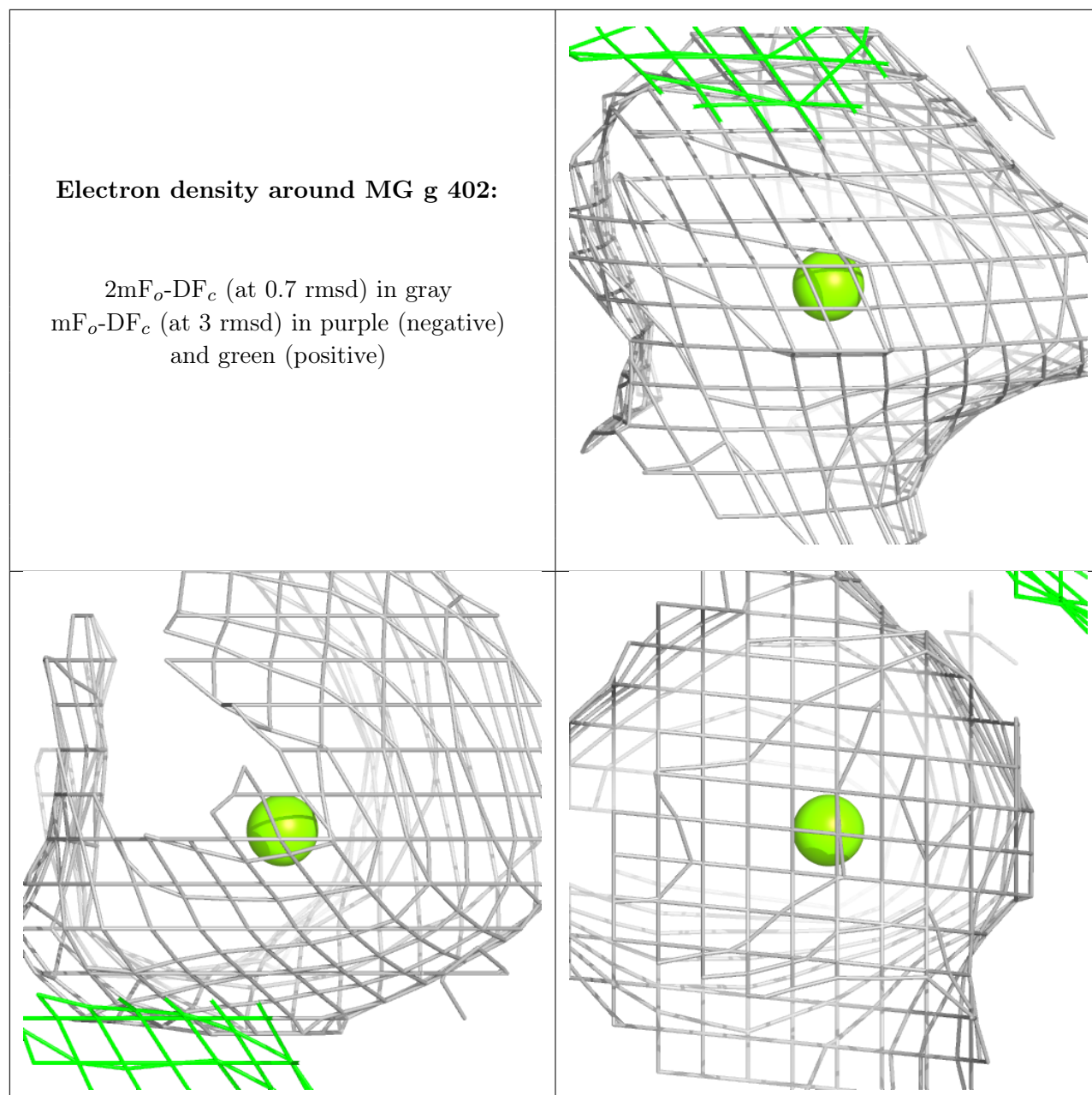
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA v 905:

$2mF_o-DF_c$ (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.