



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:27 AM UTC

PDB ID : 7WHG / pdb_00007whg
Title : Lokiarchaeota gelsolin (2DGel) bound to two molecules of rabbit actin
Authors : Robinson, R.C.; Akil, C.
Deposited on : 2021-12-30
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

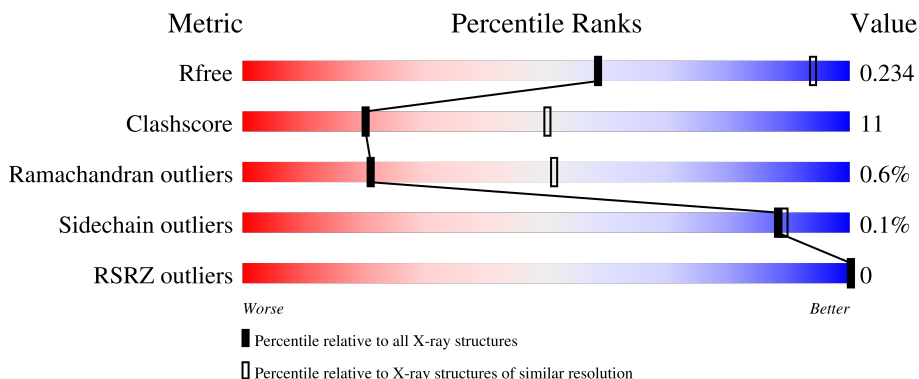
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

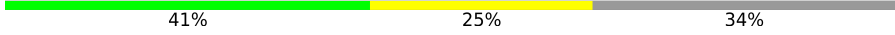
The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	377	 76% 23% .
1	B	377	 79% 19% ..
2	G	335	 41% 25% 34%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7607 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	A	371	Total	C	N	O	S	0	0	0
			2899	1833	488	558	20			
1	B	371	Total	C	N	O	S	0	0	0
			2900	1837	489	553	21			

- Molecule 2 is a protein called Lokiarchaeota gelsolin (2DGel).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	221	Total	C	N	O	S	0	0	0
			1745	1107	289	344	5			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

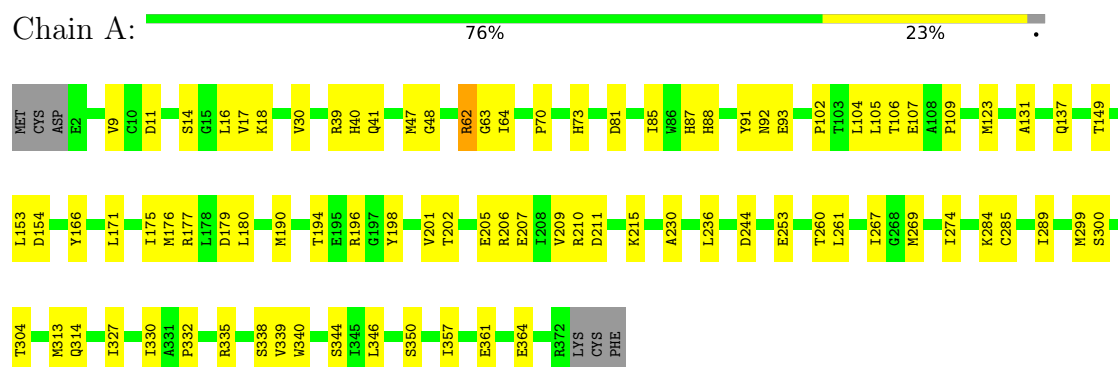
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		
4	G	6	Total	Ca	0	0
			6	6		

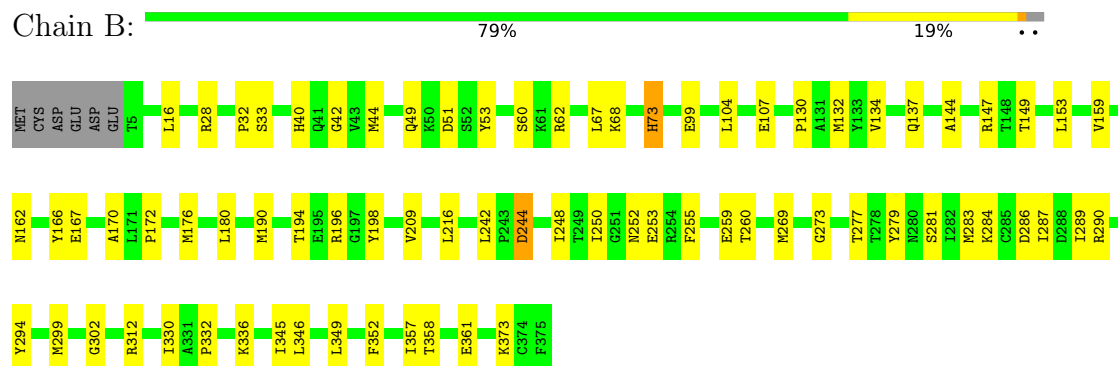
3 Residue-property plots

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.

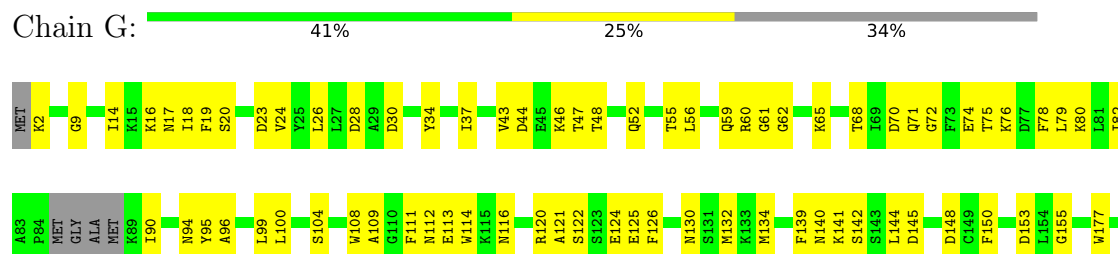
• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle



• Molecule 2: Lokiarchaeota gelsolin (2DGeI)



I181	ALA
R185	ALA
L188	PRO
D189	GLY
I200	ILE
E201	PRO
A204	GLY
A205	ARG
L206	ILE
D207	ALA
R208	ILE
K213	LEU
A217	THR
L226	GLN
GLU	LYS
GLY	THR
GLU	GLU
ASP	GLY
GLU	ARG
ASP	ARG
ASP	CYS
ARG	PRO
ILE	GLU
ALA	CYS
LYS	ASN
ALA	ILE
ILE	ASP
GLN	LYS
PRO	LYS
MET	PRO
GLU	ILE
ILE	GLN
HIS	MET
GLU	ILE
THR	HIS
THR	GLU
VAL	THR
ASP	VAL
LYS	ASP
SER	LYS
ASP	SER
VAL	ASN
THR	ILE
PRO	ILE
GLU	ILE
VAL	LEU
GLU	ASP
VAL	TYR
LYS	PRO
ALA	ARG
ASP	VAL
ILE	TYR
THR	GLY
ALA	LYS
ARG	LYS
SER	PHE
SER	LYS
SER	CYS

GLY
SER
CYS
GLY
VAL
GLU
TRP
ARG
GLU
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.66Å 72.06Å 100.39Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 20.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.25) 87.4 (20.00-3.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.29Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.175 , 0.232 0.175 , 0.234	Depositor DCC
R_{free} test set	845 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: ADP, CA, HIC

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	0.57	1/2948 (0.0%)	0.77	0/3994
1	B	0.44	0/2950	0.66	0/3994
2	G	0.48	0/1771	0.68	0/2380
All	All	0.50	1/7669 (0.0%)	0.71	0/10368

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	ASP	CA-C	5.58	1.60	1.52

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	2899	0	2861	57	1
1	B	2900	0	2872	55	1
2	G	1745	0	1731	70	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	6	0	0	0	0
All	All	7607	0	7488	171	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (171) 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:G:121:ALA:HB2	2:G:134:MET:HE3	1.49	0.94
1:B:147:ARG:NH2	2:G:70:ASP:OD1	2.10	0.85
2:G:17:ASN:HD22	2:G:82:ILE:HG23	1.47	0.79
2:G:95:TYR:HE2	2:G:226:LEU:HB3	1.48	0.79
1:A:314:GLN:NE2	1:A:327:ILE:O	2.20	0.75
2:G:44:ASP:HB2	2:G:99:LEU:HD21	1.70	0.74
1:B:287:ILE:HD12	1:B:290:ARG:HH21	1.52	0.74
1:B:180:LEU:HD11	1:B:260:THR:HG22	1.69	0.73
1:A:39:ARG:NH1	1:A:40:HIS:HB2	2.04	0.72
2:G:24:VAL:HG22	2:G:37:ILE:HA	1.72	0.71
1:B:357:ILE:HD11	1:B:373:LYS:HG3	1.77	0.66
1:B:162:ASN:HB2	1:B:176:MET:HB2	1.78	0.66
1:A:190:MET:HE2	1:A:206:ARG:HG3	1.78	0.65
1:A:335:ARG:HA	1:A:338:SER:HB3	1.77	0.64
1:B:149:THR:HG23	1:B:166:TYR:HA	1.78	0.64
1:A:107:GLU:O	1:A:137:GLN:HG3	1.97	0.64
1:B:190:MET:HG3	1:B:209:VAL:HG21	1.78	0.64
1:A:153:LEU:HD23	1:A:299:MET:HE2	1.80	0.64
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.80	0.64
2:G:43:VAL:O	2:G:47:THR:HG22	1.97	0.63
2:G:124:GLU:HG3	2:G:125:GLU:OE1	1.98	0.63
2:G:120:ARG:NH1	2:G:148:ASP:OD2	2.31	0.63
2:G:60:ARG:O	2:G:62:GLY:N	2.29	0.62
1:B:62:ARG:HB2	1:B:67:LEU:HD11	1.82	0.62
1:B:302:GLY:HA2	1:B:336:LYS:HG3	1.81	0.62
2:G:104:SER:O	2:G:112:ASN:HB3	2.01	0.61
1:A:62:ARG:HG2	1:A:63:GLY:N	2.16	0.60
1:A:39:ARG:N	1:A:64:ILE:O	2.35	0.60
1:B:107:GLU:O	1:B:137:GLN:HG3	2.01	0.60
1:A:39:ARG:HG3	1:A:40:HIS:H	1.66	0.60
1:A:11:ASP:HA	1:A:106:THR:OG1	2.01	0.59
1:A:47:MET:N	1:A:48:GLY:HA3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HH12	1:A:40:HIS:HB2	1.66	0.59
1:A:361:GLU:HA	1:A:364:GLU:HG2	1.85	0.58
1:B:196:ARG:HD2	1:B:253:GLU:OE2	2.03	0.58
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.86	0.57
1:B:345:ILE:HG21	2:G:47:THR:HG23	1.88	0.56
1:B:287:ILE:HD12	1:B:290:ARG:NH2	2.20	0.56
2:G:14:ILE:HG22	2:G:16:LYS:H	1.72	0.54
1:B:345:ILE:HD13	2:G:100:LEU:HD21	1.89	0.54
1:A:62:ARG:HG2	1:A:63:GLY:H	1.73	0.53
1:B:283:MET:HE2	1:B:294:TYR:OH	2.09	0.53
2:G:114:TRP:NE1	2:G:116:ASN:OD1	2.42	0.53
1:A:106:THR:HB	1:A:137:GLN:HG2	1.91	0.53
2:G:20:SER:OG	2:G:94:ASN:O	2.27	0.53
2:G:126:PHE:CD2	2:G:132:MET:HA	2.44	0.53
2:G:141:LYS:HD2	2:G:207:ASP:OD1	2.08	0.52
1:B:357:ILE:HG12	1:B:373:LYS:HE3	1.90	0.52
2:G:44:ASP:HB2	2:G:99:LEU:CD2	2.38	0.52
1:A:194:THR:HA	1:A:198:TYR:O	2.09	0.52
1:B:244:ASP:OD1	1:B:244:ASP:N	2.40	0.52
2:G:17:ASN:ND2	2:G:82:ILE:HG23	2.21	0.52
2:G:60:ARG:C	2:G:62:GLY:H	2.15	0.52
1:B:176:MET:HG3	1:B:281:SER:HB2	1.93	0.51
1:B:144:ALA:HA	2:G:47:THR:HB	1.93	0.50
1:B:176:MET:HE3	1:B:284:LYS:HD3	1.93	0.50
1:A:88:HIS:CD2	1:A:92:ASN:HD22	2.30	0.50
1:A:205:GLU:O	1:A:209:VAL:HG23	2.12	0.50
1:B:242:LEU:HD21	1:B:248:ILE:HD12	1.94	0.50
2:G:43:VAL:HA	2:G:46:LYS:HD3	1.93	0.50
1:B:167:GLU:OE2	2:G:65:LYS:HA	2.12	0.50
2:G:201:GLU:OE2	2:G:208:ARG:NH2	2.41	0.50
2:G:44:ASP:OD2	2:G:99:LEU:HD23	2.12	0.49
2:G:9:GLY:HA2	2:G:48:THR:HG21	1.93	0.49
2:G:122:SER:HB3	2:G:124:GLU:CG	2.43	0.49
1:B:279:TYR:HE1	1:B:283:MET:HE3	1.77	0.49
1:B:345:ILE:HG21	2:G:47:THR:CG2	2.41	0.49
1:B:153:LEU:HD23	1:B:299:MET:HE2	1.95	0.49
2:G:139:PHE:CE2	2:G:206:LEU:HA	2.48	0.49
1:A:131:ALA:HA	1:A:357:ILE:O	2.13	0.49
2:G:153:ASP:OD2	2:G:181:ILE:HD13	2.12	0.49
1:A:176:MET:HE3	1:A:284:LYS:HD2	1.93	0.49
1:B:132:MET:HE1	1:B:134:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:GLY:HA2	2:G:185:ARG:NH1	2.27	0.49
2:G:34:TYR:CE1	2:G:78:PHE:HB2	2.48	0.48
1:A:88:HIS:CE1	1:A:93:GLU:HG2	2.49	0.48
1:B:44:MET:CE	1:B:51:ASP:HA	2.44	0.48
1:B:283:MET:SD	1:B:290:ARG:NH1	2.86	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.48
2:G:144:LEU:HD22	2:G:150:PHE:CD2	2.49	0.48
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.94	0.48
1:B:16:LEU:HD23	1:B:32:PRO:HA	1.96	0.48
2:G:2:LYS:HB2	2:G:28:ASP:HB3	1.96	0.47
2:G:199:ASP:OD1	2:G:199:ASP:N	2.40	0.47
1:A:16:LEU:HB2	1:A:18:LYS:NZ	2.29	0.47
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.97	0.47
1:A:269:MET:HE2	1:A:269:MET:HB3	1.72	0.47
2:G:74:GLU:HB3	2:G:78:PHE:HD2	1.80	0.47
1:A:180:LEU:HD11	1:A:260:THR:HG22	1.97	0.47
1:A:202:THR:OG1	1:A:205:GLU:HG3	2.14	0.47
1:B:286:ASP:HB3	1:B:289:ILE:HG12	1.97	0.47
1:A:346:LEU:HA	1:A:346:LEU:HD12	1.48	0.46
1:B:287:ILE:CD1	1:B:290:ARG:HH21	2.26	0.46
1:B:279:TYR:CE1	1:B:283:MET:HE3	2.51	0.46
1:A:14:SER:OG	3:A:401:ADP:O1B	2.29	0.46
1:B:259:GLU:CD	1:B:312:ARG:HH12	2.24	0.46
2:G:95:TYR:CE2	2:G:226:LEU:HB3	2.38	0.46
1:A:180:LEU:C	1:A:180:LEU:HD23	2.41	0.46
2:G:120:ARG:NH1	2:G:122:SER:HG	2.14	0.46
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.97	0.46
1:A:180:LEU:HD12	1:A:267:ILE:HD11	1.98	0.46
1:A:211:ASP:CG	1:A:215:LYS:HZ3	2.23	0.46
1:B:68:LYS:HB2	1:B:68:LYS:HE2	1.76	0.46
1:B:49:GLN:HG3	1:B:53:TYR:OH	2.16	0.45
2:G:204:ALA:O	2:G:208:ARG:HG3	2.16	0.45
2:G:23:ASP:CG	2:G:96:ALA:H	2.23	0.45
1:A:149:THR:HG23	1:A:166:TYR:HA	1.97	0.45
1:B:345:ILE:CD1	2:G:100:LEU:HD21	2.46	0.45
2:G:75:THR:HG23	2:G:78:PHE:H	1.81	0.45
2:G:124:GLU:H	2:G:124:GLU:HG2	1.27	0.45
1:B:269:MET:HE2	1:B:269:MET:HB3	1.88	0.44
1:B:104:LEU:C	1:B:104:LEU:HD23	2.43	0.44
2:G:26:LEU:HD12	2:G:34:TYR:O	2.17	0.44
1:B:330:ILE:HG22	1:B:332:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:122:SER:HG	2:G:148:ASP:CG	2.21	0.44
1:A:177:ARG:NH1	1:A:179:ASP:OD2	2.51	0.44
1:A:207:GLU:OE1	1:A:210:ARG:NH2	2.51	0.44
1:B:147:ARG:HG2	2:G:68:THR:HG21	1.99	0.44
1:A:350:SER:N	2:G:130:ASN:OD1	2.46	0.44
1:B:73:HIC:HA	1:B:159:VAL:HB	1.99	0.44
1:A:9:VAL:HG21	1:A:344:SER:HA	1.99	0.44
1:A:153:LEU:HD22	1:A:313:MET:HE2	2.00	0.44
2:G:44:ASP:N	2:G:44:ASP:OD1	2.51	0.43
1:B:40:HIS:O	1:B:42:GLY:N	2.42	0.43
2:G:71:GLN:HG3	2:G:72:GLY:N	2.32	0.43
2:G:134:MET:SD	2:G:177:TRP:CG	3.12	0.43
1:B:194:THR:HA	1:B:198:TYR:O	2.18	0.43
2:G:79:LEU:HD23	2:G:79:LEU:HA	1.80	0.43
1:A:154:ASP:HA	1:A:300:SER:O	2.18	0.43
1:B:346:LEU:HG	1:B:352:PHE:CD2	2.54	0.43
2:G:188:LEU:H	2:G:188:LEU:HD23	1.84	0.43
1:B:99:GLU:O	1:B:130:PRO:HG3	2.19	0.43
1:B:44:MET:HE2	1:B:51:ASP:HA	2.01	0.42
1:A:304:THR:OG1	1:A:335:ARG:HD2	2.18	0.42
1:B:273:GLY:O	1:B:277:THR:HG23	2.19	0.42
1:A:16:LEU:HB2	1:A:18:LYS:HZ2	1.84	0.42
1:A:261:LEU:HB3	1:A:274:ILE:HD13	2.01	0.42
2:G:55:THR:O	2:G:59:GLN:HG3	2.20	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.75	0.42
2:G:113:GLU:H	2:G:113:GLU:HG2	1.40	0.42
1:A:102:PRO:HB3	1:A:131:ALA:HB3	2.00	0.42
2:G:140:ASN:ND2	2:G:142:SER:OG	2.53	0.42
2:G:30:ASP:O	2:G:60:ARG:NH1	2.52	0.42
2:G:108:TRP:HZ2	2:G:114:TRP:CG	2.38	0.42
1:A:340:TRP:CZ3	1:A:344:SER:HB2	2.55	0.42
1:A:105:LEU:HD11	1:A:123:MET:SD	2.59	0.41
1:A:330:ILE:HG22	1:A:332:PRO:HD3	2.02	0.41
1:B:349:LEU:HD21	2:G:48:THR:HG23	2.02	0.41
2:G:19:PHE:HB2	2:G:90:ILE:O	2.20	0.41
2:G:122:SER:HB3	2:G:124:GLU:HG2	2.02	0.41
1:A:176:MET:CE	1:A:284:LYS:HD2	2.50	0.41
1:B:216:LEU:HB3	1:B:250:ILE:HD11	2.01	0.41
2:G:145:ASP:H	2:G:150:PHE:HZ	1.68	0.41
2:G:134:MET:HE2	2:G:134:MET:HB3	1.64	0.41
2:G:76:LYS:O	2:G:80:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:OG1	1:B:361:GLU:HG3	2.20	0.41
1:B:33:SER:O	1:B:33:SER:OG	2.30	0.41
2:G:16:LYS:HB3	2:G:18:ILE:HG13	2.02	0.41
1:B:132:MET:CE	1:B:134:VAL:HG23	2.51	0.41
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.55	0.41
2:G:111:PHE:CZ	2:G:213:LYS:HD2	2.56	0.41
1:A:17:VAL:O	1:A:30:VAL:HA	2.21	0.41
1:A:81:ASP:O	1:A:85:ILE:HG12	2.20	0.41
1:A:104:LEU:C	1:A:104:LEU:HD23	2.46	0.41
2:G:52:GLN:O	2:G:56:LEU:HG	2.21	0.41
2:G:111:PHE:CE2	2:G:213:LYS:HD2	2.56	0.40
2:G:120:ARG:HG3	2:G:150:PHE:CE1	2.57	0.40
1:A:87:HIS:CE1	1:A:91:TYR:CD2	3.10	0.40
1:A:196:ARG:HD2	1:A:253:GLU:OE2	2.22	0.40
1:A:300:SER:HB2	1:A:338:SER:OG	2.21	0.40
1:B:28:ARG:NH1	2:G:109:ALA:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:NE2	1:B:99:GLU:OE1[2_555]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/377 (98%)	351 (95%)	14 (4%)	3 (1%)	16	44
1	B	368/377 (98%)	356 (97%)	11 (3%)	1 (0%)	36	66
2	G	217/335 (65%)	203 (94%)	12 (6%)	2 (1%)	14	42
All	All	953/1089 (88%)	910 (96%)	37 (4%)	6 (1%)	21	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	61	GLY
2	G	217	ALA
1	B	244	ASP
1	A	62	ARG
1	A	201	VAL
1	A	339	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/319 (98%)	313 (100%)	0	100	100
1	B	313/319 (98%)	312 (100%)	1 (0%)	86	86
2	G	186/283 (66%)	186 (100%)	0	100	100
All	All	812/921 (88%)	811 (100%)	1 (0%)	88	89

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

Mol	Chain	Res	Type
1	B	60	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	128	ASN
1	B	225	ASN
1	B	353	GLN
2	G	58	GLN
2	G	140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	A	73	1	10,11,12	2.05	3 (30%)	9,14,16	1.64	3 (33%)
1	HIC	B	73	1	10,11,12	1.76	3 (30%)	9,14,16	1.68	1 (11%)

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	A	73	1	-	3/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	4.14	1.43	1.36
1	B	73	HIC	CD2-CG	3.63	1.42	1.36
1	A	73	HIC	CD2-NE2	3.16	1.41	1.37
1	B	73	HIC	CD2-NE2	2.78	1.41	1.37
1	A	73	HIC	CE1-NE2	2.62	1.42	1.35
1	B	73	HIC	CE1-NE2	2.27	1.41	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIC	CD2-NE2-CE1	-4.19	105.06	106.71
1	A	73	HIC	CD2-NE2-CE1	-2.92	105.56	106.71
1	A	73	HIC	CA-CB-CG	-2.68	107.16	113.77
1	A	73	HIC	CB-CG-CD2	-2.09	124.91	129.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	B	73	HIC	CA-CB-CG-CD2
1	B	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	B	401	4	28,29,29	1.63	5 (17%)	43,45,45	1.91	14 (32%)
3	ADP	A	401	4	28,29,29	1.46	5 (17%)	43,45,45	2.07	14 (32%)

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	B	401	4	-	3/16/32/32	0/3/3/3
3	ADP	A	401	4	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C4	5.34	1.48	1.39
3	A	401	ADP	C5-C4	3.48	1.45	1.39
3	A	401	ADP	PA-O3A	3.32	1.63	1.59
3	A	401	ADP	C5-N7	-3.21	1.33	1.39
3	B	401	ADP	C5-C6	3.15	1.49	1.41
3	B	401	ADP	C8-N7	3.11	1.37	1.31
3	B	401	ADP	PA-O3A	2.91	1.62	1.59
3	A	401	ADP	C4-N9	-2.64	1.32	1.37
3	A	401	ADP	C8-N9	-2.42	1.33	1.37
3	B	401	ADP	C4-N9	-2.02	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C4-N9-C8	5.04	111.03	105.74
3	A	401	ADP	N3-C4-N9	4.86	135.43	127.17
3	B	401	ADP	C4-C5-N7	-4.80	105.10	110.58
3	B	401	ADP	C5-C4-N3	-4.79	120.12	126.72
3	A	401	ADP	C5-C4-N3	-4.52	120.49	126.72
3	A	401	ADP	N3-C2-N1	-3.64	123.07	128.58
3	B	401	ADP	O4'-C1'-N9	3.30	114.43	108.09
3	B	401	ADP	N3-C4-N9	3.24	132.67	127.17
3	A	401	ADP	N9-C8-N7	-3.21	109.39	113.94
3	B	401	ADP	C4-N9-C8	3.13	109.02	105.74
3	B	401	ADP	C5-N7-C8	3.09	108.31	103.45
3	A	401	ADP	C2-N3-C4	3.01	119.19	111.83
3	B	401	ADP	C2-N3-C4	2.83	118.75	111.83
3	B	401	ADP	C6-C5-N7	2.83	137.55	132.09
3	A	401	ADP	O3A-PB-O1B	-2.80	96.32	111.04
3	A	401	ADP	N6-C6-N1	2.76	124.53	118.38
3	A	401	ADP	O2A-PA-O5'	2.69	119.74	107.57
3	B	401	ADP	O3B-PB-O2B	2.52	117.27	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ADP	N9-C8-N7	-2.52	110.37	113.94
3	B	401	ADP	C2-N1-C6	2.48	122.80	118.73
3	A	401	ADP	C5-N7-C8	2.47	107.33	103.45
3	B	401	ADP	N3-C2-N1	-2.43	124.91	128.58
3	B	401	ADP	O5'-C5'-C4'	2.40	117.17	108.99
3	A	401	ADP	C5-C6-N6	-2.28	117.64	123.29
3	B	401	ADP	C4-N9-C1'	-2.19	121.52	126.63
3	A	401	ADP	C2'-C3'-C4'	2.17	106.80	102.61
3	A	401	ADP	C4-C5-N7	-2.11	108.17	110.58
3	A	401	ADP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

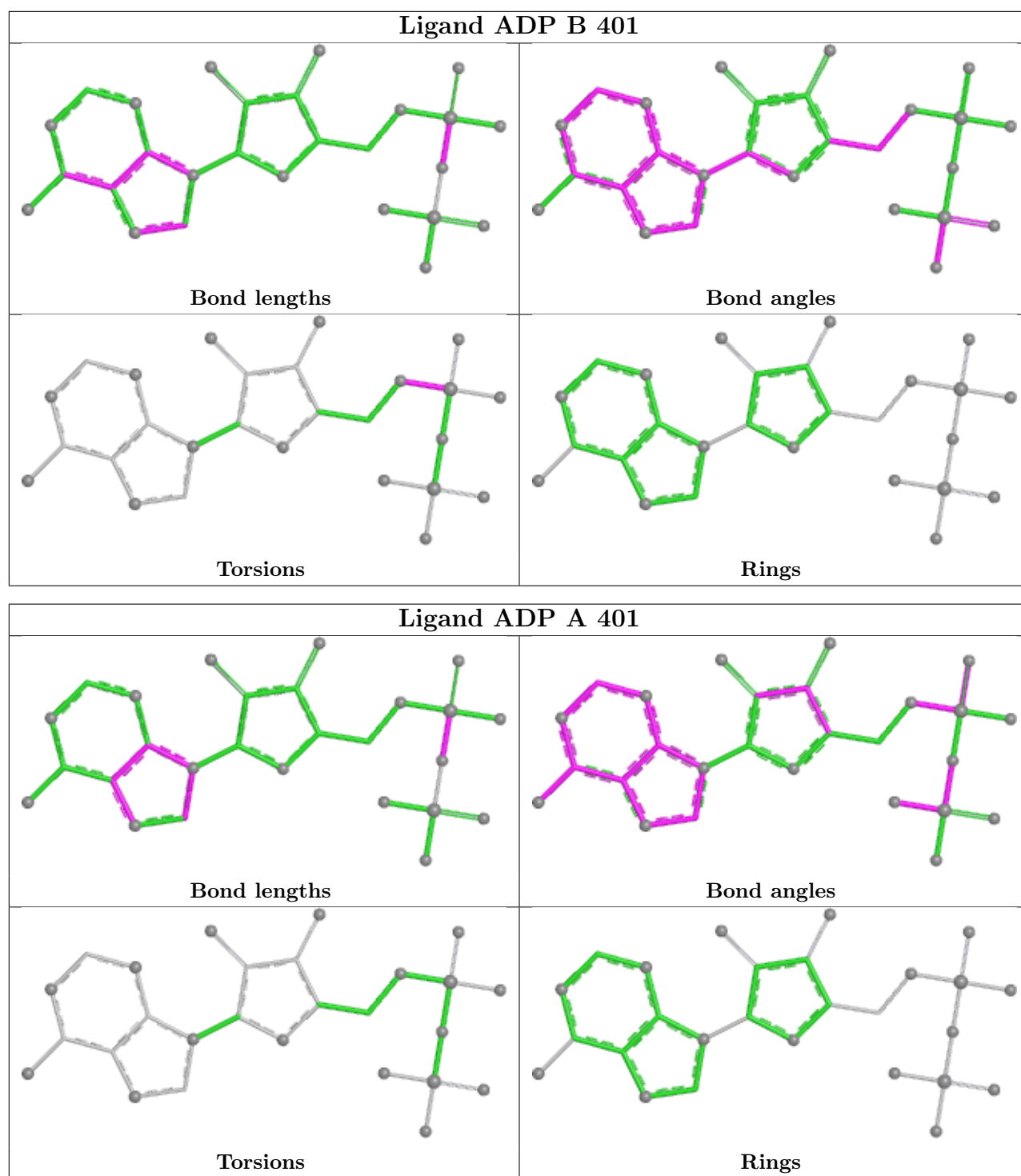
Mol	Chain	Res	Type	Atoms
3	B	401	ADP	C5'-O5'-PA-O1A
3	B	401	ADP	C5'-O5'-PA-O2A
3	B	401	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	370/377 (98%)	-0.77	0 100 100	15, 45, 91, 154	0
1	B	370/377 (98%)	-0.56	0 100 100	40, 74, 115, 144	0
2	G	221/335 (65%)	-0.40	0 100 100	35, 77, 133, 152	0
All	All	961/1089 (88%)	-0.60	0 100 100	15, 64, 118, 154	0

There are no RSRZ outliers to report.

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	B	73	11/12	0.85	0.12	79,84,86,87	0
1	HIC	A	73	11/12	0.90	0.10	40,54,64,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

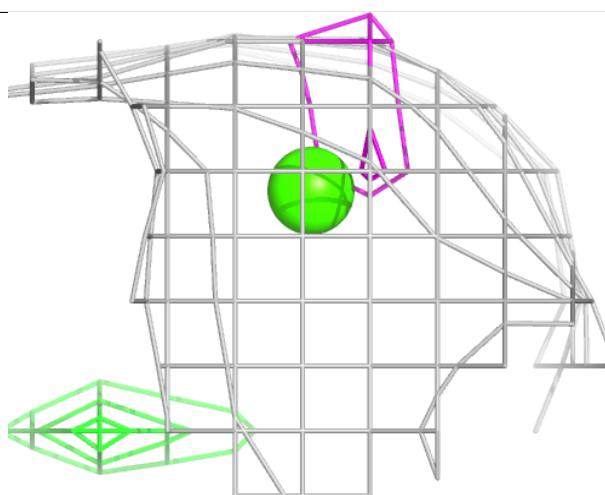
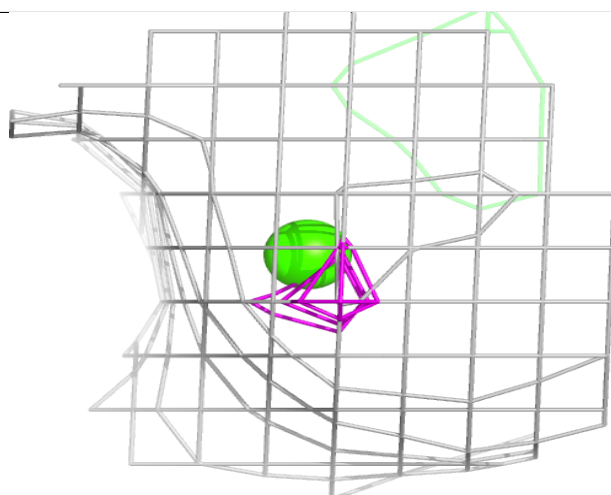
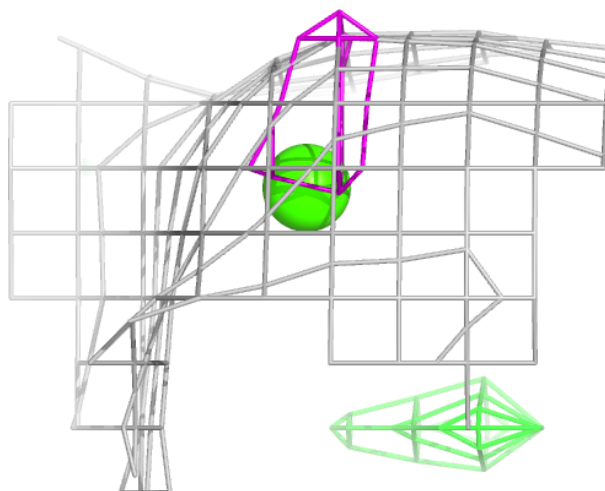
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	G	406	1/1	0.81	0.11	78,78,78,78	0
4	CA	A	403	1/1	0.91	0.06	93,93,93,93	0
4	CA	B	402	1/1	0.93	0.14	55,55,55,55	0
4	CA	G	405	1/1	0.94	0.04	116,116,116,116	0
4	CA	A	402	1/1	0.96	0.10	40,40,40,40	0
4	CA	G	402	1/1	0.97	0.03	59,59,59,59	0
4	CA	G	404	1/1	0.97	0.04	35,35,35,35	0
3	ADP	B	401	27/27	0.97	0.06	41,48,54,56	0
4	CA	G	401	1/1	0.97	0.07	82,82,82,82	0
4	CA	G	403	1/1	0.98	0.05	64,64,64,64	0
3	ADP	A	401	27/27	0.98	0.05	28,33,36,37	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.

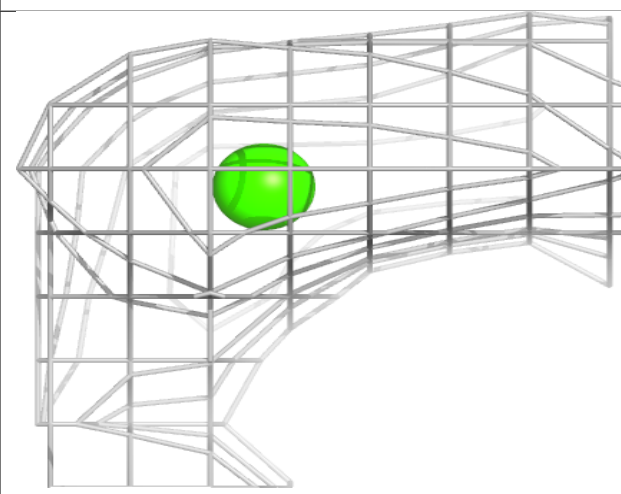
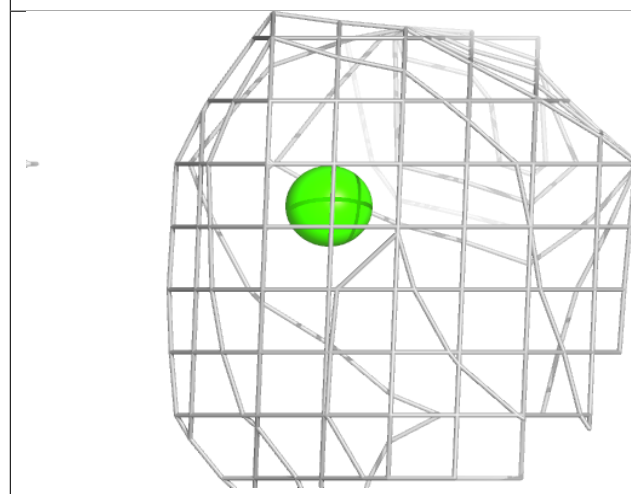
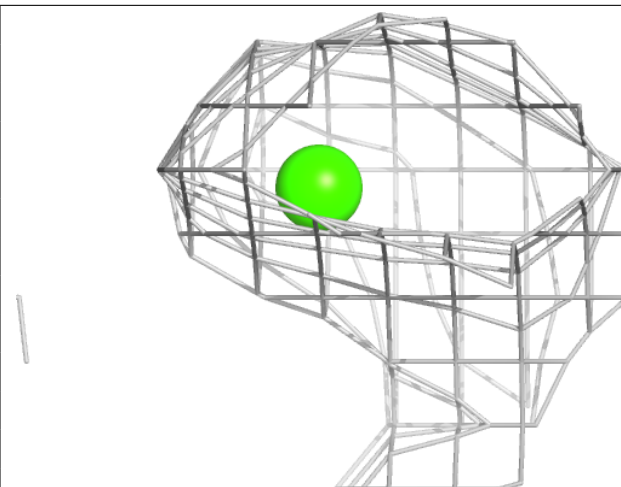
Electron density around CA G 406:

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



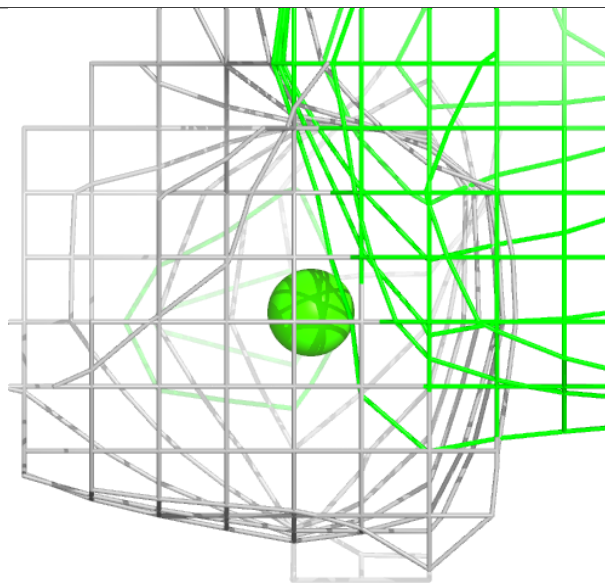
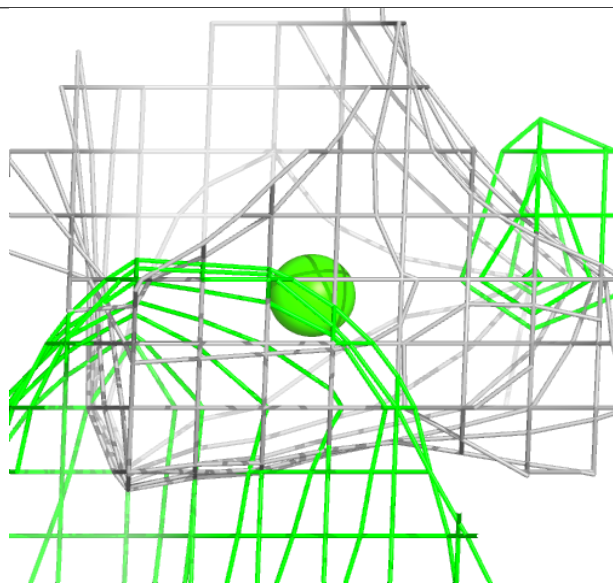
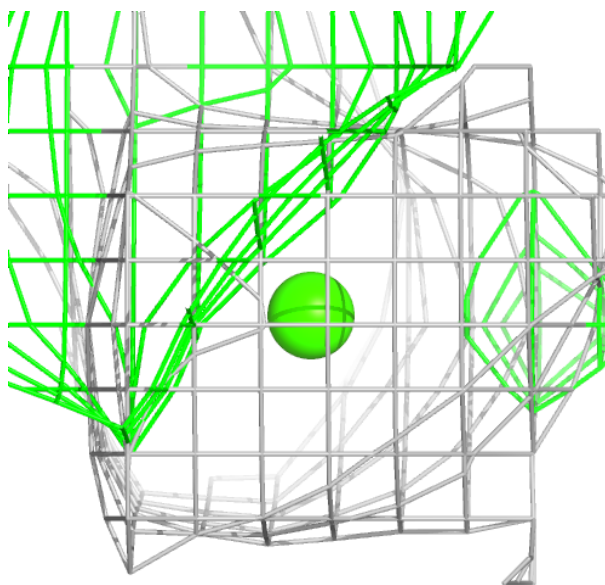
Electron density around CA A 403:

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



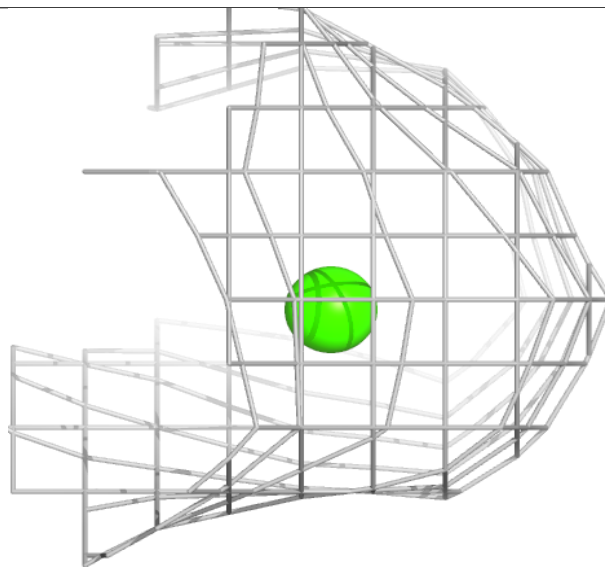
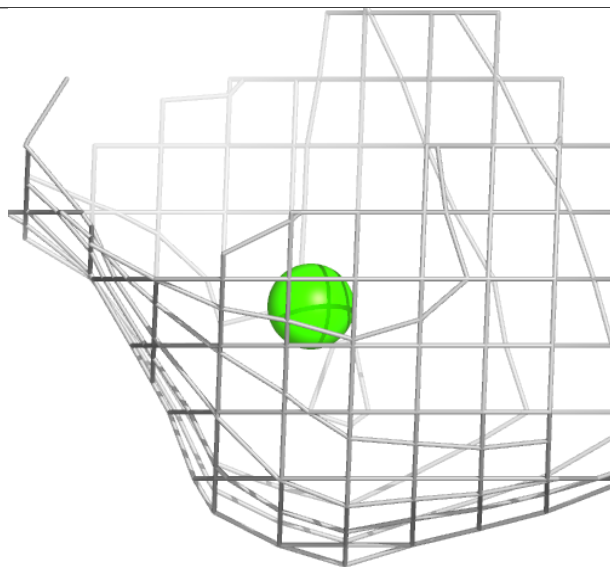
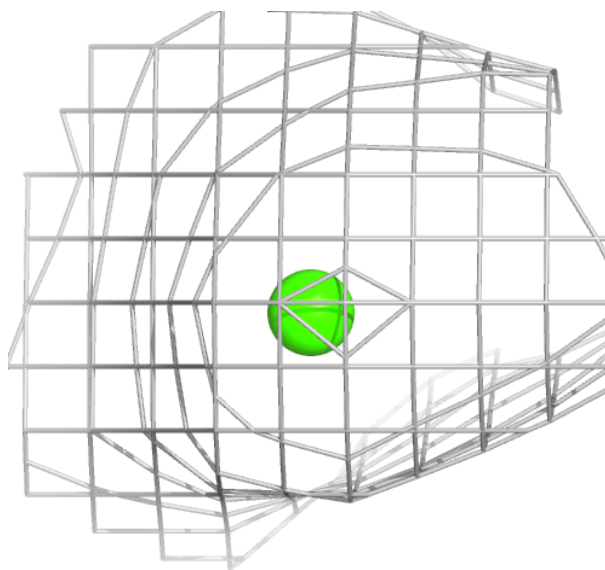
Electron density around CA B 402:

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and green (positive)



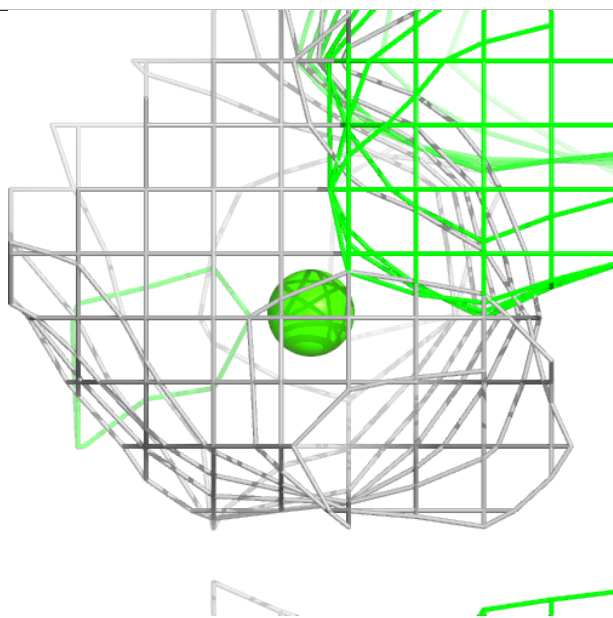
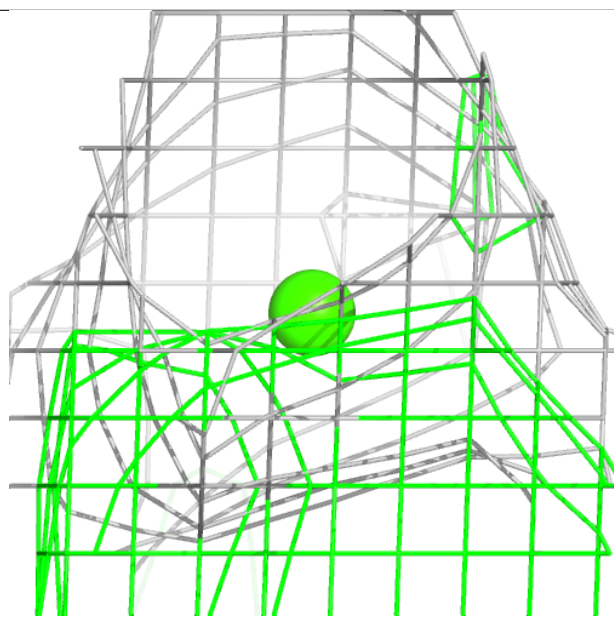
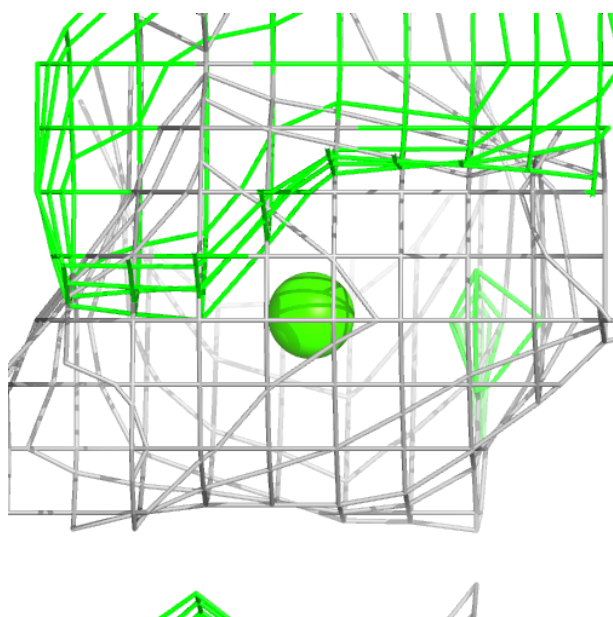
Electron density around CA G 405:

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



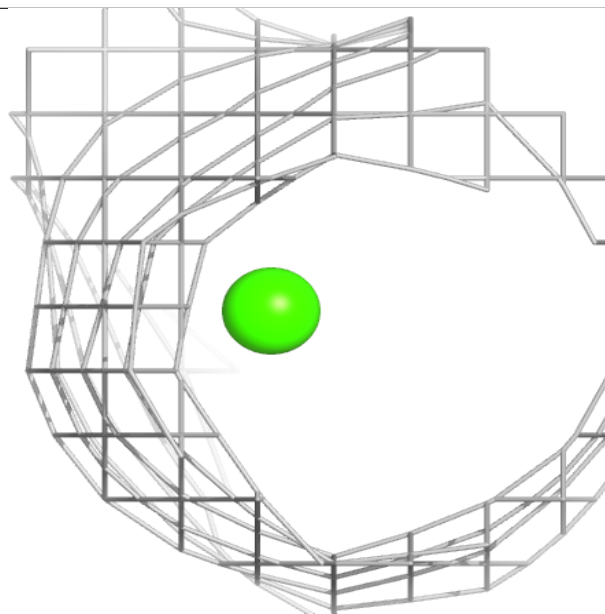
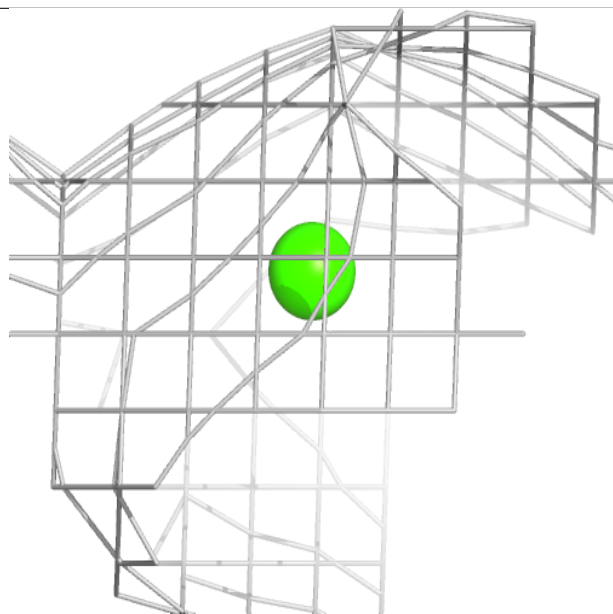
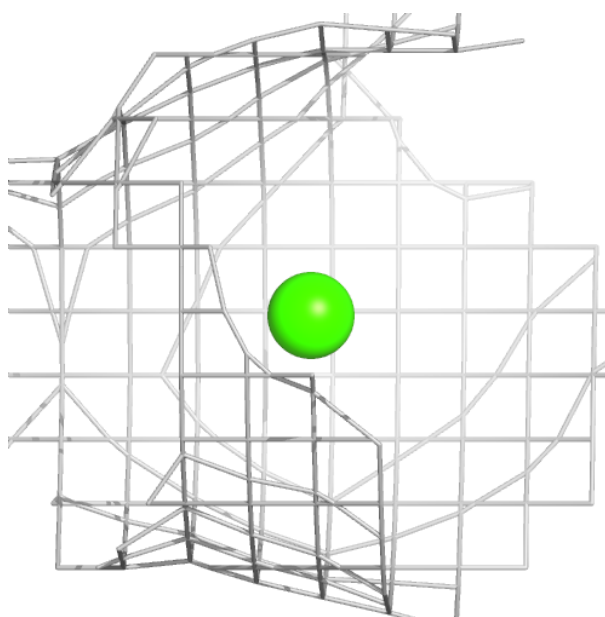
Electron density around CA A 402:

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



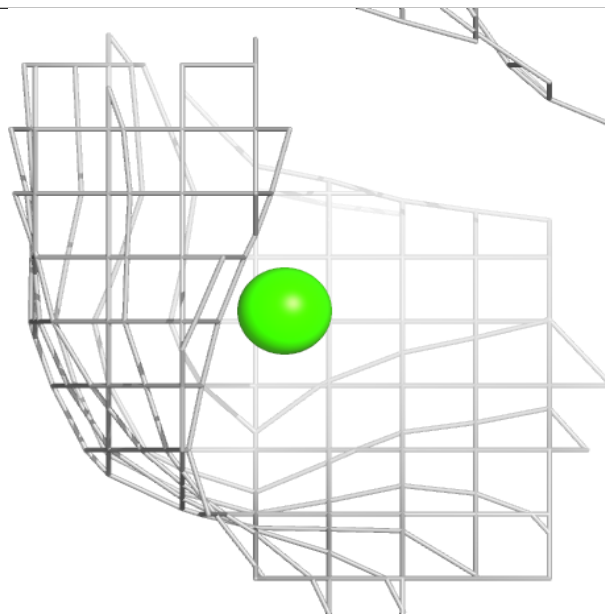
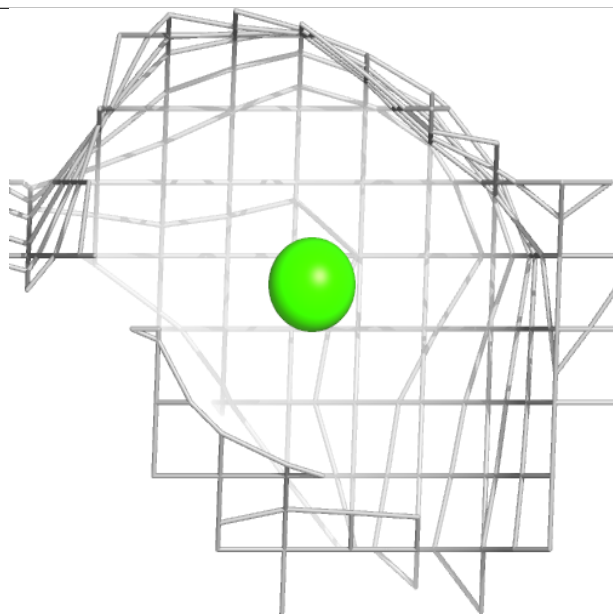
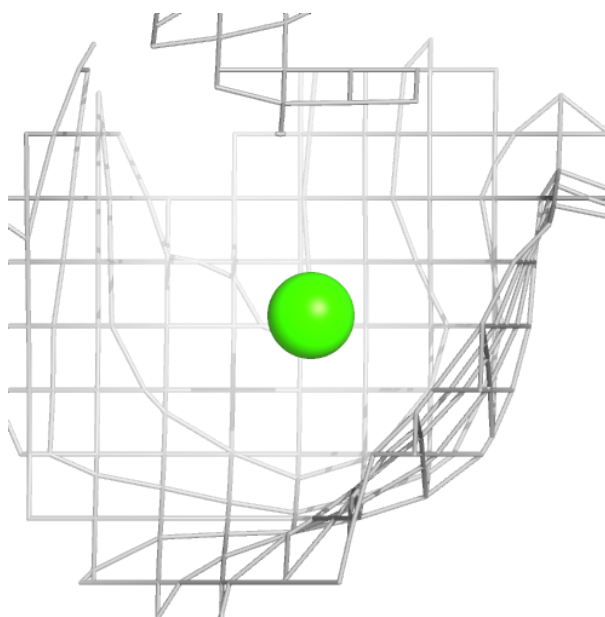
Electron density around CA G 402:

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



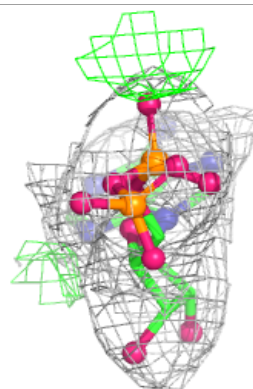
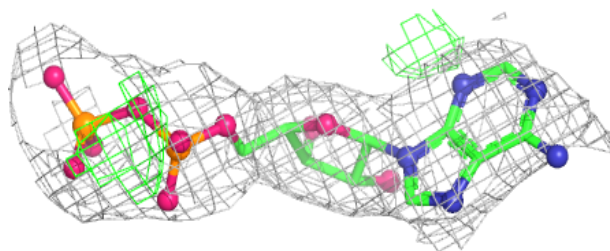
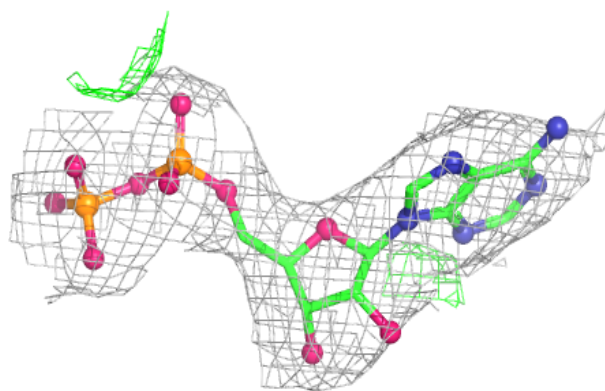
Electron density around CA G 404:

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



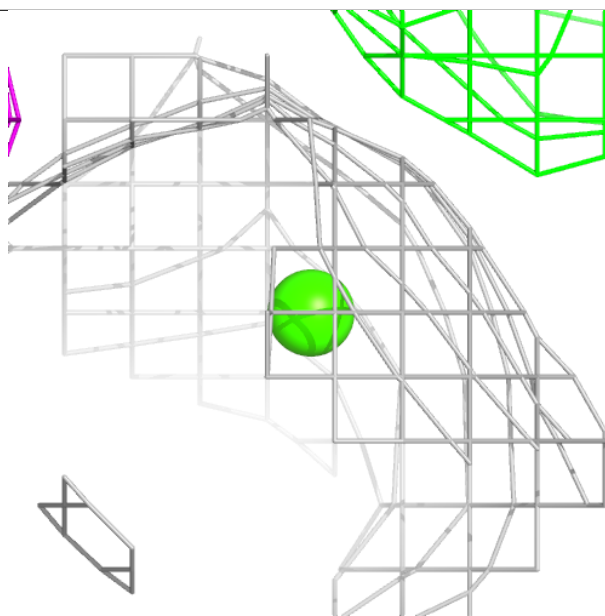
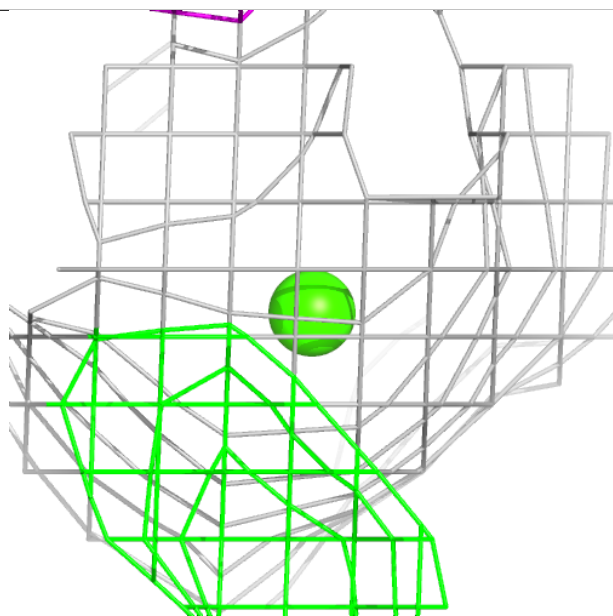
Electron density around ADP B 401:

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



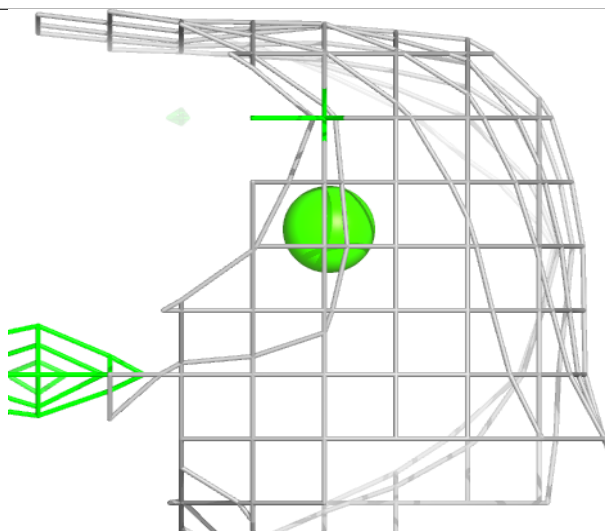
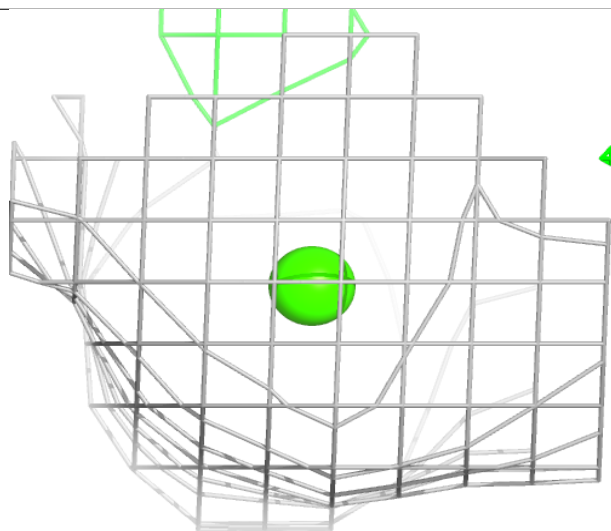
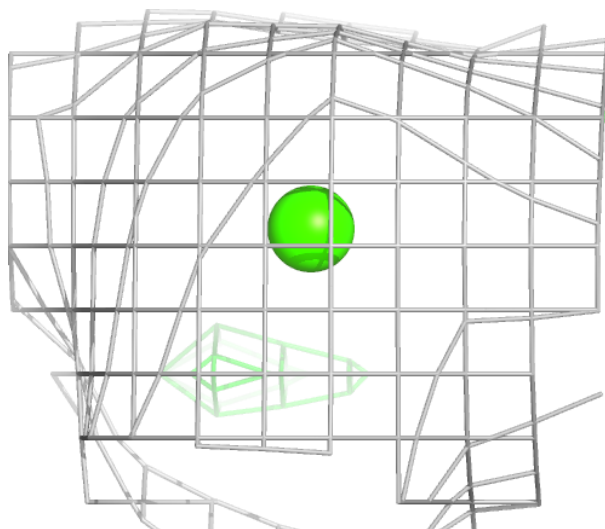
Electron density around CA G 401:

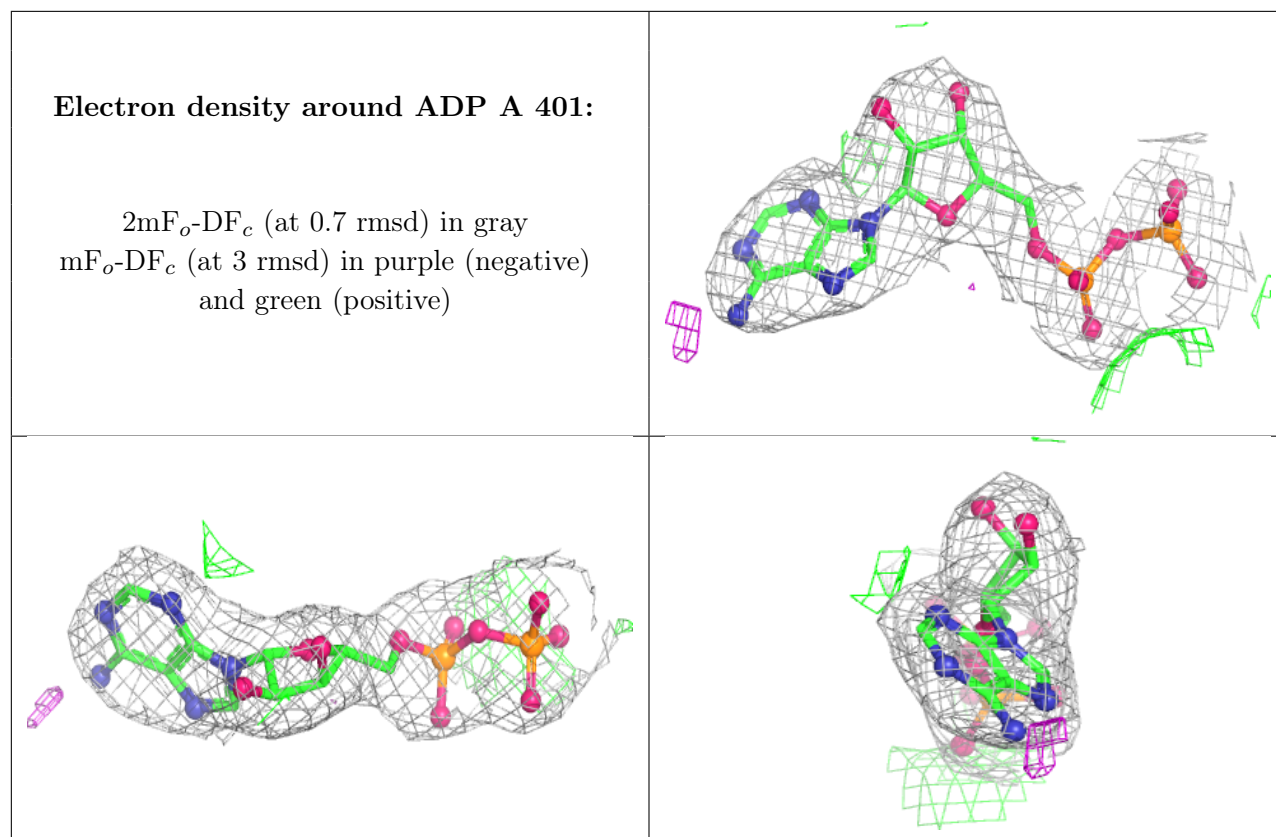
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA G 403:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.