Full wwPDB X-ray Structure Validation Report (i)

Jul 23, 2024 – 01:40 pm BST

PDB ID	:	8QCH
Title	:	Human Adenosine deaminase-like protein in complex with compound AT8001
Authors	:	Zimberger, C.; canard, B.; Ferron, F.
Deposited on	:	2023-08-26
Resolution	:	2.44 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

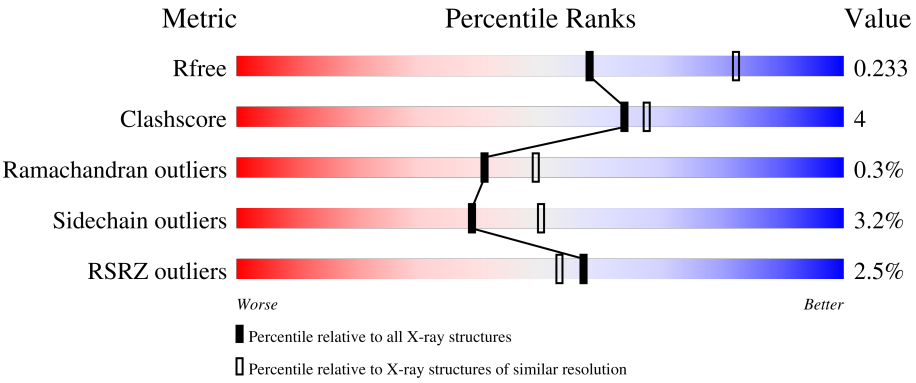
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.44 Å.

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



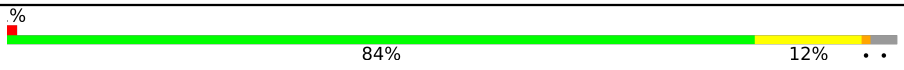
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	355	2% 86% 9%
1	B	355	3% 86% 10%
1	C	355	2% 84% 12%
1	D	355	1% 86% 10%
1	E	355	3% 87% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	355	
1	G	355	
1	H	355	

2 Entry composition (i)

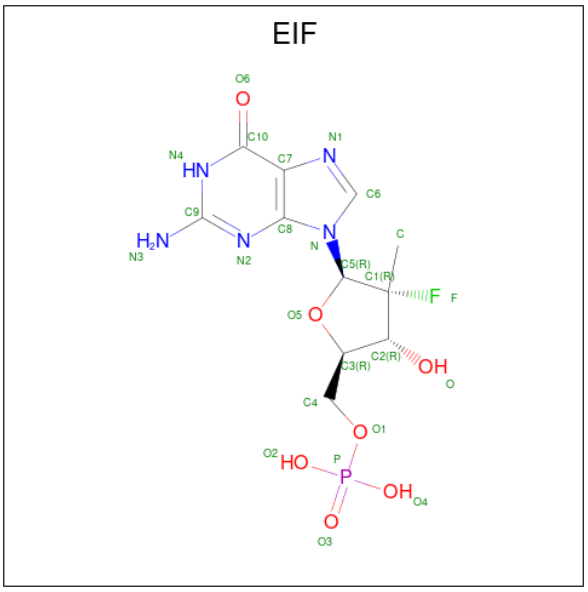
There are 7 unique types of molecules in this entry. The entry contains 23207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine deaminase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2746	1745	468	525	8			
1	B	344	Total	C	N	O	S	0	0	0
			2742	1742	467	525	8			
1	C	344	Total	C	N	O	S	0	0	0
			2746	1745	468	525	8			
1	D	346	Total	C	N	O	S	0	0	0
			2761	1754	471	527	9			
1	E	344	Total	C	N	O	S	0	0	0
			2746	1745	468	525	8			
1	F	344	Total	C	N	O	S	0	0	0
			2746	1745	468	525	8			
1	G	349	Total	C	N	O	S	0	0	0
			2786	1769	476	532	9			
1	H	350	Total	C	N	O	S	0	0	0
			2795	1774	477	535	9			

- Molecule 2 is [(2 {R},3 {R},4 {R},5 {R})-5-(2-azanyl-6-oxidanylidene-1 {H}-purin-9-yl)-4-fluoranyl-4-methyl-3-oxidanyl-oxolan-2-yl]methyl dihydrogen phosphate (three-letter code: EIF) (formula: $C_{11}H_{15}FN_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	B	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	C	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	D	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	E	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	F	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	G	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		
2	H	1	Total	C	F	N	O	P	0	0
			25	11	1	5	7	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

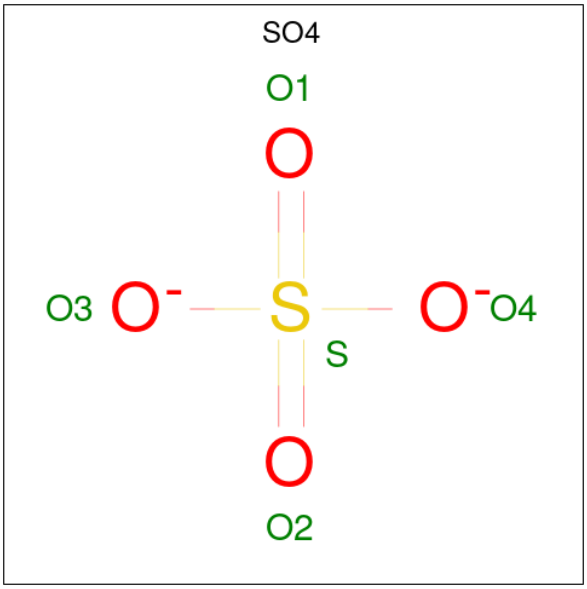
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



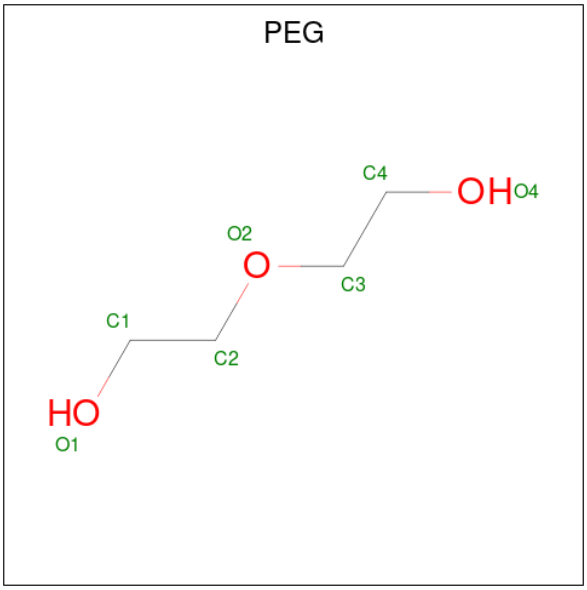
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Na 1 1	0	0

- Molecule 7 is water.

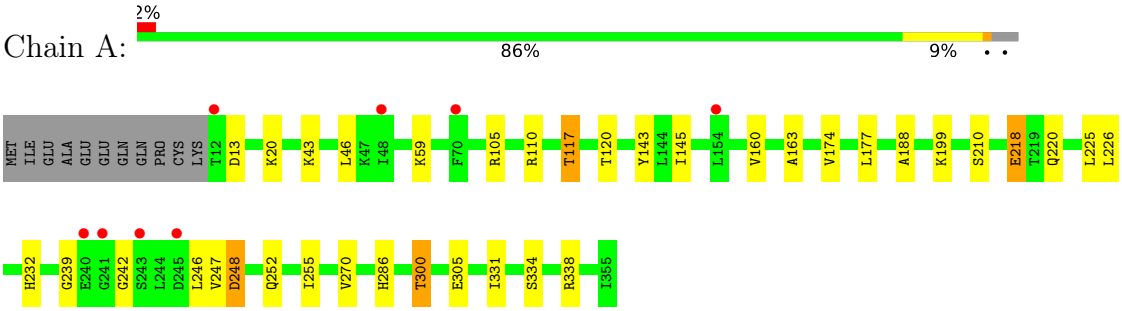
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	124	Total O 124 124	0	0
7	B	106	Total O 106 106	0	0
7	C	107	Total O 107 107	0	0
7	D	56	Total O 56 56	0	0
7	E	114	Total O 114 114	0	0
7	F	104	Total O 104 104	0	0
7	G	99	Total O 99 99	0	0
7	H	107	Total O 107 107	0	0

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.

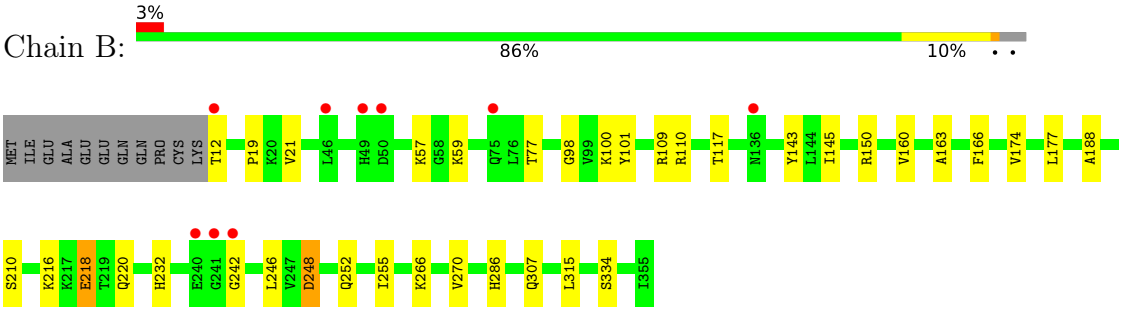
• Molecule 1: Adenosine deaminase-like protein

Chain A:



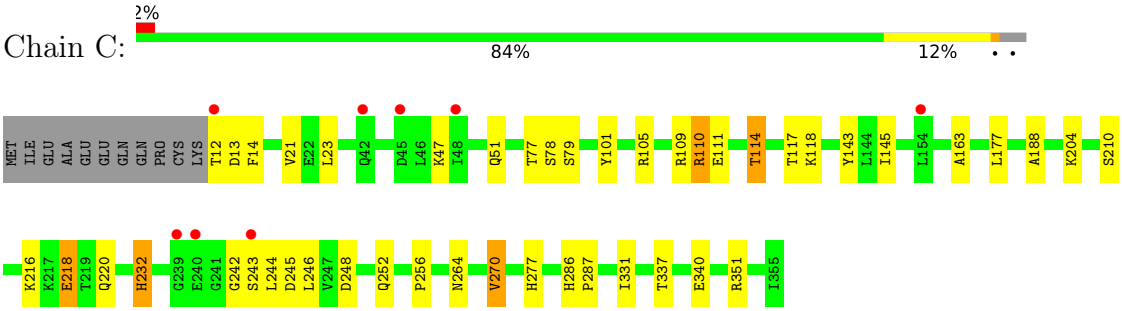
• Molecule 1: Adenosine deaminase-like protein

Chain B:



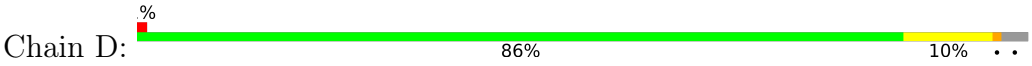
• Molecule 1: Adenosine deaminase-like protein

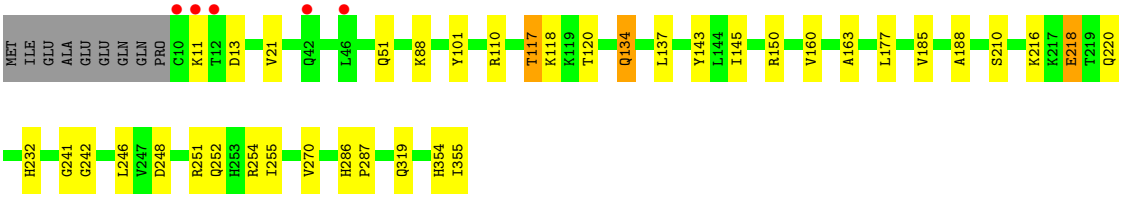
Chain C:



• Molecule 1: Adenosine deaminase-like protein

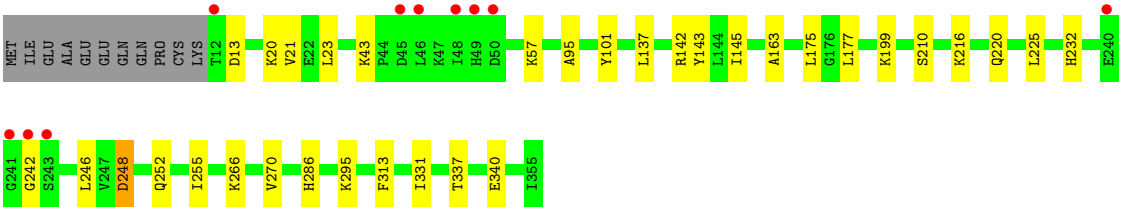
Chain D:





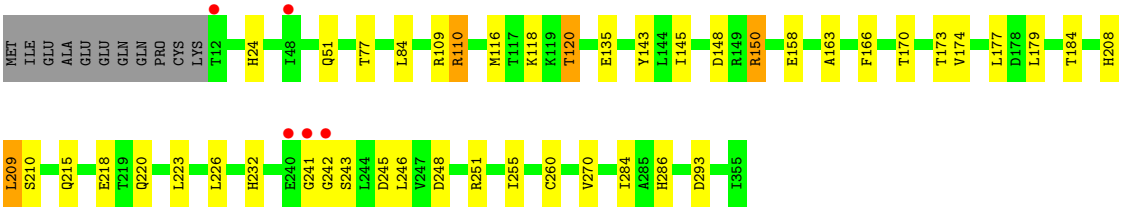
• Molecule 1: Adenosine deaminase-like protein

Chain E:



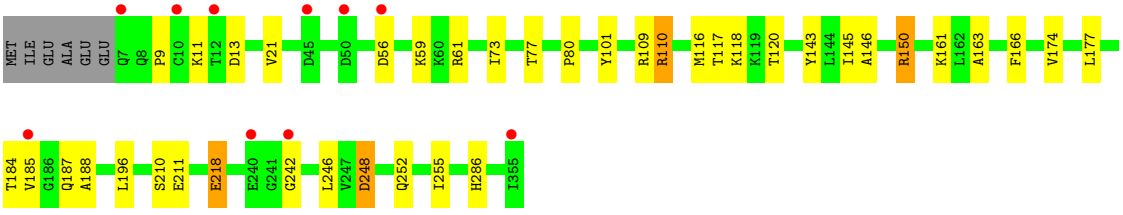
• Molecule 1: Adenosine deaminase-like protein

Chain F:



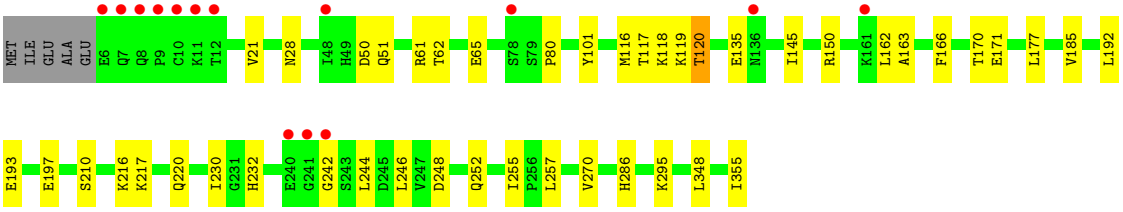
• Molecule 1: Adenosine deaminase-like protein

Chain G:



• Molecule 1: Adenosine deaminase-like protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	142.76Å 142.98Å 156.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.53 – 2.44 105.53 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (105.53-2.44) 99.7 (105.53-2.44)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.214 , 0.243 0.202 , 0.233	Depositor DCC
R_{free} test set	5715 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23207	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2556e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, EIF, NA, PEG

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	0.36	0/2801	0.54	0/3786
1	B	0.35	0/2797	0.51	0/3782
1	C	0.37	0/2801	0.54	0/3786
1	D	0.35	0/2816	0.53	0/3805
1	E	0.35	0/2801	0.52	0/3786
1	F	0.36	0/2801	0.54	0/3786
1	G	0.35	0/2842	0.53	0/3841
1	H	0.36	0/2851	0.55	0/3853
All	All	0.35	0/22510	0.53	0/30425

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

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	2746	0	2758	20	0
1	B	2742	0	2747	24	0
1	C	2746	0	2758	37	0
1	D	2761	0	2776	26	0
1	E	2746	0	2758	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2746	0	2758	24	0
1	G	2786	0	2799	20	0
1	H	2795	0	2805	18	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
2	E	25	0	0	0	0
2	F	25	0	0	0	0
2	G	25	0	0	1	0
2	H	25	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	15	0	0	1	0
4	B	10	0	0	1	0
4	C	10	0	0	1	0
4	D	10	0	0	0	0
4	E	10	0	0	1	0
4	F	20	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	D	14	0	20	3	0
5	E	7	0	10	1	0
5	G	7	0	10	0	0
6	H	1	0	0	0	0
7	A	124	0	0	6	0
7	B	106	0	0	6	0
7	C	107	0	0	8	0
7	D	56	0	0	3	0
7	E	114	0	0	9	0
7	F	104	0	0	2	0
7	G	99	0	0	2	0
7	H	107	0	0	0	0
All	All	23207	0	22199	187	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 4.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HG2	7:B:1101:HOH:O	1.17	1.27
1:G:56:ASP:HB2	1:G:59:LYS:HD3	1.44	0.98
1:C:351:ARG:HH12	1:D:134:GLN:NE2	1.65	0.91
1:F:170:THR:HG21	1:F:174:VAL:H	1.38	0.88
1:B:174:VAL:HG13	7:B:1115:HOH:O	1.78	0.83
1:F:243:SER:HB3	1:F:245:ASP:OD1	1.79	0.83
1:C:351:ARG:NH1	1:D:134:GLN:NE2	2.26	0.83
1:F:110:ARG:HE	1:F:118:LYS:H	1.28	0.76
1:A:338:ARG:NE	7:A:501:HOH:O	2.16	0.74
1:C:270:VAL:HG21	7:C:504:HOH:O	1.89	0.73
1:B:98:GLY:O	7:B:1101:HOH:O	2.06	0.72
1:H:118:LYS:HG3	1:H:162:LEU:HD22	1.72	0.71
1:E:43:LYS:NZ	7:E:502:HOH:O	2.24	0.67
1:G:73:ILE:HG22	7:G:505:HOH:O	1.95	0.66
1:C:110:ARG:HG3	1:C:117:THR:HA	1.75	0.66
1:B:145:ILE:HG13	7:B:1115:HOH:O	1.95	0.66
1:B:160:VAL:HG22	1:B:177:LEU:HD21	1.78	0.66
1:C:351:ARG:NH1	1:D:134:GLN:HE22	1.91	0.66
1:C:351:ARG:HH12	1:D:134:GLN:HE21	1.41	0.65
1:D:242:GLY:HA2	1:D:246:LEU:HD12	1.79	0.64
1:A:199:LYS:HE3	1:A:225:LEU:O	1.98	0.64
1:B:315:LEU:HD22	7:D:502:HOH:O	1.96	0.64
1:A:331:ILE:HG12	7:A:501:HOH:O	1.98	0.64
1:A:160:VAL:HG22	1:A:177:LEU:HD21	1.79	0.63
1:C:243:SER:HB3	1:C:245:ASP:OD1	1.98	0.63
1:H:242:GLY:HA2	1:H:246:LEU:HD12	1.81	0.63
1:D:319:GLN:NE2	7:D:502:HOH:O	2.31	0.62
1:E:137:LEU:HD13	7:E:517:HOH:O	1.99	0.62
1:C:277:HIS:CE1	7:C:504:HOH:O	2.52	0.62
1:D:254:ARG:HG2	5:D:401:PEG:H12	1.82	0.61
1:B:242:GLY:HA2	1:B:246:LEU:HD12	1.81	0.61
1:A:242:GLY:HA2	1:A:246:LEU:HD12	1.82	0.61
1:C:110:ARG:CG	1:C:117:THR:HA	2.29	0.61
1:F:116:MET:HG3	1:F:120:THR:HG22	1.81	0.61
1:F:242:GLY:HA2	1:F:246:LEU:HD12	1.82	0.61
1:B:59:LYS:NZ	7:B:1104:HOH:O	2.33	0.61
1:E:242:GLY:HA2	1:E:246:LEU:HD12	1.81	0.60
1:D:160:VAL:HG22	1:D:177:LEU:HD21	1.83	0.60
1:G:242:GLY:HA2	1:G:246:LEU:HD12	1.82	0.60
1:G:110:ARG:HG3	1:G:117:THR:HA	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:THR:O	1:C:109:ARG:NH2	2.36	0.59
1:C:220:GLN:HG2	1:C:246:LEU:HD21	1.85	0.59
1:E:220:GLN:HG2	1:E:246:LEU:HD21	1.85	0.58
1:G:77:THR:O	1:G:109:ARG:NH2	2.37	0.58
1:H:62:THR:HG23	1:H:65:GLU:H	1.70	0.57
1:D:110:ARG:HG3	1:D:118:LYS:HG3	1.85	0.57
1:C:79:SER:HA	1:C:114:THR:HG21	1.86	0.57
1:C:21:VAL:HG22	1:C:101:TYR:HB3	1.86	0.57
1:B:150:ARG:NH2	1:F:184:THR:OG1	2.38	0.56
1:D:241:GLY:O	7:D:501:HOH:O	2.18	0.56
1:G:21:VAL:HG22	1:G:101:TYR:HB3	1.87	0.56
1:E:21:VAL:HG22	1:E:101:TYR:HB3	1.88	0.56
1:C:264:ASN:ND2	7:C:504:HOH:O	2.31	0.56
1:F:110:ARG:NE	1:F:118:LYS:H	2.01	0.56
1:H:166:PHE:O	1:H:170:THR:HG22	2.07	0.55
1:F:170:THR:CG2	1:F:174:VAL:H	2.16	0.55
1:B:21:VAL:HG22	1:B:101:TYR:HB3	1.90	0.54
1:F:166:PHE:O	1:F:170:THR:HG22	2.08	0.54
1:C:286:HIS:CE1	7:C:501:HOH:O	2.61	0.54
1:E:57:LYS:NZ	7:E:506:HOH:O	2.40	0.54
1:G:211:GLU:OE2	2:G:402:EIF:N3	2.41	0.54
1:C:242:GLY:HA2	1:C:246:LEU:HD12	1.88	0.54
1:D:21:VAL:HG22	1:D:101:TYR:HB3	1.89	0.53
1:A:43:LYS:HB3	1:A:46:LEU:HD13	1.89	0.53
1:C:351:ARG:NH2	1:D:88:LYS:NZ	2.55	0.53
1:H:21:VAL:HG22	1:H:101:TYR:HB3	1.90	0.53
1:H:220:GLN:HG2	1:H:246:LEU:HD21	1.90	0.53
1:G:188:ALA:HB2	1:G:218:GLU:HG3	1.90	0.53
1:G:56:ASP:H	1:G:59:LYS:HZ3	1.56	0.53
1:D:220:GLN:HG2	1:D:246:LEU:HD21	1.90	0.53
1:G:146:ALA:HB1	7:G:508:HOH:O	2.09	0.53
1:B:220:GLN:HG2	1:B:246:LEU:HD21	1.90	0.52
1:D:287:PRO:HD2	5:D:401:PEG:H21	1.91	0.52
1:B:77:THR:O	1:B:109:ARG:NH2	2.43	0.52
1:H:28:ASN:ND2	2:H:401:EIF:O2	2.42	0.52
1:A:300:THR:HG21	1:A:305:GLU:OE2	2.10	0.52
1:C:110:ARG:NE	1:C:118:LYS:H	2.08	0.52
1:D:145:ILE:HD12	1:D:163:ALA:HA	1.92	0.52
1:G:145:ILE:HD12	1:G:163:ALA:HA	1.92	0.52
1:B:188:ALA:HB2	1:B:218:GLU:HG3	1.91	0.52
1:A:188:ALA:HB2	1:A:218:GLU:HG3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:GLY:O	7:F:501:HOH:O	2.19	0.51
1:F:145:ILE:HD12	1:F:163:ALA:HA	1.93	0.50
1:F:24:HIS:CE1	1:F:208:HIS:CE1	2.99	0.50
1:H:145:ILE:HD12	1:H:163:ALA:HA	1.94	0.50
1:C:270:VAL:CG2	7:C:504:HOH:O	2.55	0.50
1:D:188:ALA:HB2	1:D:218:GLU:HG3	1.94	0.50
1:F:77:THR:O	1:F:109:ARG:NH2	2.45	0.49
1:C:188:ALA:HB2	1:C:218:GLU:HG3	1.94	0.49
1:E:145:ILE:HD12	1:E:163:ALA:HA	1.93	0.49
1:A:247:VAL:HA	7:A:562:HOH:O	2.13	0.49
1:E:57:LYS:HE2	1:E:266:LYS:NZ	2.28	0.49
1:F:209:LEU:HD21	1:F:223:LEU:HG	1.95	0.49
1:A:145:ILE:HD12	1:A:163:ALA:HA	1.95	0.49
1:E:337:THR:OG1	4:E:405:SO4:O4	2.28	0.49
1:C:145:ILE:HD12	1:C:163:ALA:HA	1.95	0.48
1:E:101:TYR:HD1	7:E:503:HOH:O	1.96	0.48
1:E:142:ARG:HH11	1:E:175:LEU:HD11	1.78	0.48
1:H:117:THR:HG22	1:H:119:LYS:H	1.79	0.48
1:B:145:ILE:HD12	1:B:163:ALA:HA	1.95	0.48
1:B:255:ILE:O	1:B:286:HIS:HE1	1.97	0.48
1:D:255:ILE:O	1:D:286:HIS:HE1	1.97	0.48
1:F:255:ILE:O	1:F:286:HIS:HE1	1.96	0.48
1:D:150:ARG:HD2	1:D:185:VAL:HG11	1.96	0.48
1:D:251:ARG:HE	5:D:401:PEG:H31	1.78	0.48
1:G:150:ARG:HA	1:G:185:VAL:HG11	1.96	0.47
1:C:111:GLU:HG3	1:C:114:THR:HB	1.95	0.47
1:B:19:PRO:HA	7:B:1101:HOH:O	2.15	0.47
1:F:170:THR:OG1	1:F:173:THR:HB	2.14	0.47
1:C:78:SER:O	1:C:114:THR:HG21	2.15	0.47
1:D:117:THR:HG23	1:D:120:THR:H	1.80	0.47
1:A:334:SER:OG	4:A:405:SO4:O4	2.26	0.47
1:E:95:ALA:CB	7:E:517:HOH:O	2.63	0.47
1:B:12:THR:HG21	1:B:307:GLN:HE22	1.81	0.46
1:C:204:LYS:NZ	7:C:512:HOH:O	2.47	0.46
1:E:199:LYS:NZ	7:E:509:HOH:O	2.48	0.46
1:F:260:CYS:SG	1:F:293:ASP:HB2	2.55	0.46
1:E:248:ASP:O	1:E:252:GLN:HG2	2.16	0.45
1:G:255:ILE:O	1:G:286:HIS:HE1	1.99	0.45
1:A:248:ASP:O	1:A:252:GLN:HG2	2.17	0.45
1:E:57:LYS:HE2	1:E:266:LYS:HZ1	1.80	0.45
1:H:248:ASP:O	1:H:252:GLN:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:ASP:H	1:G:59:LYS:NZ	2.13	0.45
1:H:255:ILE:O	1:H:286:HIS:HE1	1.99	0.45
1:D:248:ASP:O	1:D:252:GLN:HG2	2.17	0.45
1:A:105:ARG:HG3	7:A:508:HOH:O	2.17	0.45
1:F:118:LYS:NZ	1:F:158:GLU:HB3	2.32	0.45
1:F:84:LEU:HA	7:F:503:HOH:O	2.16	0.44
1:B:248:ASP:O	1:B:252:GLN:HG2	2.18	0.44
1:C:351:ARG:NH2	1:D:88:LYS:HZ1	2.15	0.44
1:B:57:LYS:HE2	1:B:266:LYS:NZ	2.33	0.44
1:B:216:LYS:O	1:B:220:GLN:HG3	2.18	0.43
1:C:248:ASP:O	1:C:252:GLN:HG2	2.17	0.43
1:C:287:PRO:O	7:C:501:HOH:O	2.21	0.43
1:C:232:HIS:NE2	7:C:508:HOH:O	2.36	0.43
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.89	0.43
1:E:95:ALA:HB2	7:E:517:HOH:O	2.17	0.43
1:E:216:LYS:O	1:E:220:GLN:HG3	2.19	0.43
1:H:117:THR:HB	1:H:120:THR:HB	2.01	0.43
1:H:230:ILE:HB	1:H:257:LEU:HD23	2.00	0.43
1:A:143:TYR:CE2	1:A:145:ILE:HG12	2.54	0.43
1:E:313:PHE:HA	5:E:401:PEG:H32	1.99	0.43
1:C:256:PRO:HA	1:C:287:PRO:HB2	2.00	0.43
1:D:354:HIS:O	1:D:355:ILE:HB	2.19	0.43
1:E:23:LEU:HD21	1:E:331:ILE:HG22	2.01	0.43
1:H:244:LEU:O	1:H:248:ASP:HB2	2.19	0.42
1:D:216:LYS:O	1:D:220:GLN:HG3	2.19	0.42
1:G:117:THR:HG23	1:G:120:THR:H	1.84	0.42
1:A:255:ILE:O	1:A:286:HIS:HE1	2.02	0.42
1:B:166:PHE:HB3	1:B:174:VAL:HG21	2.02	0.42
1:E:255:ILE:O	1:E:286:HIS:HE1	2.02	0.42
1:C:12:THR:HG22	1:C:14:PHE:H	1.83	0.42
1:A:117:THR:HG23	1:A:120:THR:H	1.84	0.42
1:G:110:ARG:HE	1:G:118:LYS:H	1.68	0.42
1:G:248:ASP:O	1:G:252:GLN:HG2	2.18	0.42
1:C:110:ARG:HE	1:C:118:LYS:HB2	1.84	0.42
1:A:239:GLY:HA2	7:A:572:HOH:O	2.19	0.42
1:F:143:TYR:CE2	1:F:145:ILE:HG12	2.55	0.42
1:G:80:PRO:HA	1:G:116:MET:HE3	2.02	0.42
1:H:216:LYS:O	1:H:220:GLN:HG3	2.20	0.42
1:E:23:LEU:HD23	7:E:503:HOH:O	2.19	0.41
1:E:199:LYS:HE3	1:E:225:LEU:O	2.20	0.41
1:H:150:ARG:HA	1:H:185:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.93	0.41
1:F:251:ARG:HH11	1:F:284:ILE:HD12	1.84	0.41
1:C:244:LEU:O	1:C:248:ASP:HB2	2.21	0.41
1:E:143:TYR:CE2	1:E:145:ILE:HG12	2.56	0.41
1:F:148:ASP:OD1	1:F:150:ARG:HG2	2.21	0.41
1:C:216:LYS:O	1:C:220:GLN:HG3	2.20	0.41
1:C:337:THR:OG1	4:C:404:SO4:O1	2.27	0.41
1:H:80:PRO:HA	1:H:116:MET:HE1	2.02	0.41
1:C:23:LEU:HD21	1:C:331:ILE:HG22	2.02	0.41
1:A:174:VAL:HG12	7:A:561:HOH:O	2.20	0.41
1:B:110:ARG:NH1	1:B:117:THR:HB	2.36	0.41
1:G:143:TYR:CE2	1:G:145:ILE:HG12	2.56	0.41
1:H:117:THR:H	1:H:120:THR:HG22	1.84	0.41
1:F:215:GLN:CG	1:F:218:GLU:HB2	2.51	0.41
1:C:78:SER:O	1:C:111:GLU:HG2	2.21	0.41
1:E:20:LYS:HE2	1:E:20:LYS:HB2	1.93	0.41
1:D:143:TYR:CE2	1:D:145:ILE:HG12	2.56	0.41
1:A:20:LYS:HE2	1:A:20:LYS:HB2	1.95	0.40
1:B:334:SER:OG	4:B:1004:SO4:O3	2.30	0.40
1:B:143:TYR:CE2	1:B:145:ILE:HG12	2.56	0.40
1:C:143:TYR:CE2	1:C:145:ILE:HG12	2.56	0.40
1:G:166:PHE:HB3	1:G:174:VAL:HG21	2.03	0.40
1:D:216:LYS:HG3	1:D:246:LEU:HD11	2.04	0.40
1:E:295:LYS:HE3	7:E:578:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	342/355 (96%)	334 (98%)	7 (2%)	1 (0%)	41 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	342/355 (96%)	336 (98%)	5 (2%)	1 (0%)	41	49
1	C	342/355 (96%)	333 (97%)	8 (2%)	1 (0%)	41	49
1	D	344/355 (97%)	337 (98%)	6 (2%)	1 (0%)	41	49
1	E	342/355 (96%)	337 (98%)	4 (1%)	1 (0%)	41	49
1	F	342/355 (96%)	337 (98%)	4 (1%)	1 (0%)	41	49
1	G	347/355 (98%)	339 (98%)	7 (2%)	1 (0%)	41	49
1	H	348/355 (98%)	338 (97%)	8 (2%)	2 (1%)	25	29
All	All	2749/2840 (97%)	2691 (98%)	49 (2%)	9 (0%)	41	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	171	GLU
1	A	232	HIS
1	B	232	HIS
1	C	232	HIS
1	E	232	HIS
1	F	232	HIS
1	H	232	HIS
1	D	232	HIS
1	G	9	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/319 (97%)	299 (97%)	10 (3%)	39	50
1	B	308/319 (97%)	304 (99%)	4 (1%)	69	80
1	C	309/319 (97%)	298 (96%)	11 (4%)	35	46
1	D	311/319 (98%)	302 (97%)	9 (3%)	42	54
1	E	309/319 (97%)	303 (98%)	6 (2%)	57	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	309/319 (97%)	297 (96%)	12 (4%)	32 42
1	G	314/319 (98%)	301 (96%)	13 (4%)	30 40
1	H	315/319 (99%)	300 (95%)	15 (5%)	25 34
All	All	2484/2552 (97%)	2404 (97%)	80 (3%)	39 50

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	59	LYS
1	A	110	ARG
1	A	117	THR
1	A	210	SER
1	A	218	GLU
1	A	220	GLN
1	A	248	ASP
1	A	270	VAL
1	A	300	THR
1	B	210	SER
1	B	218	GLU
1	B	248	ASP
1	B	270	VAL
1	C	13	ASP
1	C	47	LYS
1	C	51	GLN
1	C	105	ARG
1	C	110	ARG
1	C	114	THR
1	C	177	LEU
1	C	210	SER
1	C	218	GLU
1	C	270	VAL
1	C	340	GLU
1	D	11	LYS
1	D	13	ASP
1	D	51	GLN
1	D	117	THR
1	D	134	GLN
1	D	137	LEU
1	D	210	SER
1	D	218	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	270	VAL
1	E	13	ASP
1	E	177	LEU
1	E	210	SER
1	E	248	ASP
1	E	270	VAL
1	E	340	GLU
1	F	51	GLN
1	F	110	ARG
1	F	120	THR
1	F	135	GLU
1	F	150	ARG
1	F	177	LEU
1	F	179	LEU
1	F	209	LEU
1	F	210	SER
1	F	220	GLN
1	F	248	ASP
1	F	270	VAL
1	G	11	LYS
1	G	13	ASP
1	G	61	ARG
1	G	110	ARG
1	G	150	ARG
1	G	161	LYS
1	G	177	LEU
1	G	184	THR
1	G	187	GLN
1	G	196	LEU
1	G	210	SER
1	G	218	GLU
1	G	248	ASP
1	H	50	ASP
1	H	51	GLN
1	H	61	ARG
1	H	120	THR
1	H	135	GLU
1	H	177	LEU
1	H	192	LEU
1	H	193	GLU
1	H	197	GLU
1	H	210	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	217	LYS
1	H	270	VAL
1	H	295	LYS
1	H	348	LEU
1	H	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	286	HIS
1	A	346	ASN
1	B	264	ASN
1	B	286	HIS
1	B	307	GLN
1	B	346	ASN
1	C	214	ASN
1	C	264	ASN
1	C	286	HIS
1	C	346	ASN
1	C	347	HIS
1	D	134	GLN
1	D	264	ASN
1	D	286	HIS
1	D	346	ASN
1	E	51	GLN
1	E	264	ASN
1	E	286	HIS
1	E	346	ASN
1	F	264	ASN
1	F	286	HIS
1	F	346	ASN
1	G	220	GLN
1	G	264	ASN
1	G	286	HIS
1	G	346	ASN
1	H	237	ASN
1	H	264	ASN
1	H	286	HIS
1	H	346	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 9 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
4	SO4	F	405	-	4,4,4	0.19	0	6,6,6	0.19	0
4	SO4	B	1004	-	4,4,4	0.20	0	6,6,6	0.22	0
2	EIF	B	1001	-	20,27,27	0.84	0	21,43,43	0.54	0
4	SO4	A	405	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	F	404	-	4,4,4	0.18	0	6,6,6	0.24	0
4	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.83	0
4	SO4	F	403	-	4,4,4	0.16	0	6,6,6	0.73	0
4	SO4	D	406	-	4,4,4	0.23	0	6,6,6	0.42	0
2	EIF	E	402	-	20,27,27	0.79	1 (5%)	21,43,43	0.74	0
2	EIF	D	403	-	20,27,27	0.86	2 (10%)	21,43,43	0.96	1 (4%)
2	EIF	G	402	-	20,27,27	0.79	2 (10%)	21,43,43	0.73	0
4	SO4	C	403	-	4,4,4	0.18	0	6,6,6	0.41	0
2	EIF	F	401	-	20,27,27	0.85	0	21,43,43	0.71	0
4	SO4	E	405	-	4,4,4	0.20	0	6,6,6	0.47	0
5	PEG	D	402	-	6,6,6	0.16	0	5,5,5	0.11	0
2	EIF	C	401	-	20,27,27	0.70	0	21,43,43	0.85	1 (4%)
4	SO4	E	404	-	4,4,4	0.20	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	F	406	-	4,4,4	0.21	0	6,6,6	0.43	0
5	PEG	E	401	-	6,6,6	0.19	0	5,5,5	0.08	0
4	SO4	D	405	-	4,4,4	0.19	0	6,6,6	0.70	0
2	EIF	A	401	-	20,27,27	0.88	1 (5%)	21,43,43	0.65	0
4	SO4	B	1003	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	G	404	-	4,4,4	0.16	0	6,6,6	0.80	0
5	PEG	G	401	-	6,6,6	0.14	0	5,5,5	0.16	0
2	EIF	H	401	-	20,27,27	0.81	0	21,43,43	0.81	1 (4%)
4	SO4	H	403	-	4,4,4	0.15	0	6,6,6	0.27	0
4	SO4	A	404	-	4,4,4	0.25	0	6,6,6	0.26	0
5	PEG	D	401	-	6,6,6	0.15	0	5,5,5	0.21	0
4	SO4	A	403	-	4,4,4	0.19	0	6,6,6	0.23	0

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
5	PEG	G	401	-	-	3/4/4/4	-
2	EIF	B	1001	-	-	3/6/30/30	0/3/3/3
2	EIF	H	401	-	-	4/6/30/30	0/3/3/3
2	EIF	F	401	-	-	4/6/30/30	0/3/3/3
5	PEG	D	402	-	-	2/4/4/4	-
2	EIF	C	401	-	-	4/6/30/30	0/3/3/3
2	EIF	A	401	-	-	3/6/30/30	0/3/3/3
5	PEG	E	401	-	-	3/4/4/4	-
2	EIF	E	402	-	-	3/6/30/30	0/3/3/3
2	EIF	D	403	-	-	4/6/30/30	0/3/3/3
2	EIF	G	402	-	-	4/6/30/30	0/3/3/3
5	PEG	D	401	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	EIF	C7-C10	-2.16	1.43	1.47
2	D	403	EIF	C6-N1	-2.10	1.31	1.35
2	G	402	EIF	C7-C8	-2.08	1.37	1.43
2	D	403	EIF	C7-C8	-2.06	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	402	EIF	C7-C10	-2.05	1.43	1.47
2	G	402	EIF	C6-N1	-2.04	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	403	EIF	P-O1-C4	3.24	127.22	118.30
2	C	401	EIF	P-O1-C4	2.68	125.67	118.30
2	H	401	EIF	P-O1-C4	2.54	125.29	118.30

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EIF	C4-O1-P-O3
2	A	401	EIF	C4-O1-P-O2
2	B	1001	EIF	C4-O1-P-O4
2	B	1001	EIF	C4-O1-P-O2
2	C	401	EIF	C3-C4-O1-P
2	D	403	EIF	C3-C4-O1-P
2	D	403	EIF	C4-O1-P-O3
2	D	403	EIF	C4-O1-P-O2
2	E	402	EIF	C3-C4-O1-P
2	F	401	EIF	C3-C4-O1-P
2	F	401	EIF	C4-O1-P-O3
2	F	401	EIF	C4-O1-P-O2
2	G	402	EIF	C4-O1-P-O4
2	G	402	EIF	C4-O1-P-O2
2	H	401	EIF	C3-C4-O1-P
2	A	401	EIF	C3-C4-O1-P
5	D	402	PEG	O2-C3-C4-O4
5	G	401	PEG	O1-C1-C2-O2
5	G	401	PEG	O2-C3-C4-O4
2	G	402	EIF	C3-C4-O1-P
5	D	402	PEG	O1-C1-C2-O2
5	E	401	PEG	O1-C1-C2-O2
2	B	1001	EIF	C3-C4-O1-P
5	E	401	PEG	O2-C3-C4-O4
2	C	401	EIF	C4-O1-P-O4
2	E	402	EIF	C4-O1-P-O2
2	H	401	EIF	C4-O1-P-O4
2	H	401	EIF	C4-O1-P-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	401	PEG	C1-C2-O2-C3
5	D	401	PEG	C1-C2-O2-C3
2	C	401	EIF	C4-O1-P-O3
2	E	402	EIF	C4-O1-P-O3
2	G	402	EIF	C4-O1-P-O3
2	H	401	EIF	C4-O1-P-O3
5	D	401	PEG	O1-C1-C2-O2
5	G	401	PEG	C4-C3-O2-C2
2	C	401	EIF	C4-O1-P-O2
2	D	403	EIF	C4-O1-P-O4
2	F	401	EIF	C4-O1-P-O4

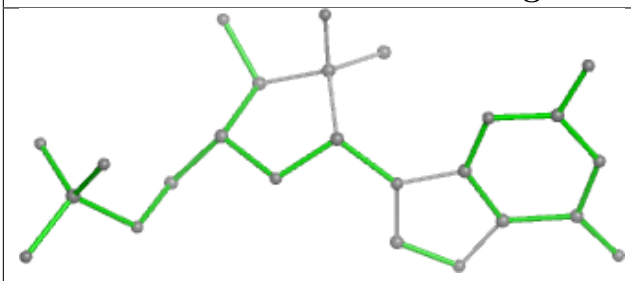
There are no ring outliers.

8 monomers are involved in 10 short contacts:

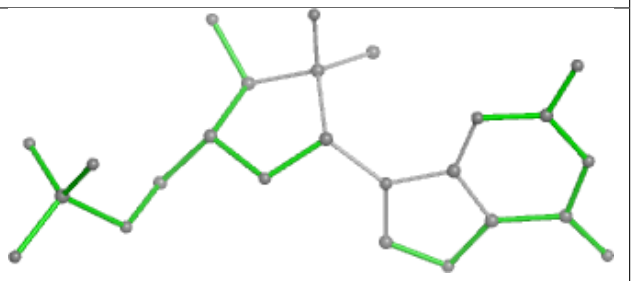
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	SO4	1	0
4	A	405	SO4	1	0
4	C	404	SO4	1	0
2	G	402	EIF	1	0
4	E	405	SO4	1	0
5	E	401	PEG	1	0
2	H	401	EIF	1	0
5	D	401	PEG	3	0

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 then 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.

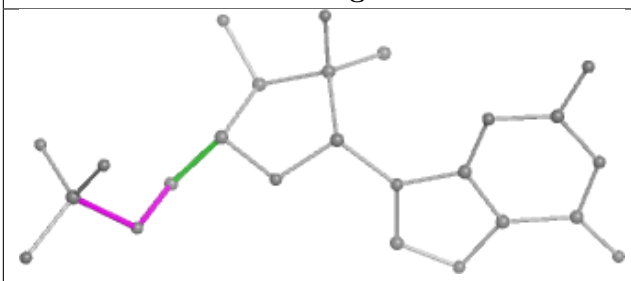
Ligand EIF B 1001



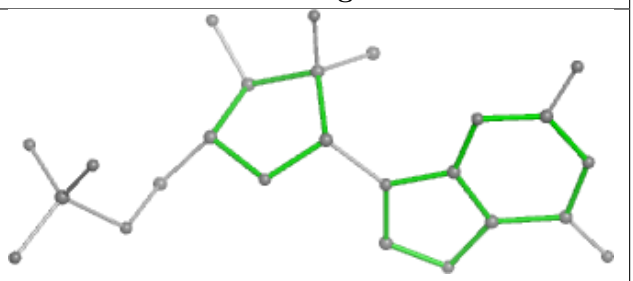
Bond lengths



Bond angles

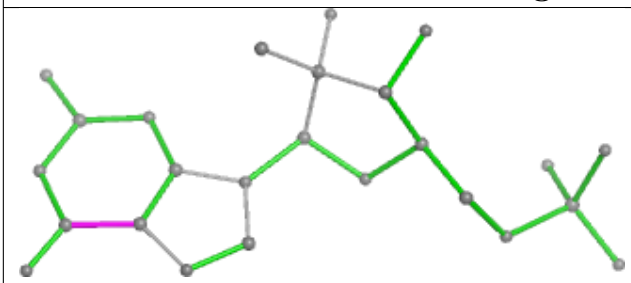


Torsions

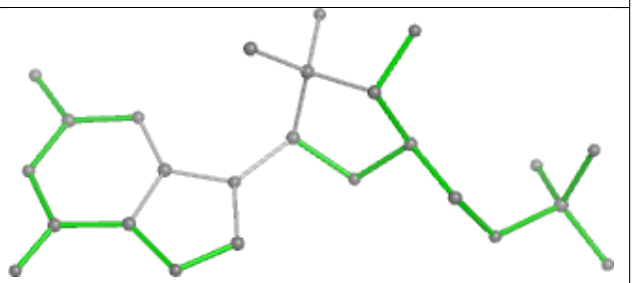


Rings

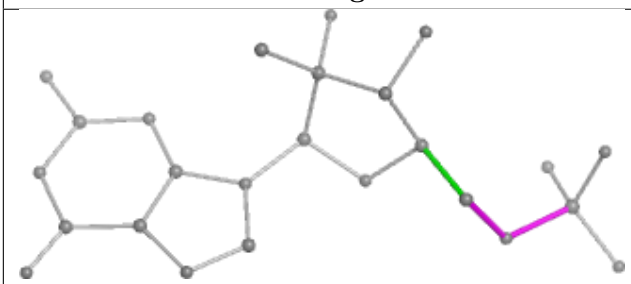
Ligand EIF E 402



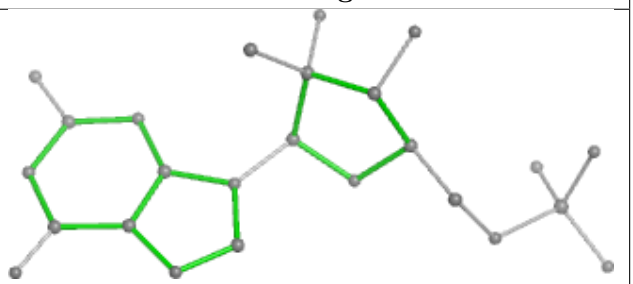
Bond lengths



Bond angles

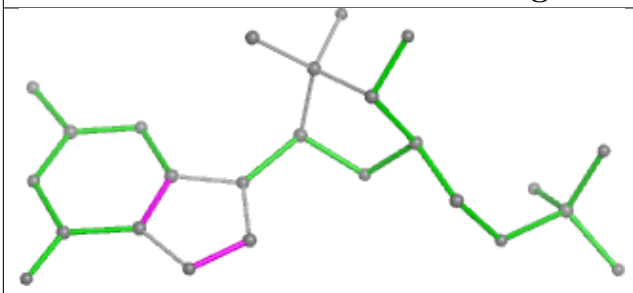


Torsions

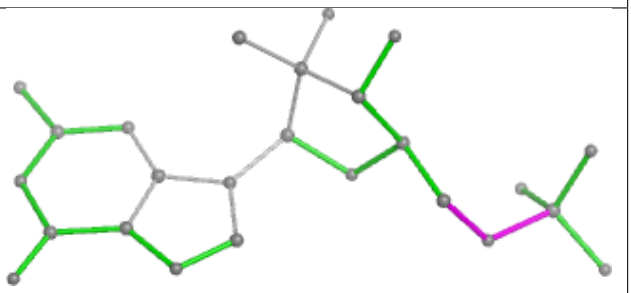


Rings

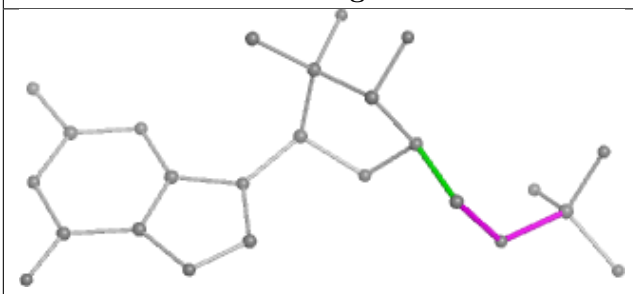
Ligand EIF D 403



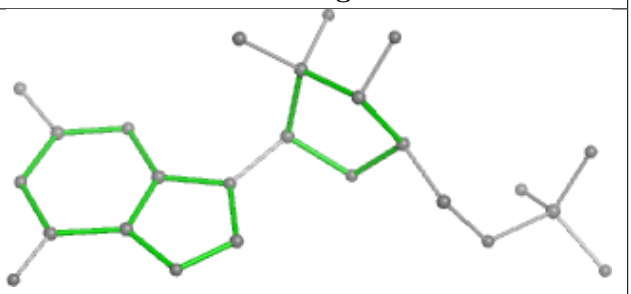
Bond lengths



Bond angles

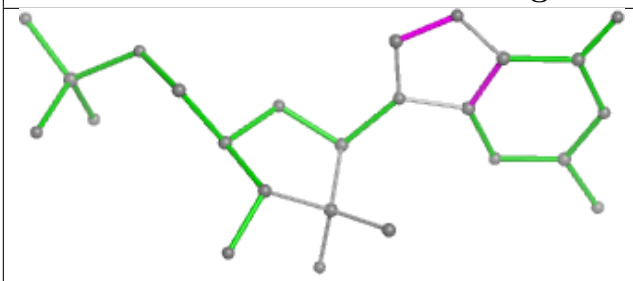


Torsions

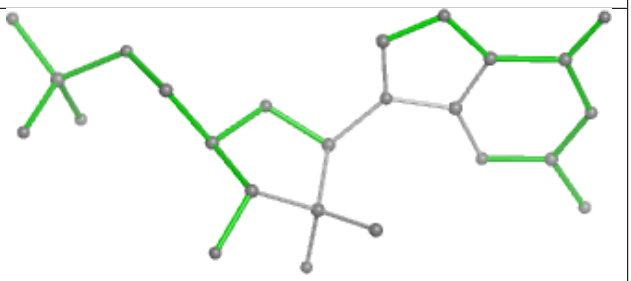


Rings

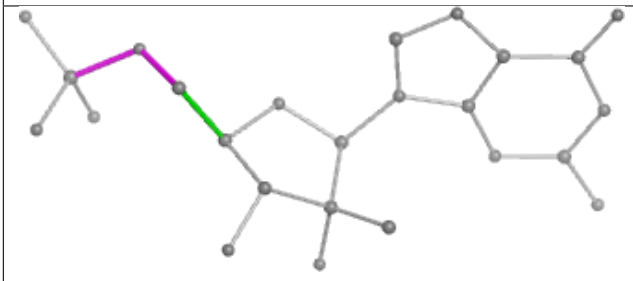
Ligand EIF G 402



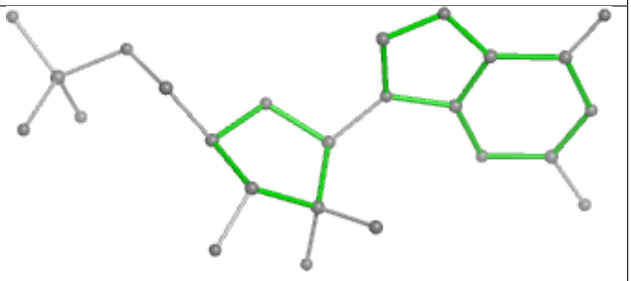
Bond lengths



Bond angles

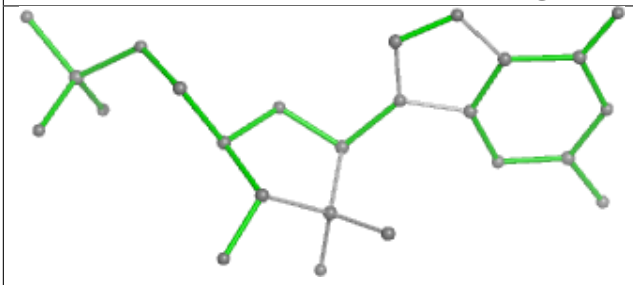


Torsions

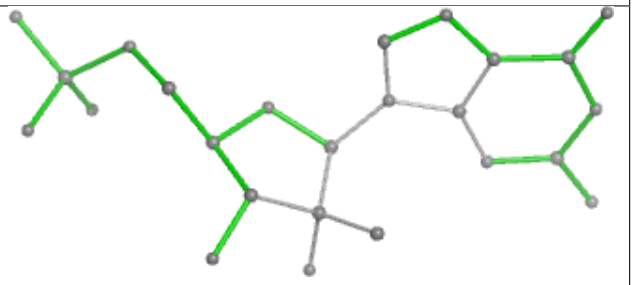


Rings

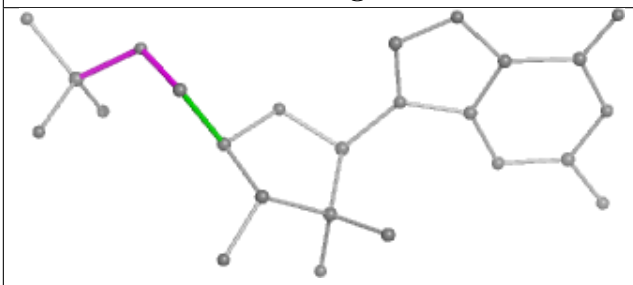
Ligand EIF F 401



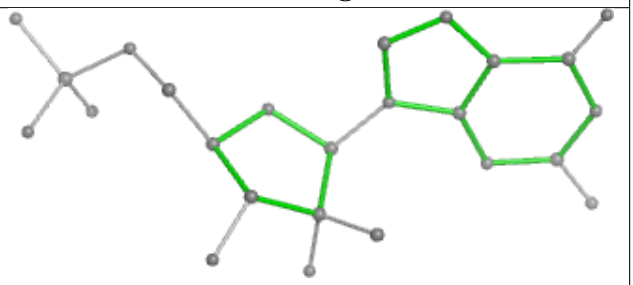
Bond lengths



Bond angles

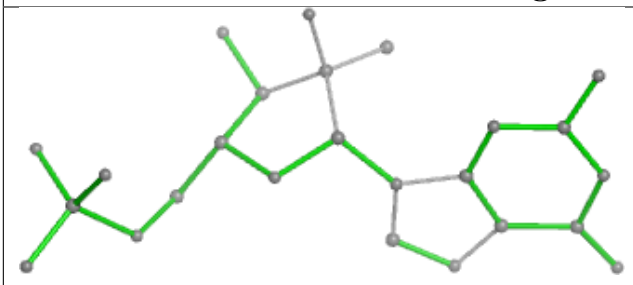


Torsions

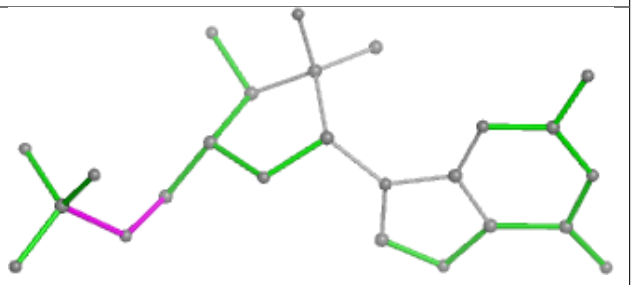


Rings

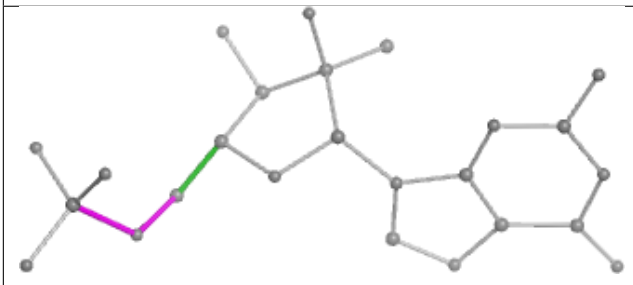
Ligand EIF C 401



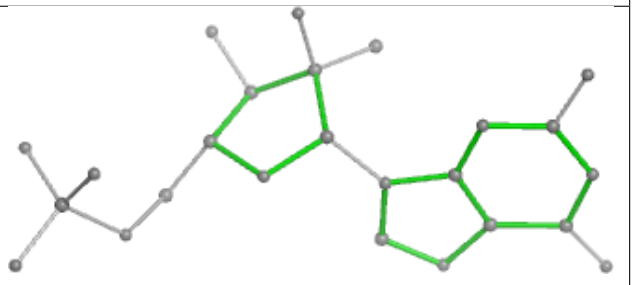
Bond lengths



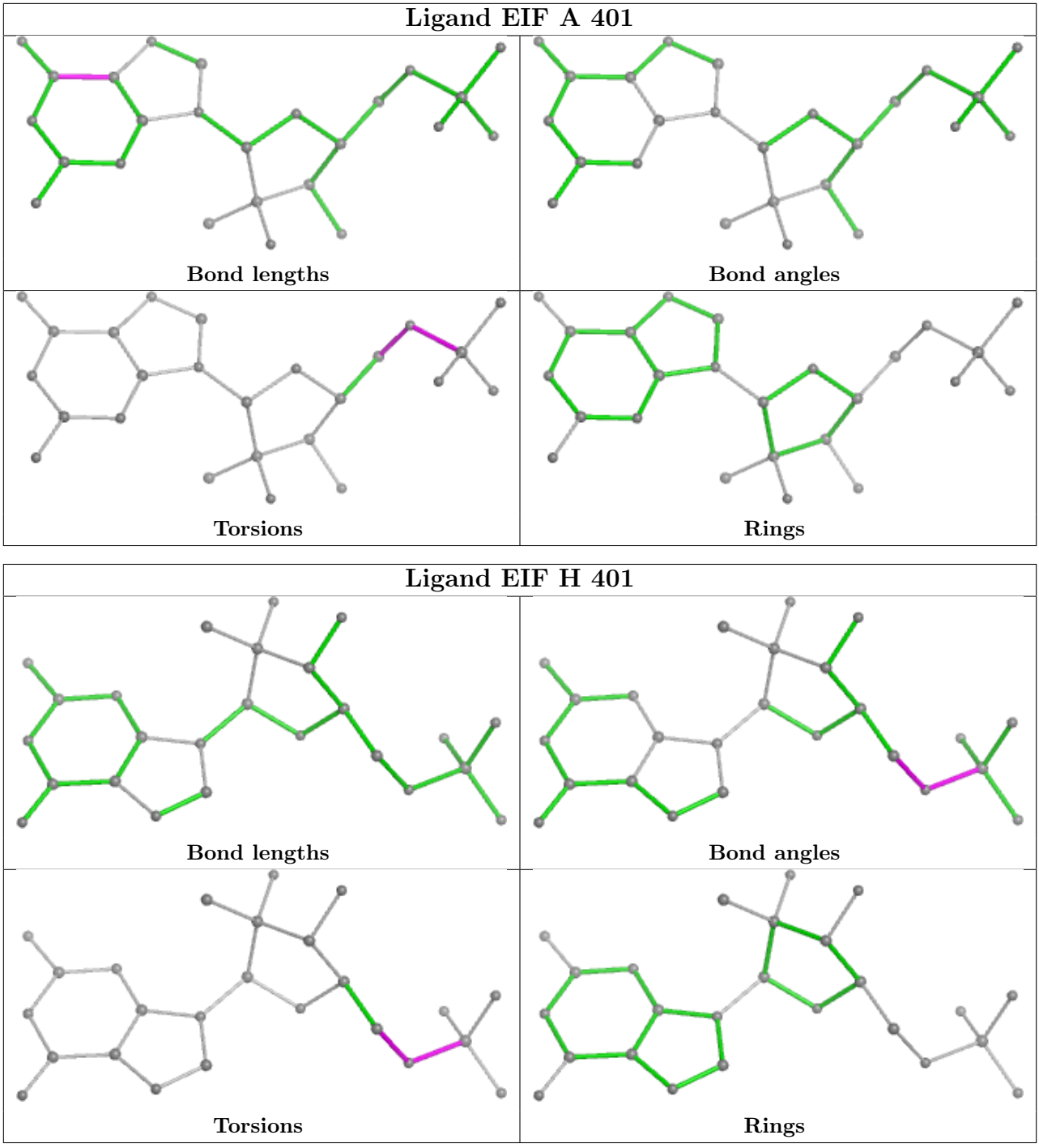
Bond angles



Torsions



Rings



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, 95^{th} 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	344/355 (96%)	0.05	8 (2%)	60	56	32, 45, 68, 87	0
1	B	344/355 (96%)	0.11	9 (2%)	56	52	32, 49, 73, 87	0
1	C	344/355 (96%)	-0.00	8 (2%)	60	56	26, 47, 66, 88	0
1	D	346/355 (97%)	0.01	5 (1%)	75	73	29, 47, 69, 88	0
1	E	344/355 (96%)	0.07	10 (2%)	51	47	30, 45, 67, 100	0
1	F	344/355 (96%)	0.05	5 (1%)	73	71	29, 47, 69, 96	0
1	G	349/355 (98%)	0.17	10 (2%)	51	47	30, 51, 74, 107	0
1	H	350/355 (98%)	0.23	14 (4%)	38	35	32, 54, 77, 111	0
All	All	2765/2840 (97%)	0.08	69 (2%)	57	53	26, 48, 73, 111	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	7	GLN	7.7
1	H	12	THR	7.3
1	G	10	CYS	6.9
1	E	46	LEU	6.2
1	H	10	CYS	6.1
1	H	9	PRO	5.9
1	G	12	THR	5.4
1	F	241	GLY	5.1
1	G	7	GLN	5.0
1	E	48	ILE	4.6
1	G	240	GLU	4.5
1	D	10	CYS	4.4
1	B	12	THR	4.4
1	D	12	THR	4.4
1	A	12	THR	4.4
1	B	242	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	136	ASN	4.1
1	H	241	GLY	3.9
1	E	12	THR	3.8
1	F	48	ILE	3.7
1	E	242	GLY	3.7
1	E	50	ASP	3.7
1	G	242	GLY	3.6
1	H	8	GLN	3.6
1	H	6	GLU	3.5
1	F	240	GLU	3.4
1	E	45	ASP	3.4
1	C	240	GLU	3.4
1	F	242	GLY	3.4
1	G	355	ILE	3.3
1	C	12	THR	3.2
1	A	241	GLY	3.2
1	D	46	LEU	3.1
1	F	12	THR	3.0
1	E	241	GLY	3.0
1	B	50	ASP	2.9
1	G	50	ASP	2.9
1	C	48	ILE	2.8
1	A	240	GLU	2.8
1	E	243	SER	2.7
1	C	239	GLY	2.7
1	E	240	GLU	2.7
1	H	78	SER	2.6
1	E	49	HIS	2.6
1	B	49	HIS	2.6
1	B	75	GLN	2.6
1	B	241	GLY	2.6
1	H	240	GLU	2.5
1	C	243	SER	2.5
1	G	185	VAL	2.5
1	A	70	PHE	2.5
1	A	154	LEU	2.4
1	A	48	ILE	2.4
1	H	48	ILE	2.4
1	H	11	LYS	2.4
1	C	154	LEU	2.4
1	H	161	LYS	2.4
1	H	136	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	242	GLY	2.3
1	D	42	GLN	2.3
1	G	56	ASP	2.2
1	C	42	GLN	2.2
1	G	45	ASP	2.1
1	C	45	ASP	2.1
1	B	46	LEU	2.1
1	A	245	ASP	2.0
1	B	240	GLU	2.0
1	D	11	LYS	2.0
1	A	243	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	SO4	A	403	5/5	0.87	0.12	109,109,109,109	0
5	PEG	D	401	7/7	0.87	0.22	50,52,55,55	0
4	SO4	F	405	5/5	0.89	0.16	123,123,123,123	0
4	SO4	D	406	5/5	0.90	0.19	92,92,92,92	0
6	NA	H	404	1/1	0.90	0.29	54,54,54,54	0
5	PEG	G	401	7/7	0.92	0.16	44,44,45,45	0
4	SO4	B	1003	5/5	0.92	0.17	78,78,78,78	0
4	SO4	A	404	5/5	0.93	0.20	76,76,76,76	0
4	SO4	H	403	5/5	0.94	0.16	77,78,78,78	0
4	SO4	E	404	5/5	0.94	0.16	80,80,80,80	0
5	PEG	D	402	7/7	0.94	0.13	45,45,46,46	0
2	EIF	C	401	25/25	0.94	0.17	44,51,52,53	0

Continued on next page...

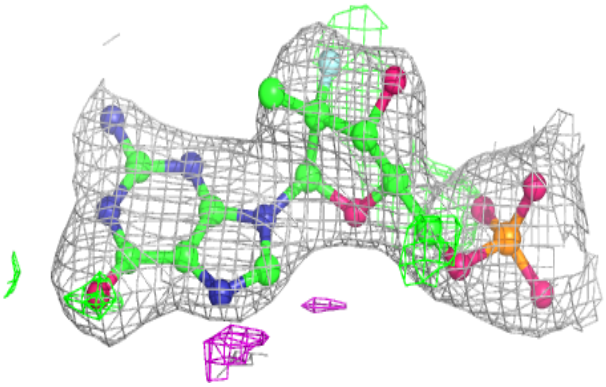
Continued from previous page...

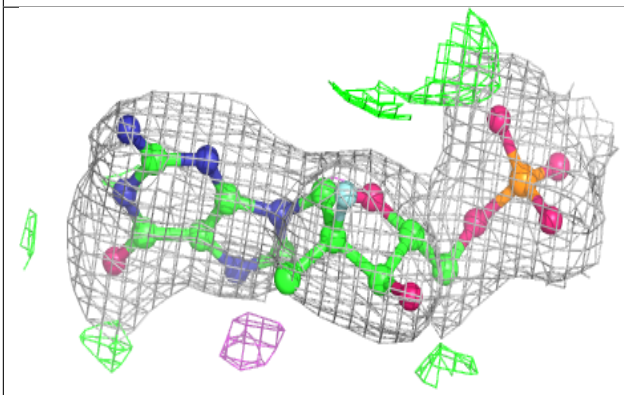
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	406	5/5	0.94	0.15	73,73,73,73	0
4	SO4	F	403	5/5	0.95	0.18	73,74,74,74	0
2	EIF	F	401	25/25	0.96	0.17	45,48,51,51	0
4	SO4	C	403	5/5	0.96	0.19	94,94,94,94	0
2	EIF	H	401	25/25	0.96	0.16	53,57,58,59	0
2	EIF	A	401	25/25	0.96	0.18	48,54,55,55	0
5	PEG	E	401	7/7	0.96	0.15	46,46,48,48	0
2	EIF	E	402	25/25	0.96	0.16	42,45,47,48	0
4	SO4	A	405	5/5	0.96	0.16	63,63,64,64	0
4	SO4	D	405	5/5	0.97	0.17	69,69,69,70	0
4	SO4	G	404	5/5	0.97	0.15	69,70,70,70	0
3	ZN	B	1002	1/1	0.97	0.08	56,56,56,56	0
2	EIF	D	403	25/25	0.97	0.17	44,47,48,50	0
4	SO4	E	405	5/5	0.97	0.14	72,72,72,72	0
2	EIF	B	1001	25/25	0.97	0.15	54,55,57,58	0
4	SO4	F	404	5/5	0.97	0.16	72,72,72,72	0
4	SO4	C	404	5/5	0.97	0.17	68,68,68,68	0
4	SO4	B	1004	5/5	0.98	0.17	69,69,69,69	0
2	EIF	G	402	25/25	0.98	0.16	48,52,53,54	0
3	ZN	H	402	1/1	0.98	0.08	59,59,59,59	0
3	ZN	F	402	1/1	0.99	0.07	53,53,53,53	0
3	ZN	G	403	1/1	0.99	0.09	53,53,53,53	0
3	ZN	A	402	1/1	0.99	0.08	51,51,51,51	0
3	ZN	C	402	1/1	0.99	0.07	53,53,53,53	0
3	ZN	E	403	1/1	0.99	0.09	50,50,50,50	0
3	ZN	D	404	1/1	1.00	0.08	50,50,50,50	0

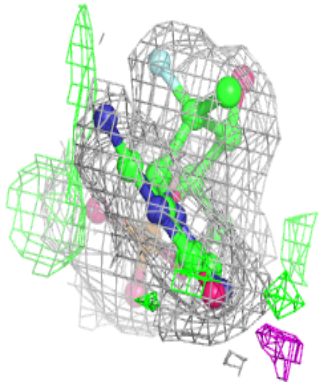
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EIF C 401:

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

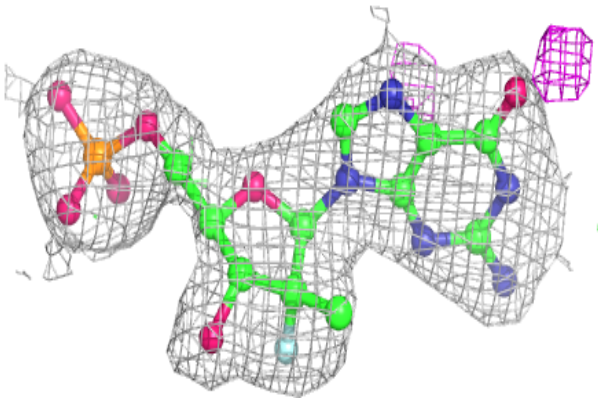


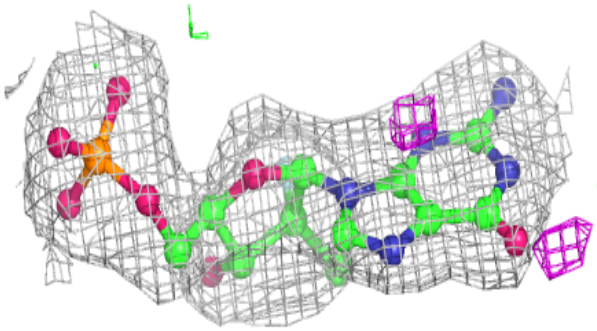


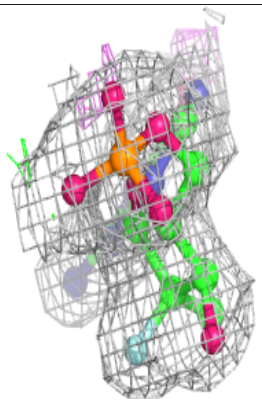


Electron density around EIF F 401:

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

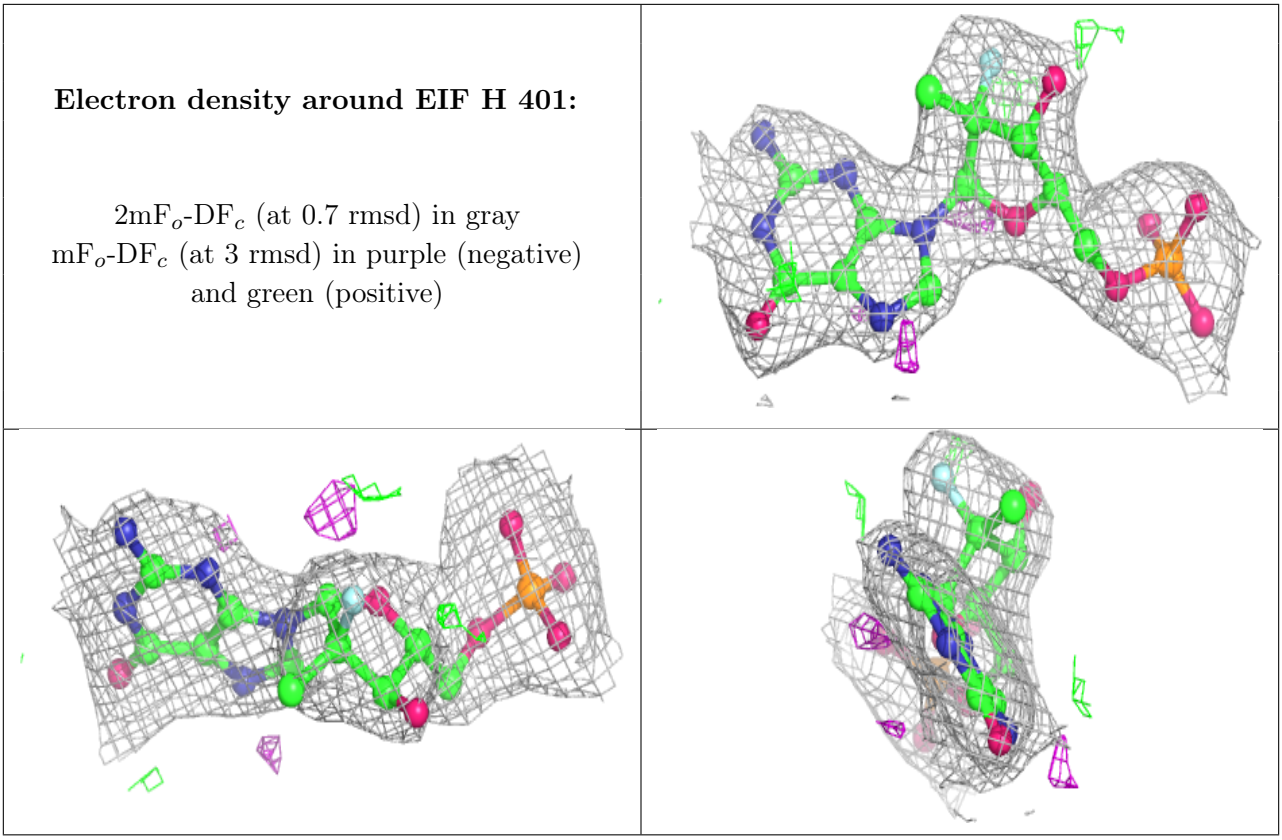






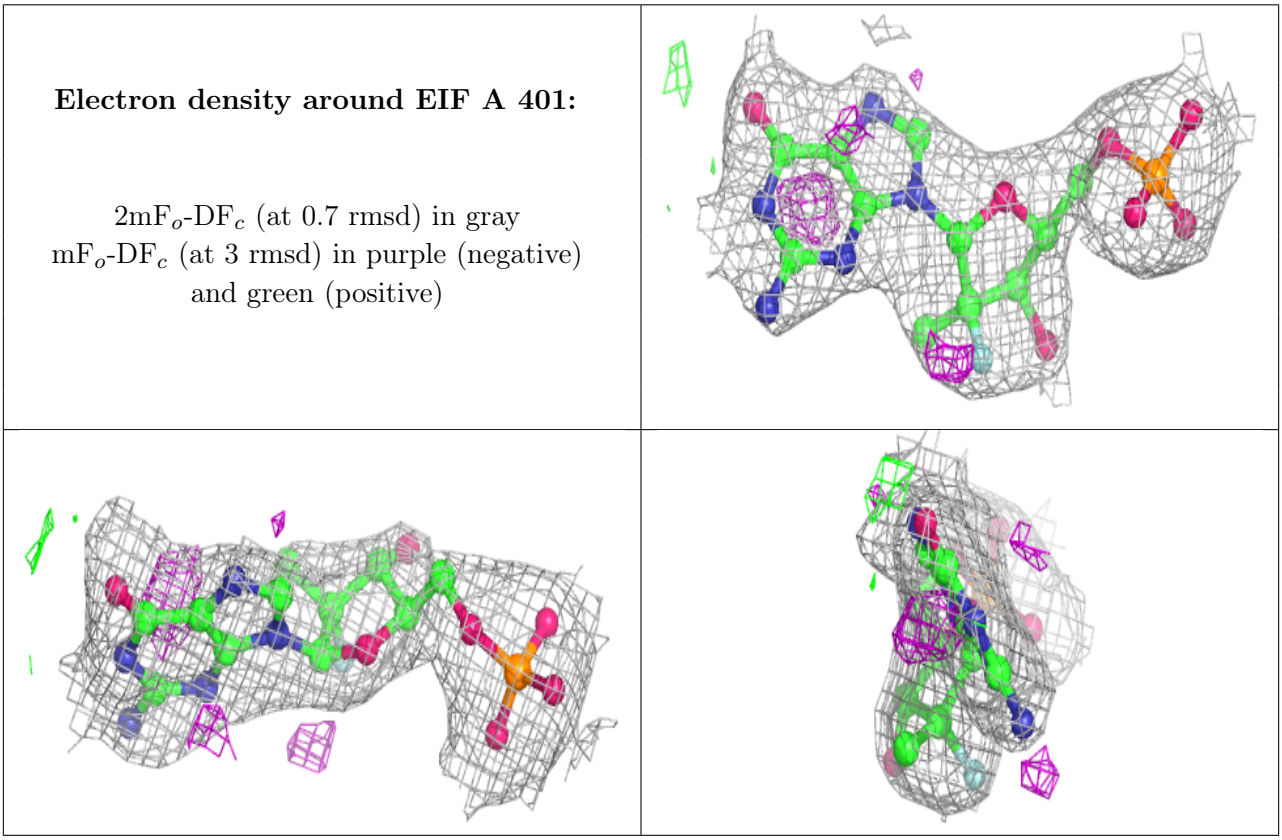
Electron density around EIF H 401:

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



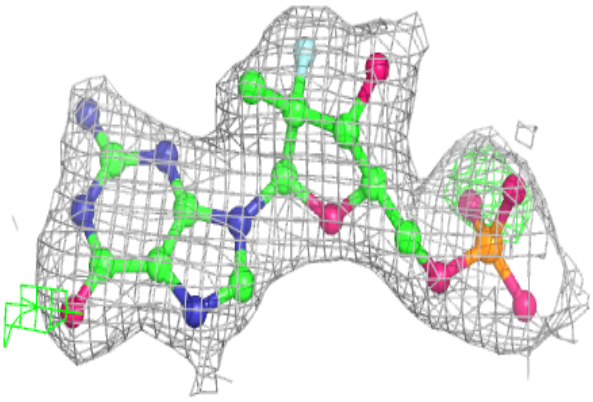
Electron density around EIF A 401:

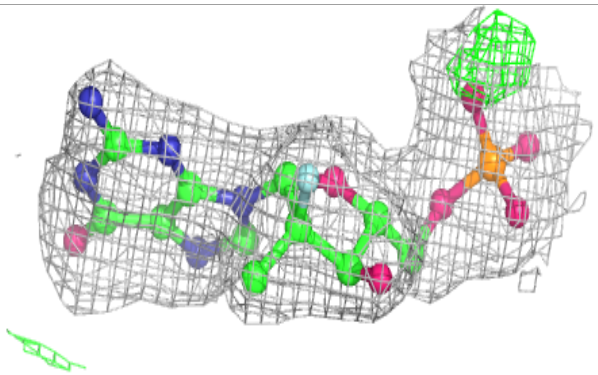
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

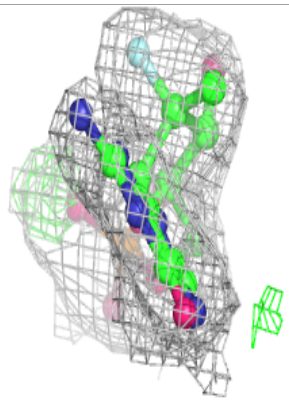


Electron density around EIF E 402:

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

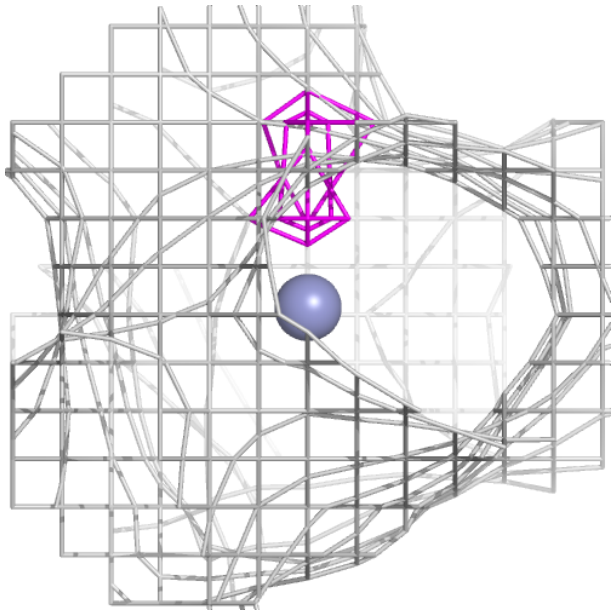


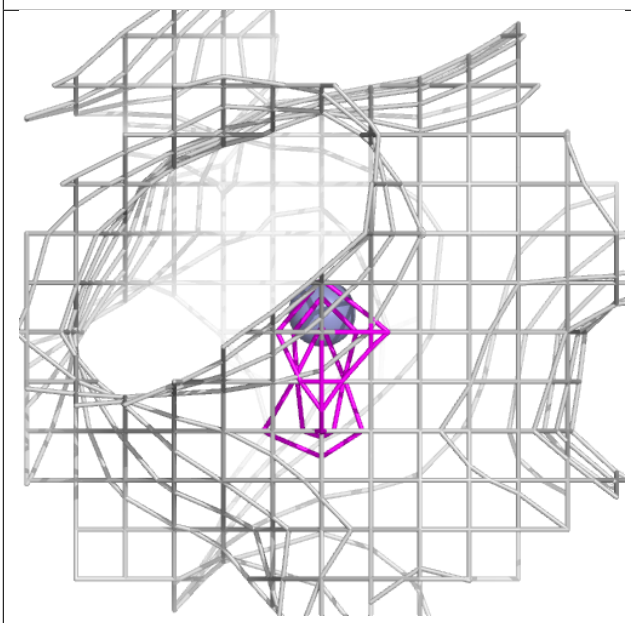


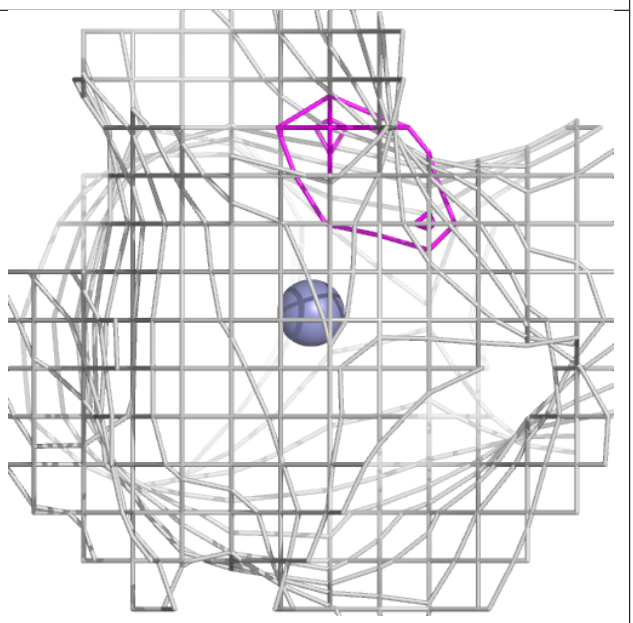


Electron density around ZN B 1002:

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

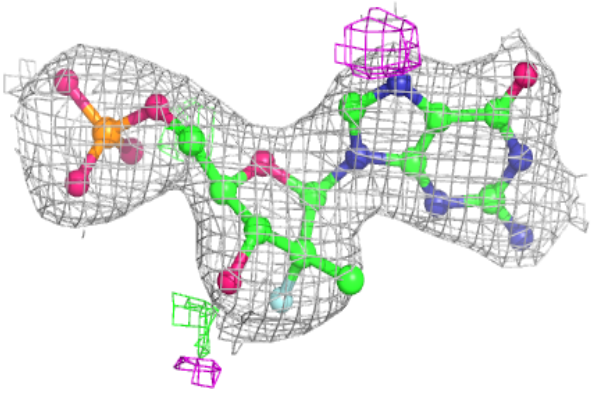


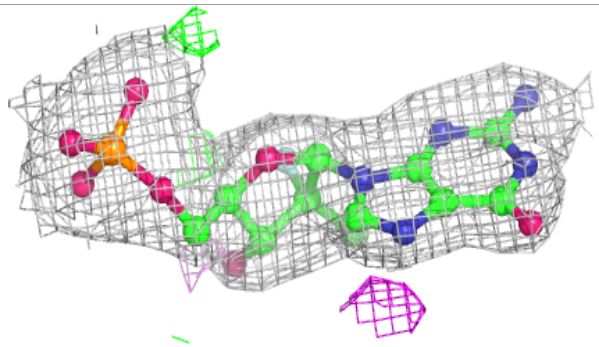


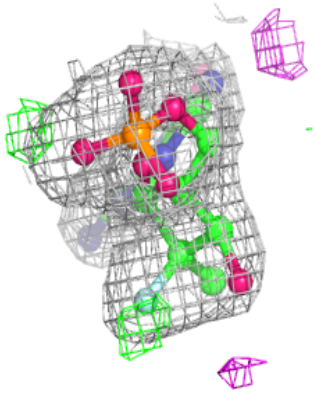


Electron density around EIF D 403:

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

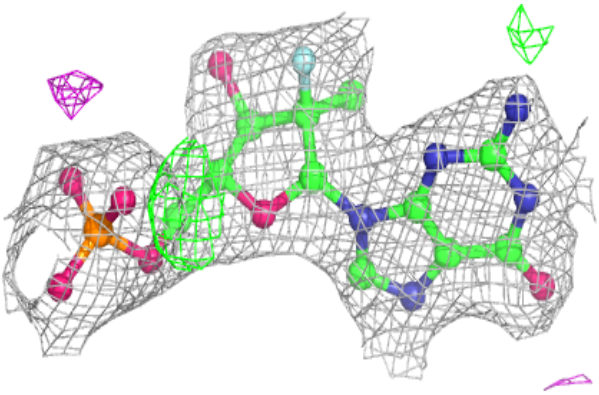


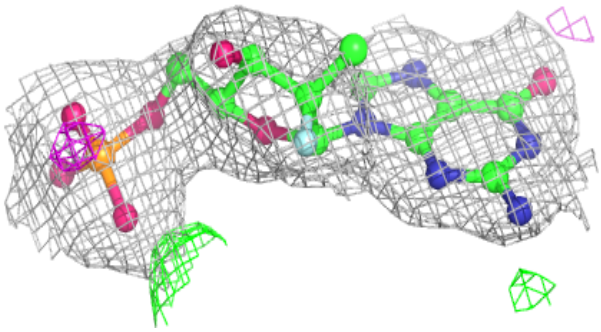


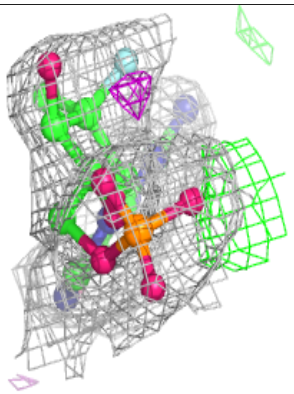


Electron density around EIF B 1001:

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

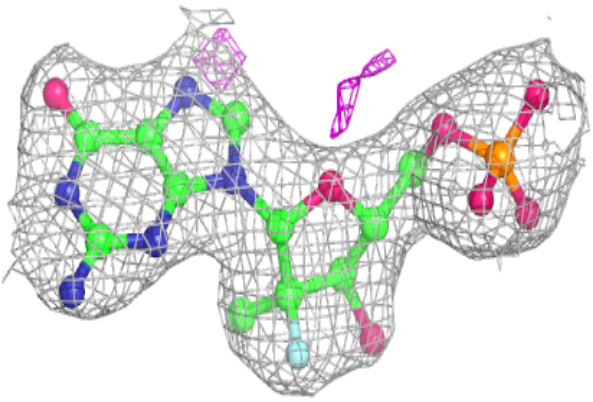


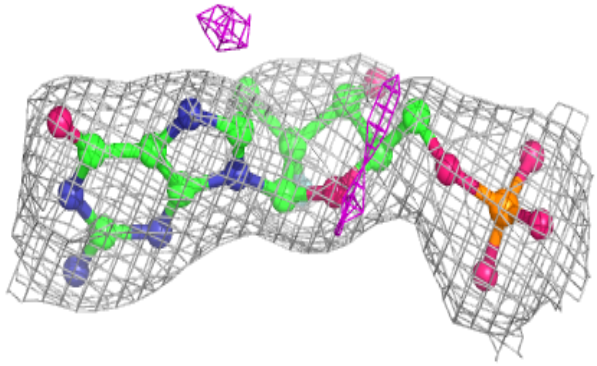


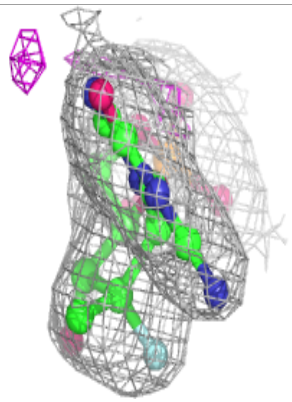


Electron density around EIF G 402:

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

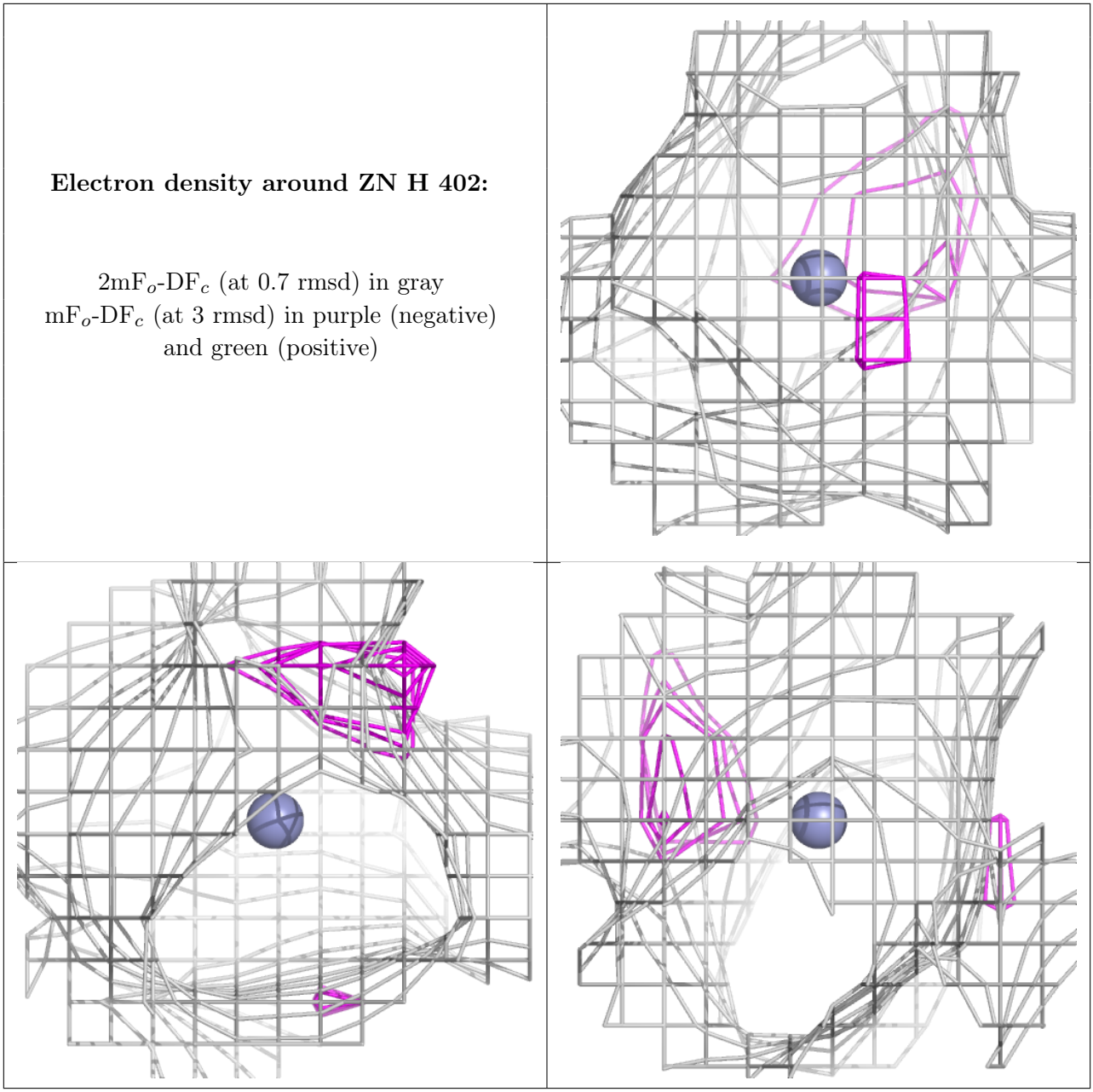






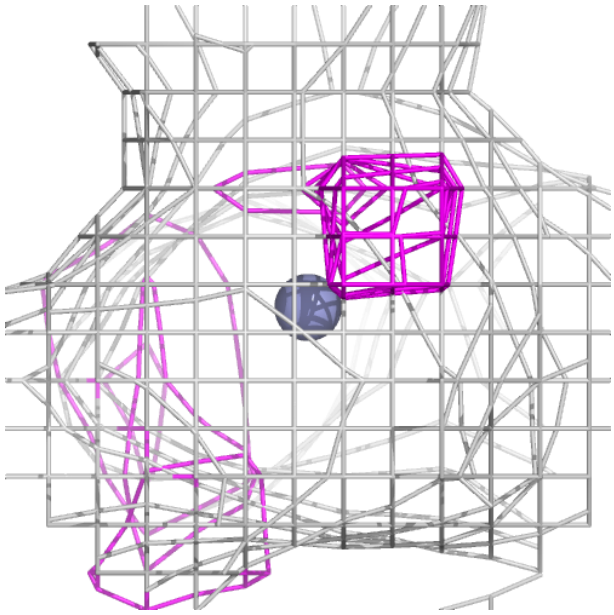
Electron density around ZN H 402:

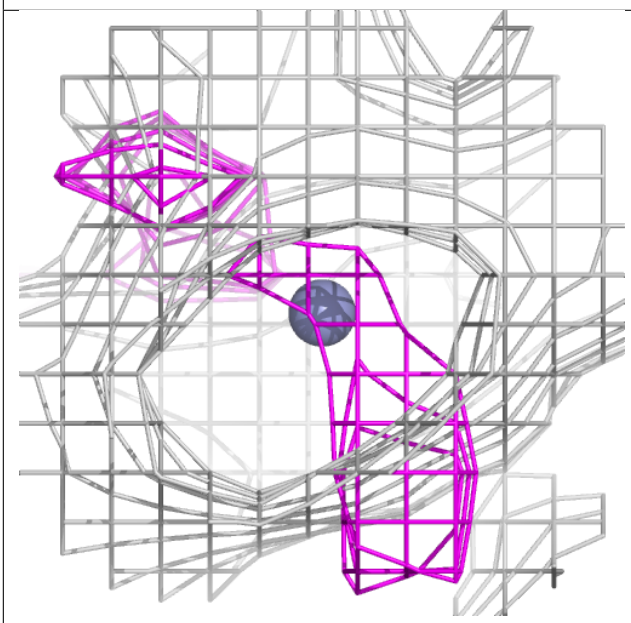
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

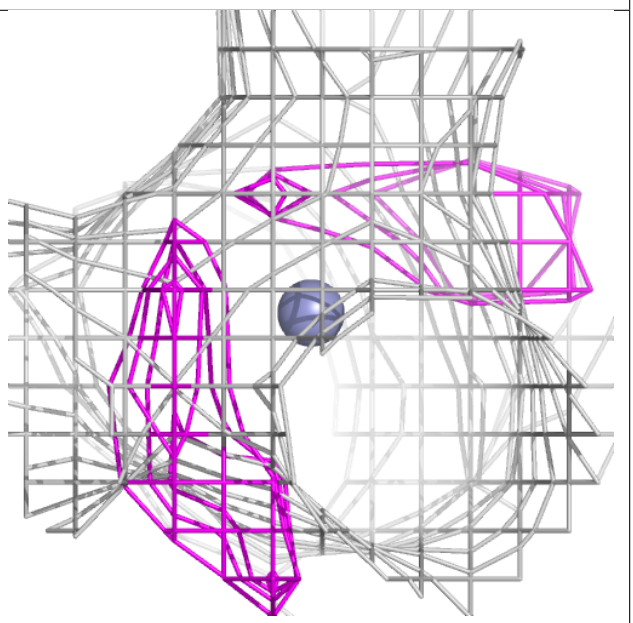


Electron density around ZN F 402:

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

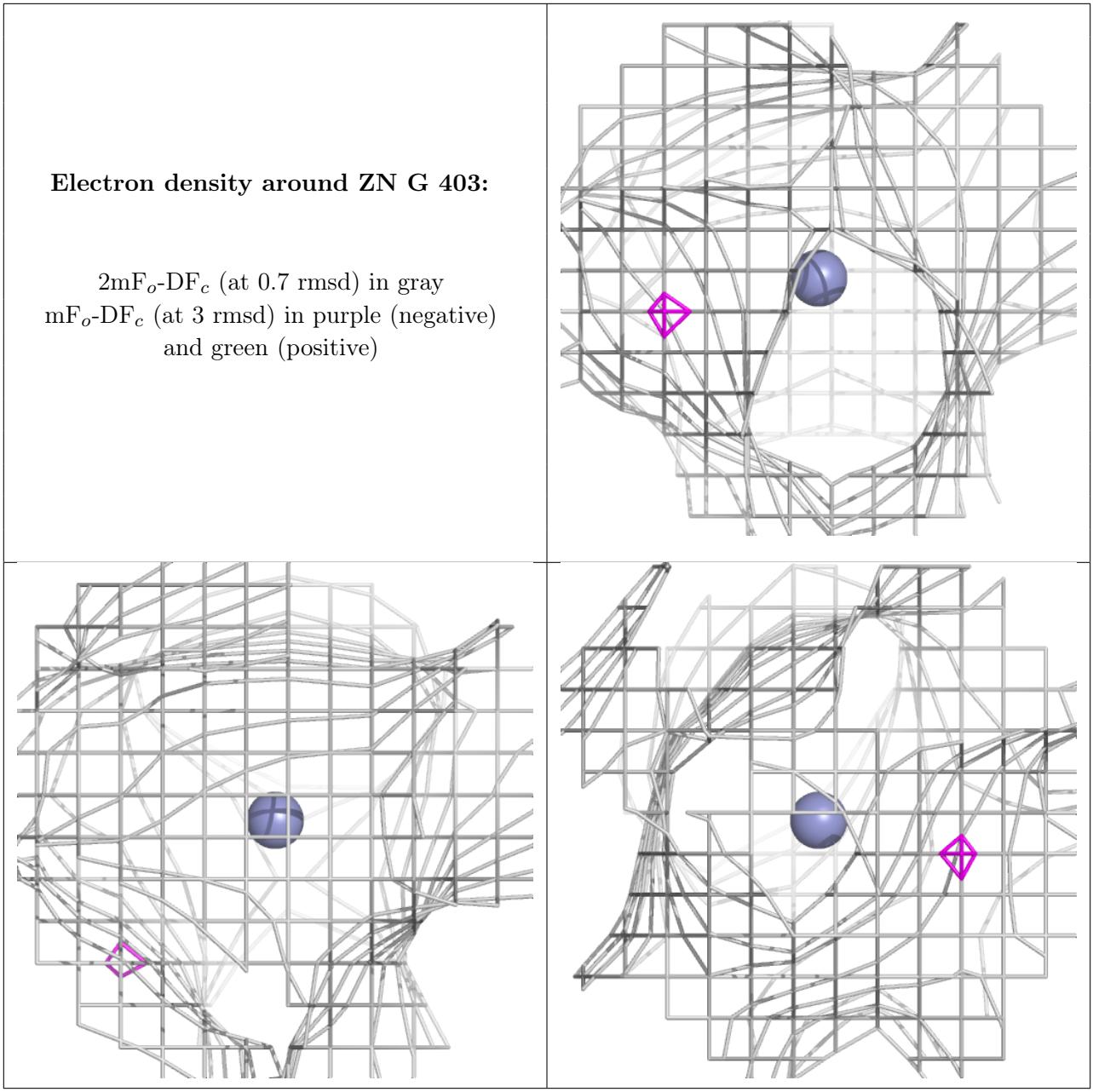






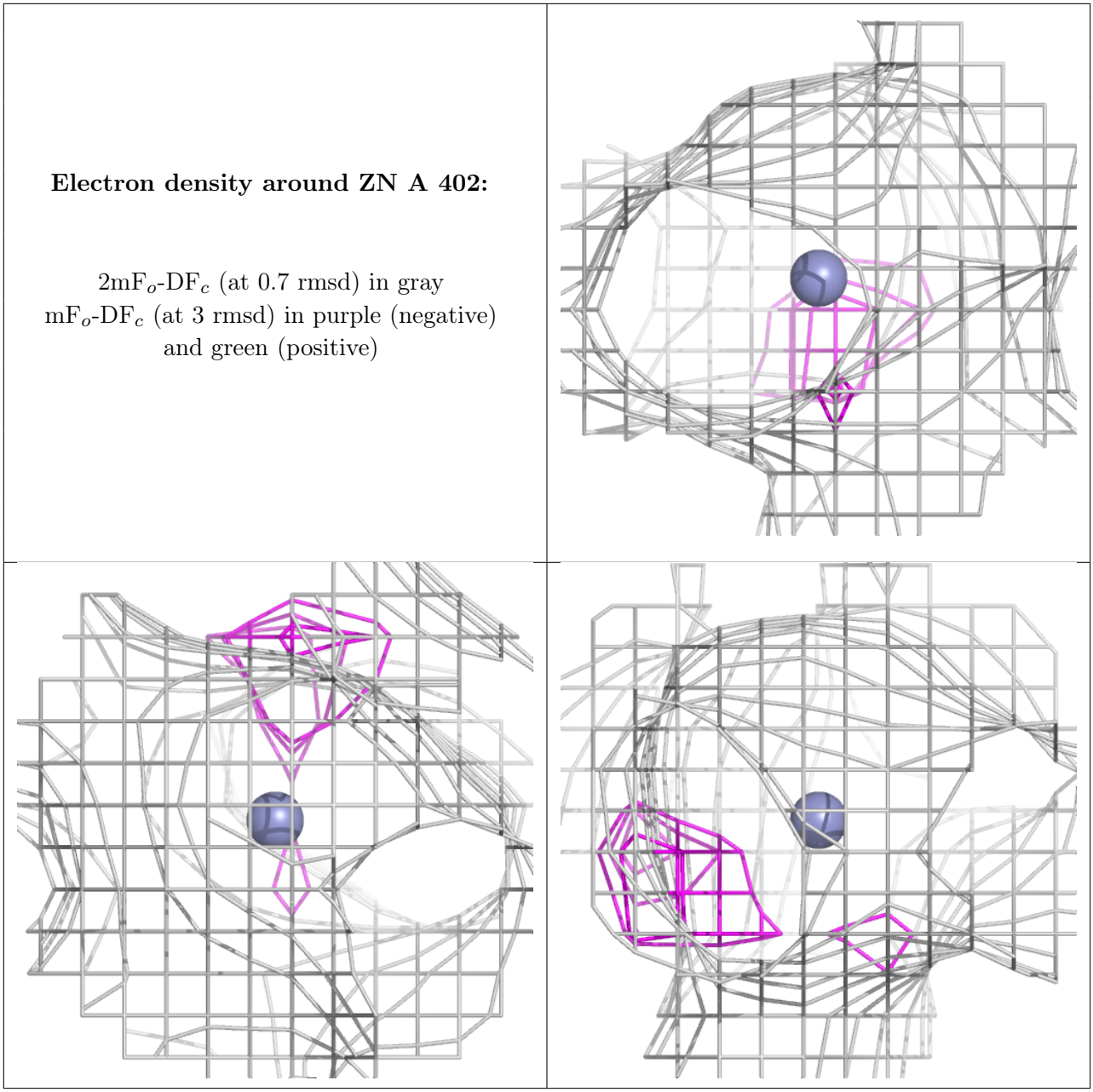
Electron density around ZN G 403:

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



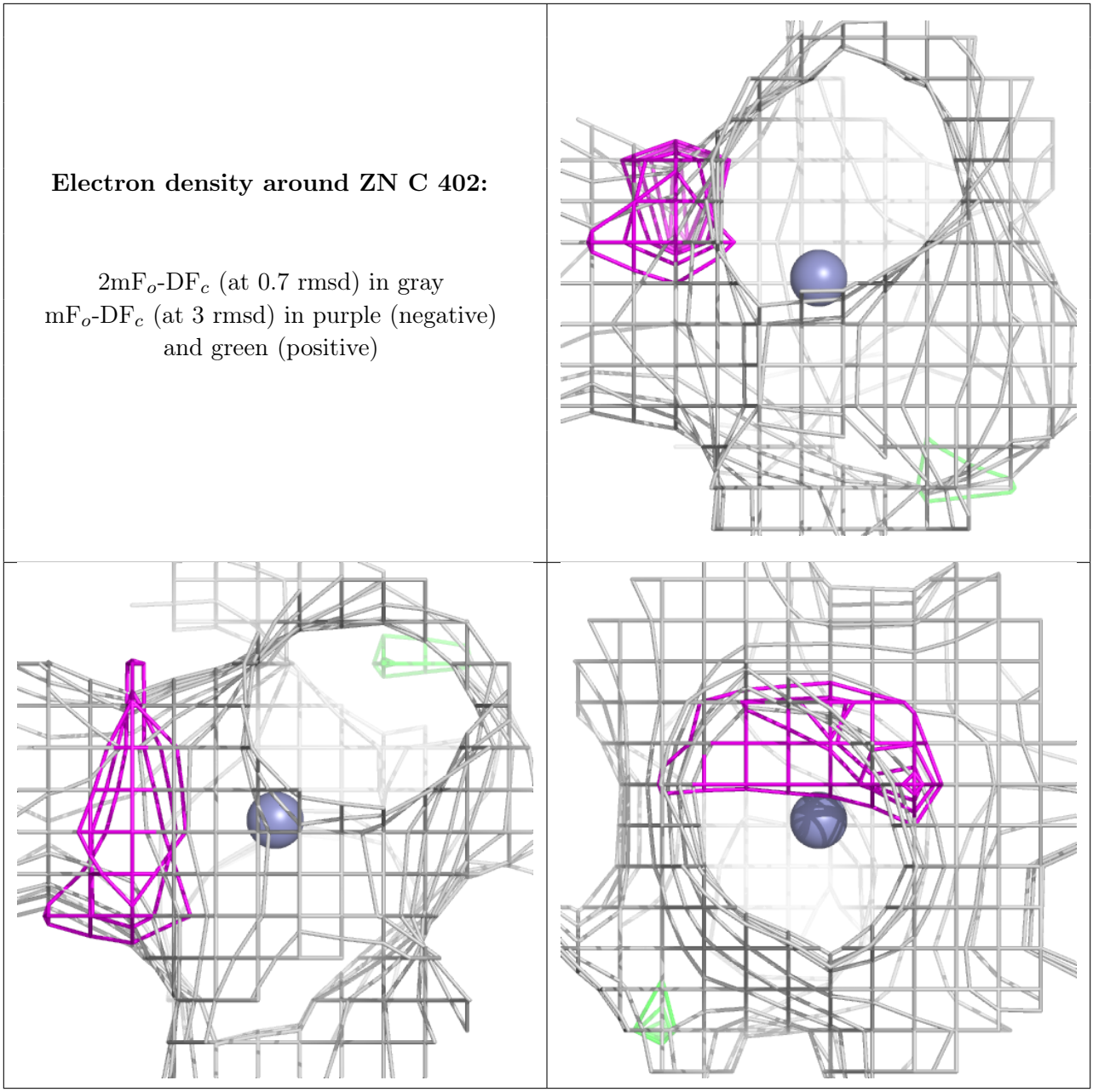
Electron density around ZN A 402:

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



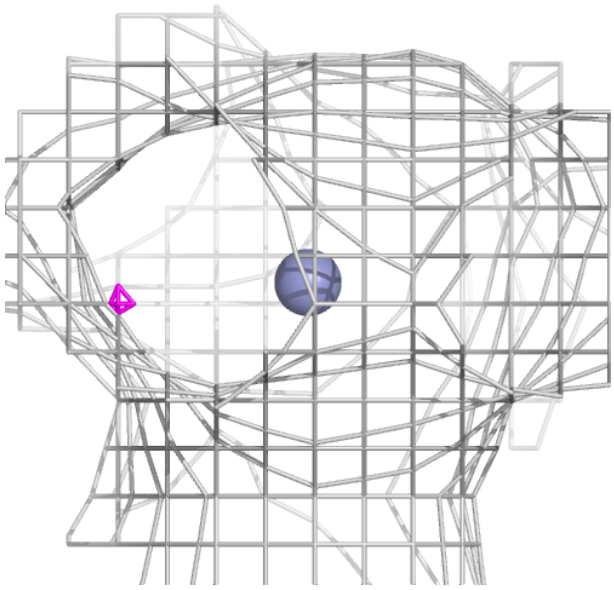
Electron density around ZN C 402:

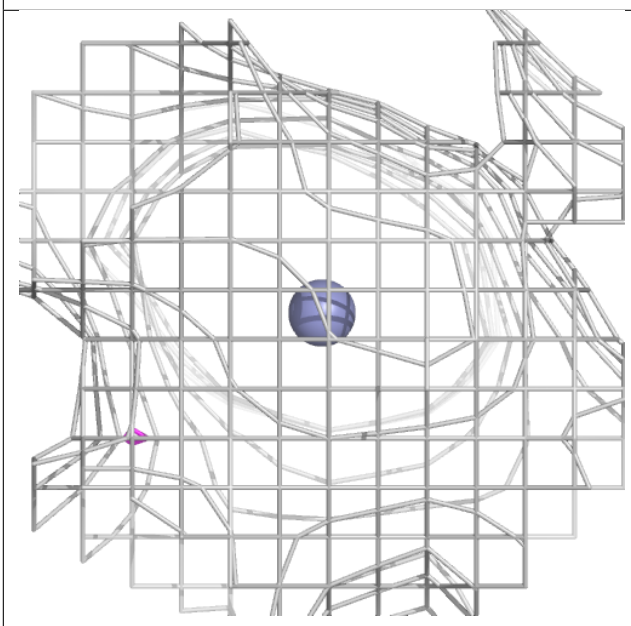
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN E 403:

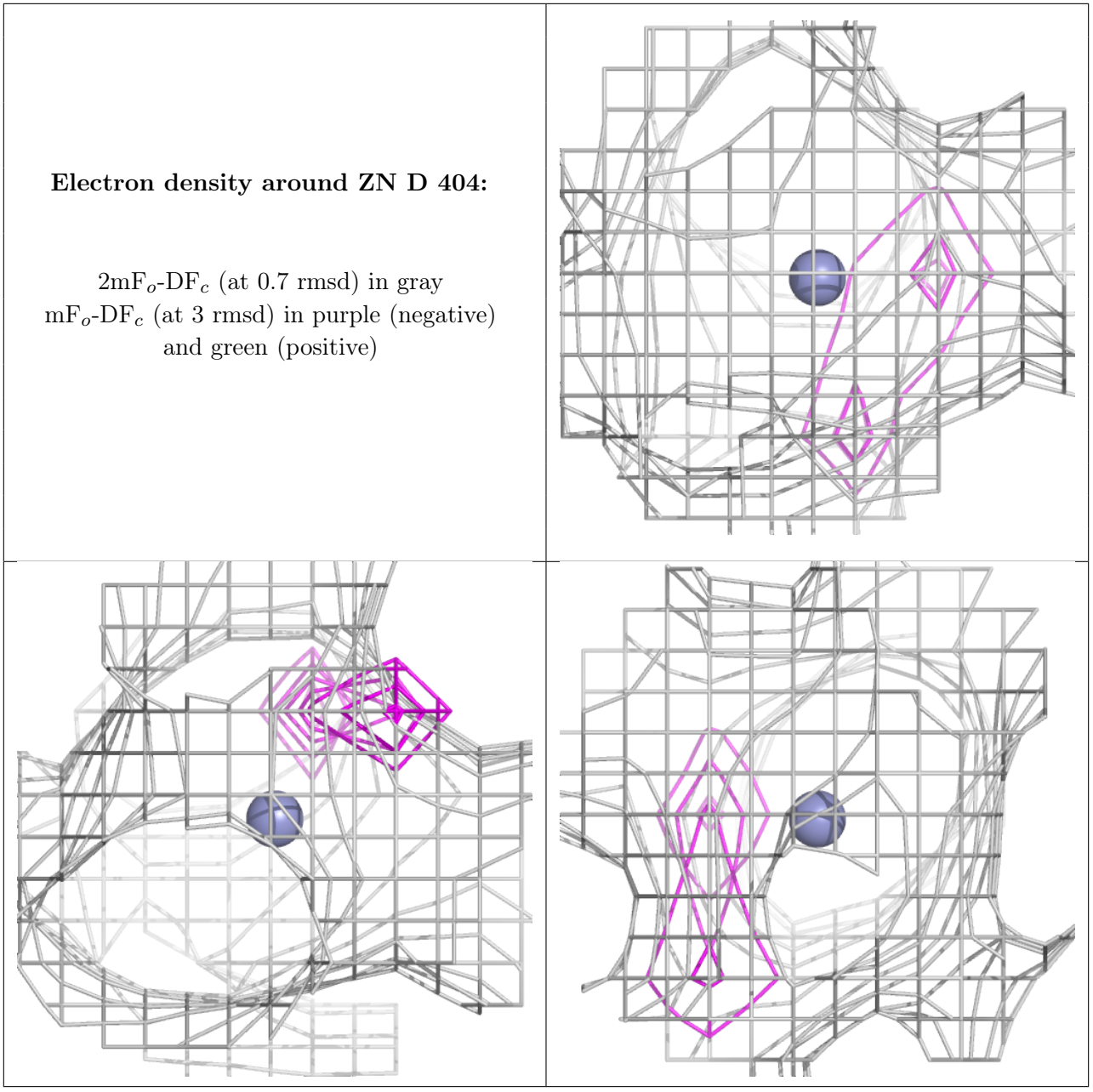
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around ZN D 404:

$2mF_o$-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.