Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2025 – 10:11 AM EDT

PDB ID	:	9MR6 / pdb_00009mr6
Title	:	X-ray crystal structure of SAMHD1 from Rhizophagus irregularis
Authors	:	Lachowicz, J.C.; Zizola, C.; Grove, T.G.
Deposited on	:	2025-01-07
Resolution	:	2.27 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:

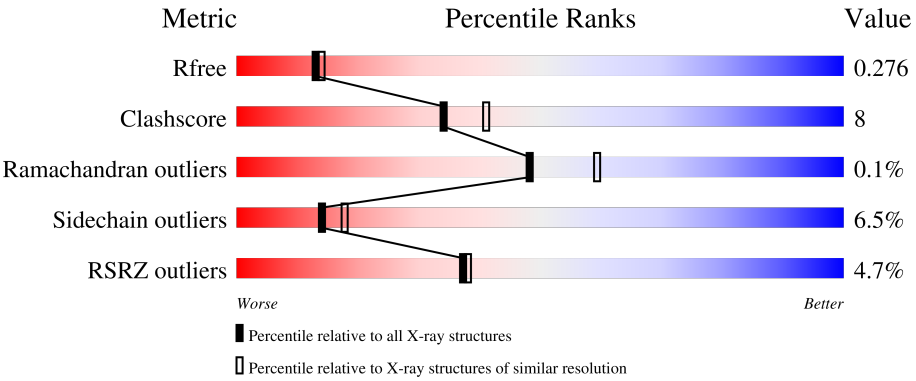
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.27 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	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	483	4% 73% 18% • 9%
1	B	483	6% 66% 23% • 9%
1	C	483	4% 71% 19% • 9%
1	D	483	4% 69% 21% • 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15052 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 HD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3685	2367	624	680	14			
1	B	440	Total	C	N	O	S	0	0	0
			3686	2369	624	679	14			
1	C	440	Total	C	N	O	S	0	0	0
			3682	2366	623	679	14			
1	D	441	Total	C	N	O	S	0	0	0
			3690	2371	626	679	14			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A015K8Z8
A	-18	GLY	-	expression tag	UNP A0A015K8Z8
A	-17	SER	-	expression tag	UNP A0A015K8Z8
A	-16	SER	-	expression tag	UNP A0A015K8Z8
A	-15	HIS	-	expression tag	UNP A0A015K8Z8
A	-14	HIS	-	expression tag	UNP A0A015K8Z8
A	-13	HIS	-	expression tag	UNP A0A015K8Z8
A	-12	HIS	-	expression tag	UNP A0A015K8Z8
A	-11	HIS	-	expression tag	UNP A0A015K8Z8
A	-10	HIS	-	expression tag	UNP A0A015K8Z8
A	-9	SER	-	expression tag	UNP A0A015K8Z8
A	-8	SER	-	expression tag	UNP A0A015K8Z8
A	-7	GLY	-	expression tag	UNP A0A015K8Z8
A	-6	LEU	-	expression tag	UNP A0A015K8Z8
A	-5	VAL	-	expression tag	UNP A0A015K8Z8
A	-4	PRO	-	expression tag	UNP A0A015K8Z8
A	-3	ARG	-	expression tag	UNP A0A015K8Z8
A	-2	GLY	-	expression tag	UNP A0A015K8Z8
A	-1	SER	-	expression tag	UNP A0A015K8Z8
A	0	HIS	-	expression tag	UNP A0A015K8Z8
B	-19	MET	-	initiating methionine	UNP A0A015K8Z8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A015K8Z8
B	-17	SER	-	expression tag	UNP A0A015K8Z8
B	-16	SER	-	expression tag	UNP A0A015K8Z8
B	-15	HIS	-	expression tag	UNP A0A015K8Z8
B	-14	HIS	-	expression tag	UNP A0A015K8Z8
B	-13	HIS	-	expression tag	UNP A0A015K8Z8
B	-12	HIS	-	expression tag	UNP A0A015K8Z8
B	-11	HIS	-	expression tag	UNP A0A015K8Z8
B	-10	HIS	-	expression tag	UNP A0A015K8Z8
B	-9	SER	-	expression tag	UNP A0A015K8Z8
B	-8	SER	-	expression tag	UNP A0A015K8Z8
B	-7	GLY	-	expression tag	UNP A0A015K8Z8
B	-6	LEU	-	expression tag	UNP A0A015K8Z8
B	-5	VAL	-	expression tag	UNP A0A015K8Z8
B	-4	PRO	-	expression tag	UNP A0A015K8Z8
B	-3	ARG	-	expression tag	UNP A0A015K8Z8
B	-2	GLY	-	expression tag	UNP A0A015K8Z8
B	-1	SER	-	expression tag	UNP A0A015K8Z8
B	0	HIS	-	expression tag	UNP A0A015K8Z8
C	-19	MET	-	initiating methionine	UNP A0A015K8Z8
C	-18	GLY	-	expression tag	UNP A0A015K8Z8
C	-17	SER	-	expression tag	UNP A0A015K8Z8
C	-16	SER	-	expression tag	UNP A0A015K8Z8
C	-15	HIS	-	expression tag	UNP A0A015K8Z8
C	-14	HIS	-	expression tag	UNP A0A015K8Z8
C	-13	HIS	-	expression tag	UNP A0A015K8Z8
C	-12	HIS	-	expression tag	UNP A0A015K8Z8
C	-11	HIS	-	expression tag	UNP A0A015K8Z8
C	-10	HIS	-	expression tag	UNP A0A015K8Z8
C	-9	SER	-	expression tag	UNP A0A015K8Z8
C	-8	SER	-	expression tag	UNP A0A015K8Z8
C	-7	GLY	-	expression tag	UNP A0A015K8Z8
C	-6	LEU	-	expression tag	UNP A0A015K8Z8
C	-5	VAL	-	expression tag	UNP A0A015K8Z8
C	-4	PRO	-	expression tag	UNP A0A015K8Z8
C	-3	ARG	-	expression tag	UNP A0A015K8Z8
C	-2	GLY	-	expression tag	UNP A0A015K8Z8
C	-1	SER	-	expression tag	UNP A0A015K8Z8
C	0	HIS	-	expression tag	UNP A0A015K8Z8
D	-19	MET	-	initiating methionine	UNP A0A015K8Z8
D	-18	GLY	-	expression tag	UNP A0A015K8Z8
D	-17	SER	-	expression tag	UNP A0A015K8Z8

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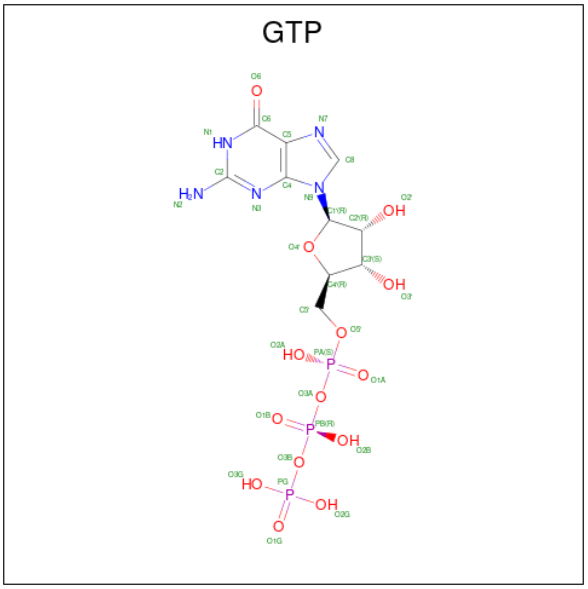
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A015K8Z8
D	-15	HIS	-	expression tag	UNP A0A015K8Z8
D	-14	HIS	-	expression tag	UNP A0A015K8Z8
D	-13	HIS	-	expression tag	UNP A0A015K8Z8
D	-12	HIS	-	expression tag	UNP A0A015K8Z8
D	-11	HIS	-	expression tag	UNP A0A015K8Z8
D	-10	HIS	-	expression tag	UNP A0A015K8Z8
D	-9	SER	-	expression tag	UNP A0A015K8Z8
D	-8	SER	-	expression tag	UNP A0A015K8Z8
D	-7	GLY	-	expression tag	UNP A0A015K8Z8
D	-6	LEU	-	expression tag	UNP A0A015K8Z8
D	-5	VAL	-	expression tag	UNP A0A015K8Z8
D	-4	PRO	-	expression tag	UNP A0A015K8Z8
D	-3	ARG	-	expression tag	UNP A0A015K8Z8
D	-2	GLY	-	expression tag	UNP A0A015K8Z8
D	-1	SER	-	expression tag	UNP A0A015K8Z8
D	0	HIS	-	expression tag	UNP A0A015K8Z8

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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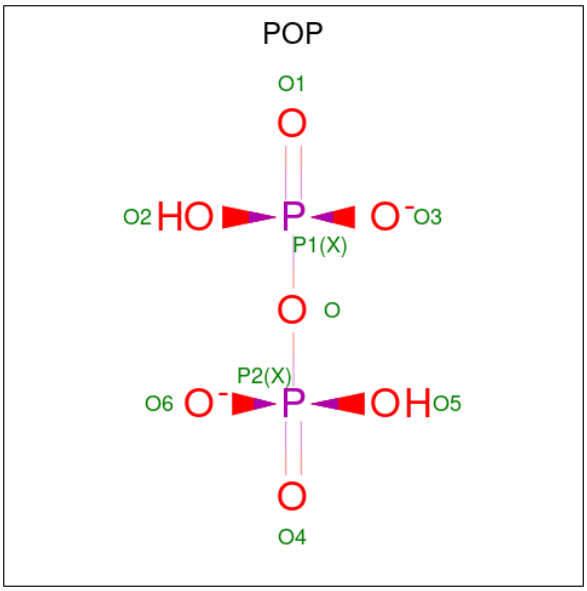
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O P 32 10 5 14 3	0	0
2	D	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $H_2O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0
3	D	1	Total O P 9 7 2	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

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

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

- Molecule 6 is water.

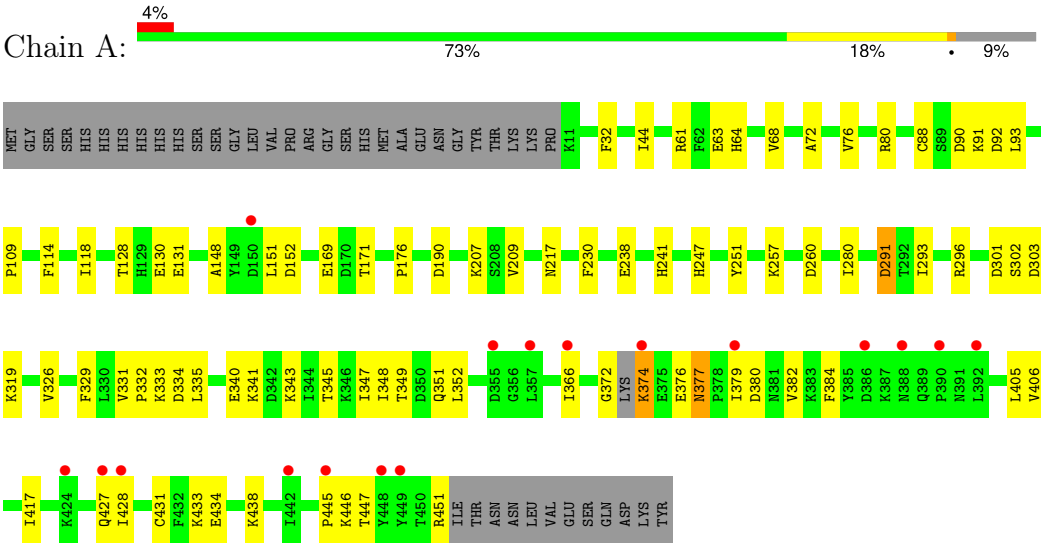
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	24	Total O 24 24	0	0
6	C	42	Total O 42 42	0	0
6	D	33	Total O 33 33	0	0

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.

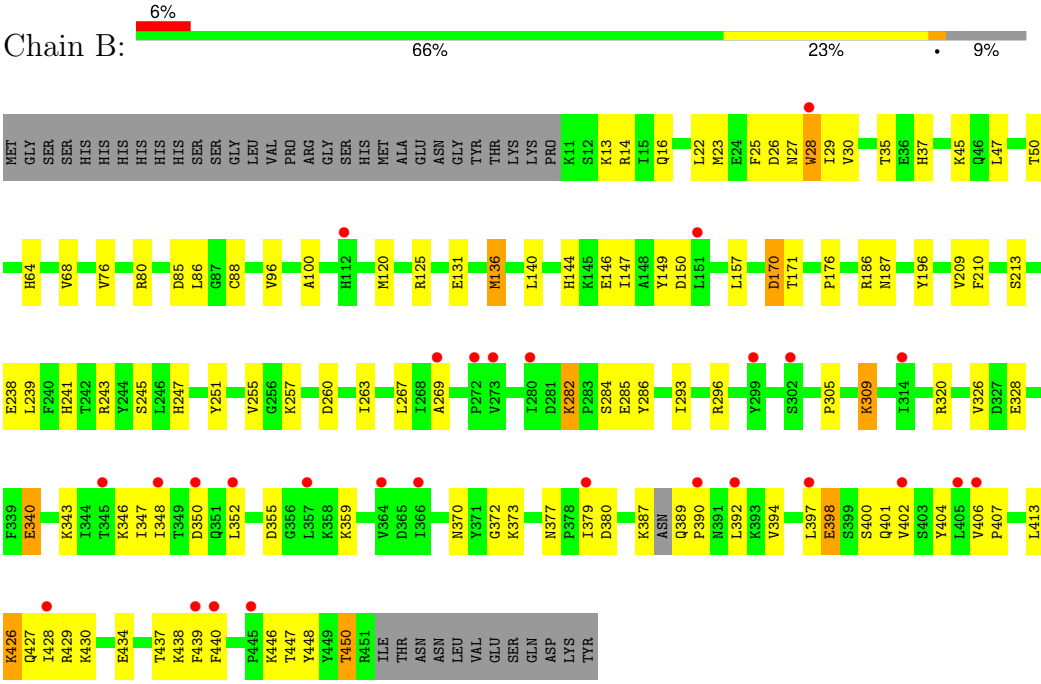
• Molecule 1: HD domain-containing protein

Chain A:



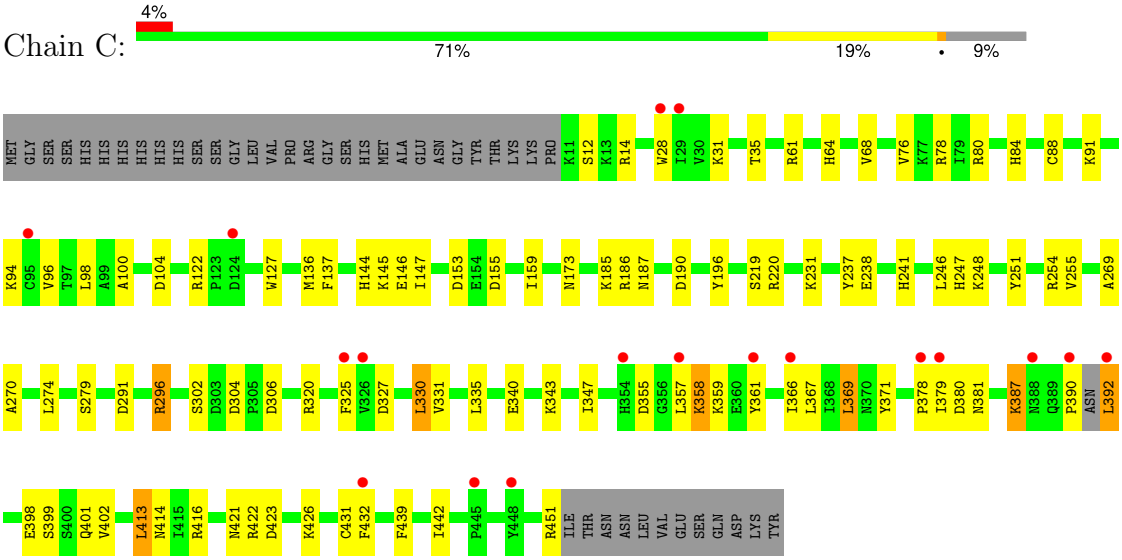
• Molecule 1: HD domain-containing protein

Chain B:



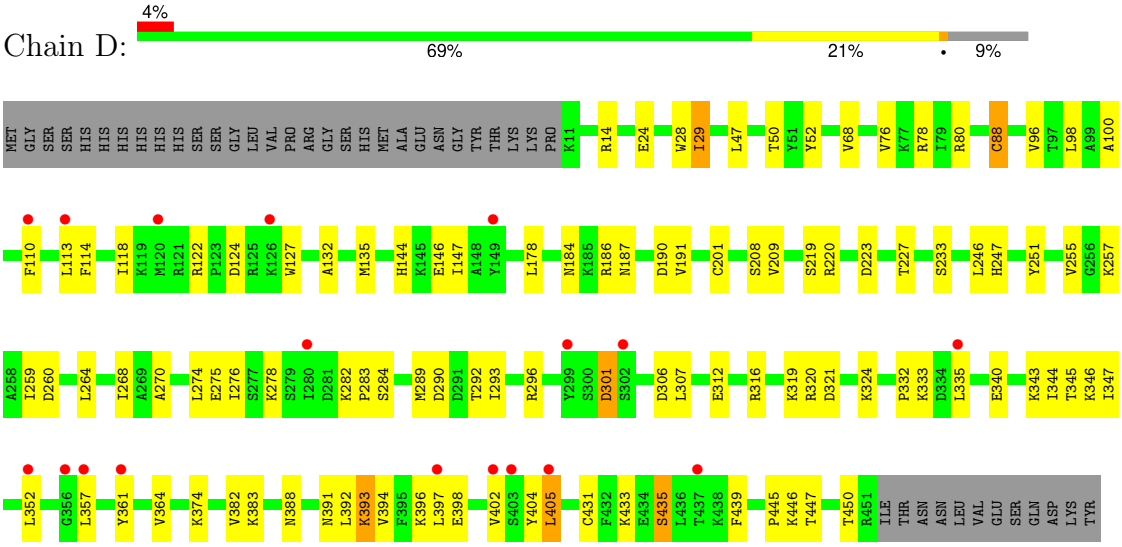
• Molecule 1: HD domain-containing protein

Chain C:



• Molecule 1: HD domain-containing protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.36Å 85.42Å 87.03Å 104.58° 111.65° 99.51°	Depositor
Resolution (Å)	41.50 – 2.27 41.50 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.0 (41.50-2.27) 93.0 (41.50-2.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.220 , 0.280 0.218 , 0.276	Depositor DCC
R_{free} test set	4789 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15052	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GTP, POP, MN, CA

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	0.25	0/3767	0.47	0/5064
1	B	0.29	0/3768	0.49	0/5064
1	C	0.26	0/3764	0.47	0/5060
1	D	0.28	0/3773	0.49	0/5073
All	All	0.27	0/15072	0.48	0/20261

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	3685	0	3683	47	0
1	B	3686	0	3690	70	0
1	C	3682	0	3679	56	0
1	D	3690	0	3693	59	0
2	A	64	0	24	1	0
2	D	64	0	24	4	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	38	0	0	0	0
6	B	24	0	0	0	0
6	C	42	0	0	1	0
6	D	33	0	0	1	0
All	All	15052	0	14793	224	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 8.

All (224) 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:387:LYS:C	1:B:389:GLN:N	2.31	0.83
1:C:390:PRO:C	1:C:392:LEU:N	2.32	0.82
1:B:426:LYS:HE3	1:B:427:GLN:HE22	1.50	0.75
1:A:405:LEU:HG	1:D:405:LEU:HD12	1.69	0.75
1:B:398:GLU:HG3	1:B:401:GLN:HB2	1.69	0.74
1:D:433:LYS:HG2	1:D:445:PRO:HG2	1.71	0.73
1:D:118:ILE:HG21	1:D:127:TRP:HB3	1.71	0.72
1:C:340:GLU:HB3	1:C:343:LYS:HB2	1.74	0.69
1:B:397:LEU:HD13	1:B:402:VAL:HG11	1.75	0.69
1:B:14:ARG:HB3	1:B:22:LEU:HD22	1.73	0.69
1:A:80:ARG:NH2	1:A:90:ASP:OD1	2.28	0.66
1:D:340:GLU:HB2	1:D:343:LYS:HE3	1.78	0.66
1:A:351:GLN:HE22	1:A:434:GLU:HB3	1.62	0.65
1:B:293:ILE:HA	1:B:296:ARG:HG3	1.78	0.64
1:B:347:ILE:HD13	1:B:439:PHE:HB2	1.78	0.64
1:B:247:HIS:HA	1:B:251:TYR:HB2	1.77	0.64
1:C:68:VAL:HG12	1:C:100:ALA:HB1	1.79	0.64
1:C:331:VAL:HG22	1:C:413:LEU:HB3	1.80	0.63
1:B:406:VAL:HG22	1:B:407:PRO:HD2	1.81	0.63
1:D:398:GLU:N	1:D:398:GLU:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:OE1	1:A:130:GLU:N	2.24	0.62
1:C:61:ARG:NH1	1:C:104:ASP:OD2	2.33	0.61
1:A:68:VAL:HG12	1:A:100:ALA:HB1	1.81	0.61
1:B:447:THR:O	1:C:401:GLN:NE2	2.33	0.61
1:D:290:ASP:OD1	1:D:292:THR:OG1	2.18	0.61
1:A:379:ILE:HD11	1:A:384:PHE:HZ	1.66	0.61
1:A:372:GLY:O	1:A:374:LYS:N	2.33	0.61
1:D:431:CYS:O	1:D:435:SER:OG	2.19	0.61
1:B:27:ASN:HA	1:B:30:VAL:HB	1.83	0.60
1:A:302:SER:HB3	1:A:307:LEU:HD12	1.82	0.60
1:C:76:VAL:HG21	1:C:96:VAL:HG11	1.83	0.60
1:B:448:TYR:OH	1:C:231:LYS:NZ	2.29	0.59
1:C:255:VAL:HG11	2:D:601:GTP:H5"	1.83	0.59
1:C:371:TYR:HE2	1:C:378:PRO:HG3	1.68	0.58
1:D:187:ASN:ND2	6:D:704:HOH:O	2.35	0.58
2:A:603:GTP:H5"	1:B:255:VAL:HG21	1.85	0.58
1:A:345:THR:O	1:A:349:THR:OG1	2.19	0.58
1:D:301:ASP:OD1	1:D:301:ASP:N	2.36	0.58
1:D:14:ARG:HG2	1:D:24:GLU:HG2	1.86	0.57
1:C:347:ILE:HD13	1:C:439:PHE:HB2	1.85	0.57
1:D:80:ARG:HG2	1:D:88:CYS:HB3	1.87	0.57
1:C:78:ARG:NH2	1:C:219:SER:OG	2.38	0.56
1:A:351:GLN:NE2	1:A:434:GLU:HB3	2.20	0.56
1:C:357:LEU:HD23	1:C:361:TYR:HE2	1.69	0.56
1:A:148:ALA:HB1	1:A:151:LEU:HD23	1.87	0.56
1:B:430:LYS:O	1:B:434:GLU:HG2	2.06	0.55
1:D:264:LEU:O	1:D:268:ILE:HD12	2.07	0.55
1:A:169:GLU:OE1	1:A:169:GLU:N	2.40	0.54
1:C:35:THR:HA	1:D:319:LYS:HZ2	1.72	0.54
1:C:320:ARG:HH21	2:D:601:GTP:H5'	1.72	0.54
1:B:68:VAL:HG12	1:B:100:ALA:HB1	1.90	0.54
1:A:247:HIS:HA	1:A:251:TYR:HB2	1.90	0.54
1:B:170:ASP:N	1:B:170:ASP:OD1	2.41	0.54
1:C:390:PRO:O	1:C:392:LEU:N	2.40	0.54
1:A:379:ILE:HD11	1:A:384:PHE:CZ	2.43	0.54
1:B:45:LYS:HA	1:B:60:ASN:HD22	1.72	0.53
1:D:52:TYR:O	1:D:320:ARG:NH2	2.41	0.53
1:B:76:VAL:HG21	1:B:96:VAL:HG11	1.90	0.53
1:C:247:HIS:HA	1:C:251:TYR:HB2	1.90	0.53
1:C:220:ARG:NH1	1:C:220:ARG:HB3	2.23	0.53
1:D:357:LEU:HB3	1:D:361:TYR:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HA	1:A:296:ARG:HG3	1.91	0.53
1:B:23:MET:HE3	1:B:25:PHE:HE2	1.74	0.52
1:B:328:GLU:HG2	1:B:448:TYR:HB2	1.91	0.52
1:D:122:ARG:CZ	1:D:122:ARG:HA	2.39	0.52
1:B:326:VAL:HG12	1:B:429:ARG:HG3	1.90	0.52
1:A:428:ILE:H	1:A:428:ILE:HD12	1.75	0.52
1:B:282:LYS:HD3	1:B:284:SER:H	1.75	0.52
1:D:127:TRP:HE1	1:D:132:ALA:HB2	1.75	0.52
1:D:76:VAL:HG21	1:D:96:VAL:HG11	1.92	0.51
1:A:329:PHE:CE2	1:A:331:VAL:HG12	2.46	0.51
1:B:171:THR:HB	1:B:176:PRO:HB3	1.93	0.51
1:B:186:ARG:HG2	1:B:187:ASN:OD1	2.12	0.50
1:A:76:VAL:HG13	1:A:93:LEU:HD12	1.93	0.50
1:B:400:SER:HB2	1:C:330:LEU:HD22	1.94	0.50
1:C:254:ARG:HG2	1:C:325:PHE:HE2	1.76	0.50
1:B:426:LYS:HE3	1:B:427:GLN:NE2	2.24	0.50
1:D:282:LYS:HD2	1:D:284:SER:OG	2.11	0.50
1:A:348:ILE:O	1:A:352:LEU:HD23	2.12	0.50
1:B:227:THR:HG21	1:B:394:VAL:HG11	1.94	0.50
1:A:80:ARG:HG2	1:A:88:CYS:HB3	1.94	0.50
1:B:326:VAL:O	1:B:429:ARG:NH1	2.45	0.49
1:C:367:LEU:HB3	1:C:414:ASN:HB2	1.95	0.49
1:A:340:GLU:HG3	1:A:343:LYS:H	1.76	0.49
1:C:392:LEU:HD23	1:C:392:LEU:HA	1.68	0.49
1:B:210:PHE:CZ	1:B:239:LEU:HD12	2.47	0.48
1:B:340:GLU:HB3	1:B:343:LYS:HB2	1.95	0.48
1:B:419:THR:HG21	1:B:428:ILE:HD12	1.95	0.48
1:D:282:LYS:HD3	1:D:283:PRO:HD2	1.95	0.48
1:A:347:ILE:HD11	1:A:438:LYS:HB3	1.96	0.48
1:A:351:GLN:HE21	1:A:431:CYS:HA	1.78	0.48
1:B:370:ASN:HB3	1:B:372:GLY:O	2.14	0.48
1:C:237:TYR:CE1	1:C:379:ILE:HG13	2.49	0.48
1:C:371:TYR:CE2	1:C:378:PRO:HG3	2.48	0.48
1:D:343:LYS:HD2	1:D:439:PHE:CE2	2.49	0.48
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.65	0.48
1:D:28:TRP:CE2	1:D:29:ILE:HG12	2.49	0.48
1:A:377:ASN:OD1	1:A:379:ILE:HG22	2.13	0.47
1:B:125:ARG:NH1	1:B:131:GLU:OE2	2.32	0.47
1:B:47:LEU:HB3	1:B:50:THR:HB	1.96	0.47
1:D:135:MET:SD	1:D:283:PRO:HG3	2.54	0.47
1:D:312:GLU:O	1:D:316:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG21	2:D:602:GTP:H5'	1.96	0.47
1:A:61:ARG:NH1	1:A:104:ASP:OD2	2.39	0.47
1:A:451:ARG:HE	1:A:451:ARG:HA	1.78	0.47
1:B:28:TRP:NE1	1:B:29:ILE:HG23	2.29	0.47
1:A:209:VAL:HG23	1:D:209:VAL:HG23	1.96	0.47
1:C:220:ARG:HB3	1:C:220:ARG:HH11	1.79	0.47
1:D:347:ILE:HG22	1:D:435:SER:HB3	1.96	0.47
1:D:255:VAL:O	1:D:259:ILE:HG13	2.15	0.47
1:A:238:GLU:HA	1:A:241:HIS:HB2	1.98	0.46
1:B:434:GLU:HA	1:B:437:THR:HG22	1.98	0.46
1:D:270:ALA:HB1	1:D:274:LEU:HD23	1.96	0.46
1:A:118:ILE:HD13	1:A:280:ILE:HD13	1.97	0.46
1:B:352:LEU:HD11	1:B:428:ILE:HG23	1.98	0.46
1:B:347:ILE:HG13	1:B:348:ILE:N	2.31	0.46
1:C:335:LEU:HD11	1:C:442:ILE:HD11	1.98	0.46
1:A:433:LYS:HB3	1:A:445:PRO:HG3	1.96	0.46
1:C:270:ALA:HB1	1:C:274:LEU:HD12	1.98	0.46
1:C:304:ASP:OD2	1:C:306:ASP:HB2	2.16	0.46
1:A:32:PHE:CZ	1:A:148:ALA:HB2	2.51	0.46
1:C:155:ASP:O	1:C:159:ILE:HG13	2.16	0.45
1:C:296:ARG:HD3	1:D:296:ARG:HD3	1.99	0.45
1:B:355:ASP:OD1	1:B:355:ASP:N	2.48	0.45
1:A:64:HIS:O	1:A:68:VAL:HG23	2.16	0.45
1:B:326:VAL:HG21	1:B:419:THR:HG23	1.99	0.45
1:B:413:LEU:HD12	1:B:413:LEU:HA	1.84	0.45
1:D:374:LYS:HA	1:D:374:LYS:HD3	1.82	0.45
1:B:257:LYS:HA	1:B:260:ASP:HB2	1.98	0.45
1:D:247:HIS:HA	1:D:251:TYR:HB2	1.97	0.45
1:A:44:ILE:HA	1:A:291:ASP:OD1	2.15	0.45
1:D:47:LEU:HB3	1:D:50:THR:HB	1.97	0.45
1:A:91:LYS:HE3	1:A:91:LYS:HB2	1.75	0.44
1:B:387:LYS:HD2	1:B:387:LYS:HA	1.79	0.44
1:C:127:TRP:NE1	6:C:601:HOH:O	2.28	0.44
1:B:136:MET:HE2	1:B:286:TYR:HD2	1.83	0.44
1:A:72:ALA:O	1:A:76:VAL:HG12	2.17	0.44
1:C:325:PHE:HE1	1:C:327:ASP:C	2.20	0.44
1:D:346:LYS:HE3	1:D:347:ILE:HG12	1.99	0.44
1:C:387:LYS:HB2	1:C:387:LYS:HE2	1.56	0.44
1:D:307:LEU:HD23	1:D:307:LEU:HA	1.80	0.44
1:A:379:ILE:HD12	1:A:379:ILE:HA	1.80	0.44
1:C:146:GLU:CD	1:C:146:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:HG12	1:D:100:ALA:HB1	1.98	0.44
1:A:109:PRO:HD2	1:A:114:PHE:CD1	2.53	0.44
1:A:341:LYS:HD2	1:A:366:ILE:HG12	1.99	0.44
1:D:227:THR:HG21	1:D:394:VAL:HG11	2.00	0.44
1:B:243:ARG:HH22	1:B:372:GLY:HA2	1.82	0.43
1:C:358:LYS:NZ	1:C:361:TYR:OH	2.48	0.43
1:D:276:ILE:HG23	1:D:289:MET:HE3	1.99	0.43
1:D:447:THR:HG22	1:D:450:THR:OG1	2.18	0.43
1:A:257:LYS:HA	1:A:260:ASP:HB2	2.00	0.43
1:D:257:LYS:HA	1:D:257:LYS:HD3	1.75	0.43
1:D:392:LEU:HD13	1:D:393:LYS:O	2.18	0.43
1:B:263:ILE:O	1:B:267:LEU:HG	2.19	0.43
1:C:28:TRP:CE2	1:C:94:LYS:HD3	2.54	0.43
1:C:64:HIS:CE1	1:C:196:TYR:HB3	2.54	0.43
1:C:327:ASP:HB3	1:C:432:PHE:HD2	1.83	0.43
1:D:78:ARG:NH2	1:D:219:SER:OG	2.50	0.43
1:B:13:LYS:HG3	1:B:30:VAL:HG21	2.01	0.43
1:B:150:ASP:OD1	1:B:150:ASP:N	2.41	0.43
1:B:309:LYS:H	1:B:309:LYS:HG2	1.58	0.43
1:B:447:THR:HG22	1:B:450:THR:HG23	1.99	0.43
1:B:80:ARG:HG2	1:B:88:CYS:HB3	2.00	0.43
1:D:397:LEU:HD22	1:D:402:VAL:HG22	2.01	0.43
1:B:25:PHE:HB3	1:B:29:ILE:HD11	2.01	0.42
1:D:110:PHE:HB2	1:D:113:LEU:HB3	2.01	0.42
1:C:144:HIS:O	1:C:147:ILE:HG12	2.19	0.42
1:D:144:HIS:O	1:D:147:ILE:HG12	2.18	0.42
1:D:343:LYS:HD2	1:D:439:PHE:HE2	1.84	0.42
1:B:86:LEU:HD11	1:B:221:VAL:HB	2.01	0.42
1:B:269:ALA:HB1	1:B:309:LYS:HG3	2.00	0.42
1:C:247:HIS:HB3	1:C:369:LEU:HD21	2.01	0.42
1:B:144:HIS:O	1:B:147:ILE:HG12	2.18	0.42
1:A:171:THR:HB	1:A:176:PRO:HB3	2.00	0.42
1:A:326:VAL:HB	1:A:417:ILE:HG22	2.02	0.42
1:A:351:GLN:HG2	1:A:431:CYS:HB3	2.02	0.42
1:B:328:GLU:O	1:B:447:THR:OG1	2.35	0.42
1:C:80:ARG:HG3	1:C:88:CYS:HB3	2.00	0.42
1:C:343:LYS:O	1:C:347:ILE:HG22	2.19	0.42
1:C:421:ASN:OD1	1:C:423:ASP:HB2	2.19	0.42
1:C:367:LEU:HD22	1:C:416:ARG:CZ	2.49	0.42
1:D:324:LYS:HD2	1:D:324:LYS:HA	1.84	0.42
1:D:332:PRO:HD2	1:D:335:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:HIS:HB2	1:B:140:LEU:HD12	2.01	0.42
1:C:136:MET:HB3	1:C:136:MET:HE3	1.86	0.42
1:C:366:ILE:HD12	1:C:366:ILE:O	2.19	0.42
1:D:275:GLU:HB3	1:D:278:LYS:HD3	2.01	0.42
1:D:346:LYS:HE2	1:D:346:LYS:HB3	1.78	0.42
1:B:64:HIS:CE1	1:B:196:TYR:HB3	2.54	0.42
1:C:269:ALA:O	1:C:306:ASP:HB3	2.20	0.41
1:D:397:LEU:HB3	1:D:402:VAL:HG21	2.01	0.41
1:C:31:LYS:HD2	1:C:31:LYS:HA	1.71	0.41
1:D:340:GLU:O	1:D:344:ILE:HG22	2.20	0.41
2:D:602:GTP:O1A	2:D:602:GTP:N2	2.54	0.41
1:B:379:ILE:H	1:B:379:ILE:HD12	1.86	0.41
1:D:68:VAL:HG13	1:D:191:VAL:HG23	2.01	0.41
1:D:98:LEU:HD23	1:D:98:LEU:HA	1.94	0.41
1:A:332:PRO:HD2	1:A:335:LEU:HD12	2.02	0.41
1:B:377:ASN:HB3	1:B:380:ASP:OD2	2.20	0.41
1:B:305:PRO:O	1:B:309:LYS:NZ	2.48	0.41
1:B:28:TRP:CD1	1:B:29:ILE:HG23	2.56	0.41
1:B:238:GLU:HA	1:B:241:HIS:HB3	2.03	0.41
1:B:338:LYS:HE2	1:B:440:PHE:HB3	2.03	0.41
1:D:316:ARG:HB3	1:D:321:ASP:HB3	2.02	0.41
1:A:128:THR:HG23	1:A:131:GLU:H	1.86	0.41
1:A:332:PRO:HB2	1:A:334:ASP:OD1	2.20	0.41
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.89	0.41
1:C:186:ARG:HG3	1:C:381:ASN:HD22	1.84	0.41
1:B:392:LEU:HD23	1:C:451:ARG:HH12	1.86	0.41
1:C:246:LEU:HD23	1:C:246:LEU:HA	1.90	0.41
1:D:201:CYS:SG	1:D:246:LEU:HD21	2.61	0.41
1:C:137:PHE:HZ	1:C:159:ILE:HD12	1.86	0.40
1:C:238:GLU:HA	1:C:241:HIS:HB2	2.02	0.40
1:B:257:LYS:HA	1:B:257:LYS:HD2	1.82	0.40
1:C:187:ASN:HD22	1:C:187:ASN:HA	1.64	0.40
1:B:35:THR:HG21	1:B:140:LEU:HD21	2.03	0.40
1:C:254:ARG:HG2	1:C:325:PHE:CE2	2.56	0.40
1:D:184:ASN:OD1	1:D:186:ARG:HG3	2.21	0.40
1:D:293:ILE:HA	1:D:296:ARG:HG3	2.03	0.40
1:A:63:GLU:HB3	1:B:55:PRO:HB2	2.04	0.40
1:B:146:GLU:HA	1:B:149:TYR:CZ	2.57	0.40
1:B:434:GLU:O	1:B:438:LYS:HB2	2.21	0.40
1:D:345:THR:HG23	1:D:364:VAL:HG21	2.04	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	436/483 (90%)	421 (97%)	15 (3%)	0	100 100
1	B	436/483 (90%)	418 (96%)	17 (4%)	1 (0%)	44 53
1	C	436/483 (90%)	420 (96%)	16 (4%)	0	100 100
1	D	439/483 (91%)	420 (96%)	19 (4%)	0	100 100
All	All	1747/1932 (90%)	1679 (96%)	67 (4%)	1 (0%)	48 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	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	411/449 (92%)	389 (95%)	22 (5%)	18 24
1	B	411/449 (92%)	383 (93%)	28 (7%)	13 16
1	C	410/449 (91%)	380 (93%)	30 (7%)	11 14
1	D	411/449 (92%)	385 (94%)	26 (6%)	15 19
All	All	1643/1796 (92%)	1537 (94%)	106 (6%)	14 18

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	152	ASP
1	A	190	ASP
1	A	217	ASN
1	A	230	PHE
1	A	291	ASP
1	A	301	ASP
1	A	303	ASP
1	A	306	ASP
1	A	319	LYS
1	A	333	LYS
1	A	374	LYS
1	A	376	GLU
1	A	377	ASN
1	A	380	ASP
1	A	382	VAL
1	A	406	VAL
1	A	408	GLU
1	A	413	LEU
1	A	427	GLN
1	A	446	LYS
1	A	447	THR
1	B	16	GLN
1	B	26	ASP
1	B	28	TRP
1	B	85	ASP
1	B	120	MET
1	B	136	MET
1	B	157	LEU
1	B	170	ASP
1	B	209	VAL
1	B	213	SER
1	B	245	SER
1	B	282	LYS
1	B	285	GLU
1	B	309	LYS
1	B	320	ARG
1	B	333	LYS
1	B	334	ASP
1	B	338	LYS
1	B	340	GLU
1	B	346	LYS
1	B	350	ASP

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Mol	Chain	Res	Type
1	B	359	LYS
1	B	373	LYS
1	B	398	GLU
1	B	404	TYR
1	B	426	LYS
1	B	446	LYS
1	B	450	THR
1	C	12	SER
1	C	14	ARG
1	C	84	HIS
1	C	91	LYS
1	C	122	ARG
1	C	145	LYS
1	C	153	ASP
1	C	173	ASN
1	C	185	LYS
1	C	190	ASP
1	C	248	LYS
1	C	279	SER
1	C	291	ASP
1	C	296	ARG
1	C	302	SER
1	C	330	LEU
1	C	355	ASP
1	C	358	LYS
1	C	359	LYS
1	C	369	LEU
1	C	380	ASP
1	C	387	LYS
1	C	392	LEU
1	C	398	GLU
1	C	399	SER
1	C	402	VAL
1	C	413	LEU
1	C	422	ARG
1	C	426	LYS
1	C	431	CYS
1	D	29	ILE
1	D	88	CYS
1	D	114	PHE
1	D	124	ASP
1	D	146	GLU

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Mol	Chain	Res	Type
1	D	178	LEU
1	D	190	ASP
1	D	208	SER
1	D	220	ARG
1	D	223	ASP
1	D	233	SER
1	D	260	ASP
1	D	301	ASP
1	D	306	ASP
1	D	333	LYS
1	D	352	LEU
1	D	382	VAL
1	D	383	LYS
1	D	388	ASN
1	D	391	ASN
1	D	393	LYS
1	D	396	LYS
1	D	404	TYR
1	D	405	LEU
1	D	435	SER
1	D	446	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	351	GLN
1	B	60	ASN
1	B	187	ASN
1	B	427	GLN
1	C	83	GLN
1	C	187	ASN
1	C	381	ASN
1	C	389	GLN
1	D	129	HIS
1	D	217	ASN
1	D	389	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	POP	D	603	4	6,8,8	0.85	0	12,13,13	0.73	0
2	GTP	D	601	5	29,34,34	1.24	1 (3%)	35,54,54	1.27	4 (11%)
2	GTP	A	601	5	29,34,34	1.23	3 (10%)	35,54,54	1.26	4 (11%)
2	GTP	D	602	5	29,34,34	1.30	5 (17%)	35,54,54	1.33	5 (14%)
3	POP	A	602	4	6,8,8	0.80	0	12,13,13	0.79	0
3	POP	B	501	4	6,8,8	0.79	0	12,13,13	0.79	0
2	GTP	A	603	5	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
3	POP	C	501	4	6,8,8	0.80	0	12,13,13	0.78	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
3	POP	D	603	4	-	0/6/6/6	-
2	GTP	D	601	5	-	5/18/38/38	0/3/3/3
2	GTP	A	601	5	-	1/18/38/38	0/3/3/3
2	GTP	D	602	5	-	4/18/38/38	0/3/3/3
3	POP	A	602	4	-	0/6/6/6	-
3	POP	B	501	4	-	0/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	A	603	5	-	2/18/38/38	0/3/3/3
3	POP	C	501	4	-	0/6/6/6	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	GTP	C5-C6	-4.19	1.39	1.47
2	D	601	GTP	C5-C6	-4.14	1.39	1.47
2	D	602	GTP	C5-C6	-4.11	1.39	1.47
2	A	601	GTP	C5-C6	-4.00	1.39	1.47
2	D	602	GTP	PB-O3B	2.32	1.62	1.59
2	D	602	GTP	PA-O3A	2.26	1.61	1.59
2	A	601	GTP	PB-O3B	2.25	1.61	1.59
2	D	602	GTP	C2-N3	2.24	1.38	1.33
2	A	601	GTP	C2-N3	2.18	1.38	1.33
2	D	602	GTP	PB-O3A	2.17	1.61	1.59
2	A	603	GTP	C2-N3	2.15	1.38	1.33
2	A	603	GTP	PA-O3A	2.04	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	GTP	C8-N7-C5	3.62	108.72	102.55
2	A	603	GTP	C8-N7-C5	3.55	108.59	102.55
2	D	602	GTP	C8-N7-C5	3.51	108.53	102.55
2	D	601	GTP	C8-N7-C5	3.37	108.28	102.55
2	D	602	GTP	C2-N1-C6	-2.97	119.68	125.11
2	D	602	GTP	C5-C6-N1	2.96	119.71	114.07
2	A	601	GTP	C5-C6-N1	2.92	119.65	114.07
2	D	601	GTP	C5-C6-N1	2.89	119.58	114.07
2	A	601	GTP	C2-N1-C6	-2.89	119.82	125.11
2	A	603	GTP	C2-N1-C6	-2.86	119.88	125.11
2	A	603	GTP	C5-C6-N1	2.85	119.50	114.07
2	D	601	GTP	C2-N1-C6	-2.81	119.97	125.11
2	D	602	GTP	O6-C6-C5	-2.29	119.79	124.32
2	A	603	GTP	O6-C6-C5	-2.28	119.80	124.32
2	A	601	GTP	O3G-PG-O3B	2.18	111.94	104.64
2	D	601	GTP	C4'-O4'-C1'	2.09	111.84	109.92
2	D	602	GTP	O4'-C1'-N9	2.09	111.51	108.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	GTP	C5'-O5'-PA-O1A
2	A	603	GTP	O4'-C4'-C5'-O5'
2	A	603	GTP	C3'-C4'-C5'-O5'
2	D	602	GTP	PB-O3A-PA-O1A
2	D	601	GTP	C5'-O5'-PA-O3A
2	D	601	GTP	C5'-O5'-PA-O2A
2	D	602	GTP	C5'-O5'-PA-O3A
2	D	602	GTP	C5'-O5'-PA-O1A
2	A	601	GTP	PB-O3B-PG-O1G
2	D	601	GTP	PB-O3A-PA-O2A
2	D	602	GTP	C4'-C5'-O5'-PA
2	D	601	GTP	PB-O3A-PA-O1A

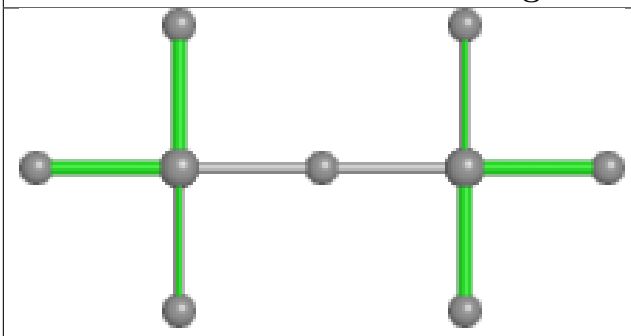
There are no ring outliers.

3 monomers are involved in 5 short contacts:

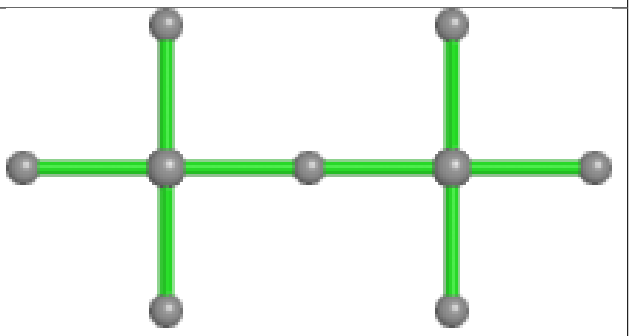
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GTP	2	0
2	D	602	GTP	2	0
2	A	603	GTP	1	0

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 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.

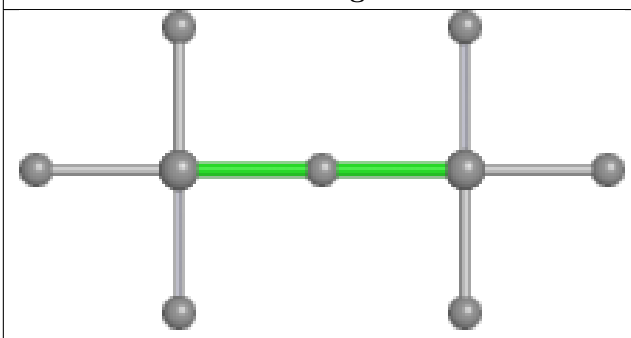
Ligand POP D 603



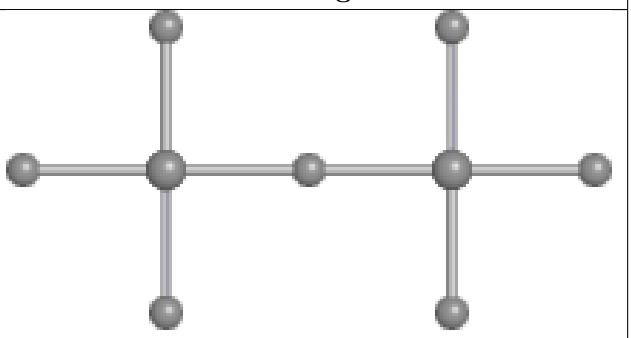
Bond lengths



Bond angles

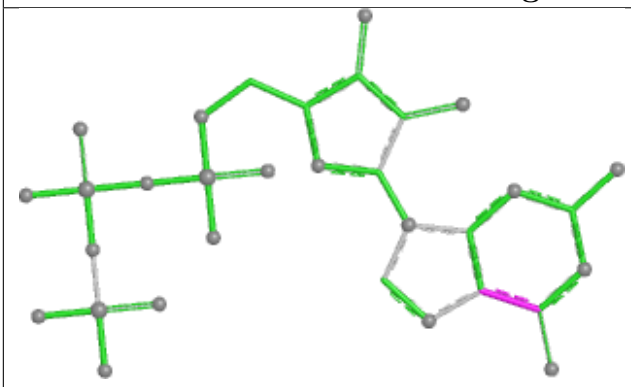


Torsions

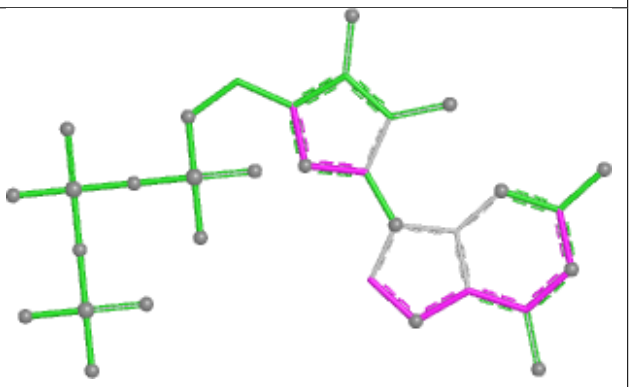


Rings

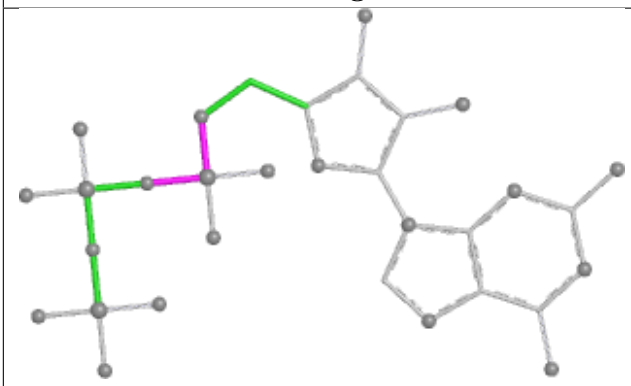
Ligand GTP D 601



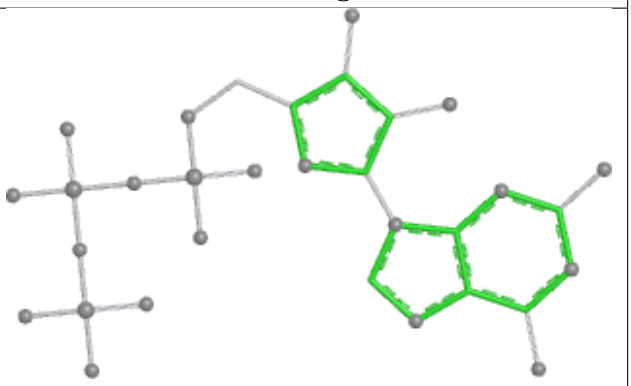
Bond lengths



Bond angles

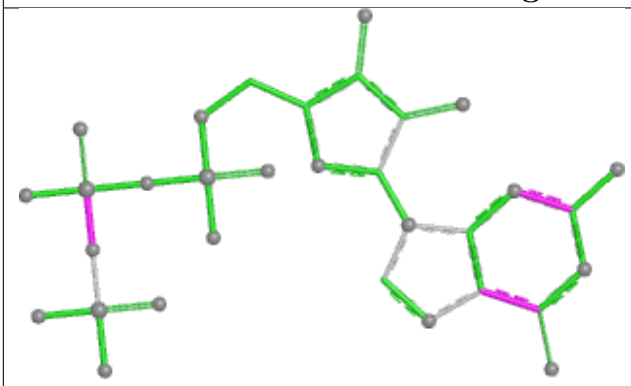


Torsions

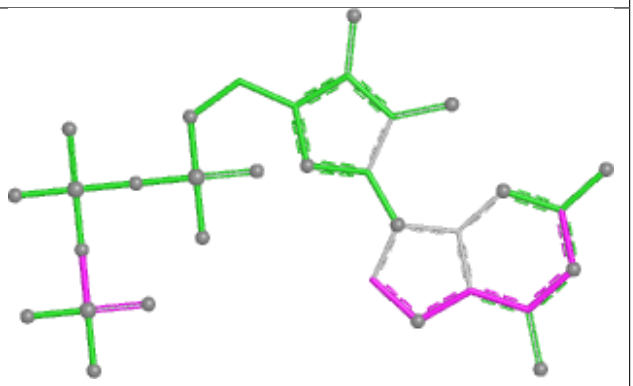


Rings

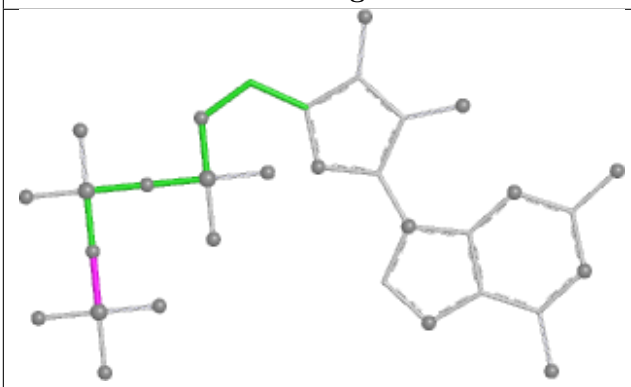
Ligand GTP A 601



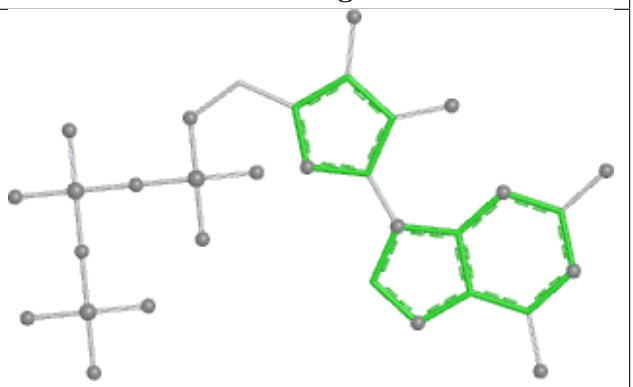
Bond lengths



Bond angles

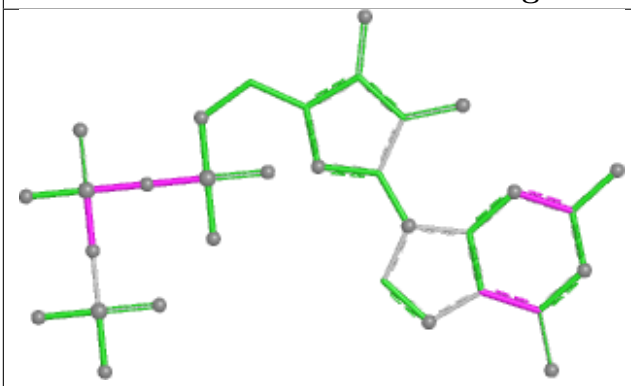


Torsions

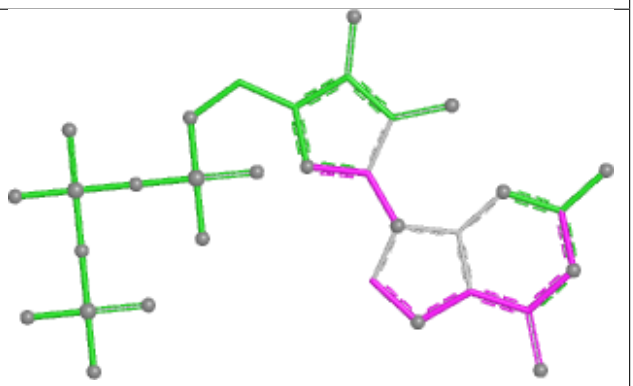


Rings

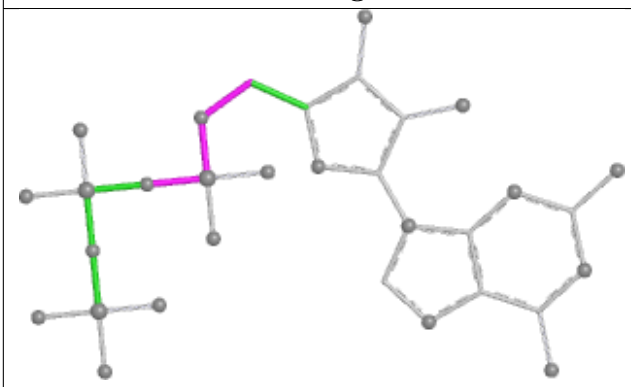
Ligand GTP D 602



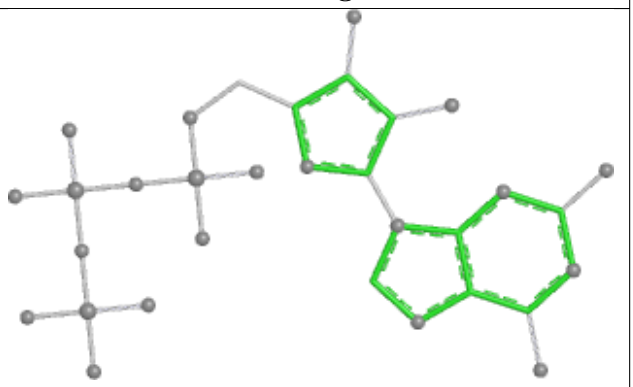
Bond lengths



Bond angles

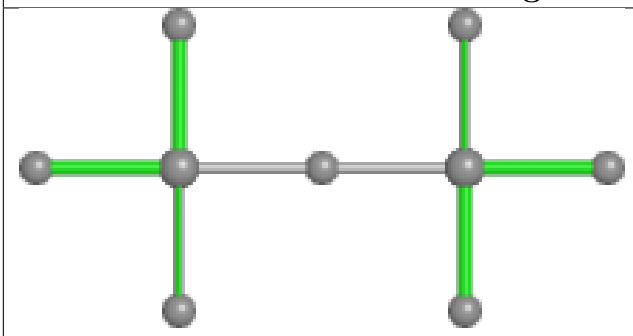


Torsions

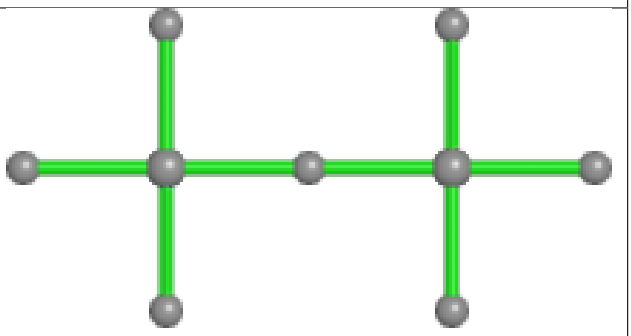


Rings

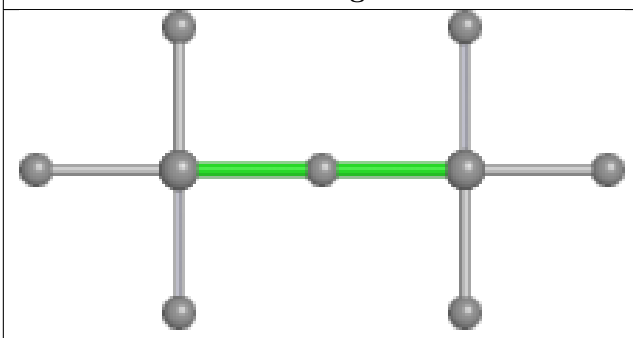
Ligand POP A 602



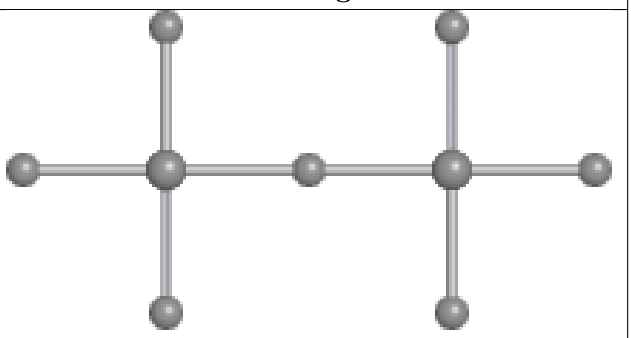
Bond lengths



Bond angles

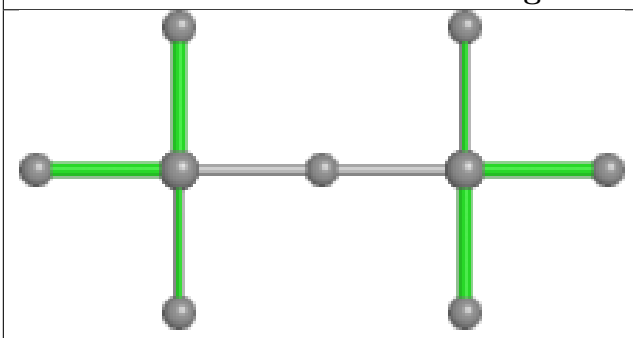


Torsions

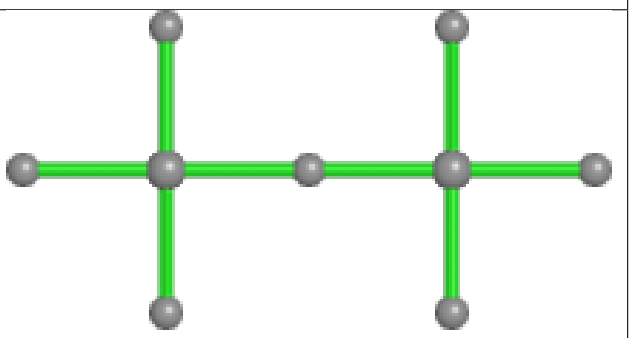


Rings

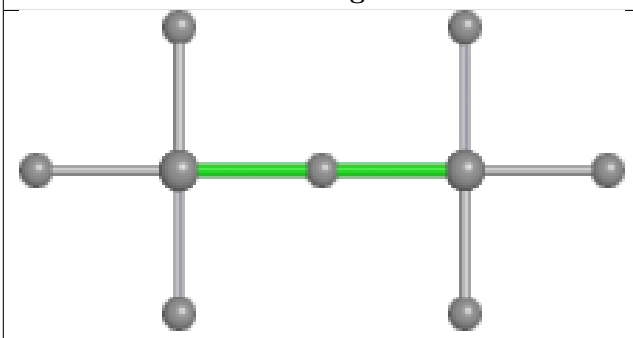
Ligand POP B 501



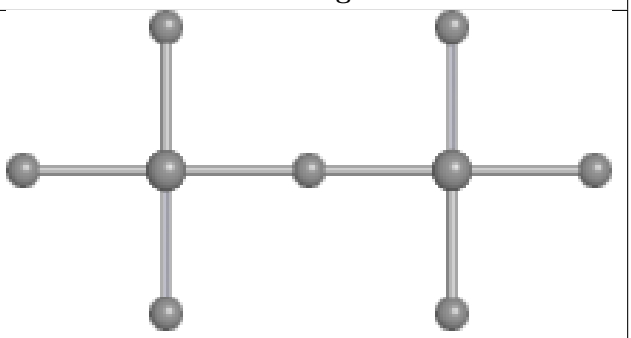
Bond lengths



Bond angles

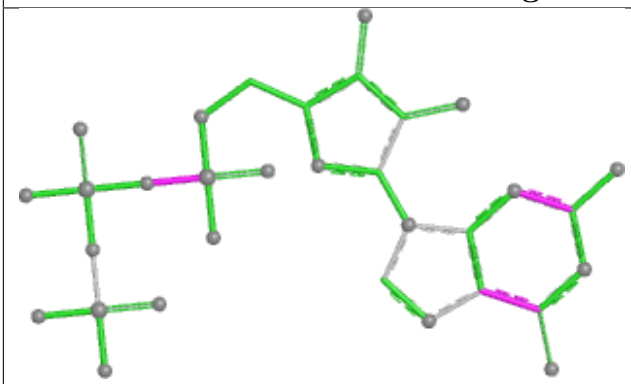


Torsions

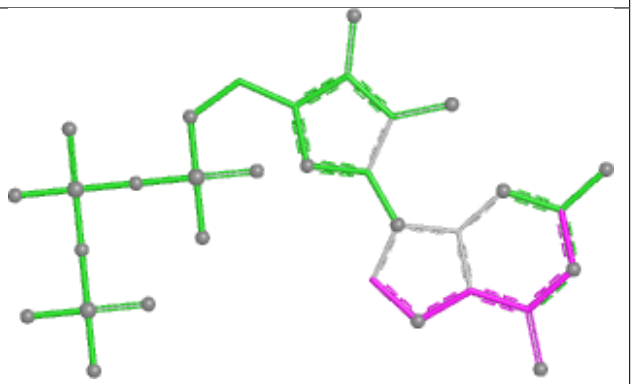


Rings

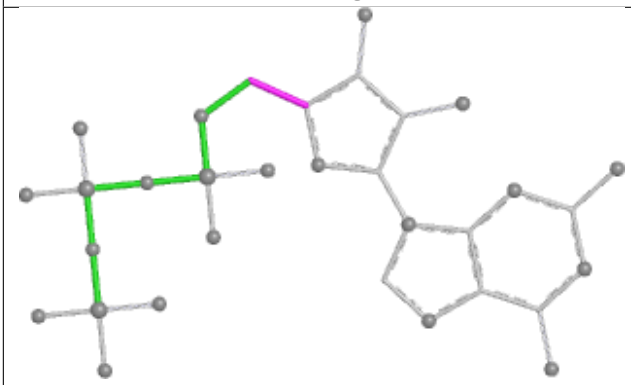
Ligand GTP A 603



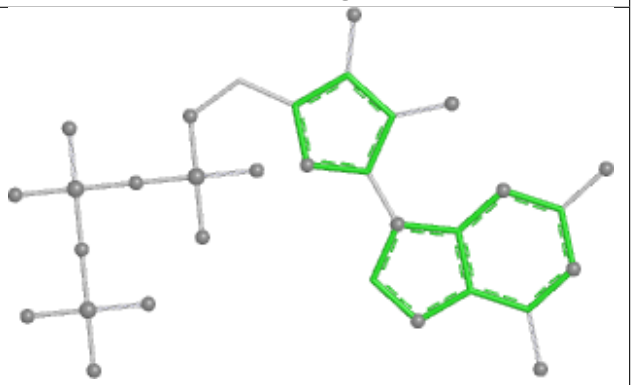
Bond lengths



Bond angles

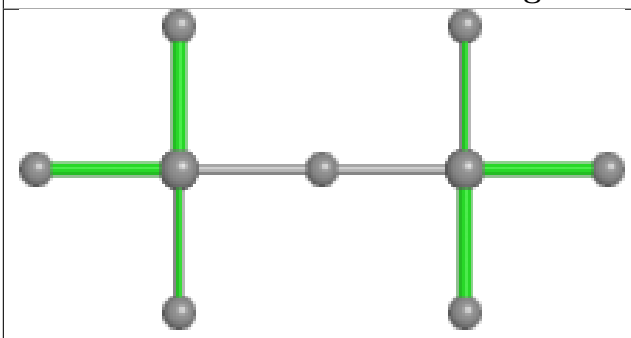


Torsions

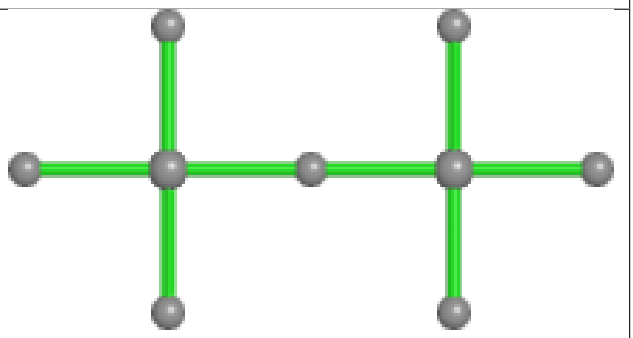


Rings

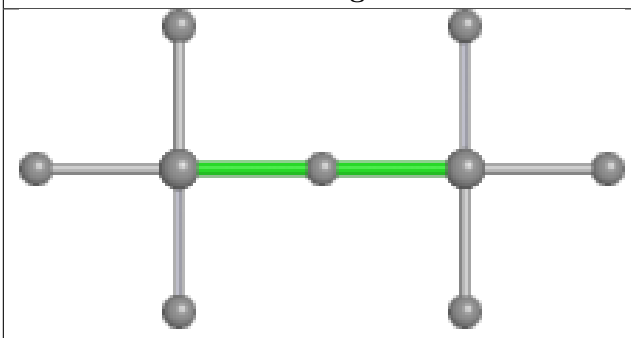
Ligand POP C 501



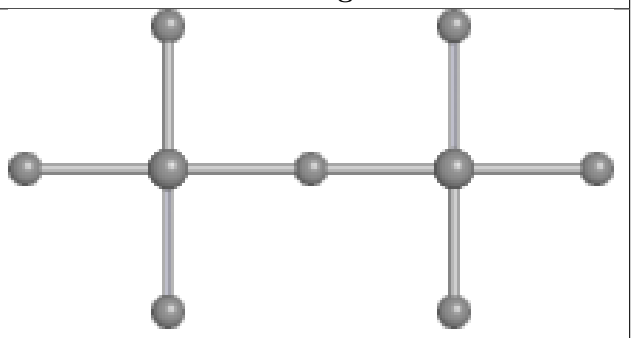
Bond lengths



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	440/483 (91%)	0.41	17 (3%)	44	45	28, 57, 106, 137	0
1	B	440/483 (91%)	0.64	30 (6%)	25	26	34, 65, 109, 131	0
1	C	440/483 (91%)	0.53	18 (4%)	42	43	33, 63, 103, 132	0
1	D	441/483 (91%)	0.43	18 (4%)	42	43	30, 57, 106, 135	0
All	All	1761/1932 (91%)	0.50	83 (4%)	37	38	28, 61, 106, 137	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	405	LEU	4.9
1	D	357	LEU	4.2
1	A	388	ASN	4.1
1	D	280	ILE	3.8
1	A	427	GLN	3.7
1	D	299	TYR	3.6
1	B	348	ILE	3.3
1	B	28	TRP	3.3
1	B	445	PRO	3.2
1	B	366	ILE	3.1
1	A	386	ASP	3.1
1	A	448	TYR	3.0
1	C	366	ILE	2.9
1	B	397	LEU	2.9
1	C	379	ILE	2.9
1	D	113	LEU	2.9
1	A	445	PRO	2.9
1	B	428	ILE	2.9
1	B	406	VAL	2.8
1	A	392	LEU	2.8
1	C	361	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	302	SER	2.7
1	D	302	SER	2.7
1	D	397	LEU	2.7
1	A	150	ASP	2.7
1	D	361	TYR	2.7
1	C	357	LEU	2.6
1	D	402	VAL	2.6
1	B	425	ILE	2.6
1	B	439	PHE	2.5
1	C	95	CYS	2.5
1	B	272	PRO	2.5
1	B	299	TYR	2.4
1	B	357	LEU	2.4
1	A	390	PRO	2.4
1	B	364	VAL	2.3
1	C	28	TRP	2.3
1	B	273	VAL	2.3
1	D	120	MET	2.3
1	D	403	SER	2.3
1	A	449	TYR	2.3
1	C	388	ASN	2.3
1	B	402	VAL	2.3
1	C	390	PRO	2.3
1	D	437	THR	2.3
1	B	112	HIS	2.3
1	A	379	ILE	2.3
1	C	29	ILE	2.3
1	D	356	GLY	2.3
1	B	151	LEU	2.2
1	C	445	PRO	2.2
1	B	440	PHE	2.2
1	B	379	ILE	2.2
1	A	424	LYS	2.2
1	B	405	LEU	2.2
1	B	390	PRO	2.2
1	C	432	PHE	2.2
1	A	355	ASP	2.2
1	C	325	PHE	2.2
1	B	350	ASP	2.2
1	B	392	LEU	2.2
1	C	392	LEU	2.2
1	D	352	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	448	TYR	2.2
1	D	149	TYR	2.2
1	B	345	THR	2.2
1	A	428	ILE	2.1
1	D	335	LEU	2.1
1	D	126	LYS	2.1
1	C	378	PRO	2.1
1	A	374	LYS	2.1
1	B	269	ALA	2.1
1	C	124	ASP	2.1
1	A	442	ILE	2.1
1	A	366	ILE	2.1
1	B	314	ILE	2.1
1	B	55	PRO	2.1
1	C	326	VAL	2.0
1	D	110	PHE	2.0
1	C	354	HIS	2.0
1	A	357	LEU	2.0
1	B	280	ILE	2.0
1	B	352	LEU	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
3	POP	C	501	9/9	0.76	0.19	74,74,74,74	9
5	CA	A	605	1/1	0.76	0.12	76,76,76,76	0
3	POP	A	602	9/9	0.82	0.16	69,69,69,69	9

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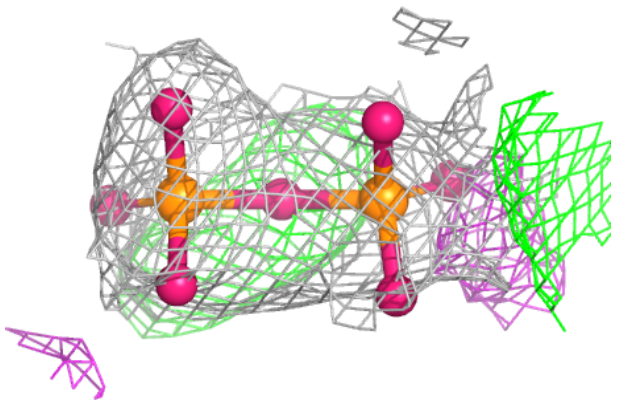
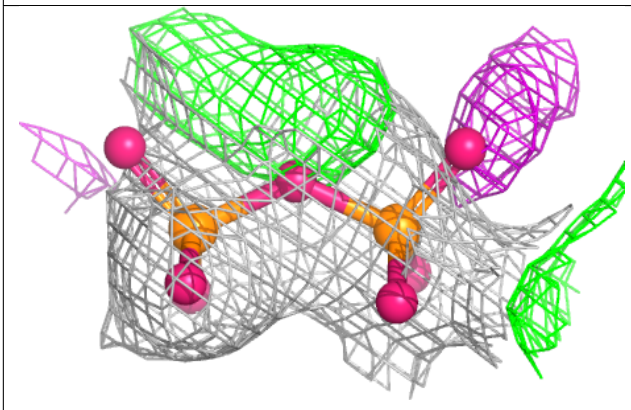
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	POP	B	501	9/9	0.84	0.19	66,66,66,66	9
3	POP	D	603	9/9	0.85	0.20	62,62,62,62	9
5	CA	B	503	1/1	0.87	0.10	82,82,82,82	0
5	CA	C	503	1/1	0.91	0.09	81,81,81,81	0
2	GTP	D	602	32/32	0.92	0.10	39,63,84,94	0
2	GTP	A	603	32/32	0.94	0.09	46,56,79,81	0
2	GTP	D	601	32/32	0.94	0.08	28,45,74,81	0
2	GTP	A	601	32/32	0.95	0.09	41,54,82,90	0
5	CA	D	605	1/1	0.96	0.08	80,80,80,80	0
4	MN	B	502	1/1	0.99	0.03	42,42,42,42	0
4	MN	C	502	1/1	0.99	0.06	44,44,44,44	0
4	MN	A	604	1/1	0.99	0.05	40,40,40,40	0
4	MN	D	604	1/1	1.00	0.05	36,36,36,36	0

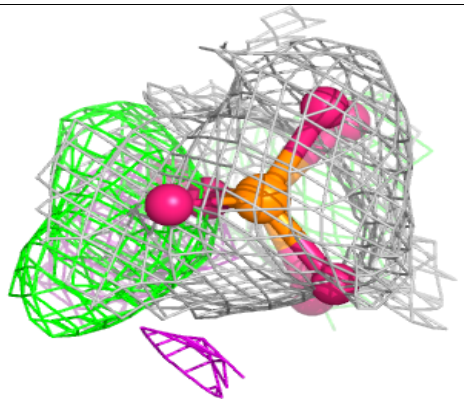
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around POP C 501:

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

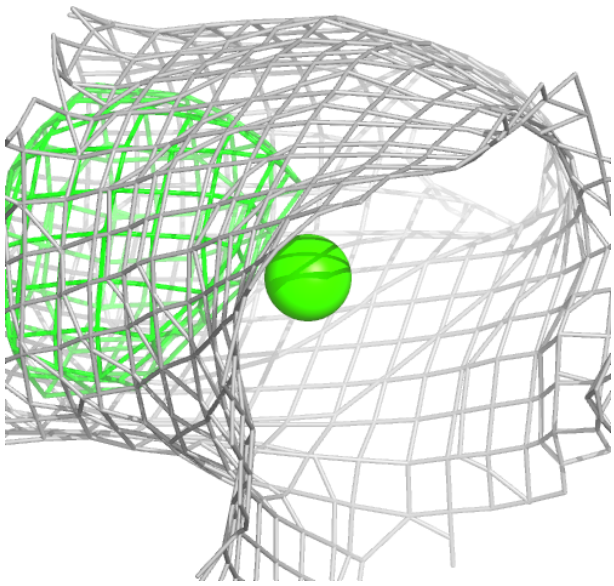


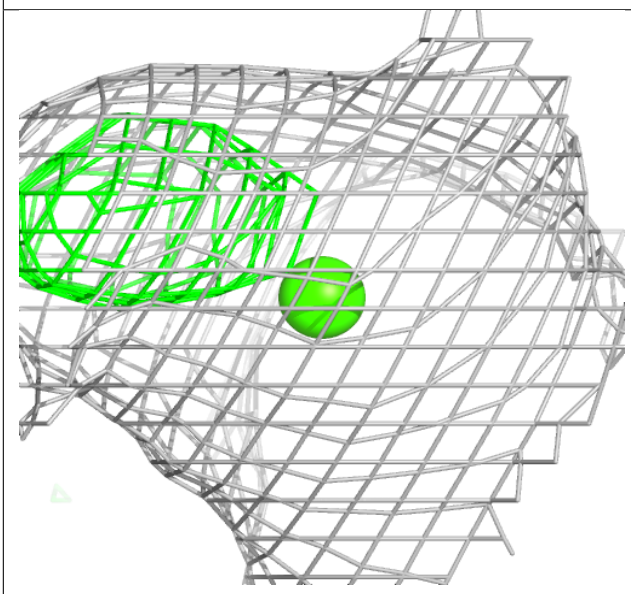


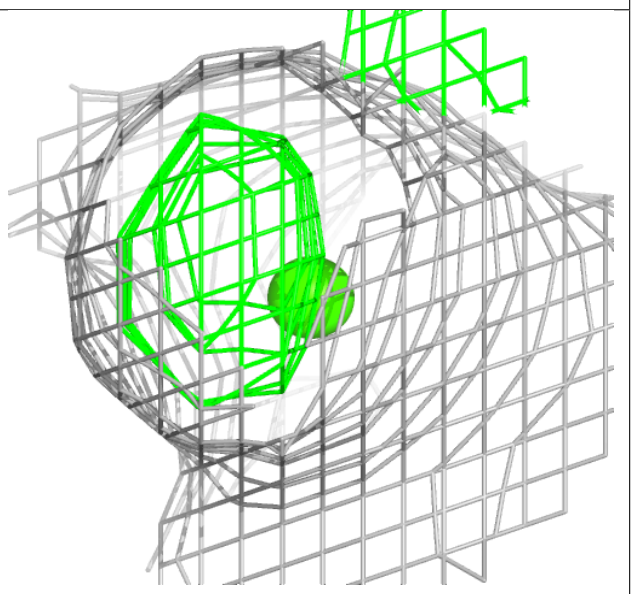


Electron density around CA A 605:

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

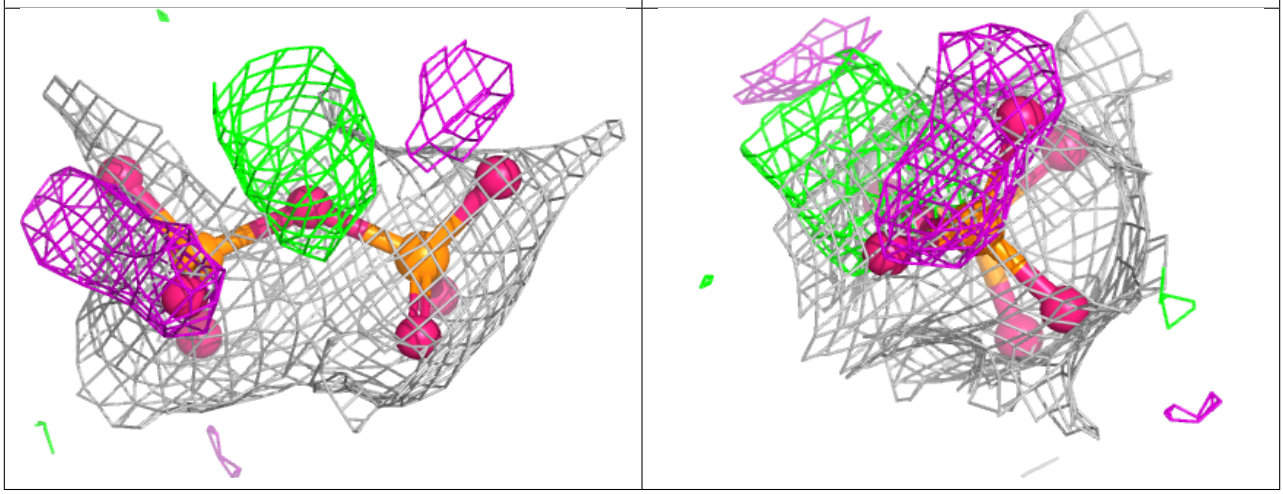






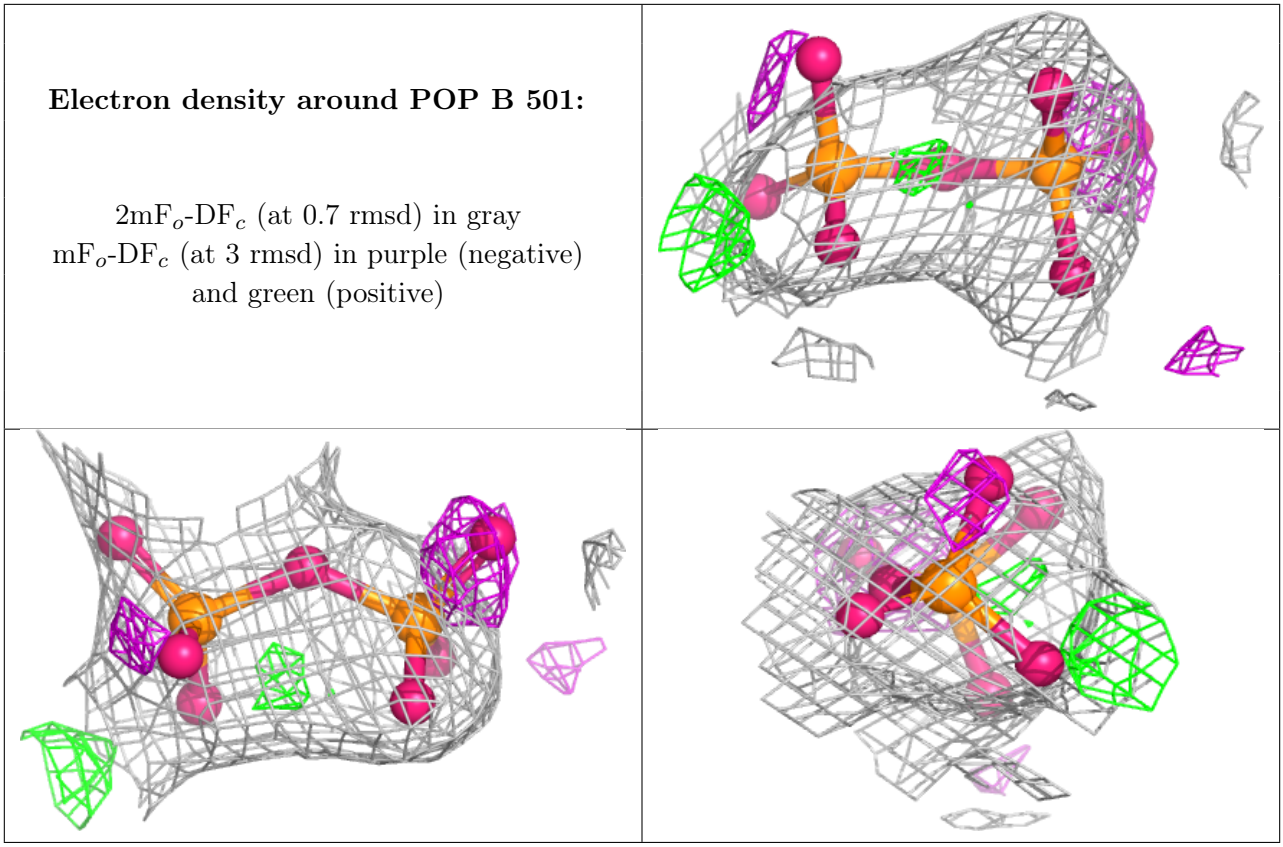
Electron density around POP A 602:

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



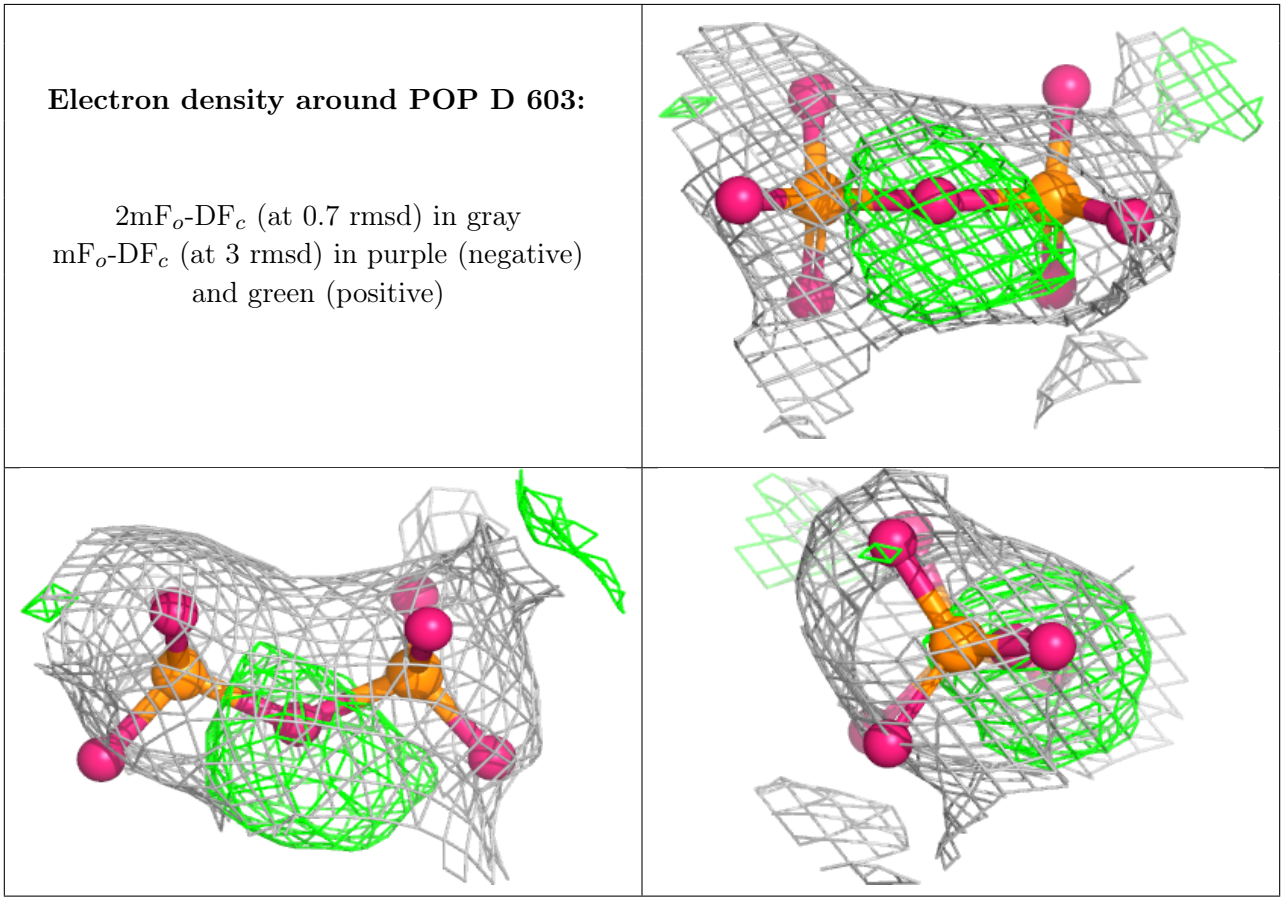
Electron density around POP B 501:

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



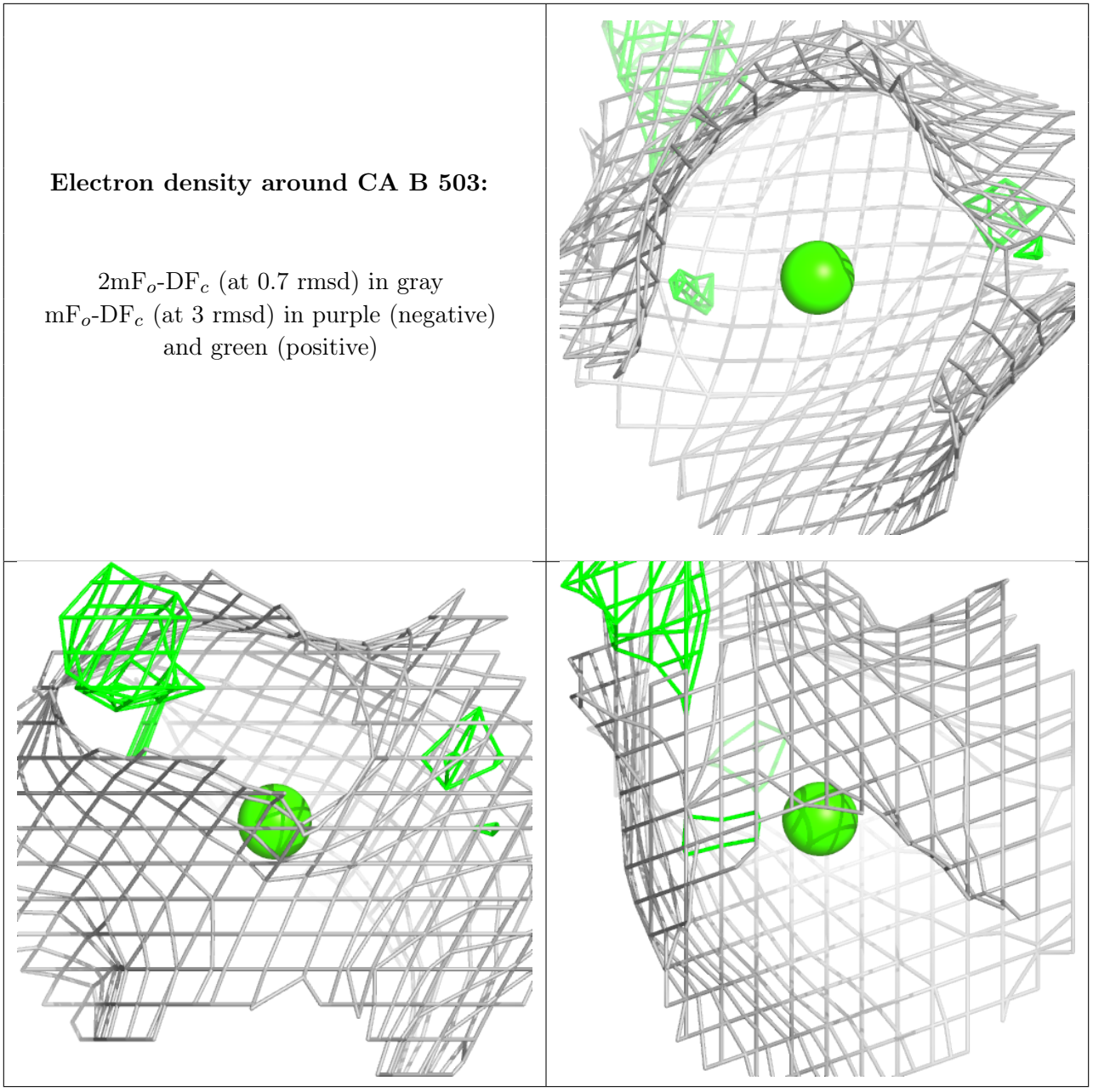
Electron density around POP D 603:

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



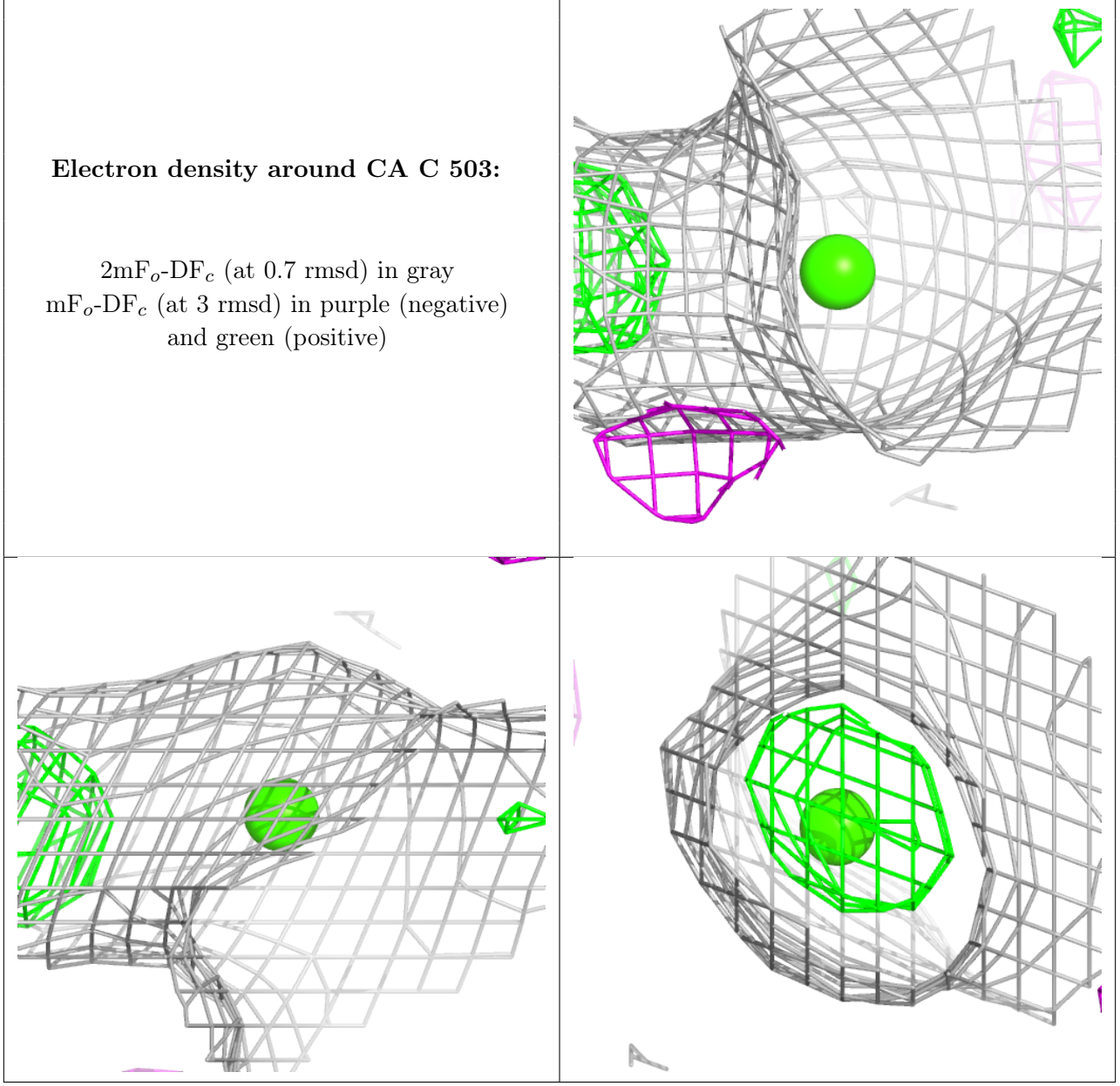
Electron density around CA B 503:

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



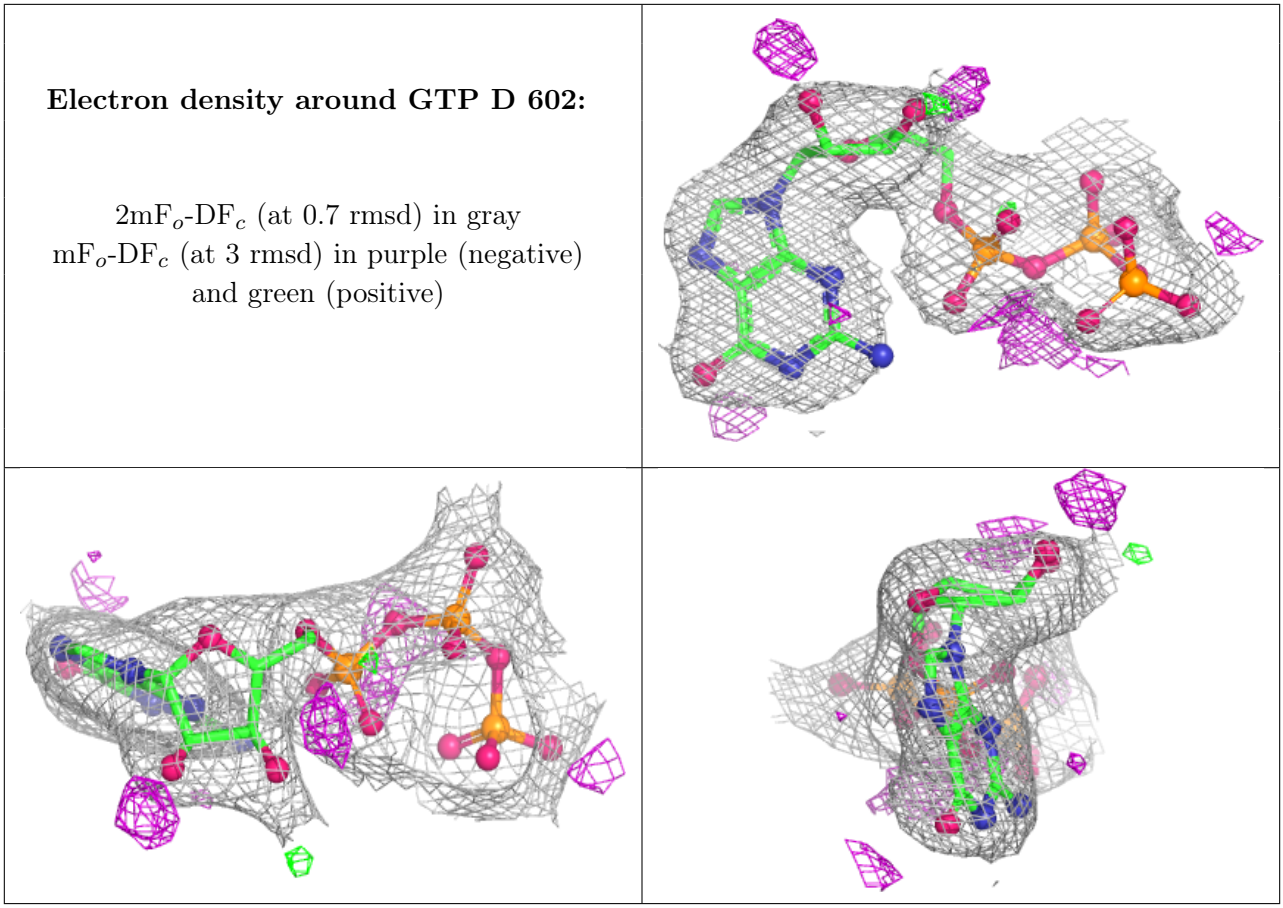
Electron density around CA C 503:

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



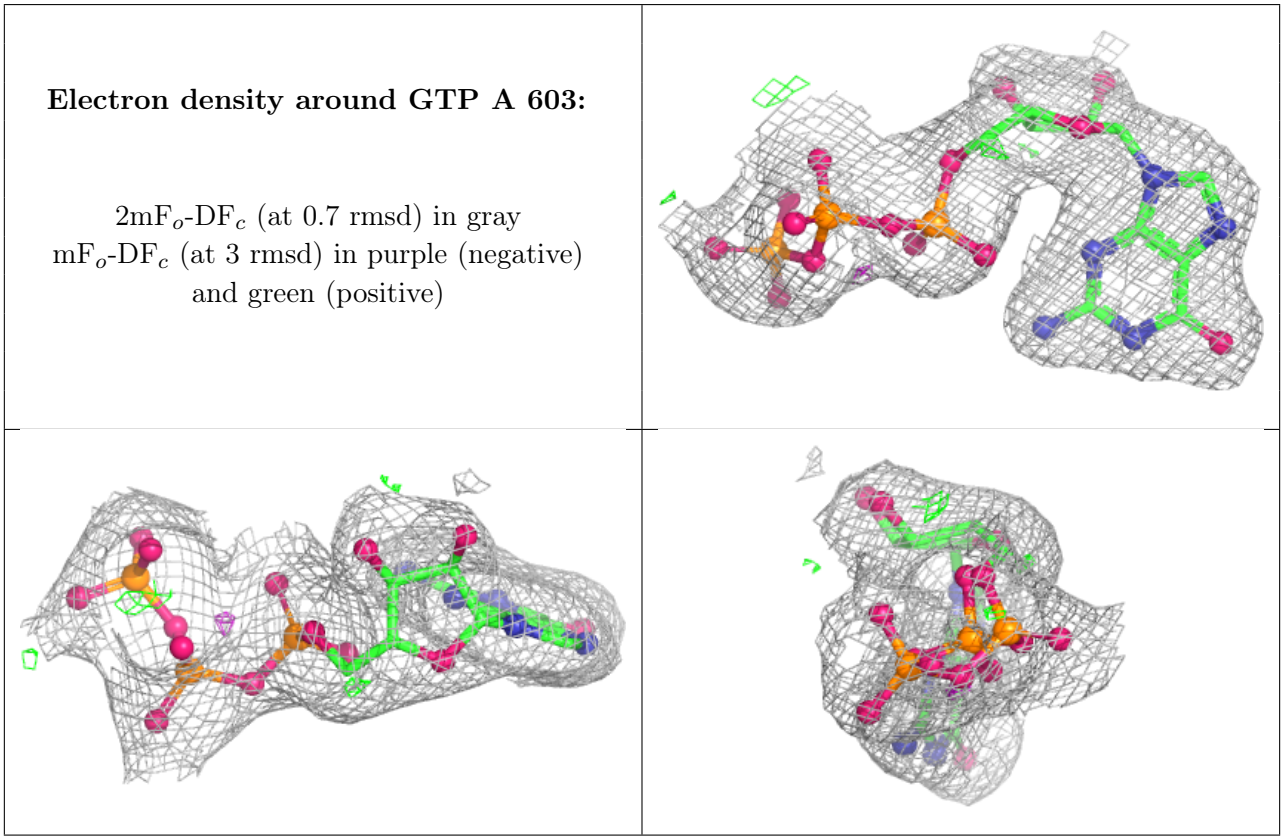
Electron density around GTP D 602:

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



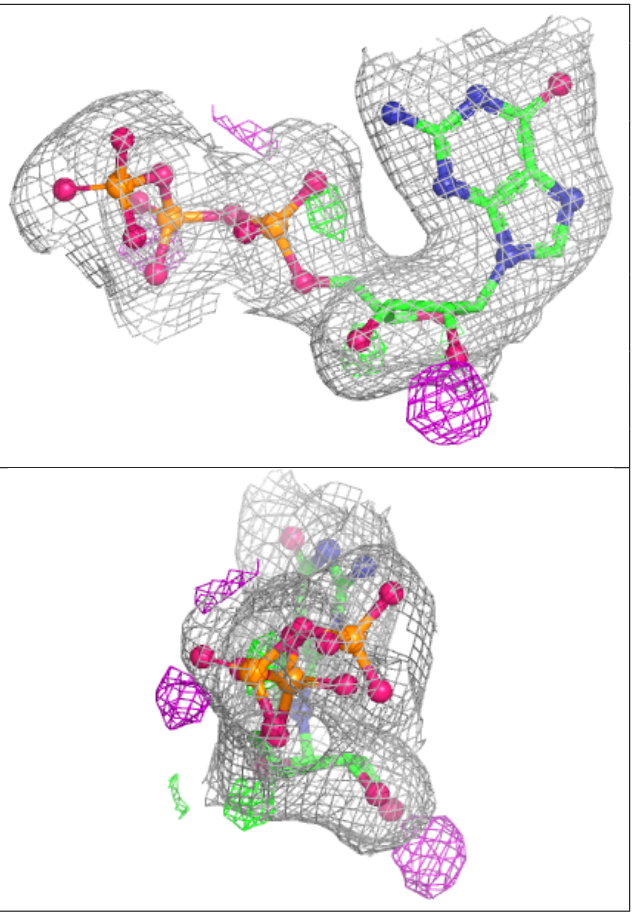
Electron density around GTP A 603:

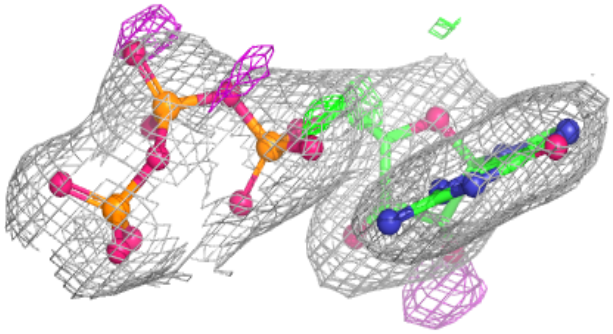
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP D 601:

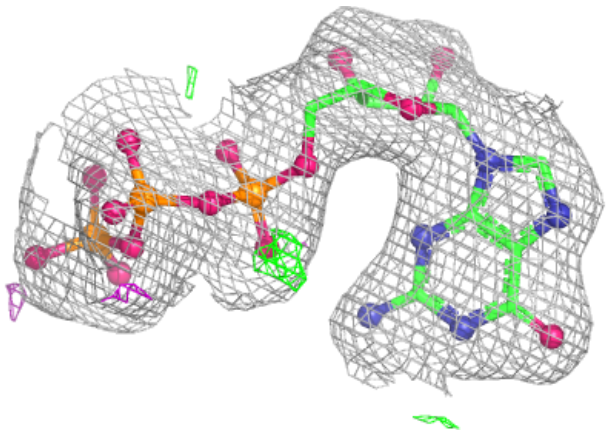
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

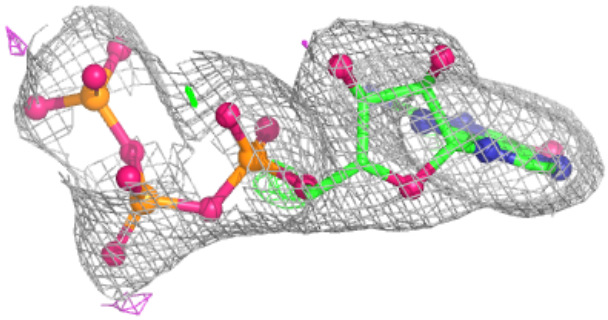


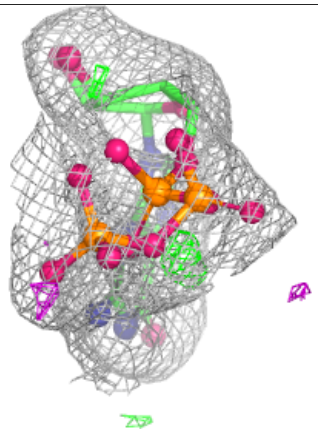


Electron density around GTP A 601:

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

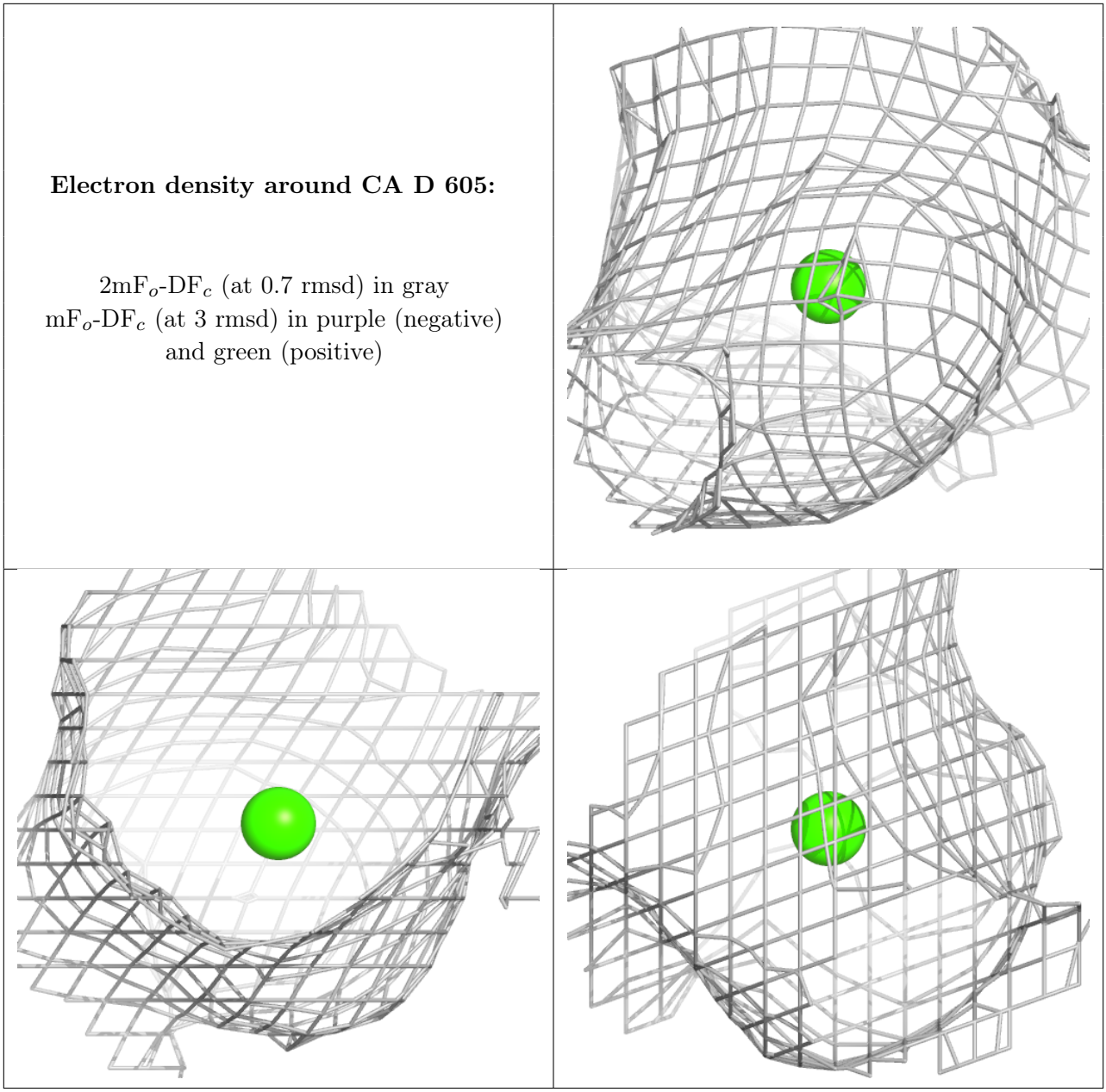






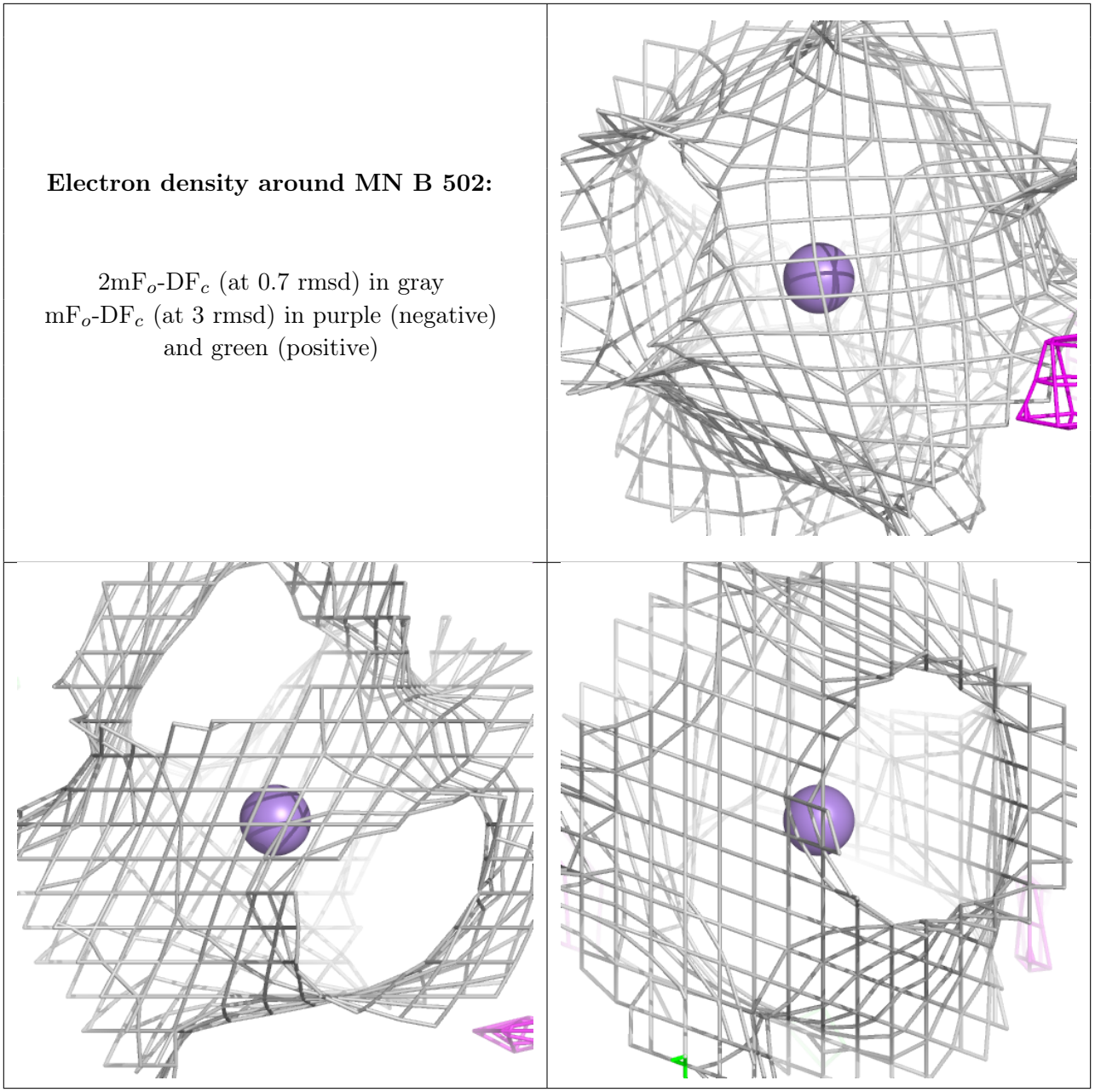
Electron density around CA D 605:

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



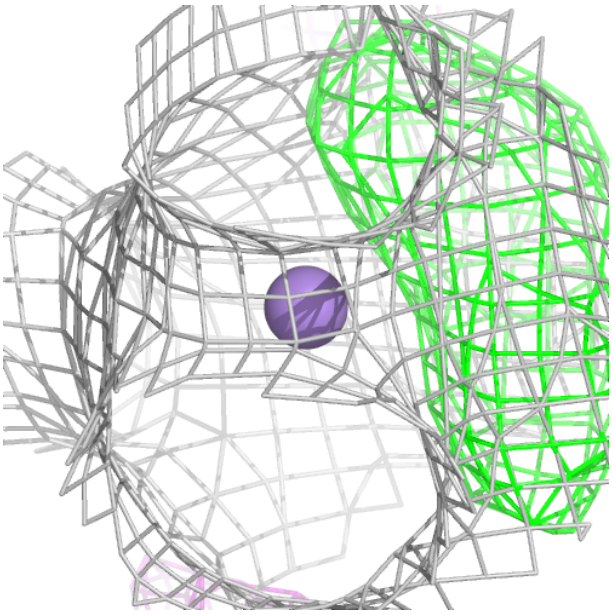
Electron density around MN B 502:

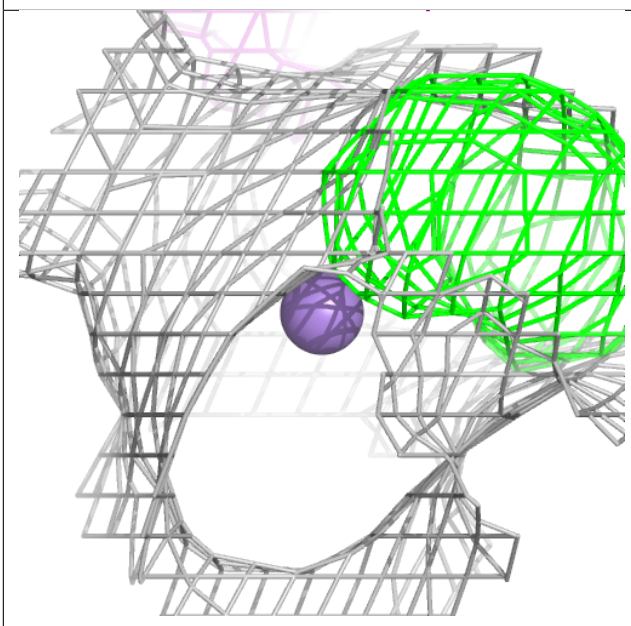
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

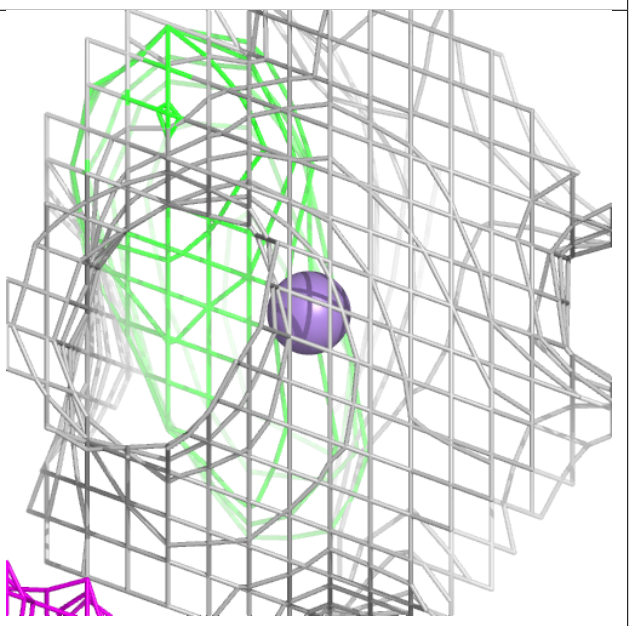


Electron density around MN C 502:

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

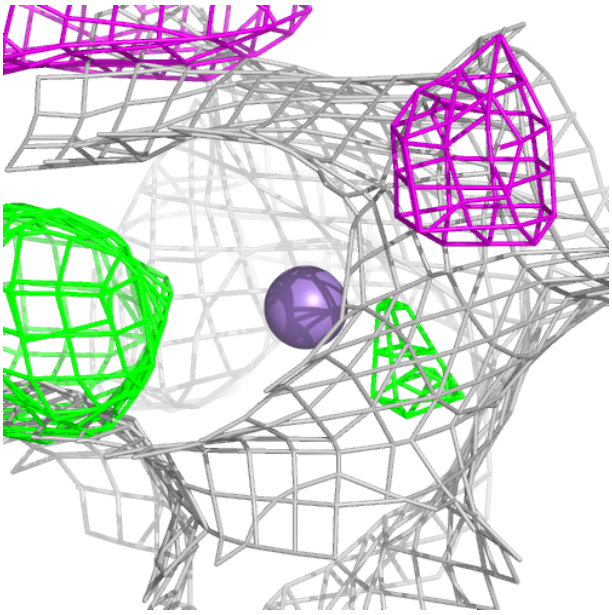


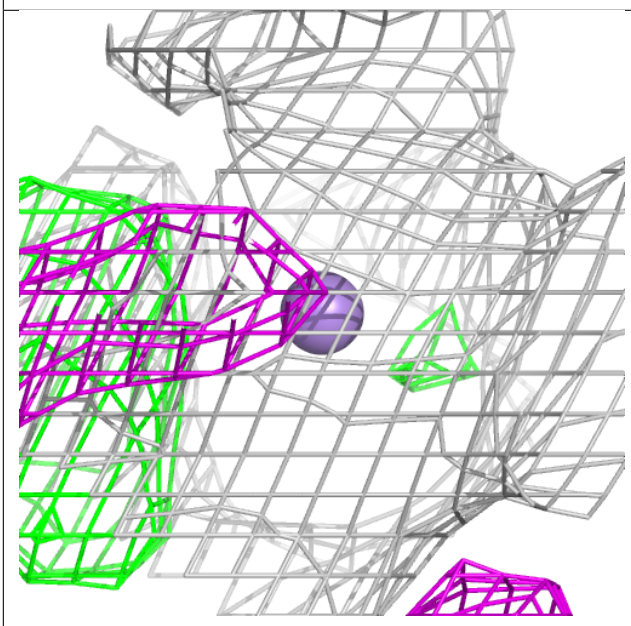


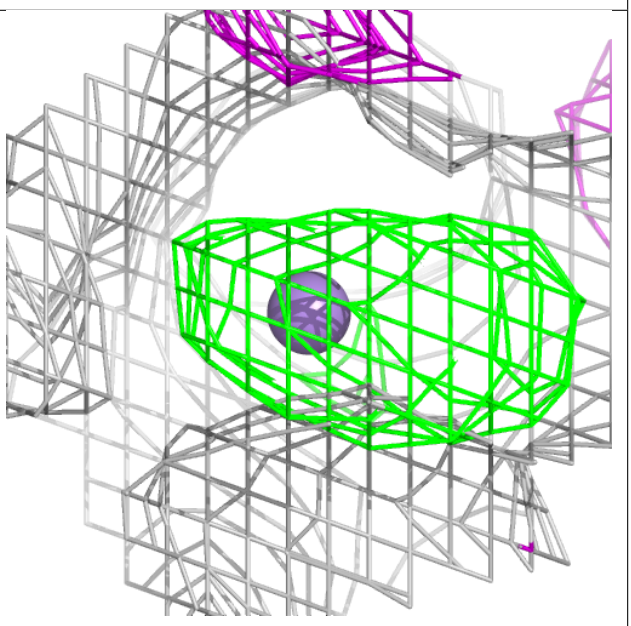


Electron density around MN A 604:

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

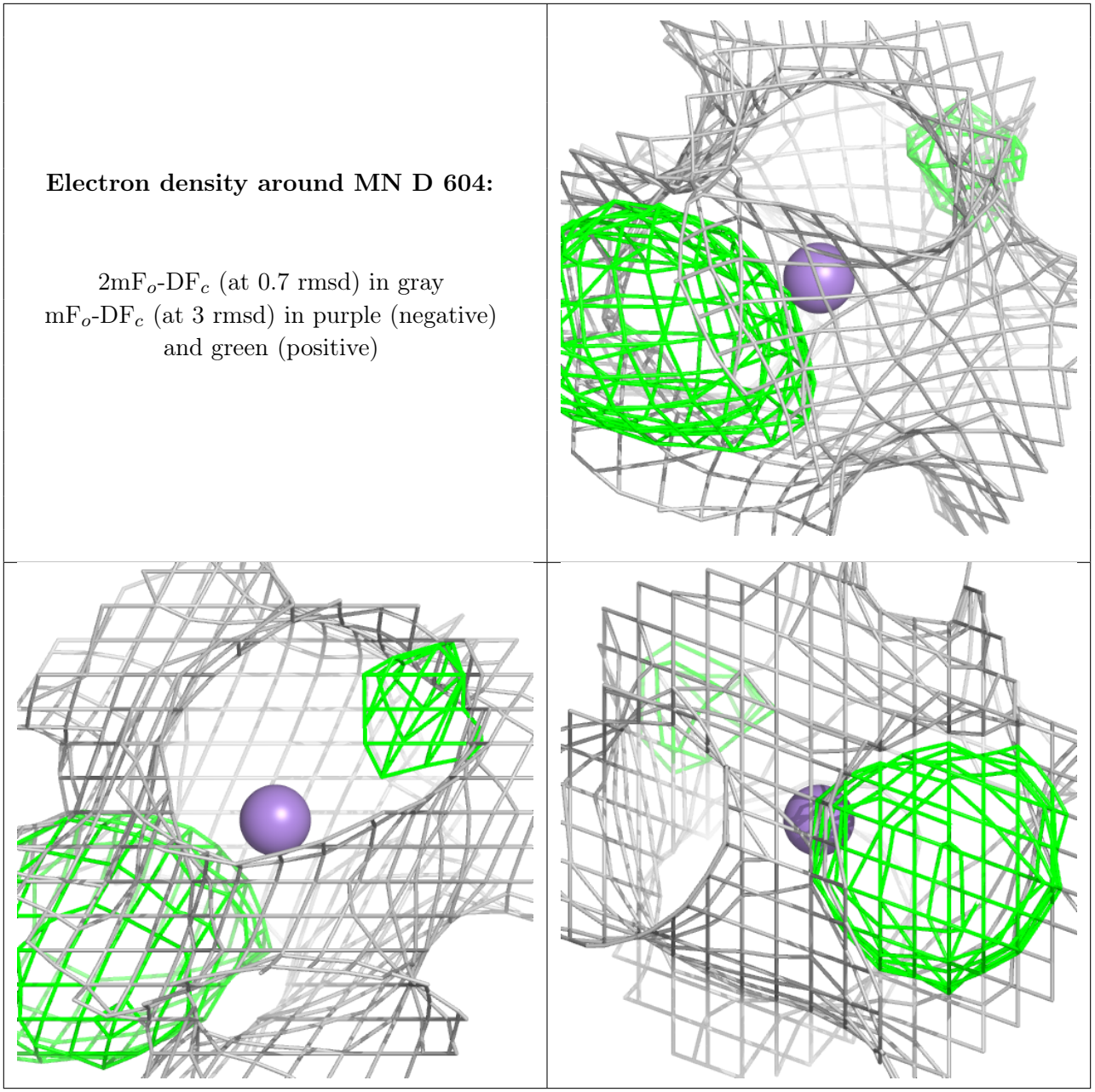






Electron density around MN D 604:

$2mF_o$-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.