Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 01:30 pm GMT

PDB ID	:	9QZ8 / pdb_00009qz8
Title	:	Crystal structure of sulfoacetaldehyde acetyltransferase in complex with ATP and inactive cofactor 3-deaza-ThDP
Authors	:	Zahn, M.; Rohwerder, T.
Deposited on	:	2025-04-22
Resolution	:	1.85 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:

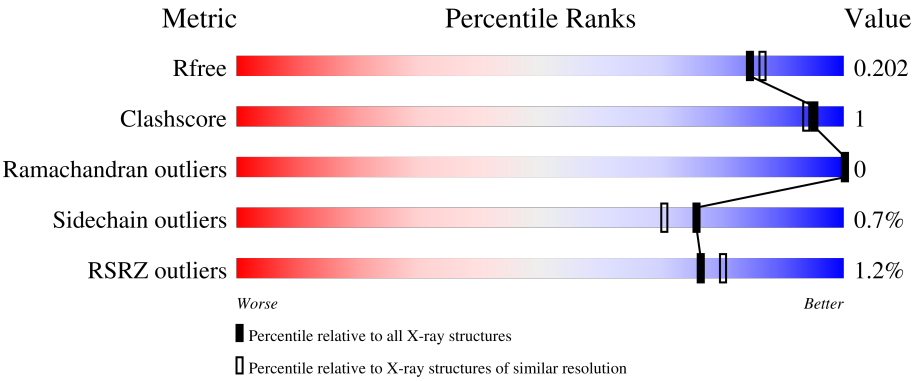
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.85 Å.

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



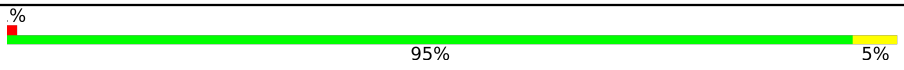
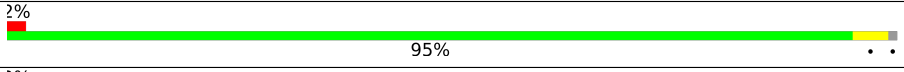
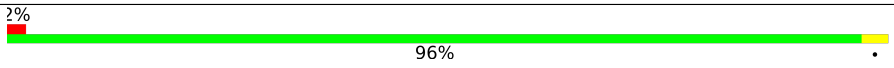
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	603	95%
1	B	603	96%
1	C	603	95%
1	D	603	95% 5%
1	E	603	94% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	603	
1	G	603	
1	H	603	

2 Entry composition (i)

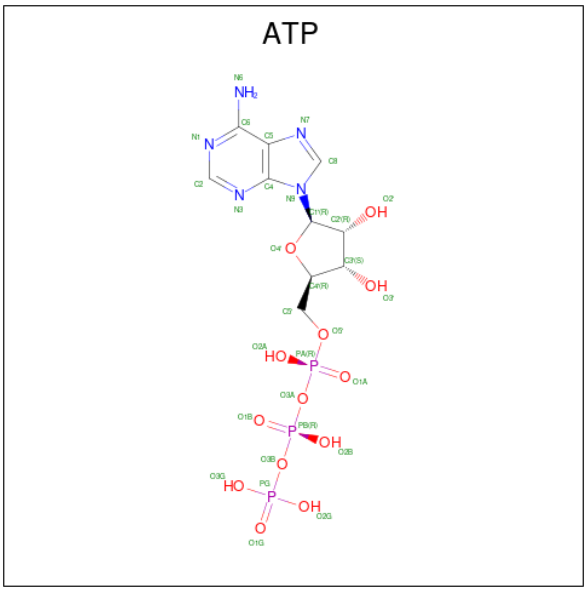
There are 6 unique types of molecules in this entry. The entry contains 39578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sulfoacetaldehyde acetyltransferase.

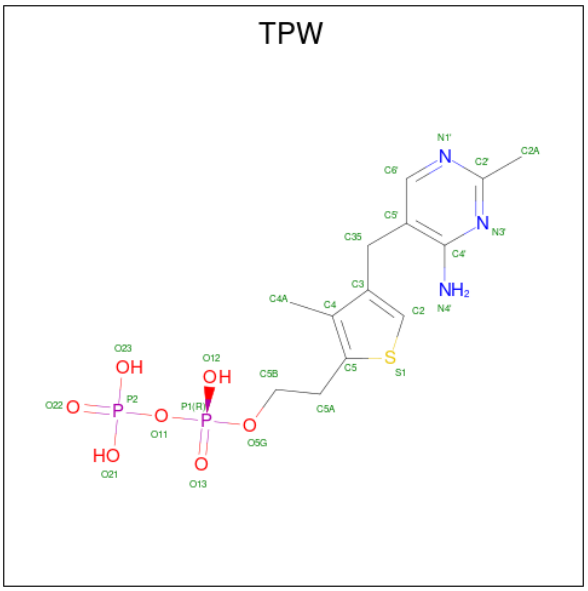
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4556	2870	799	848	39			
1	B	600	Total	C	N	O	S	0	0	0
			4556	2870	799	848	39			
1	C	599	Total	C	N	O	S	0	0	0
			4549	2866	798	846	39			
1	D	599	Total	C	N	O	S	0	0	0
			4549	2866	798	846	39			
1	E	599	Total	C	N	O	S	0	0	0
			4549	2866	798	846	39			
1	F	600	Total	C	N	O	S	0	1	0
			4559	2872	799	849	39			
1	G	599	Total	C	N	O	S	0	0	0
			4549	2866	798	846	39			
1	H	600	Total	C	N	O	S	0	0	0
			4556	2870	799	848	39			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TPW) (formula: $C_{13}H_{19}N_3O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	G	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
3	H	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

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

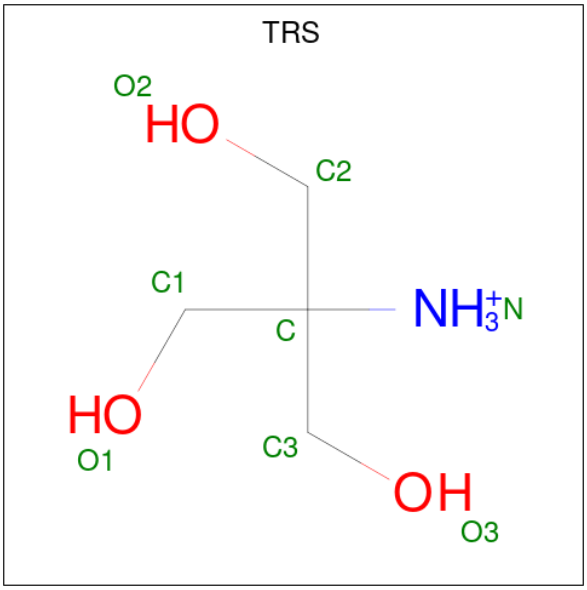
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	424	Total O 424 424	0	0
6	B	422	Total O 422 422	0	0
6	C	367	Total O 367 367	0	0

Continued on next page...

Continued from previous page...

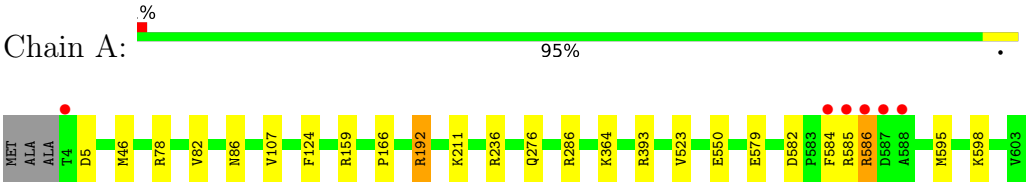
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	358	Total O 358 358	0	0
6	E	312	Total O 312 312	0	0
6	F	354	Total O 354 354	0	0
6	G	247	Total O 247 247	0	0
6	H	199	Total O 199 199	0	0

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.

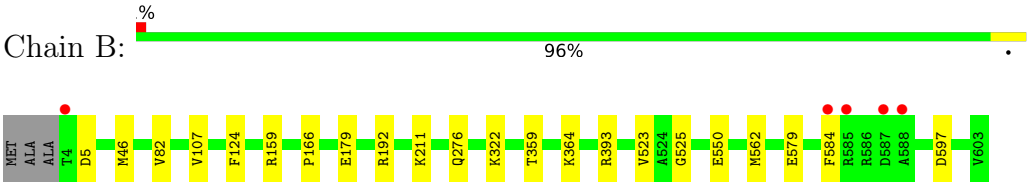
• Molecule 1: Sulfoacetaldehyde acetyltransferase

Chain A:



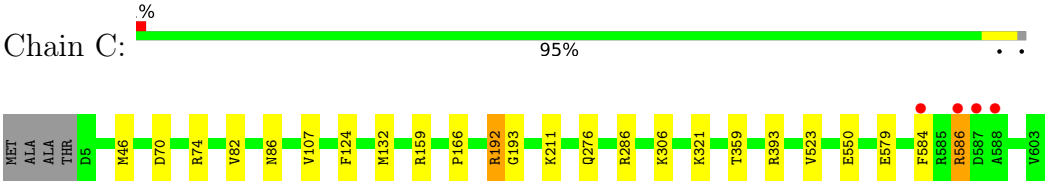
• Molecule 1: Sulfoacetaldehyde acetyltransferase

Chain B:



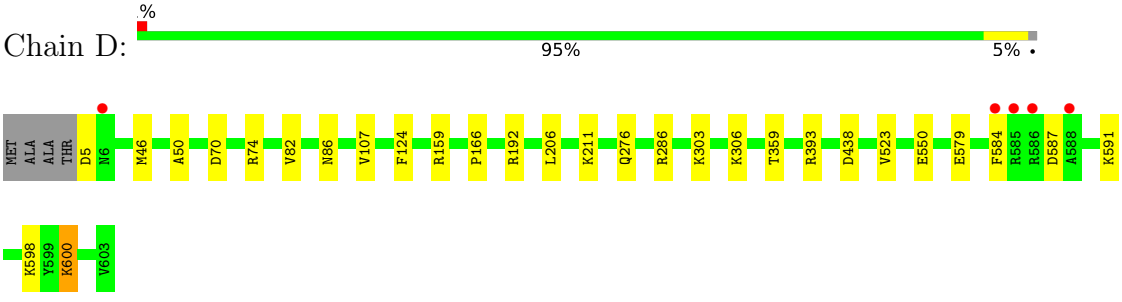
• Molecule 1: Sulfoacetaldehyde acetyltransferase

Chain C:



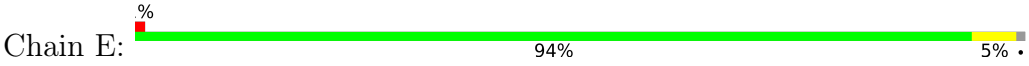
• Molecule 1: Sulfoacetaldehyde acetyltransferase

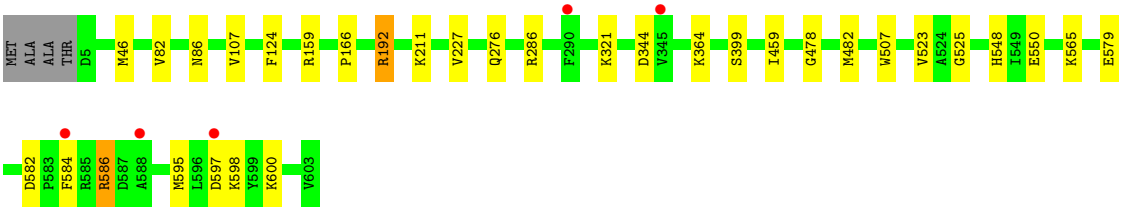
Chain D:



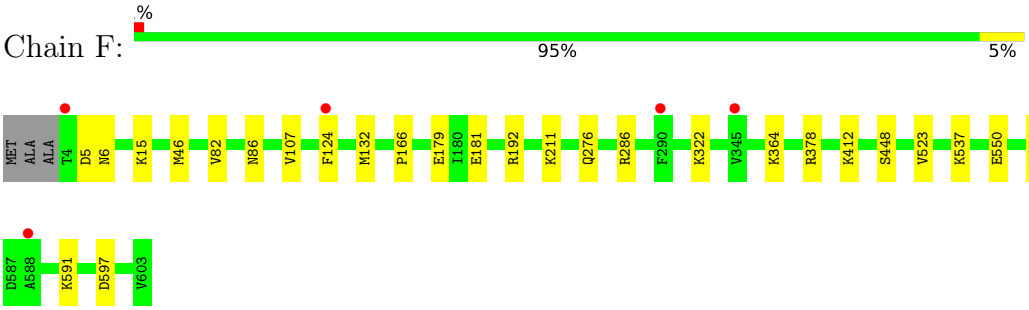
• Molecule 1: Sulfoacetaldehyde acetyltransferase

Chain E:

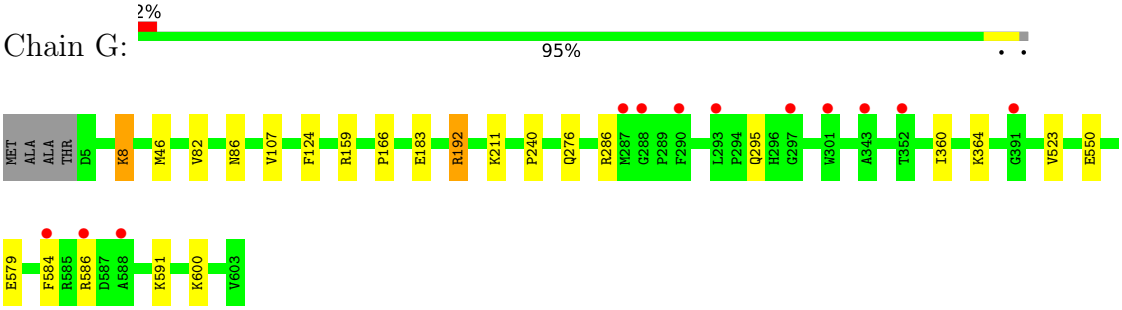




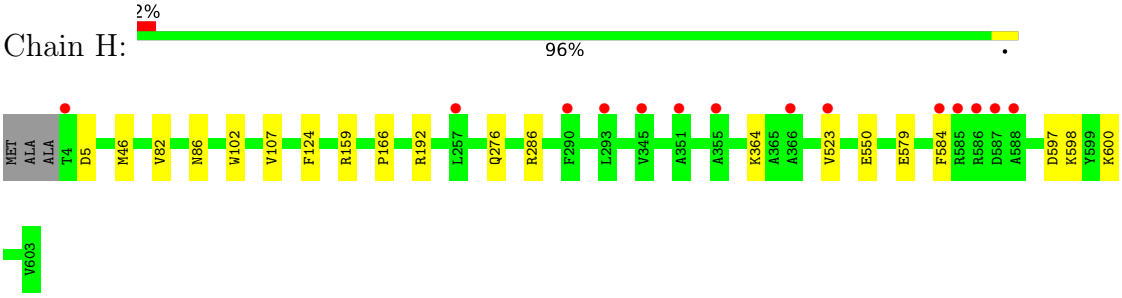
• Molecule 1: Sulfoacetaldehyde acetyltransferase



• Molecule 1: Sulfoacetaldehyde acetyltransferase



• Molecule 1: Sulfoacetaldehyde acetyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	360.08Å 81.59Å 174.82Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	174.82 – 1.85 174.82 – 1.85	Depositor EDS
% Data completeness (in resolution range)	65.9 (174.82-1.85) 65.9 (174.82-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.170 , 0.202 0.170 , 0.202	Depositor DCC
R_{free} test set	14243 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	39578	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: ATP, TRS, TPW, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/4655	1.06	9/6295 (0.1%)
1	B	0.64	0/4655	1.06	13/6295 (0.2%)
1	C	0.61	0/4648	1.05	10/6285 (0.2%)
1	D	0.62	0/4648	1.04	13/6285 (0.2%)
1	E	0.59	0/4648	1.04	9/6285 (0.1%)
1	F	0.60	0/4661	1.05	15/6303 (0.2%)
1	G	0.58	0/4648	1.04	11/6285 (0.2%)
1	H	0.57	0/4655	1.03	9/6295 (0.1%)
All	All	0.61	0/37218	1.05	89/50328 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	4
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	4
1	H	0	2
All	All	0	18

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	579	GLU	CB-CA-C	-9.48	93.99	109.72
1	A	579	GLU	CB-CA-C	-9.43	94.07	109.72
1	D	579	GLU	CB-CA-C	-9.29	94.31	109.72
1	H	579	GLU	CB-CA-C	-9.05	94.69	109.72
1	F	124	PHE	N-CA-CB	-8.96	96.81	109.97
1	F	579	GLU	CB-CA-C	-8.93	94.89	109.72
1	D	124	PHE	N-CA-CB	-8.85	96.97	109.97
1	B	124	PHE	N-CA-CB	-8.81	96.76	110.06
1	A	124	PHE	N-CA-CB	-8.77	97.07	109.97
1	E	579	GLU	CB-CA-C	-8.73	95.23	109.72
1	G	124	PHE	N-CA-CB	-8.71	97.16	109.97
1	H	124	PHE	N-CA-CB	-8.69	97.20	109.97
1	E	124	PHE	N-CA-CB	-8.60	97.08	110.06
1	C	124	PHE	N-CA-CB	-8.47	97.52	109.97
1	A	192	ARG	CA-C-N	-8.29	113.43	122.55
1	A	192	ARG	C-N-CA	-8.29	113.43	122.55
1	E	192	ARG	CA-C-N	-7.94	113.82	122.55
1	E	192	ARG	C-N-CA	-7.94	113.82	122.55
1	F	378	ARG	CG-CD-NE	-7.68	95.11	112.00
1	D	192	ARG	N-CA-C	7.51	119.55	111.36
1	C	192	ARG	CA-C-N	-7.09	113.67	122.75
1	C	192	ARG	C-N-CA	-7.09	113.67	122.75
1	G	192	ARG	CA-C-N	-7.06	113.71	122.75
1	G	192	ARG	C-N-CA	-7.06	113.71	122.75
1	D	393	ARG	CA-CB-CG	7.02	128.15	114.10
1	D	600	LYS	CG-CD-CE	6.76	126.84	111.30
1	G	591	LYS	CG-CD-CE	6.57	126.41	111.30
1	H	550	GLU	CB-CG-CD	6.53	123.71	112.60
1	B	5	ASP	CA-CB-CG	6.45	119.05	112.60
1	G	8	LYS	CG-CD-CE	6.35	125.91	111.30
1	G	600	LYS	CG-CD-CE	-6.22	97.00	111.30
1	G	550	GLU	CB-CG-CD	6.20	123.14	112.60
1	F	192	ARG	N-CA-C	6.18	118.09	111.36
1	H	192	ARG	N-CA-C	6.16	118.07	111.36
1	D	550	GLU	CB-CG-CD	6.06	122.90	112.60
1	B	550	GLU	CB-CG-CD	6.03	122.84	112.60
1	B	584	PHE	CA-CB-CG	6.03	119.83	113.80
1	E	550	GLU	CB-CG-CD	6.03	122.84	112.60
1	A	550	GLU	CB-CG-CD	6.00	122.80	112.60
1	D	584	PHE	CA-CB-CG	5.95	119.75	113.80
1	G	600	LYS	CB-CG-CD	5.87	124.80	111.30
1	G	584	PHE	CA-CB-CG	5.87	119.67	113.80
1	H	192	ARG	CA-C-N	-5.86	113.57	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	192	ARG	C-N-CA	-5.86	113.57	122.06
1	H	5	ASP	CA-CB-CG	5.80	118.40	112.60
1	F	550	GLU	CB-CG-CD	5.80	122.45	112.60
1	C	584	PHE	CA-CB-CG	5.76	119.56	113.80
1	C	393	ARG	CB-CG-CD	5.73	124.47	111.30
1	F	5	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	550	GLU	CB-CG-CD	5.66	122.23	112.60
1	F	192	ARG	CA-C-N	-5.63	113.90	122.06
1	F	192	ARG	C-N-CA	-5.63	113.90	122.06
1	H	584	PHE	CA-CB-CG	5.60	119.40	113.80
1	F	276	GLN	CB-CA-C	-5.54	100.83	110.09
1	B	192	ARG	CA-C-N	-5.51	114.06	122.06
1	B	192	ARG	C-N-CA	-5.51	114.06	122.06
1	E	227	VAL	N-CA-CB	5.51	117.00	110.55
1	A	584	PHE	CA-CB-CG	5.49	119.29	113.80
1	G	276	GLN	CB-CA-C	-5.48	100.93	110.09
1	C	359	THR	CA-CB-OG1	-5.44	101.44	109.60
1	D	600	LYS	CB-CG-CD	5.43	123.79	111.30
1	B	276	GLN	CB-CA-C	-5.39	101.08	110.09
1	A	5	ASP	CA-CB-CG	5.36	117.96	112.60
1	E	584	PHE	CA-CB-CG	5.35	119.15	113.80
1	H	276	GLN	CB-CA-C	-5.34	101.17	110.09
1	A	276	GLN	CB-CA-C	-5.34	101.18	110.09
1	F	378	ARG	CD-NE-CZ	5.32	131.85	124.40
1	B	579	GLU	CG-CD-OE1	-5.29	106.23	118.40
1	B	562	MET	CB-CA-C	-5.27	102.04	110.79
1	C	276	GLN	CB-CA-C	-5.27	101.29	110.09
1	B	322	LYS	N-CA-CB	-5.26	101.89	109.83
1	E	211	LYS	CB-CA-C	-5.24	100.21	110.11
1	B	211	LYS	CB-CA-C	-5.23	100.23	110.11
1	C	211	LYS	CB-CA-C	-5.22	100.24	110.11
1	F	584	PHE	CA-CB-CG	5.22	119.03	113.80
1	D	211	LYS	CB-CA-C	-5.21	100.25	110.11
1	E	276	GLN	CB-CA-C	-5.19	101.42	110.09
1	G	211	LYS	CB-CA-C	-5.17	100.35	110.11
1	D	5	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	359	THR	CA-CB-OG1	-5.13	101.90	109.60
1	F	132	MET	CB-CA-C	-5.13	102.27	110.79
1	B	359	THR	CA-CB-OG1	-5.13	101.91	109.60
1	F	378	ARG	CB-CG-CD	-5.13	99.51	111.30
1	D	587	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	132	MET	CB-CA-C	-5.08	102.35	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LYS	CB-CA-C	-5.07	100.52	110.11
1	F	211	LYS	CB-CA-C	-5.07	100.53	110.11
1	D	276	GLN	CB-CA-C	-5.06	101.64	110.09
1	F	412	LYS	CG-CD-CE	5.01	122.82	111.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain
1	A	286	ARG	Sidechain
1	B	159	ARG	Sidechain
1	C	159	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	579	GLU	Sidechain
1	C	586	ARG	Sidechain
1	D	159	ARG	Sidechain
1	D	286	ARG	Sidechain
1	E	159	ARG	Sidechain
1	E	286	ARG	Sidechain
1	F	286	ARG	Sidechain
1	G	159	ARG	Sidechain
1	G	286	ARG	Sidechain
1	G	579	GLU	Sidechain
1	G	586	ARG	Sidechain
1	H	159	ARG	Sidechain
1	H	286	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4556	0	4504	15	0
1	B	4556	0	4504	7	0
1	C	4549	0	4497	11	0
1	D	4549	0	4497	12	0
1	E	4549	0	4497	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4559	0	4509	13	0
1	G	4549	0	4497	10	0
1	H	4556	0	4504	7	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	1	0
2	G	31	0	12	0	0
2	H	31	0	12	1	0
3	A	26	0	16	0	0
3	B	26	0	16	0	0
3	C	26	0	16	0	0
3	D	26	0	16	0	0
3	E	26	0	16	0	0
3	F	26	0	16	0	0
3	G	26	0	16	0	0
3	H	26	0	16	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
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	C	8	0	12	0	0
6	A	424	0	0	7	0
6	B	422	0	0	3	0
6	C	367	0	0	6	0
6	D	358	0	0	4	0
6	E	312	0	0	9	0
6	F	354	0	0	4	0
6	G	247	0	0	5	0
6	H	199	0	0	1	0
All	All	39578	0	36245	84	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 1.

All (84) 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:E:482:MET:HE1	1:E:507:TRP:CH2	1.86	1.11
1:E:482:MET:HE1	1:E:507:TRP:HH2	1.09	1.09
1:C:192:ARG:HD3	6:C:815:HOH:O	1.54	1.08
1:E:482:MET:CE	1:E:507:TRP:HH2	1.76	0.97
1:A:393:ARG:HD3	6:A:1117:HOH:O	1.65	0.97
1:G:192:ARG:HD3	6:G:802:HOH:O	1.66	0.93
1:A:192:ARG:HD3	6:A:803:HOH:O	1.70	0.92
1:E:478:GLY:O	1:E:482:MET:HE3	1.75	0.87
1:C:321:LYS:HE2	6:C:1112:HOH:O	1.74	0.86
1:F:322:LYS:NZ	1:G:183:GLU:OE1	2.11	0.83
1:G:295:GLN:OE1	6:G:801:HOH:O	2.01	0.79
6:C:879:HOH:O	1:D:598:LYS:HE3	1.87	0.73
1:G:46:MET:HE3	1:H:523:VAL:HG23	1.70	0.72
1:E:482:MET:CE	1:E:507:TRP:CH2	2.59	0.71
1:C:193:GLY:N	6:C:801:HOH:O	2.08	0.71
1:E:321:LYS:HE2	6:E:1063:HOH:O	1.92	0.68
1:F:585:ARG:O	1:F:586:ARG:HB2	1.93	0.67
1:G:46:MET:HE3	1:H:523:VAL:CG2	2.25	0.67
1:E:192:ARG:O	6:E:801:HOH:O	2.13	0.66
1:D:303:LYS:HE2	6:D:863:HOH:O	1.97	0.64
1:A:585:ARG:HA	6:A:808:HOH:O	1.98	0.62
1:E:523:VAL:HG13	1:F:46:MET:HE3	1.80	0.62
1:B:364:LYS:NZ	6:B:803:HOH:O	2.33	0.61
1:H:364:LYS:NZ	6:H:802:HOH:O	2.33	0.60
1:A:46:MET:HE3	1:B:523:VAL:HG23	1.83	0.60
1:A:598:LYS:HE3	6:B:962:HOH:O	2.02	0.59
1:A:523:VAL:HG13	1:B:46:MET:HE3	1.83	0.59
6:G:899:HOH:O	1:H:598:LYS:HE3	2.01	0.59
1:F:585:ARG:O	1:F:586:ARG:CB	2.51	0.58
1:A:582:ASP:HB3	1:A:586:ARG:HH12	1.69	0.57
1:E:582:ASP:HB3	1:E:586:ARG:HH12	1.68	0.57
1:C:306:LYS:HD3	6:C:1123:HOH:O	2.06	0.54
1:C:46:MET:HE3	1:D:523:VAL:HG23	1.89	0.53
1:F:364:LYS:NZ	6:F:806:HOH:O	2.35	0.53
1:E:344:ASP:N	6:E:803:HOH:O	2.31	0.52
1:C:523:VAL:HG23	1:D:46:MET:HE3	1.91	0.52
1:E:482:MET:HE1	1:E:507:TRP:CZ3	2.39	0.52
1:A:595:MET:SD	1:B:179:GLU:HG2	2.50	0.52
1:C:46:MET:HE3	1:D:523:VAL:CG2	2.40	0.51
1:F:537:LYS:HE3	6:F:988:HOH:O	2.11	0.51
1:E:597:ASP:HA	1:E:600:LYS:HG2	1.94	0.50
1:C:192:ARG:NH1	6:C:802:HOH:O	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:MET:HE3	1:F:523:VAL:HG23	1.94	0.49
1:A:78:ARG:HD2	6:A:1179:HOH:O	2.12	0.48
1:E:46:MET:HE3	1:F:523:VAL:CG2	2.43	0.48
1:E:598:LYS:HE3	6:F:970:HOH:O	2.13	0.48
1:F:15:LYS:HG2	1:F:181:GLU:HG2	1.96	0.47
1:A:46:MET:HE3	1:B:523:VAL:CG2	2.45	0.47
1:G:523:VAL:HG13	1:H:46:MET:HE3	1.96	0.46
1:A:585:ARG:CA	6:A:808:HOH:O	2.58	0.46
1:C:523:VAL:CG2	1:D:46:MET:HE3	2.46	0.45
1:A:393:ARG:HH11	1:A:393:ARG:HG3	1.81	0.45
1:D:591:LYS:HB3	6:D:803:HOH:O	2.16	0.45
1:E:595:MET:SD	1:F:179:GLU:HG2	2.57	0.45
1:G:364:LYS:NZ	6:G:805:HOH:O	2.44	0.45
1:D:438:ASP:OD1	6:D:801:HOH:O	2.21	0.44
1:C:107:VAL:O	1:C:166:PRO:HA	2.18	0.44
1:B:107:VAL:O	1:B:166:PRO:HA	2.18	0.44
1:E:107:VAL:O	1:E:166:PRO:HA	2.17	0.44
1:E:344:ASP:HB2	6:E:803:HOH:O	2.18	0.43
1:H:107:VAL:O	1:H:166:PRO:HA	2.18	0.43
1:F:107:VAL:O	1:F:166:PRO:HA	2.19	0.43
1:G:107:VAL:O	1:G:166:PRO:HA	2.19	0.43
1:D:50:ALA:HA	6:D:916:HOH:O	2.18	0.43
1:F:448[A]:SER:OG	2:F:702:ATP:O1G	2.33	0.43
1:A:236:ARG:HB2	6:A:1013:HOH:O	2.19	0.43
1:D:206:LEU:CD2	1:D:306:LYS:HD2	2.48	0.43
1:E:364:LYS:NZ	6:E:817:HOH:O	2.49	0.43
1:B:525:GLY:HA3	6:B:1044:HOH:O	2.18	0.42
1:D:107:VAL:O	1:D:166:PRO:HA	2.20	0.42
1:E:399:SER:HB2	6:E:954:HOH:O	2.19	0.42
1:E:565:LYS:HZ2	1:E:565:LYS:HG3	1.63	0.42
1:A:364:LYS:NZ	6:A:815:HOH:O	2.46	0.42
1:E:548:HIS:HD2	6:E:808:HOH:O	2.00	0.42
1:F:591:LYS:HB3	6:F:874:HOH:O	2.19	0.42
1:A:107:VAL:O	1:A:166:PRO:HA	2.20	0.42
1:E:548:HIS:CD2	6:E:808:HOH:O	2.72	0.42
1:C:70:ASP:O	1:C:74:ARG:HG3	2.21	0.41
1:G:192:ARG:CD	6:G:802:HOH:O	2.43	0.41
1:E:525:GLY:HA3	6:E:905:HOH:O	2.20	0.41
1:H:102:TRP:O	2:H:702:ATP:O2G	2.39	0.41
1:D:70:ASP:O	1:D:74:ARG:HG3	2.22	0.40
1:G:240:PRO:HD3	1:G:360:ILE:HD11	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:ILE:HD12	1:E:459:ILE:HA	2.01	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	598/603 (99%)	583 (98%)	15 (2%)	0	100	100
1	B	598/603 (99%)	584 (98%)	14 (2%)	0	100	100
1	C	597/603 (99%)	582 (98%)	15 (2%)	0	100	100
1	D	597/603 (99%)	585 (98%)	12 (2%)	0	100	100
1	E	597/603 (99%)	584 (98%)	13 (2%)	0	100	100
1	F	599/603 (99%)	582 (97%)	17 (3%)	0	100	100
1	G	597/603 (99%)	581 (97%)	16 (3%)	0	100	100
1	H	598/603 (99%)	586 (98%)	12 (2%)	0	100	100
All	All	4781/4824 (99%)	4667 (98%)	114 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	466/467 (100%)	463 (99%)	3 (1%)	78	73
1	B	466/467 (100%)	463 (99%)	3 (1%)	78	73
1	C	465/467 (100%)	462 (99%)	3 (1%)	78	73
1	D	465/467 (100%)	462 (99%)	3 (1%)	78	73
1	E	465/467 (100%)	462 (99%)	3 (1%)	78	73
1	F	467/467 (100%)	463 (99%)	4 (1%)	70	64
1	G	465/467 (100%)	462 (99%)	3 (1%)	78	73
1	H	466/467 (100%)	462 (99%)	4 (1%)	70	64
All	All	3725/3736 (100%)	3699 (99%)	26 (1%)	76	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	86	ASN
1	A	586	ARG
1	B	82	VAL
1	B	393	ARG
1	B	597	ASP
1	C	82	VAL
1	C	86	ASN
1	C	586	ARG
1	D	82	VAL
1	D	86	ASN
1	D	600	LYS
1	E	82	VAL
1	E	86	ASN
1	E	586	ARG
1	F	6	ASN
1	F	82	VAL
1	F	86	ASN
1	F	597	ASP
1	G	8	LYS
1	G	82	VAL
1	G	86	ASN
1	H	82	VAL
1	H	86	ASN
1	H	597	ASP
1	H	600	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	A	548	HIS
1	B	134	GLN
1	B	194	HIS
1	B	405	GLN
1	B	548	HIS
1	C	134	GLN
1	C	328	ASN
1	C	548	HIS
1	D	328	ASN
1	D	548	HIS
1	E	29	ASN
1	E	134	GLN
1	E	140	GLN
1	E	232	GLN
1	E	405	GLN
1	E	548	HIS
1	F	134	GLN
1	F	140	GLN
1	F	194	HIS
1	F	548	HIS
1	G	134	GLN
1	G	140	GLN
1	G	548	HIS
1	H	328	ASN
1	H	548	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
2	ATP	A	701	-	29,33,33	0.63	1 (3%)	44,52,52	0.89	1 (2%)
2	ATP	H	702	-	29,33,33	0.52	0	44,52,52	0.83	0
3	TPW	F	701	4	25,27,27	1.69	3 (12%)	34,40,40	1.30	3 (8%)
2	ATP	D	702	-	29,33,33	0.47	0	44,52,52	0.78	1 (2%)
3	TPW	G	702	4	25,27,27	1.30	2 (8%)	34,40,40	1.08	3 (8%)
3	TPW	A	702	4	25,27,27	1.28	1 (4%)	34,40,40	1.74	5 (14%)
2	ATP	C	701	-	29,33,33	0.55	0	44,52,52	0.79	0
3	TPW	D	701	4	25,27,27	1.63	3 (12%)	34,40,40	1.77	5 (14%)
3	TPW	B	701	4	25,27,27	1.41	4 (16%)	34,40,40	1.25	4 (11%)
5	TRS	C	703	-	7,7,7	0.16	0	9,9,9	0.45	0
3	TPW	C	702	4	25,27,27	1.42	4 (16%)	34,40,40	1.45	6 (17%)
2	ATP	E	701	-	29,33,33	0.60	0	44,52,52	1.01	2 (4%)
2	ATP	G	701	-	29,33,33	0.57	0	44,52,52	0.90	3 (6%)
3	TPW	E	702	4	25,27,27	1.55	3 (12%)	34,40,40	1.22	1 (2%)
3	TPW	H	701	4	25,27,27	1.20	1 (4%)	34,40,40	1.23	3 (8%)
2	ATP	B	702	-	29,33,33	0.58	0	44,52,52	0.82	1 (2%)
2	ATP	F	702	-	29,33,33	0.57	0	44,52,52	0.79	1 (2%)

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
2	ATP	A	701	-	-	3/22/38/38	0/3/3/3
2	ATP	H	702	-	-	3/22/38/38	0/3/3/3
3	TPW	F	701	4	-	2/17/17/17	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	702	-	-	3/22/38/38	0/3/3/3
3	TPW	G	702	4	-	3/17/17/17	0/2/2/2
3	TPW	A	702	4	-	1/17/17/17	0/2/2/2
2	ATP	C	701	-	-	3/22/38/38	0/3/3/3
3	TPW	D	701	4	-	1/17/17/17	0/2/2/2
3	TPW	B	701	4	-	0/17/17/17	0/2/2/2
5	TRS	C	703	-	-	9/9/9/9	-
3	TPW	C	702	4	-	2/17/17/17	0/2/2/2
2	ATP	E	701	-	-	2/22/38/38	0/3/3/3
2	ATP	G	701	-	-	3/22/38/38	0/3/3/3
3	TPW	E	702	4	-	2/17/17/17	0/2/2/2
3	TPW	H	701	4	-	1/17/17/17	0/2/2/2
2	ATP	B	702	-	-	3/22/38/38	0/3/3/3
2	ATP	F	702	-	-	3/22/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	701	TPW	C2-C3	5.69	1.41	1.36
3	D	701	TPW	C2-C3	5.17	1.41	1.36
3	A	702	TPW	C4'-N4'	4.85	1.46	1.34
3	F	701	TPW	C4'-N4'	4.79	1.46	1.34
3	D	701	TPW	C4'-N4'	4.75	1.46	1.34
3	G	702	TPW	C4'-N4'	4.70	1.45	1.34
3	E	702	TPW	C2-C3	4.67	1.40	1.36
3	E	702	TPW	C4'-N4'	4.67	1.45	1.34
3	H	701	TPW	C4'-N4'	4.55	1.45	1.34
3	C	702	TPW	C4'-N4'	4.23	1.44	1.34
3	B	701	TPW	C2-C3	3.91	1.39	1.36
3	B	701	TPW	C4'-N4'	3.77	1.43	1.34
3	G	702	TPW	C2-C3	3.11	1.39	1.36
3	C	702	TPW	C2-C3	3.02	1.39	1.36
3	B	701	TPW	C5-C4	2.55	1.40	1.36
3	C	702	TPW	C5-C4	2.50	1.40	1.36
3	F	701	TPW	C5-C4	2.17	1.39	1.36
3	E	702	TPW	C5-C4	2.15	1.39	1.36
3	D	701	TPW	C5-C4	2.11	1.39	1.36
3	B	701	TPW	C5'-C4'	-2.06	1.39	1.42
3	C	702	TPW	C5'-C4'	-2.06	1.39	1.42
2	A	701	ATP	PG-O1G	2.04	1.57	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	TPW	C2-C3-C4	-5.80	107.79	111.89
3	D	701	TPW	C2-S1-C5	5.43	97.47	92.36
3	A	702	TPW	C5-C4-C3	4.75	115.94	112.50
3	C	702	TPW	C2-C3-C4	-4.69	108.57	111.89
3	D	701	TPW	C5-C4-C3	4.61	115.84	112.50
3	F	701	TPW	C2-S1-C5	4.02	96.14	92.36
3	E	702	TPW	C2-S1-C5	3.26	95.44	92.36
3	A	702	TPW	C2-S1-C5	3.25	95.42	92.36
3	D	701	TPW	C4A-C4-C3	-3.23	118.60	125.60
3	G	702	TPW	C2-C3-C4	-3.19	109.63	111.89
3	H	701	TPW	C2-S1-C5	3.18	95.36	92.36
3	D	701	TPW	C2-C3-C4	-3.11	109.69	111.89
3	C	702	TPW	C5-C4-C3	2.97	114.65	112.50
3	F	701	TPW	C2-C3-C4	-2.86	109.86	111.89
3	D	701	TPW	O5G-P1-O13	-2.84	97.98	109.07
3	G	702	TPW	C2-S1-C5	2.71	94.92	92.36
3	C	702	TPW	C5A-C5-C4	2.64	134.00	130.95
3	A	702	TPW	C4A-C4-C3	-2.56	120.07	125.60
2	E	701	ATP	C4'-O4'-C1'	-2.47	104.03	109.47
3	B	701	TPW	C4A-C4-C3	-2.47	120.27	125.60
3	F	701	TPW	C5-C4-C3	2.40	114.24	112.50
3	B	701	TPW	C2-C3-C4	-2.34	110.23	111.89
2	D	702	ATP	O3G-PG-O2G	2.23	116.15	107.64
3	B	701	TPW	C2A-C2'-N1'	2.22	119.58	117.14
2	B	702	ATP	C4'-O4'-C1'	-2.17	104.68	109.47
3	C	702	TPW	C5A-C5-S1	-2.15	115.73	120.89
2	G	701	ATP	O2'-C2'-C3'	2.15	118.76	111.82
3	C	702	TPW	O23-P2-O21	2.14	115.82	107.64
2	G	701	ATP	O3'-C3'-C2'	2.14	118.74	111.82
3	H	701	TPW	C2-C3-C4	-2.12	110.39	111.89
3	H	701	TPW	C4A-C4-C3	-2.12	121.02	125.60
3	G	702	TPW	C5-C4-C3	2.11	114.03	112.50
3	C	702	TPW	C2A-C2'-N1'	2.11	119.45	117.14
2	E	701	ATP	PA-O3A-PB	2.10	140.03	132.83
3	B	701	TPW	C5A-C5-C4	-2.09	128.53	130.95
2	G	701	ATP	O2G-PG-O3B	2.08	111.60	104.64
3	A	702	TPW	C6'-N1'-C2'	2.07	119.49	115.96
2	F	702	ATP	O4'-C1'-C2'	-2.03	102.21	106.64
2	A	701	ATP	O3G-PG-O3B	2.02	111.40	104.64

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	PB-O3B-PG-O2G
2	A	701	ATP	PB-O3B-PG-O3G
2	C	701	ATP	PB-O3B-PG-O2G
2	D	702	ATP	PB-O3B-PG-O3G
2	E	701	ATP	PB-O3B-PG-O2G
2	F	702	ATP	PB-O3B-PG-O3G
2	G	701	ATP	PB-O3B-PG-O2G
2	G	701	ATP	PB-O3B-PG-O3G
2	H	702	ATP	PB-O3B-PG-O3G
3	E	702	TPW	P1-O11-P2-O21
5	C	703	TRS	C1-C-C2-O2
5	C	703	TRS	C3-C-C2-O2
5	C	703	TRS	N-C-C2-O2
5	C	703	TRS	C2-C-C3-O3
5	C	703	TRS	C3-C-C1-O1
5	C	703	TRS	C1-C-C3-O3
2	B	702	ATP	PB-O3B-PG-O1G
3	A	702	TPW	P1-O11-P2-O22
3	C	702	TPW	P1-O11-P2-O22
3	G	702	TPW	P1-O11-P2-O22
3	E	702	TPW	P1-O11-P2-O22
2	B	702	ATP	PB-O3B-PG-O3G
2	C	701	ATP	PB-O3B-PG-O3G
2	E	701	ATP	PB-O3B-PG-O3G
3	G	702	TPW	P1-O11-P2-O21
2	B	702	ATP	C5'-O5'-PA-O3A
2	D	702	ATP	C5'-O5'-PA-O3A
3	G	702	TPW	C5-C5A-C5B-O5G
5	C	703	TRS	N-C-C1-O1
5	C	703	TRS	N-C-C3-O3
2	F	702	ATP	PB-O3B-PG-O1G
2	A	701	ATP	C4'-C5'-O5'-PA
2	G	701	ATP	C4'-C5'-O5'-PA
5	C	703	TRS	C2-C-C1-O1
2	H	702	ATP	PB-O3B-PG-O1G
2	F	702	ATP	C4'-C5'-O5'-PA
2	H	702	ATP	C4'-C5'-O5'-PA
2	D	702	ATP	PB-O3B-PG-O1G
3	F	701	TPW	P1-O11-P2-O21
3	C	702	TPW	C5-C5A-C5B-O5G
3	D	701	TPW	C5-C5A-C5B-O5G
3	F	701	TPW	C5-C5A-C5B-O5G

Continued on next page...

Continued from previous page...

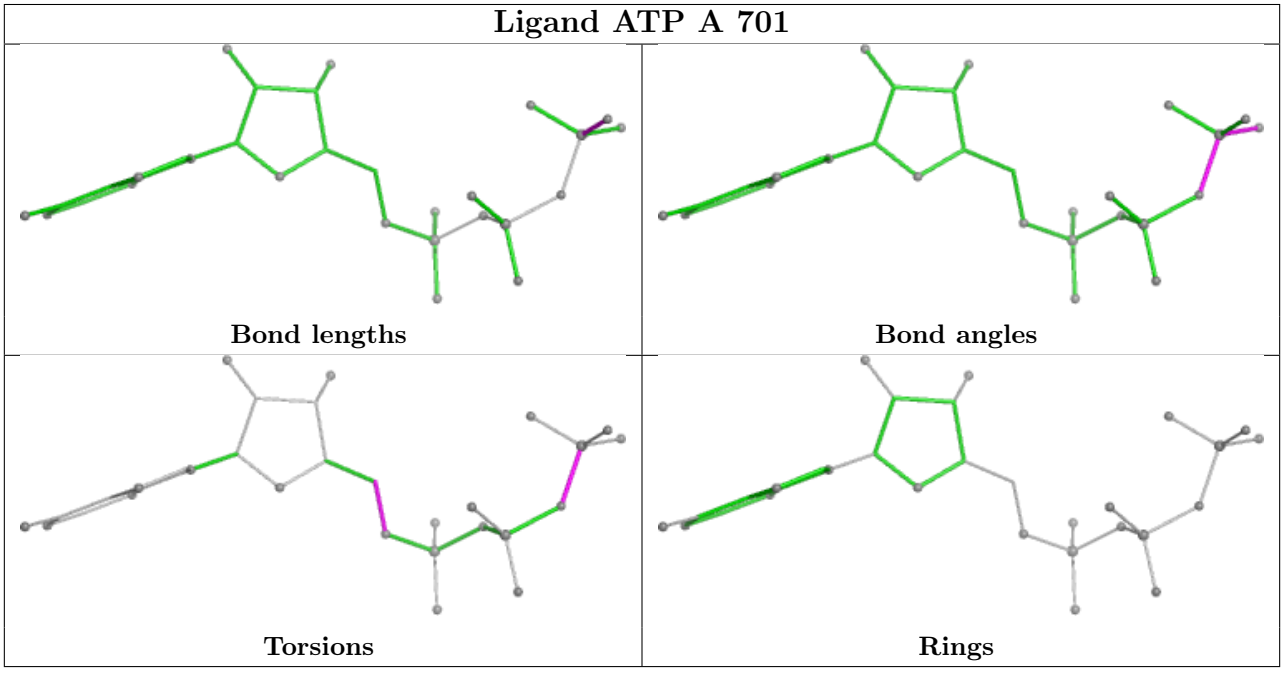
Mol	Chain	Res	Type	Atoms
3	H	701	TPW	C5-C5A-C5B-O5G
2	C	701	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

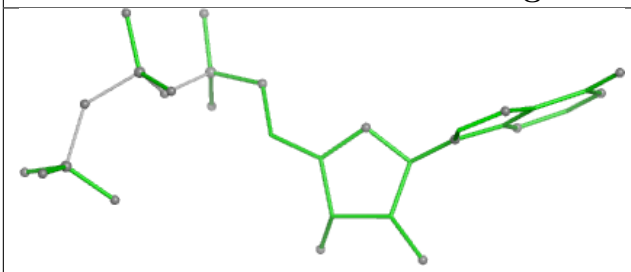
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	702	ATP	1	0
2	F	702	ATP	1	0

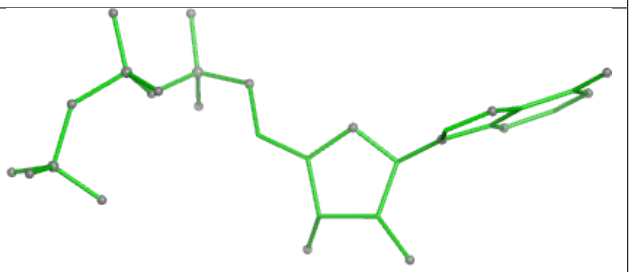
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



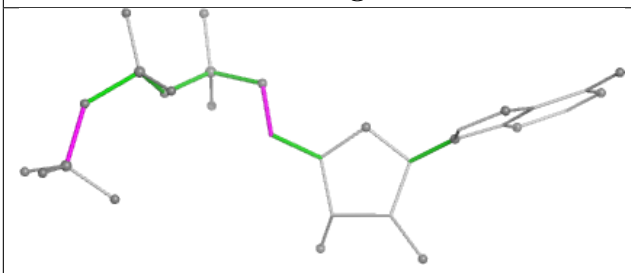
Ligand ATP H 702



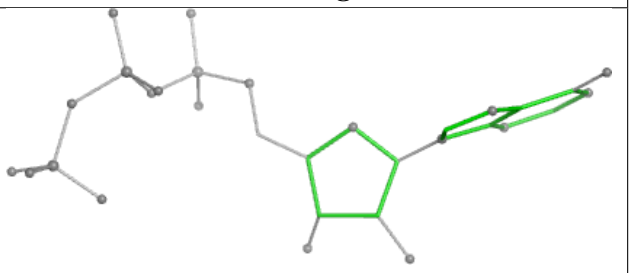
Bond lengths



Bond angles

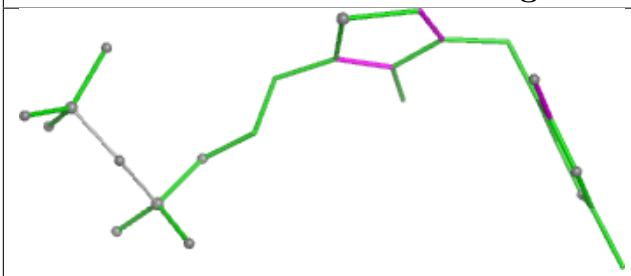


Torsions

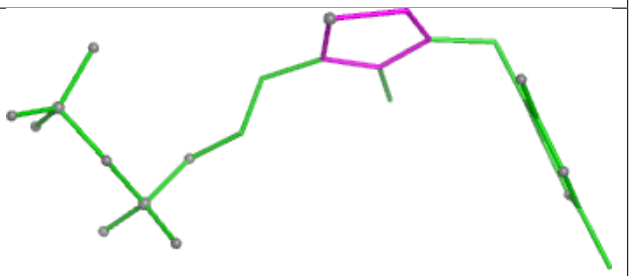


Rings

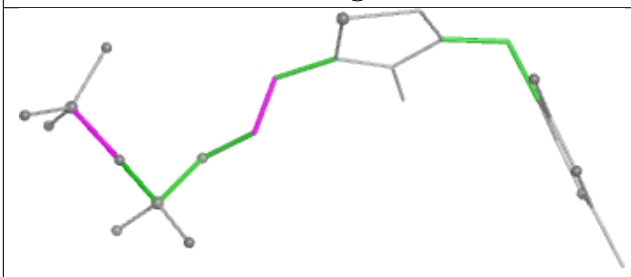
Ligand TPW F 701



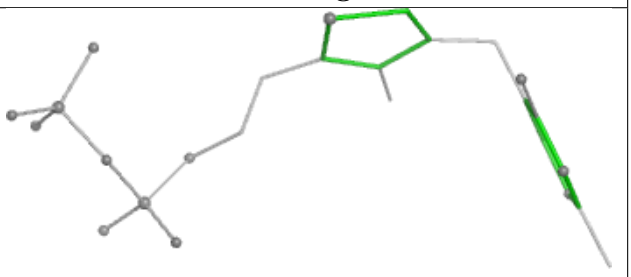
Bond lengths



Bond angles

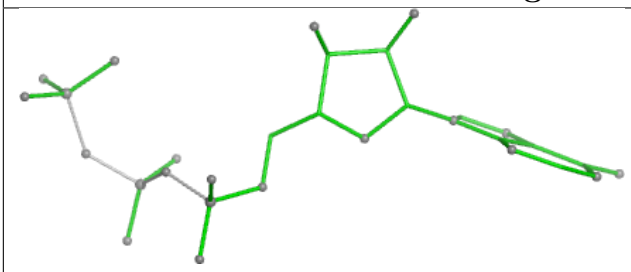


Torsions

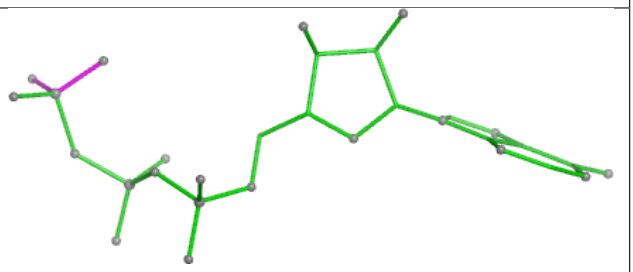


Rings

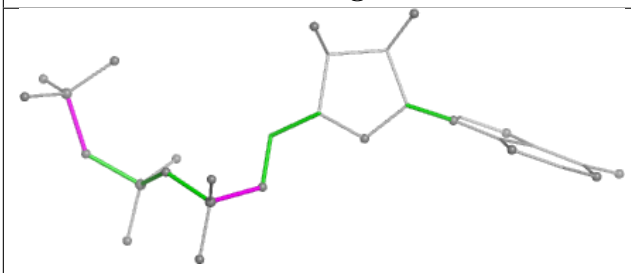
Ligand ATP D 702



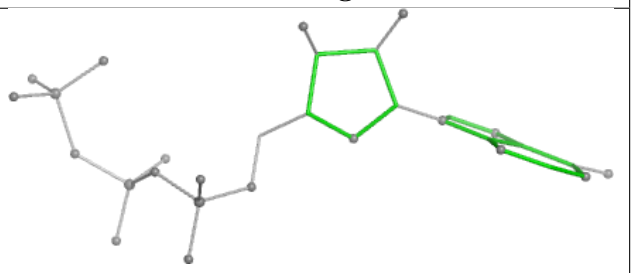
Bond lengths



Bond angles

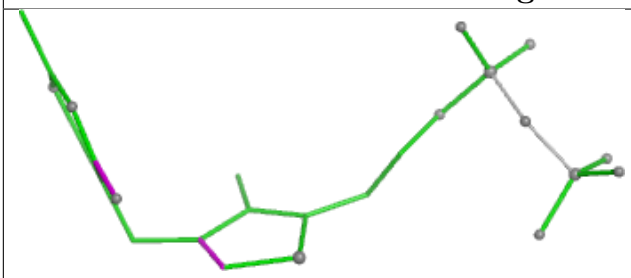


Torsions

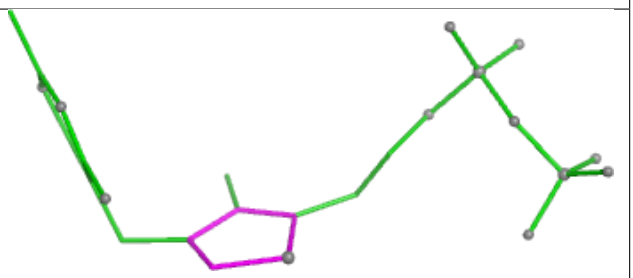


Rings

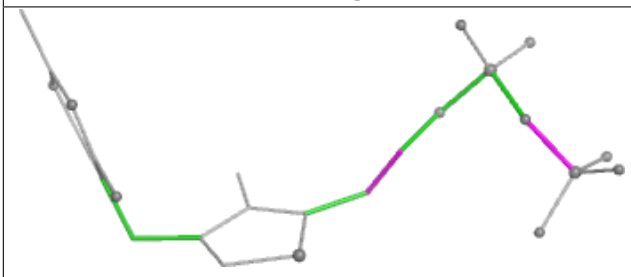
Ligand TPW G 702



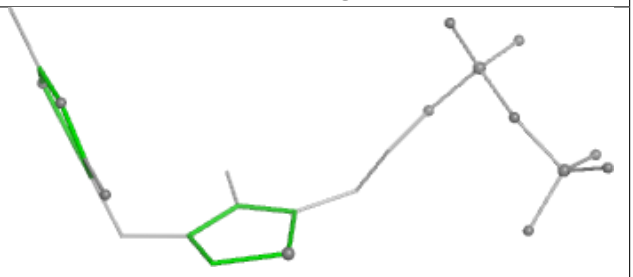
Bond lengths



Bond angles

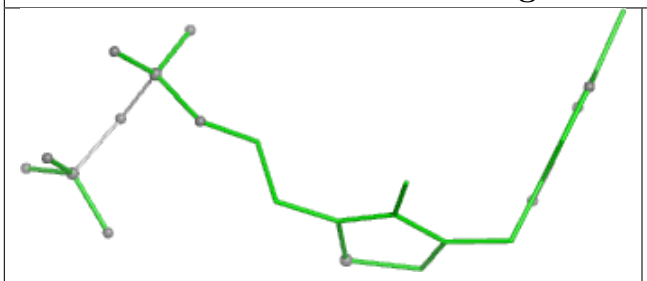


Torsions

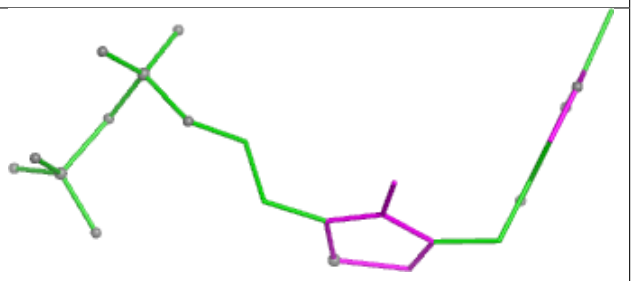


Rings

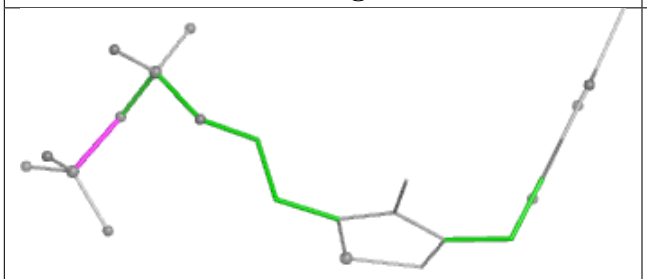
Ligand TPW A 702



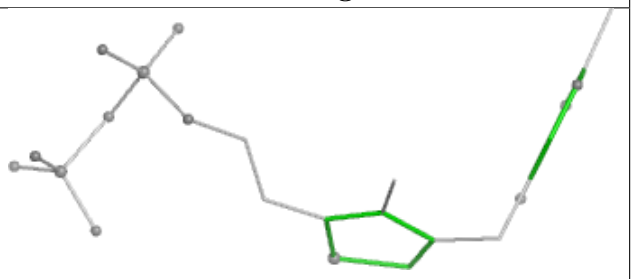
Bond lengths



Bond angles

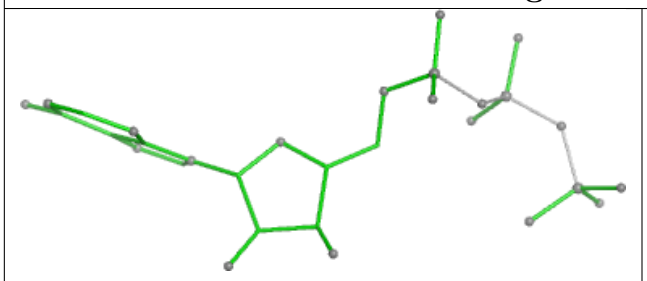


Torsions

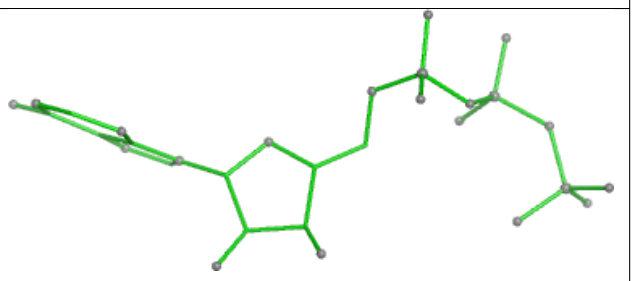


Rings

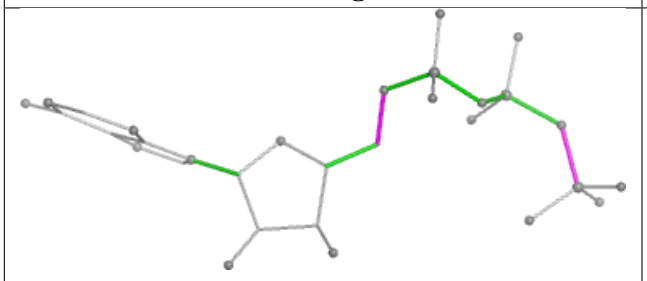
Ligand ATP C 701



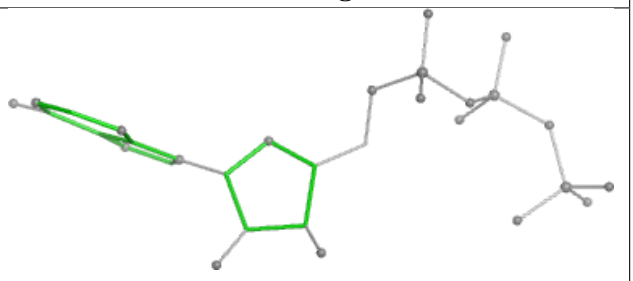
Bond lengths



Bond angles

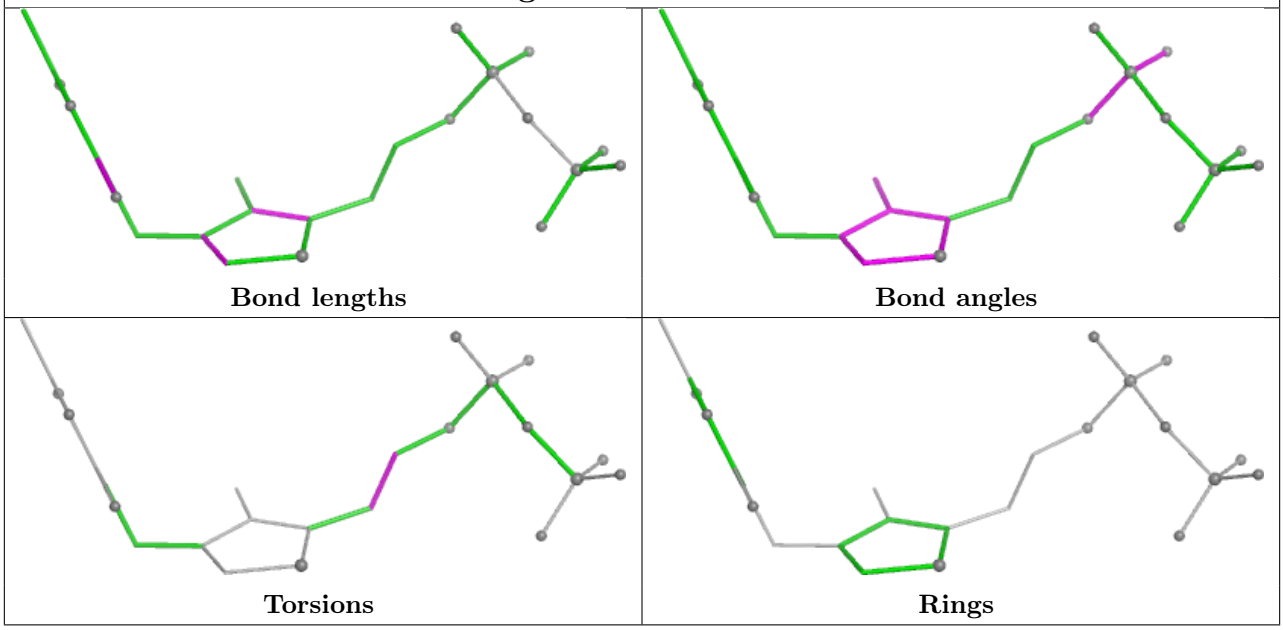


Torsions

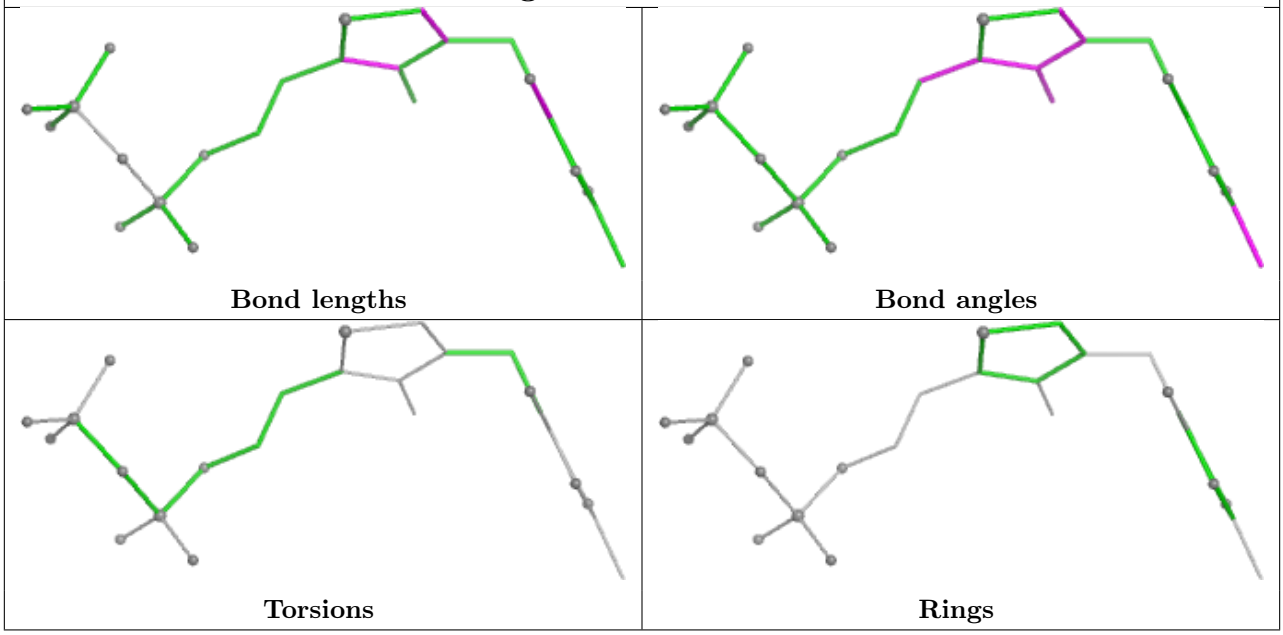


Rings

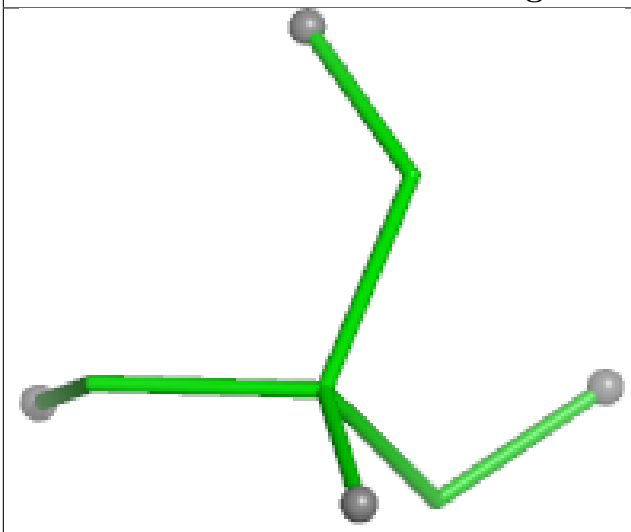
Ligand TPW D 701



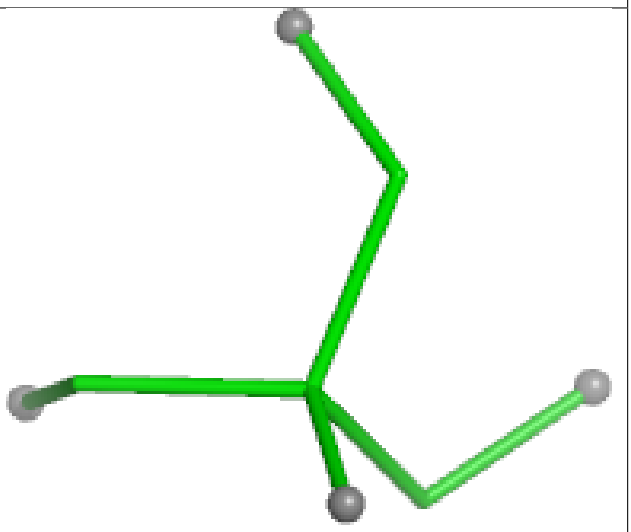
Ligand TPW B 701



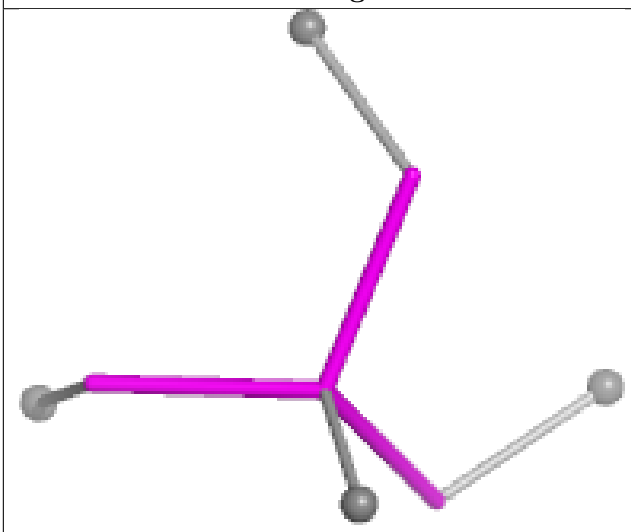
Ligand TRS C 703



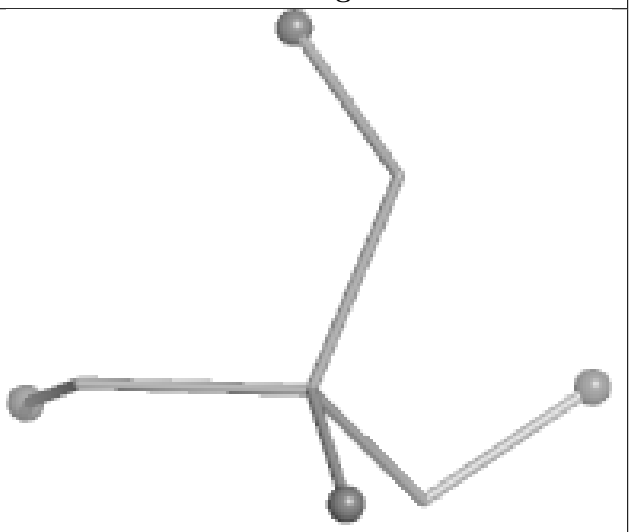
Bond lengths



Bond angles

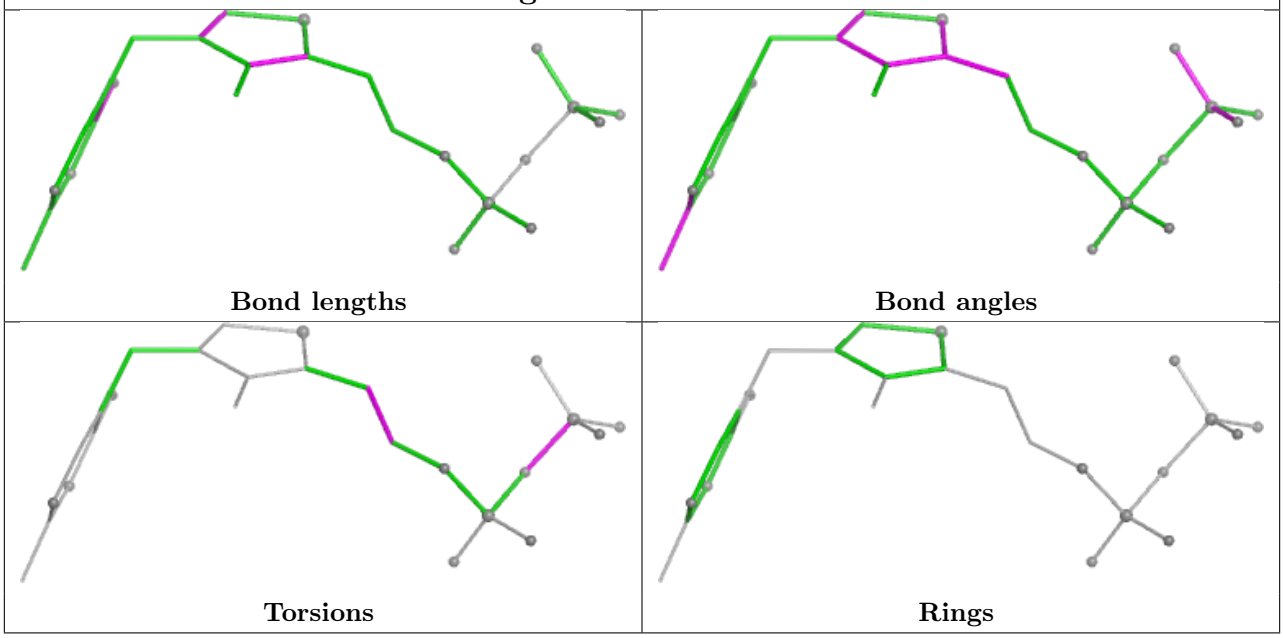


Torsions

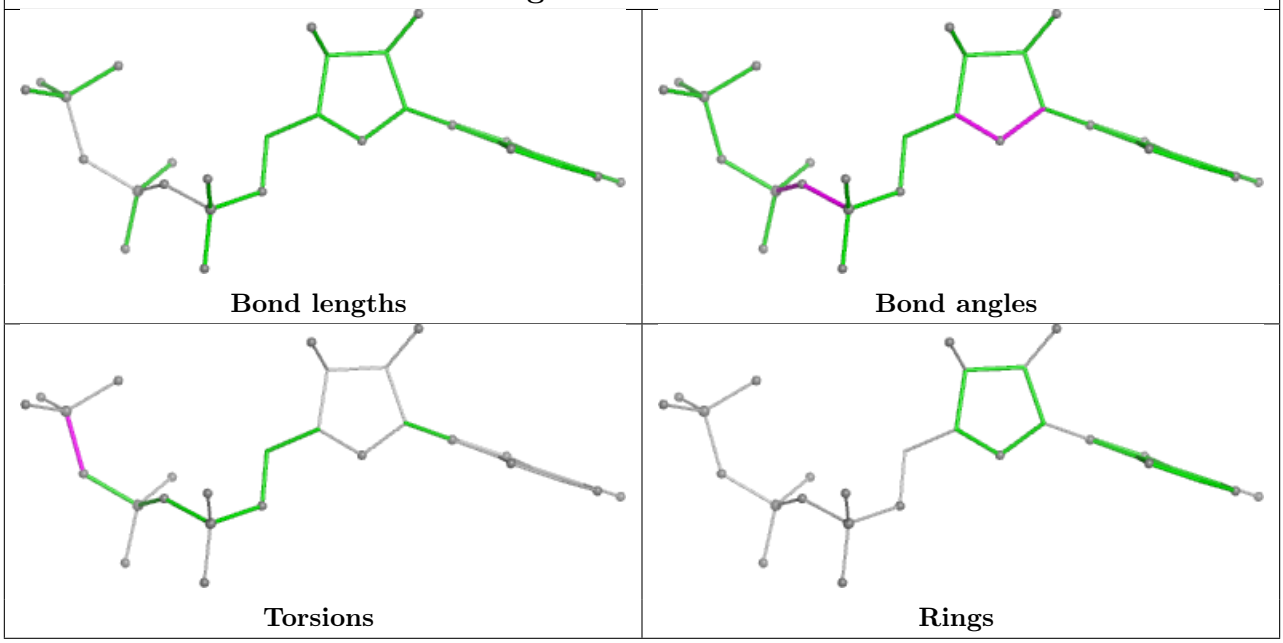


Rings

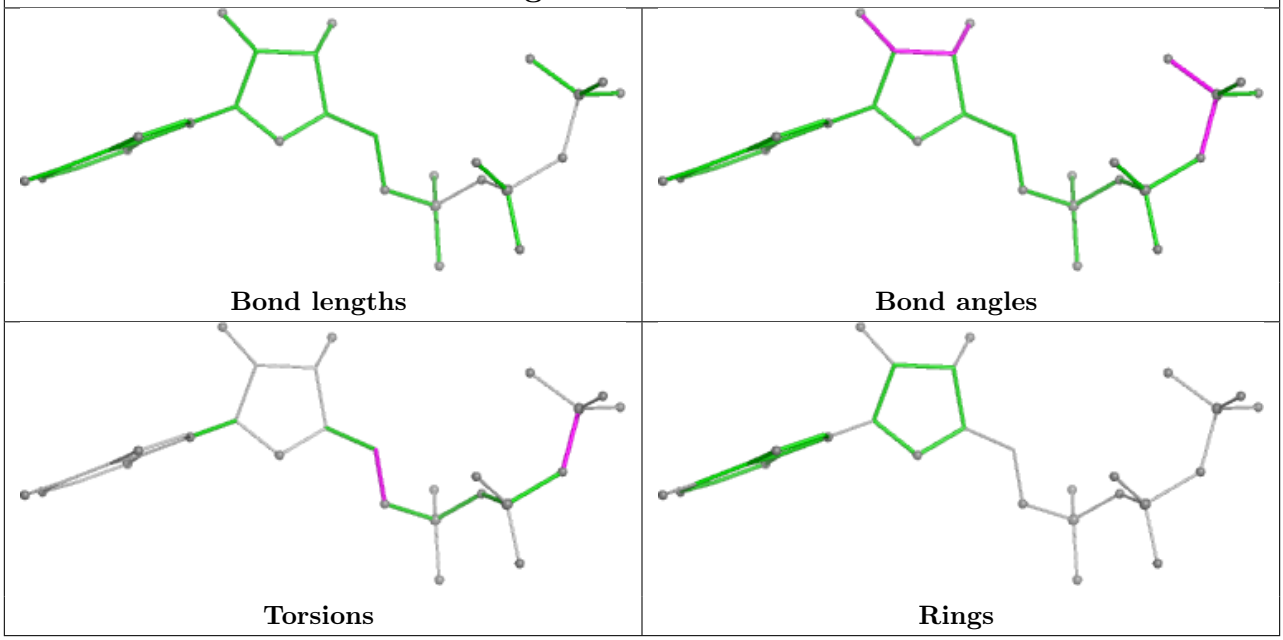
Ligand TPW C 702



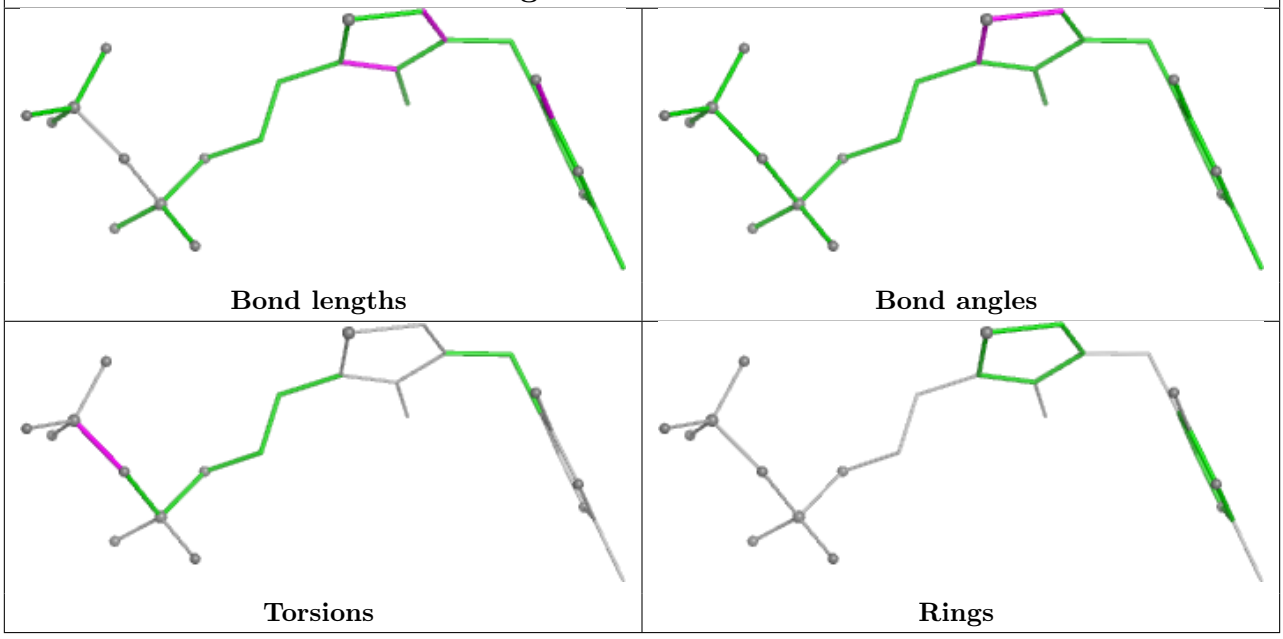
Ligand ATP E 701



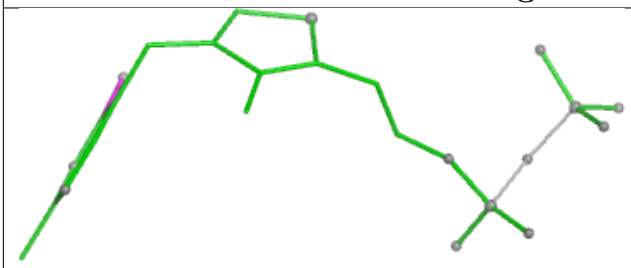
Ligand ATP G 701



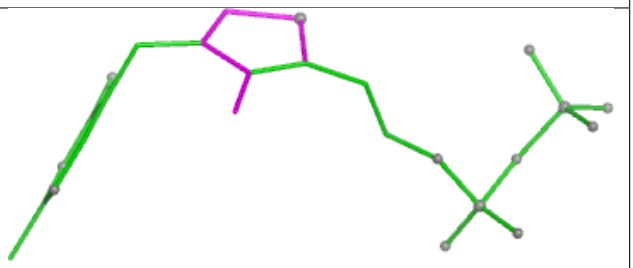
Ligand TPW E 702



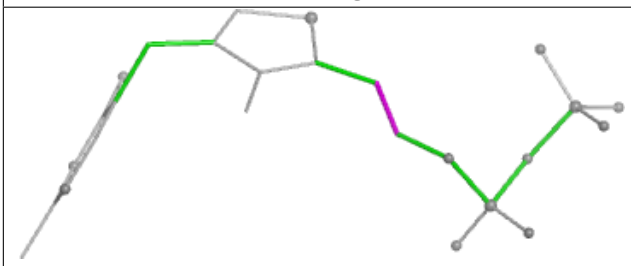
Ligand TPW H 701



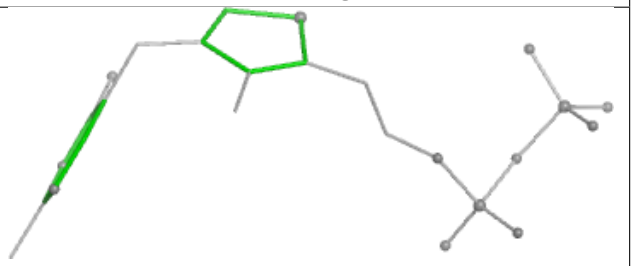
Bond lengths



Bond angles

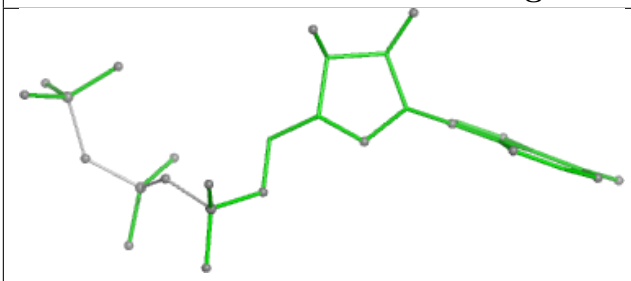


Torsions

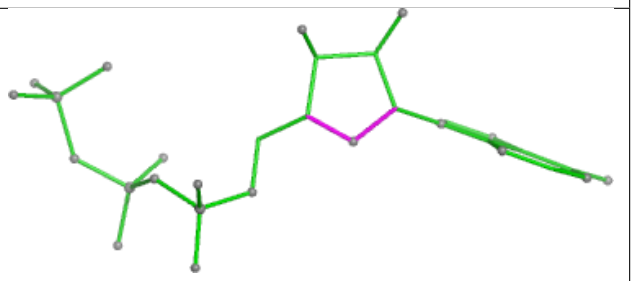


Rings

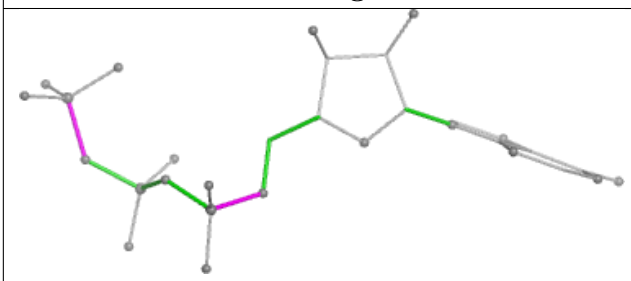
Ligand ATP B 702



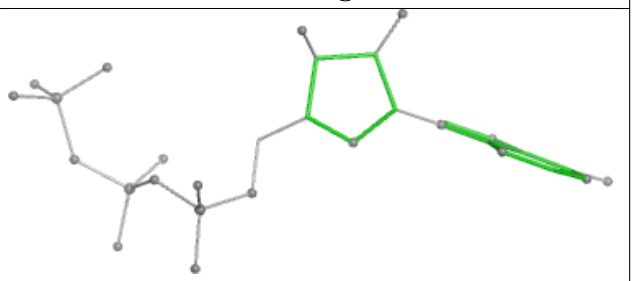
Bond lengths



Bond angles

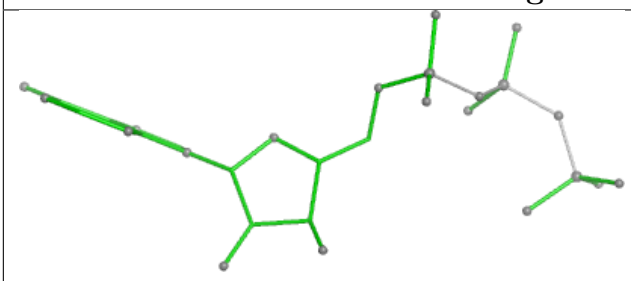


Torsions

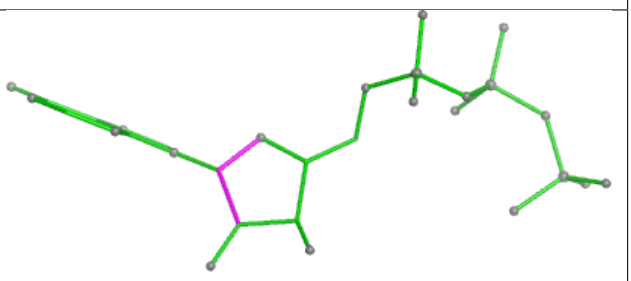


Rings

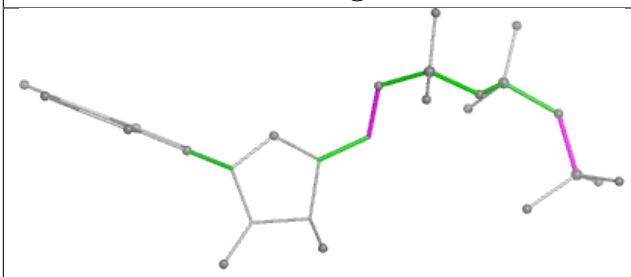
Ligand ATP F 702



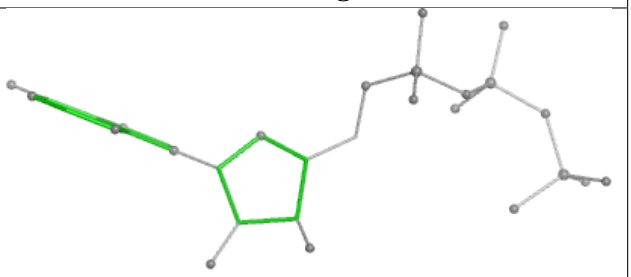
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	600/603 (99%)	-0.54	6 (1%)	79	83	10, 19, 37, 84	0
1	B	600/603 (99%)	-0.42	5 (0%)	82	86	11, 21, 39, 73	0
1	C	599/603 (99%)	-0.38	4 (0%)	84	87	14, 24, 40, 74	0
1	D	599/603 (99%)	-0.27	5 (0%)	82	86	13, 25, 43, 82	0
1	E	599/603 (99%)	-0.08	5 (0%)	82	86	19, 30, 47, 80	0
1	F	600/603 (99%)	-0.13	8 (1%)	75	79	15, 28, 45, 89	1 (0%)
1	G	599/603 (99%)	0.21	12 (2%)	65	68	23, 36, 53, 89	0
1	H	600/603 (99%)	0.45	14 (2%)	61	64	23, 39, 57, 96	0
All	All	4796/4824 (99%)	-0.14	59 (1%)	76	80	10, 28, 49, 96	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	584	PHE	5.6
1	C	584	PHE	5.3
1	D	584	PHE	4.8
1	H	588	ALA	4.1
1	A	586	ARG	3.9
1	H	351	ALA	3.8
1	F	4	THR	3.8
1	A	584	PHE	3.7
1	E	584	PHE	3.6
1	B	587	ASP	3.4
1	F	584	PHE	3.4
1	G	584	PHE	3.3
1	B	4	THR	3.3
1	G	588	ALA	3.2
1	C	588	ALA	3.1
1	H	290	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	588	ALA	3.1
1	A	4	THR	3.1
1	H	4	THR	3.0
1	A	588	ALA	3.0
1	H	586	ARG	3.0
1	E	290	PHE	3.0
1	H	355	ALA	2.8
1	H	345	VAL	2.8
1	B	584	PHE	2.8
1	A	587	ASP	2.7
1	G	290	PHE	2.7
1	H	293	LEU	2.7
1	B	585	ARG	2.6
1	H	366	ALA	2.6
1	F	290	PHE	2.5
1	H	587	ASP	2.5
1	A	585	ARG	2.4
1	C	587	ASP	2.4
1	H	585	ARG	2.4
1	B	588	ALA	2.4
1	F	588	ALA	2.3
1	E	588	ALA	2.3
1	D	586	ARG	2.3
1	G	293	LEU	2.3
1	H	523	VAL	2.2
1	G	301	TRP	2.2
1	F	585	ARG	2.2
1	F	345	VAL	2.2
1	G	287	MET	2.2
1	E	345	VAL	2.2
1	D	585	ARG	2.2
1	F	124	PHE	2.1
1	E	597	ASP	2.1
1	G	391	GLY	2.1
1	C	586	ARG	2.1
1	G	288	GLY	2.1
1	G	586	ARG	2.1
1	G	297	GLY	2.0
1	H	257	LEU	2.0
1	F	586	ARG	2.0
1	G	343	ALA	2.0
1	G	352	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	6	ASN	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	TRS	C	703	8/8	0.83	0.15	48,58,59,68	0
2	ATP	H	702	31/31	0.96	0.07	31,37,42,43	0
2	ATP	G	701	31/31	0.96	0.07	33,35,40,41	0
3	TPW	G	702	26/26	0.97	0.06	31,32,34,34	0
3	TPW	H	701	26/26	0.97	0.06	30,36,39,40	0
2	ATP	E	701	31/31	0.97	0.06	27,31,35,37	0
2	ATP	D	702	31/31	0.98	0.05	22,24,27,32	0
3	TPW	D	701	26/26	0.98	0.04	16,19,23,25	0
3	TPW	E	702	26/26	0.98	0.06	24,26,28,31	0
3	TPW	F	701	26/26	0.98	0.04	18,20,21,22	0
2	ATP	B	702	31/31	0.98	0.04	20,22,23,24	0
2	ATP	F	702	31/31	0.98	0.05	25,28,31,32	0
4	MG	E	703	1/1	0.98	0.02	21,21,21,21	0
2	ATP	C	701	31/31	0.98	0.05	21,23,26,26	0
3	TPW	C	702	26/26	0.99	0.03	15,17,19,22	0
2	ATP	A	701	31/31	0.99	0.04	17,19,21,22	0
4	MG	A	703	1/1	0.99	0.01	13,13,13,13	0
4	MG	B	703	1/1	0.99	0.04	13,13,13,13	0
4	MG	C	704	1/1	0.99	0.04	17,17,17,17	0
4	MG	D	703	1/1	0.99	0.01	19,19,19,19	0
3	TPW	A	702	26/26	0.99	0.03	9,12,14,15	0
4	MG	F	703	1/1	0.99	0.02	18,18,18,18	0

Continued on next page...

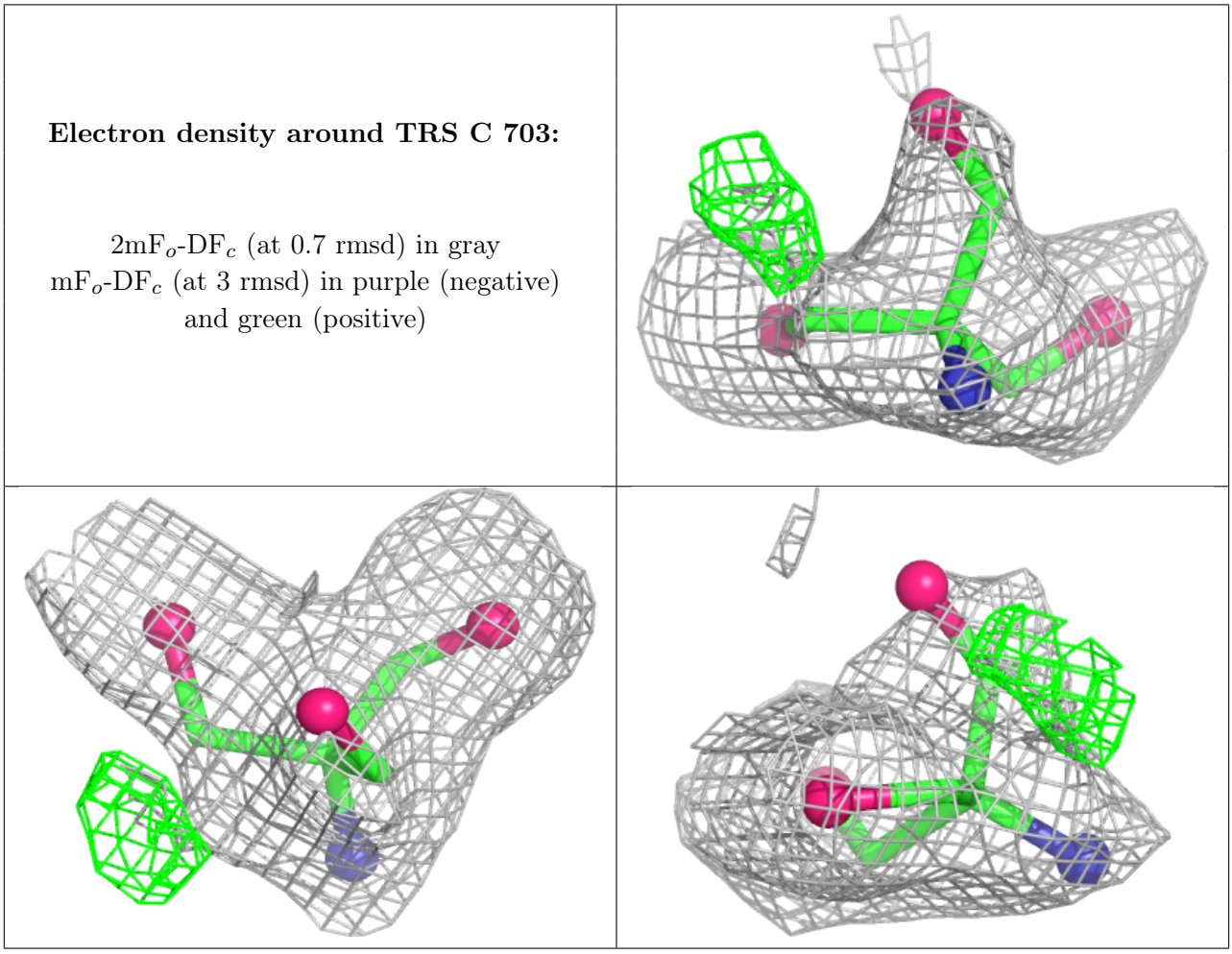
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	G	703	1/1	0.99	0.06	22,22,22,22	0
4	MG	H	703	1/1	0.99	0.04	30,30,30,30	0
3	TPW	B	701	26/26	0.99	0.03	11,14,19,19	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.

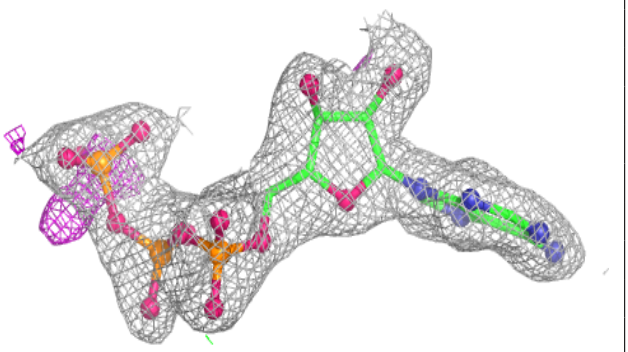
Electron density around TRS C 703:

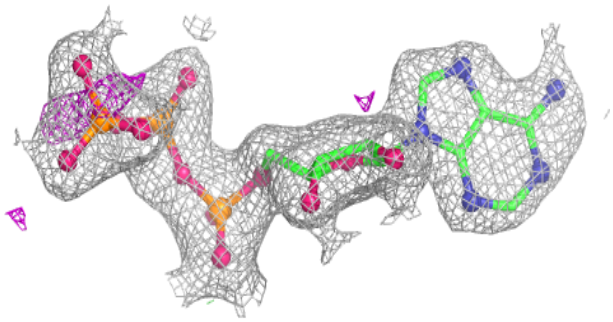
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

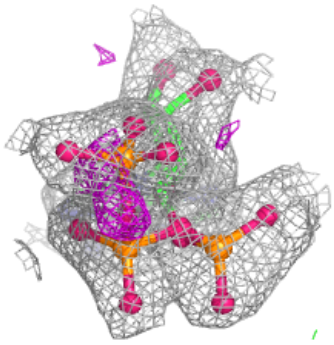


Electron density around ATP H 702:

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

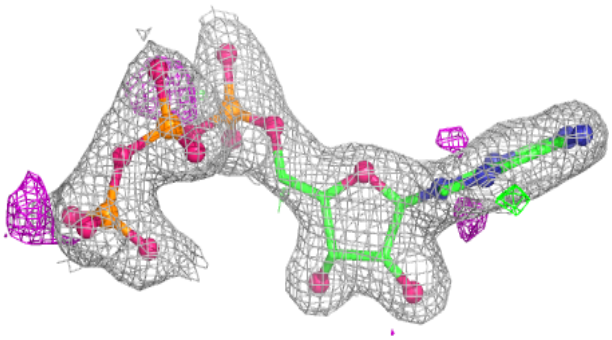


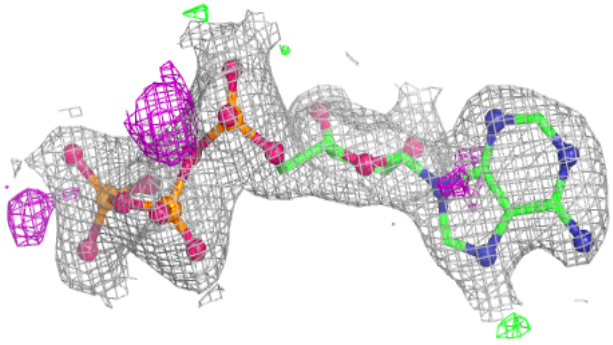


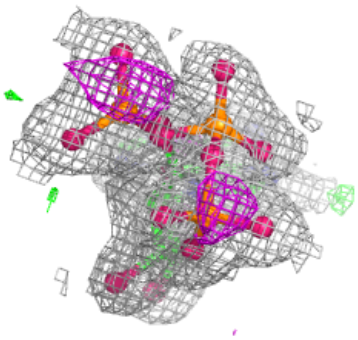


Electron density around ATP G 701:

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

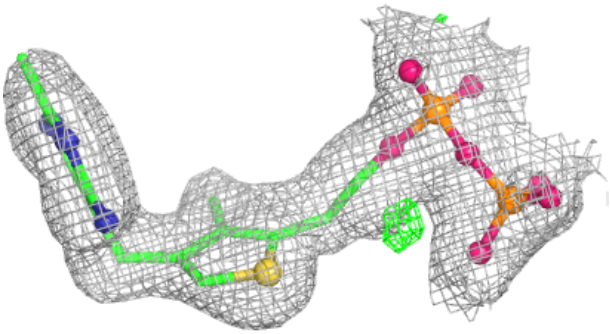


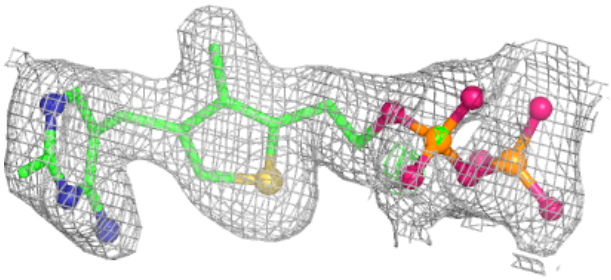


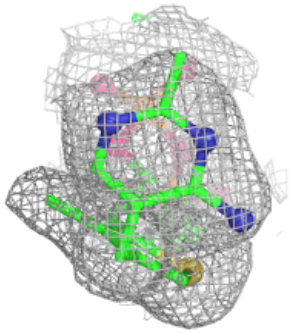


Electron density around TPW G 702:

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

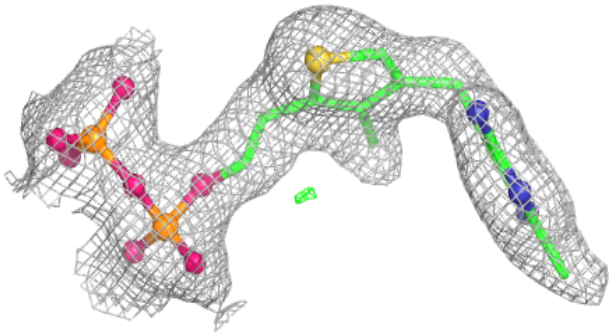


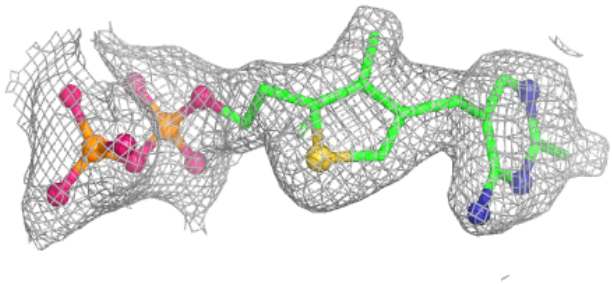


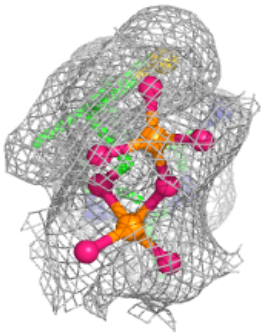


Electron density around TPW H 701:

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

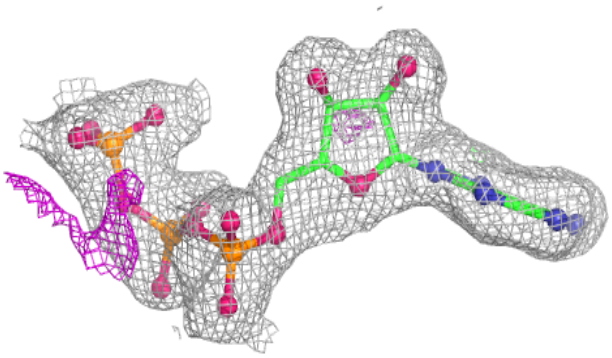


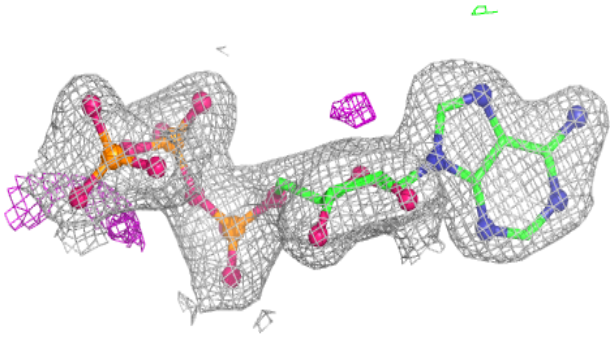


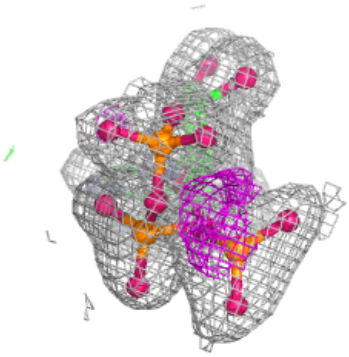


Electron density around ATP E 701:

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

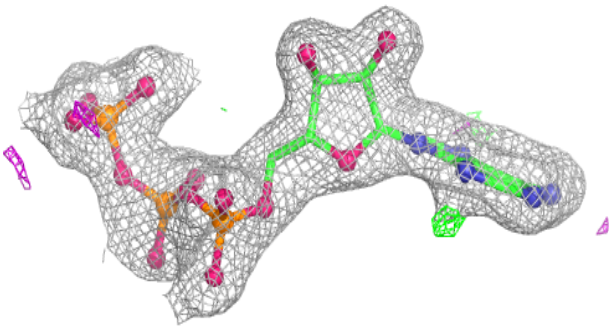


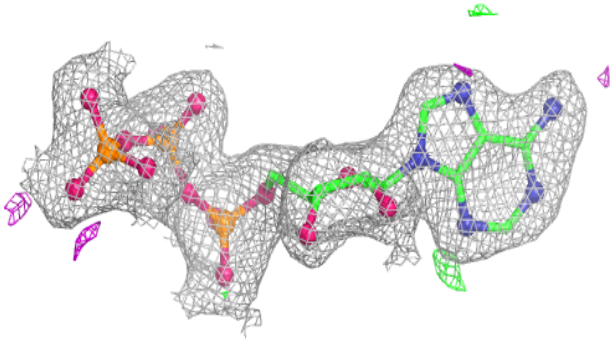


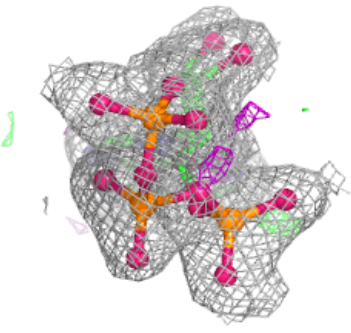


Electron density around ATP D 702:

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

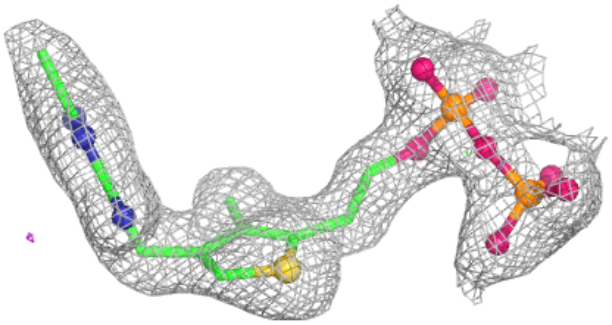


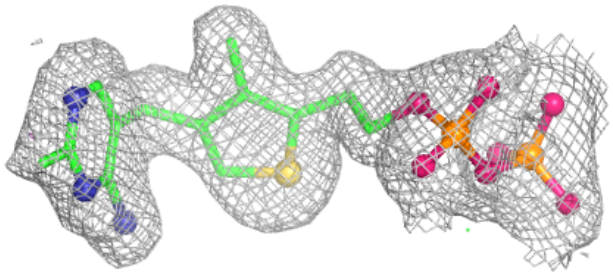


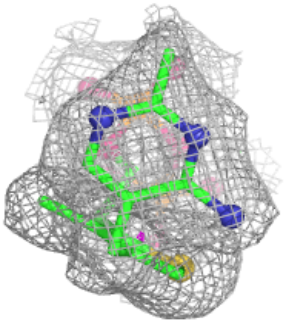


Electron density around TPW D 701:

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

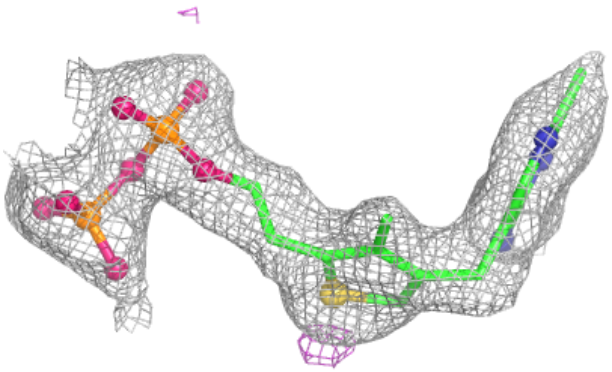


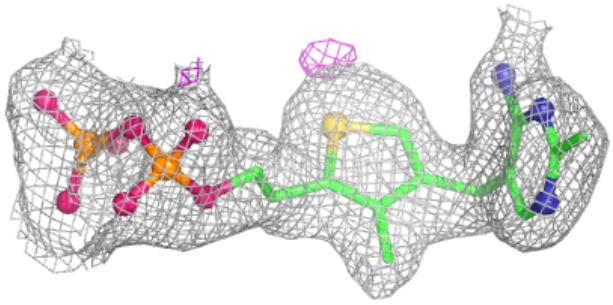


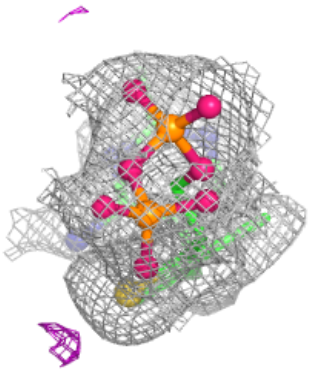


Electron density around TPW E 702:

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

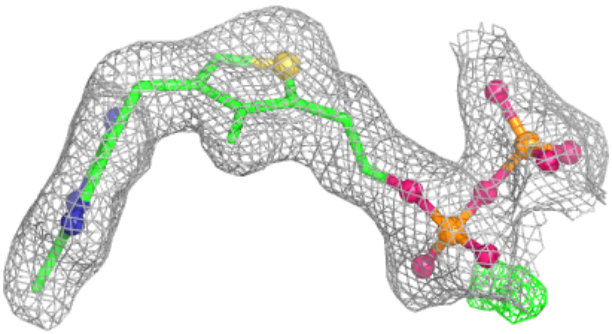


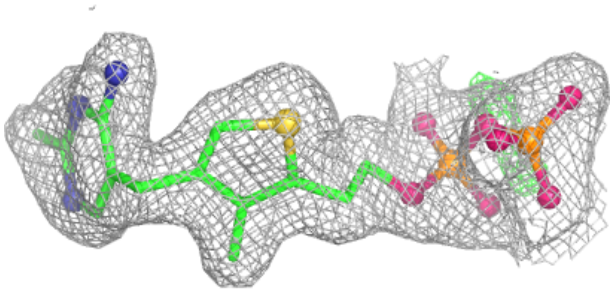


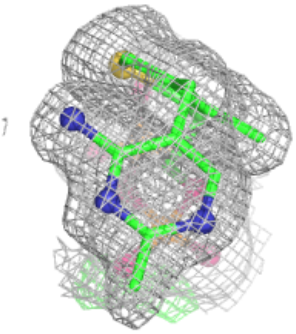


Electron density around TPW F 701:

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

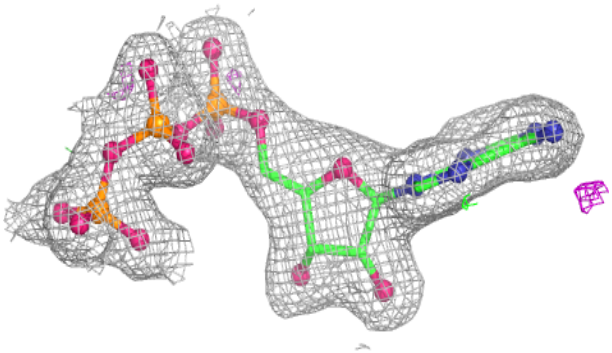


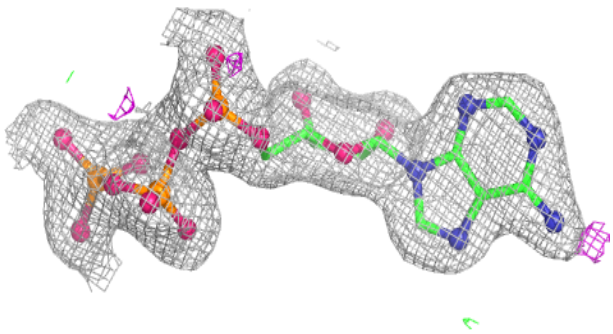


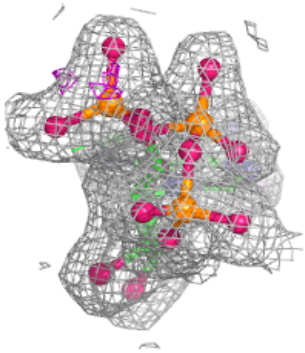


Electron density around ATP B 702:

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

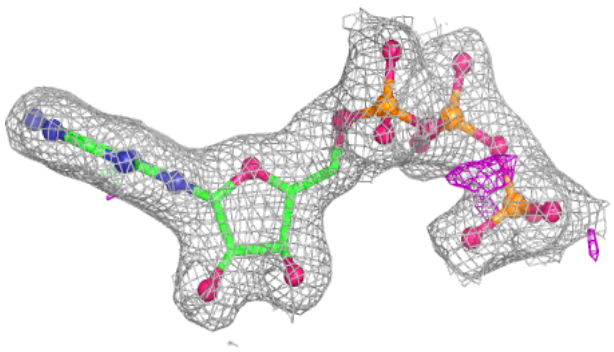


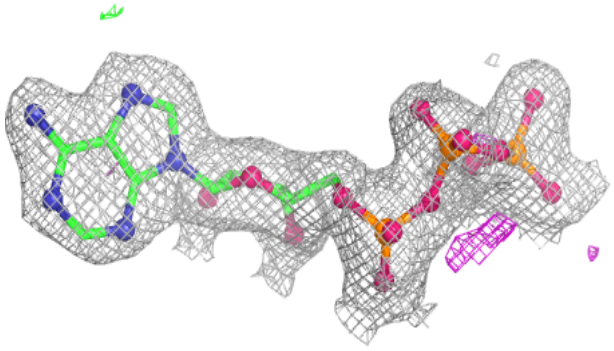


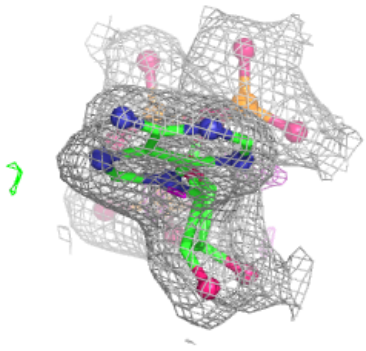


Electron density around ATP F 702:

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

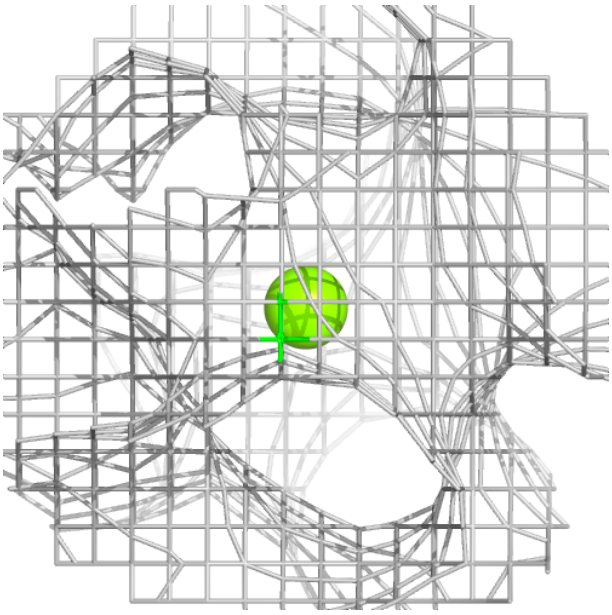


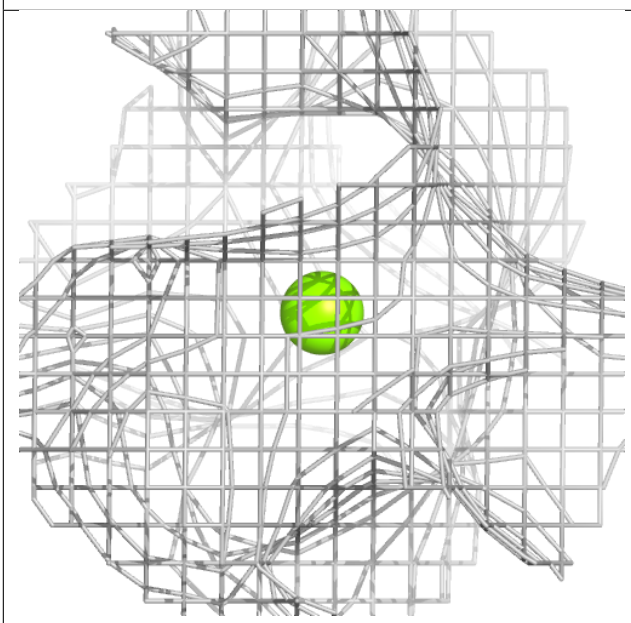


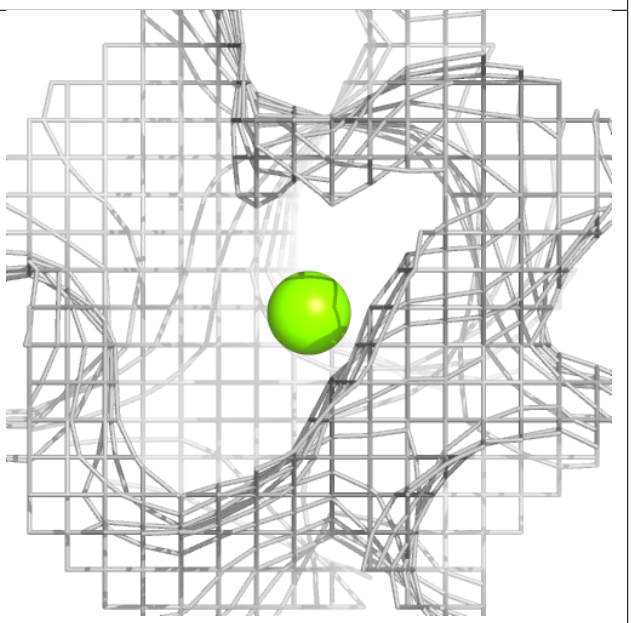


Electron density around MG E 703:

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

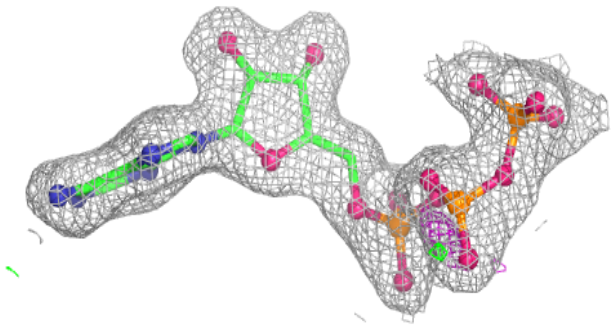


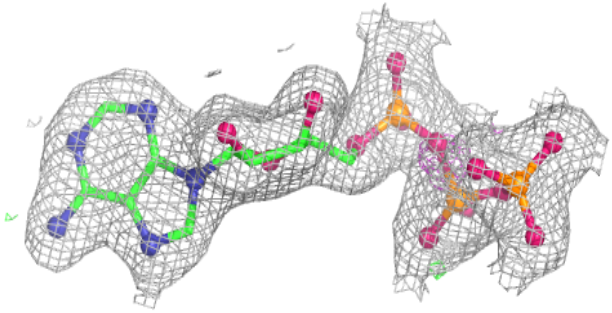


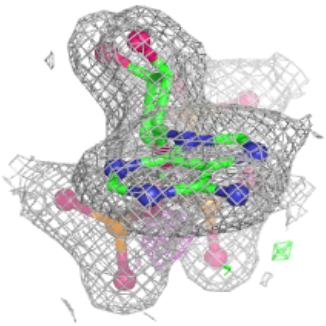


Electron density around ATP C 701:

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

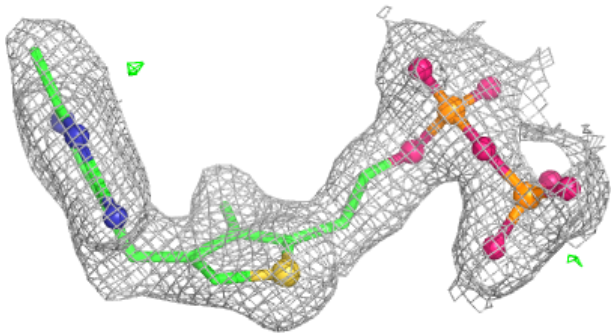


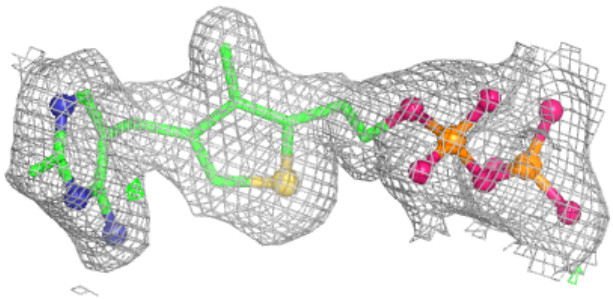


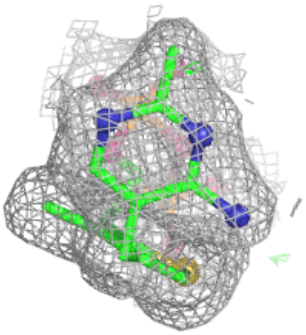


Electron density around TPW C 702:

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

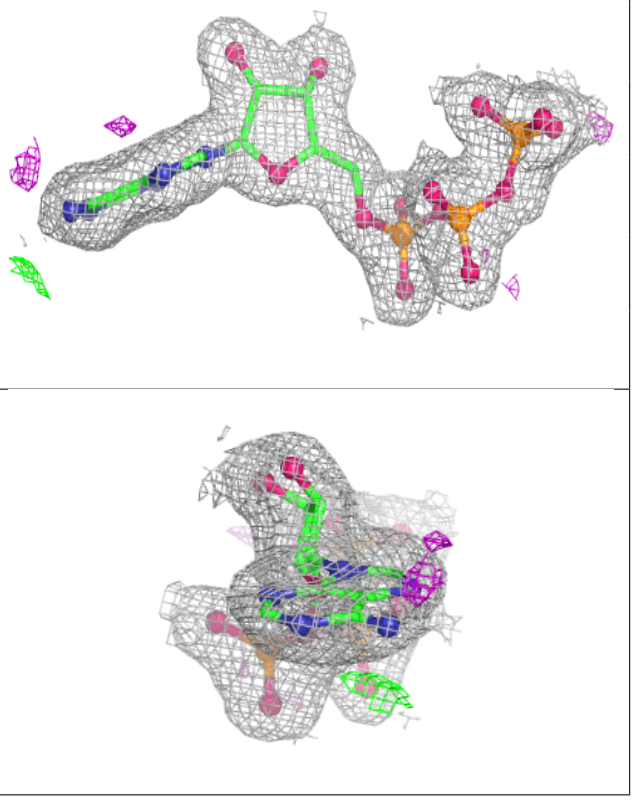


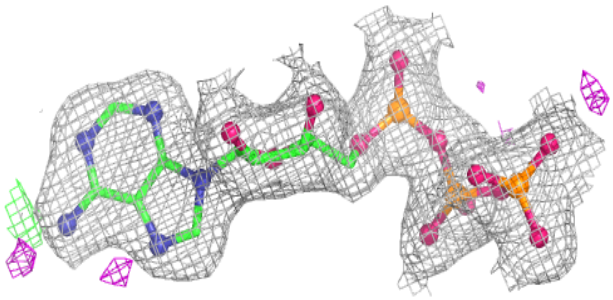




Electron density around ATP A 701:

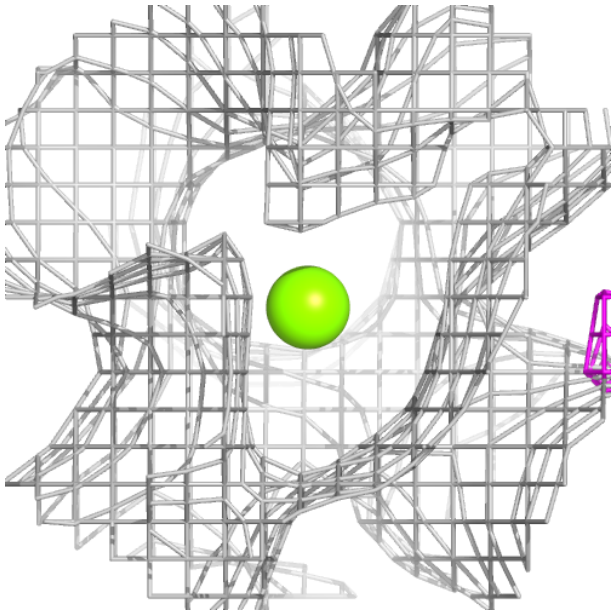
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

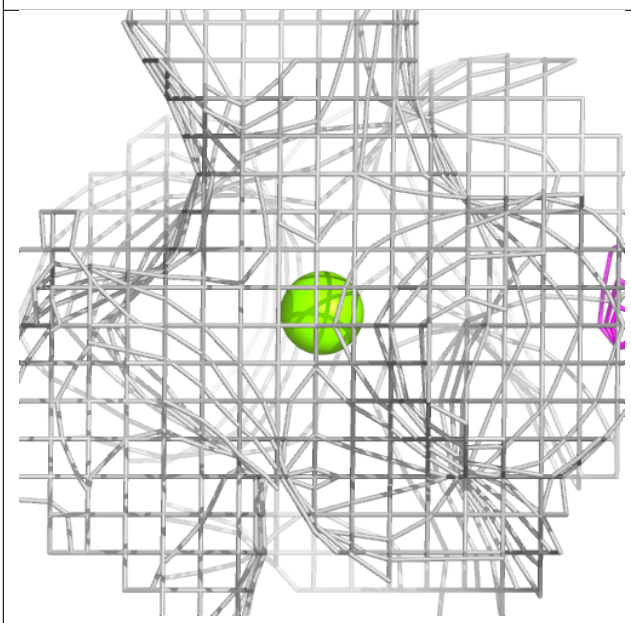


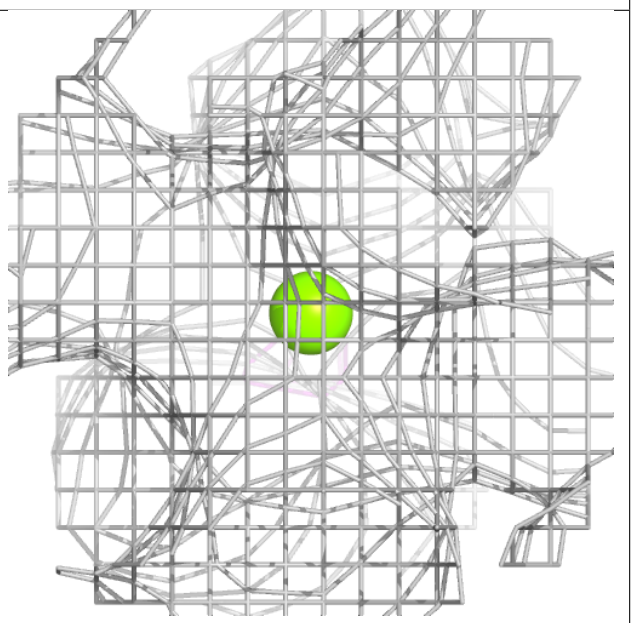


Electron density around MG A 703:

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

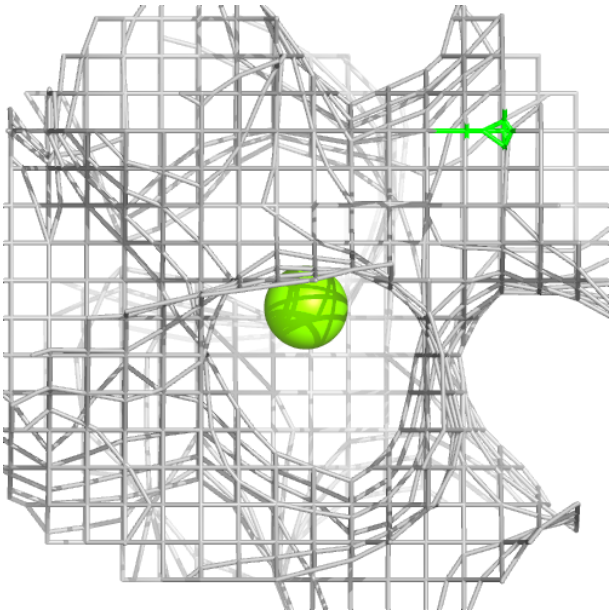


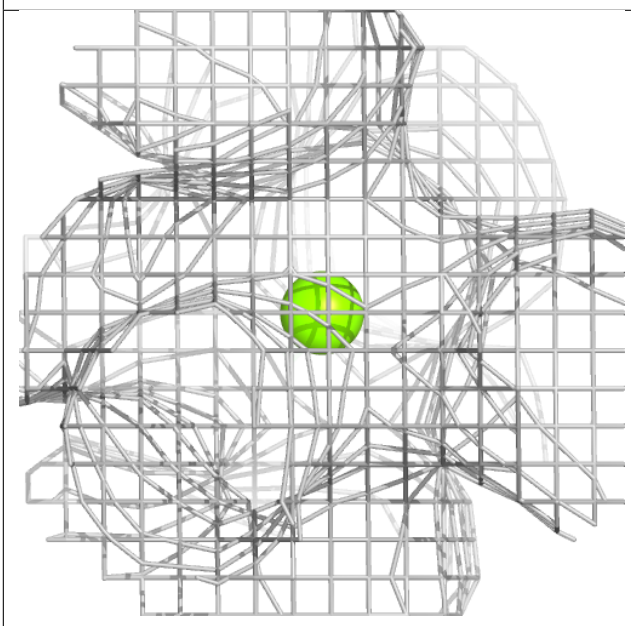


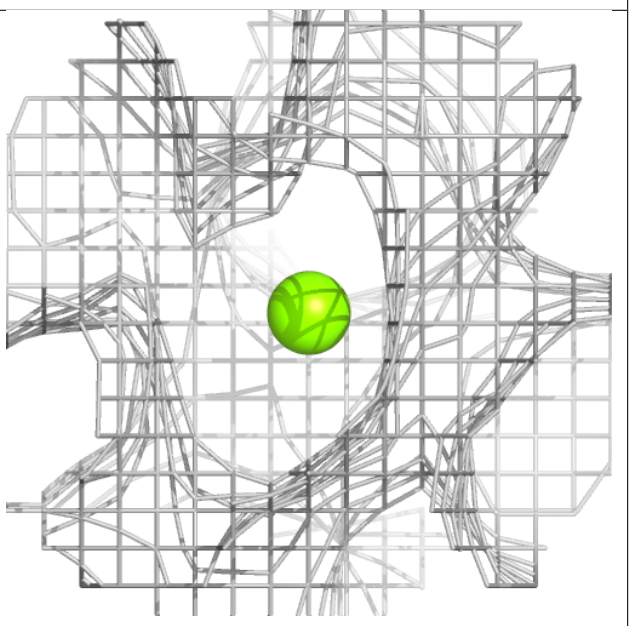


Electron density around MG B 703:

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

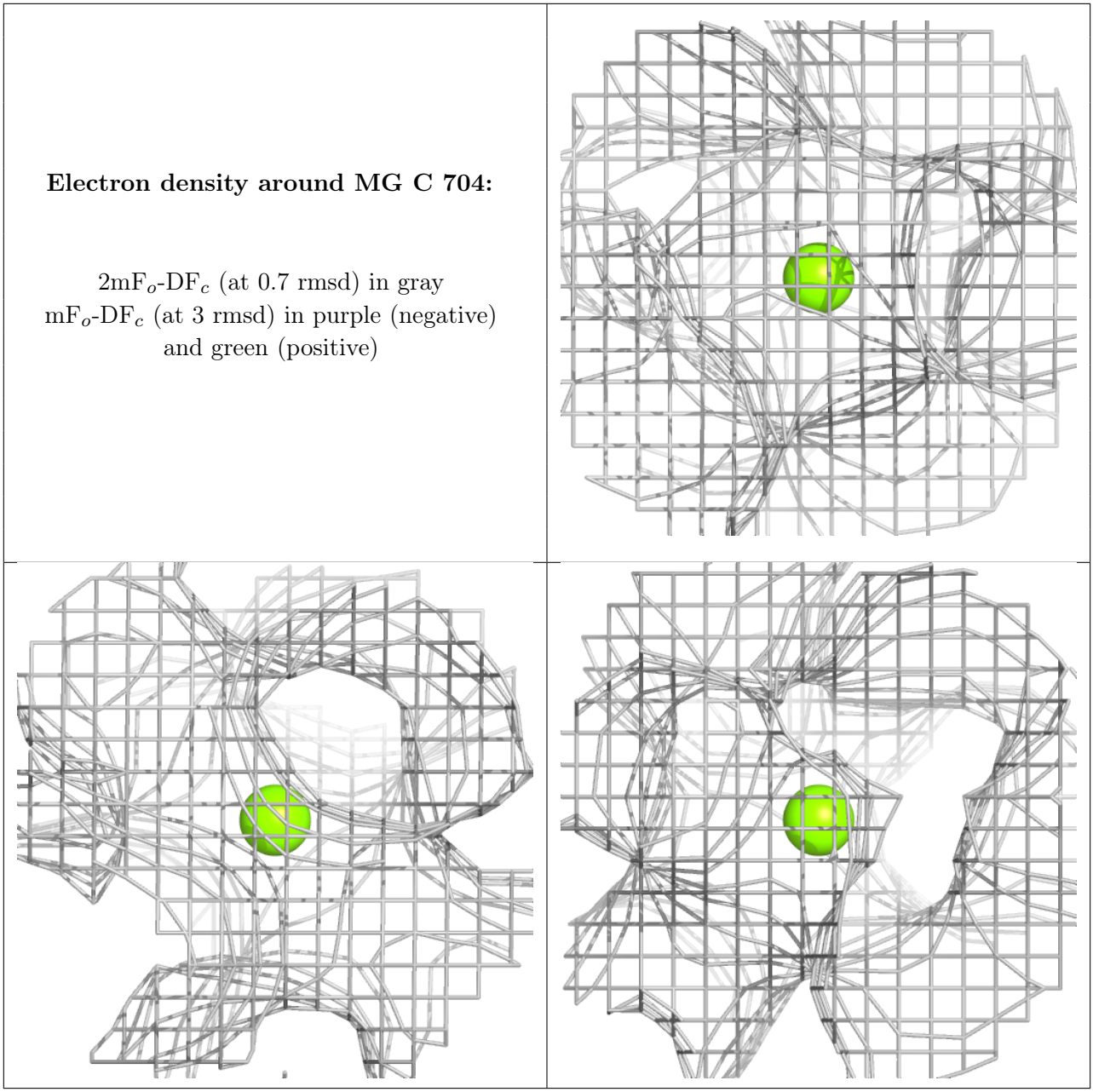






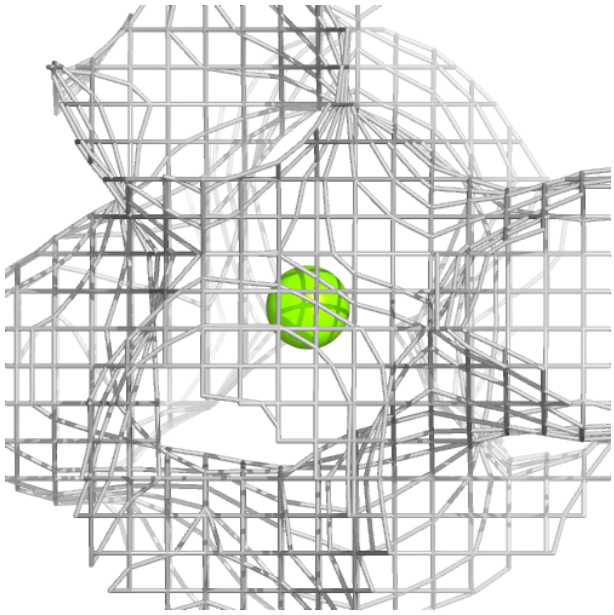
Electron density around MG C 704:

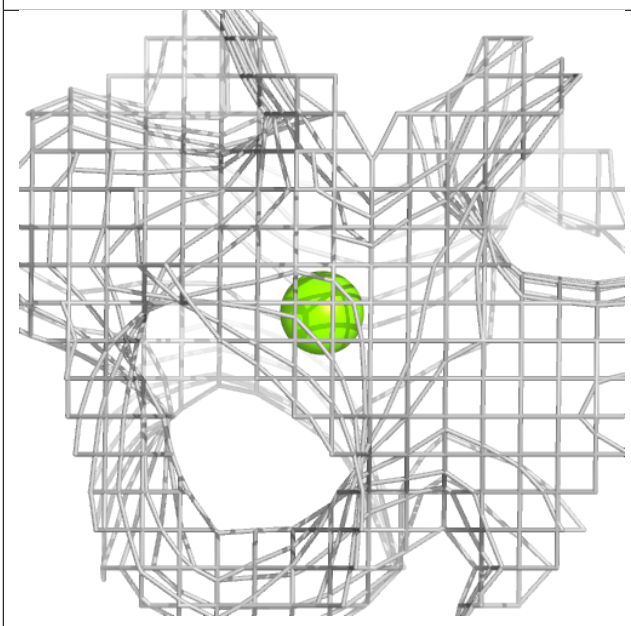
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

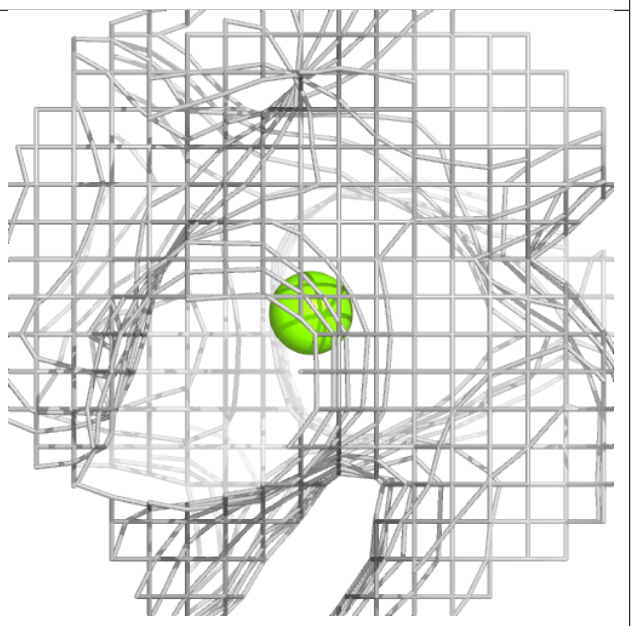


Electron density around MG D 703:

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

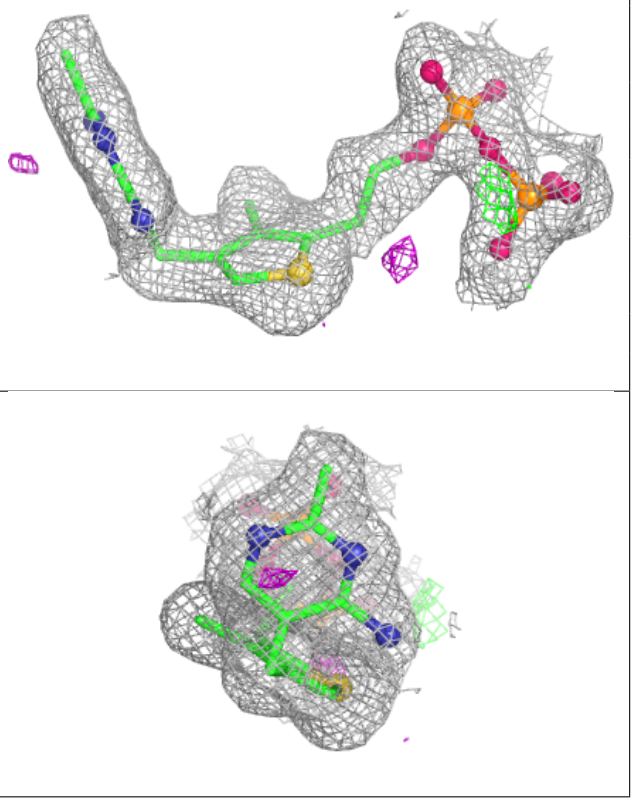


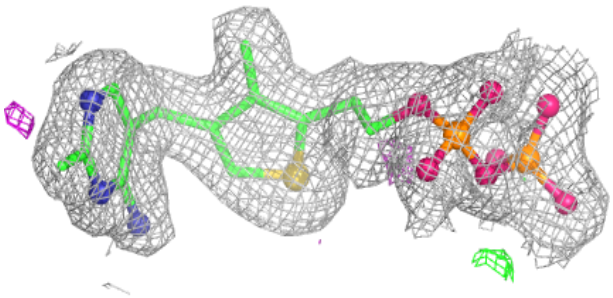




Electron density around TPW A 702:

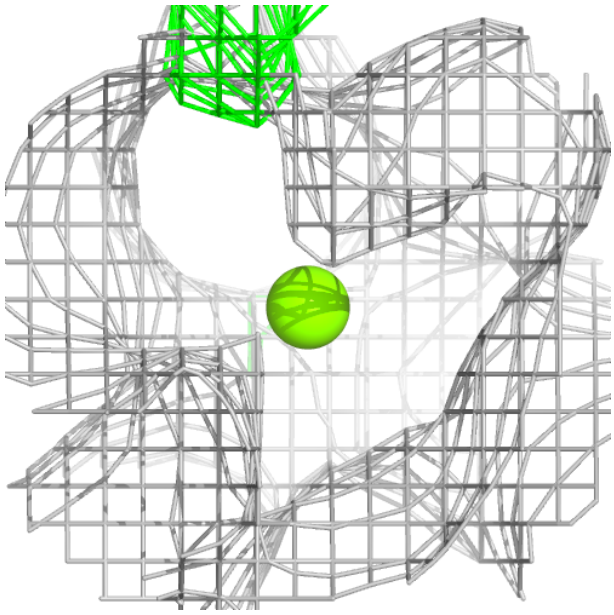
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

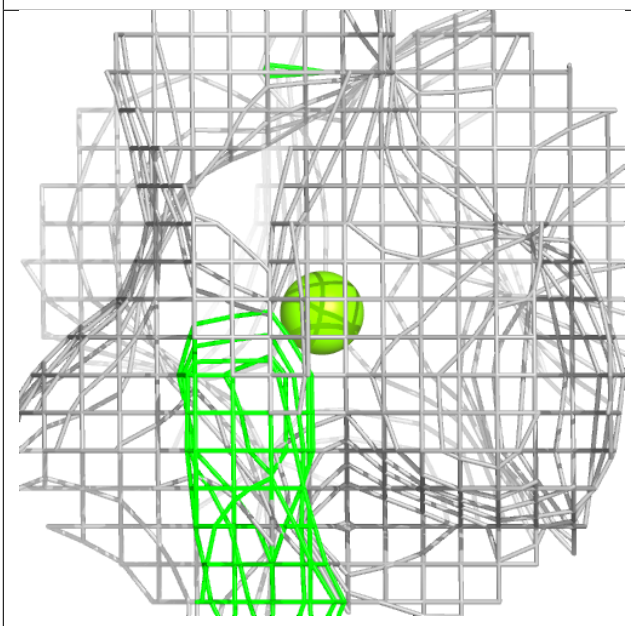


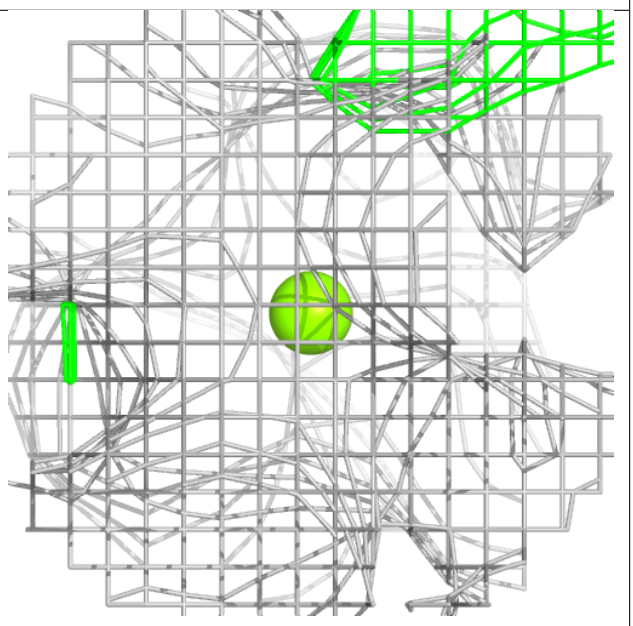


Electron density around MG F 703:

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

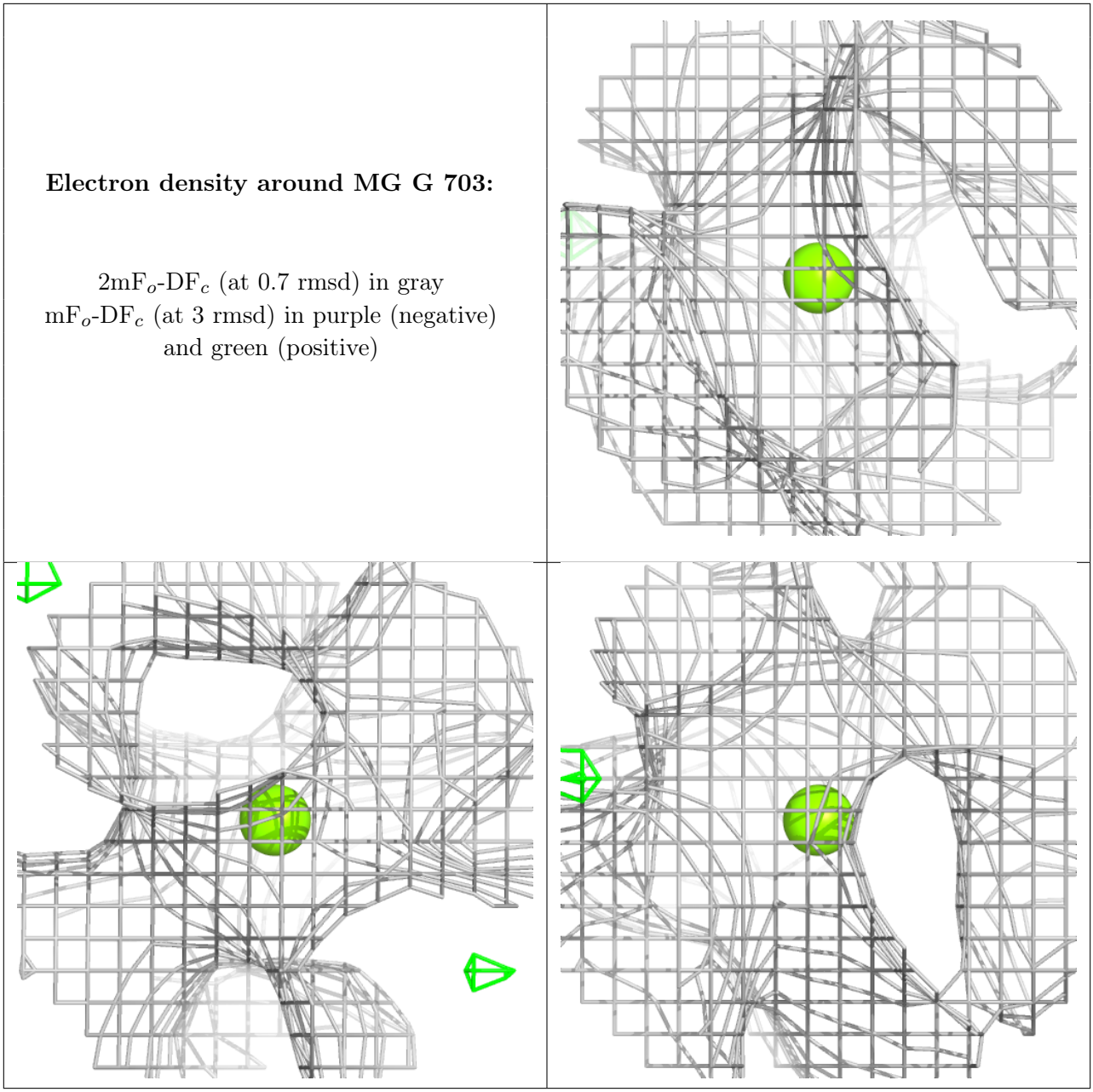






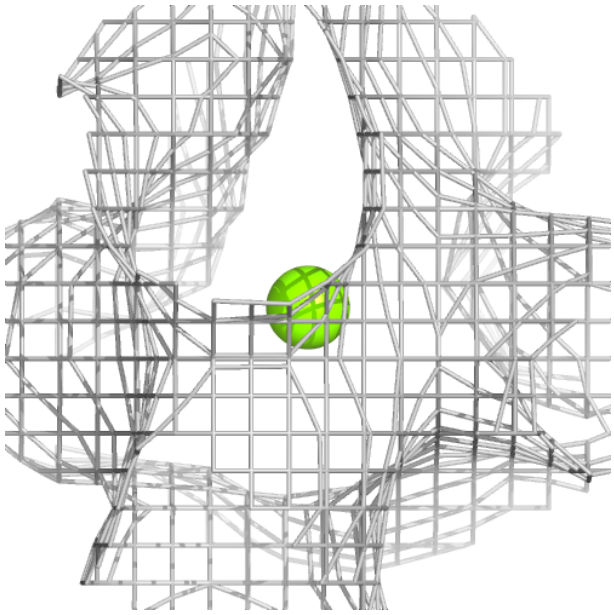
Electron density around MG G 703:

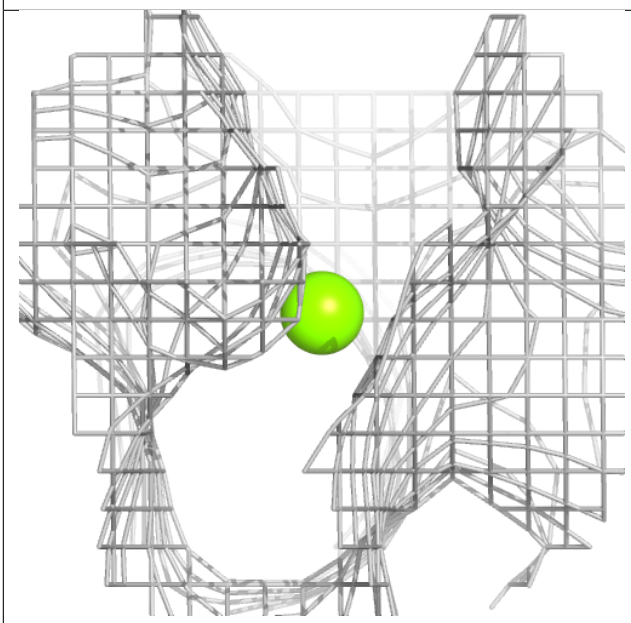
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

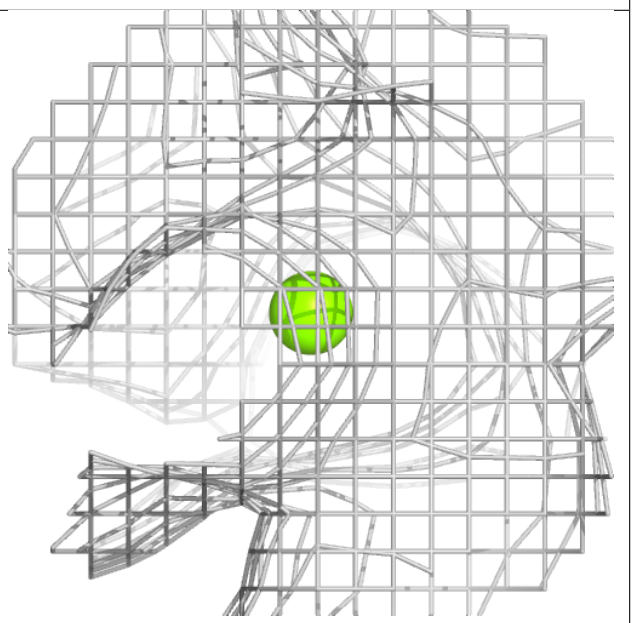


Electron density around MG H 703:

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

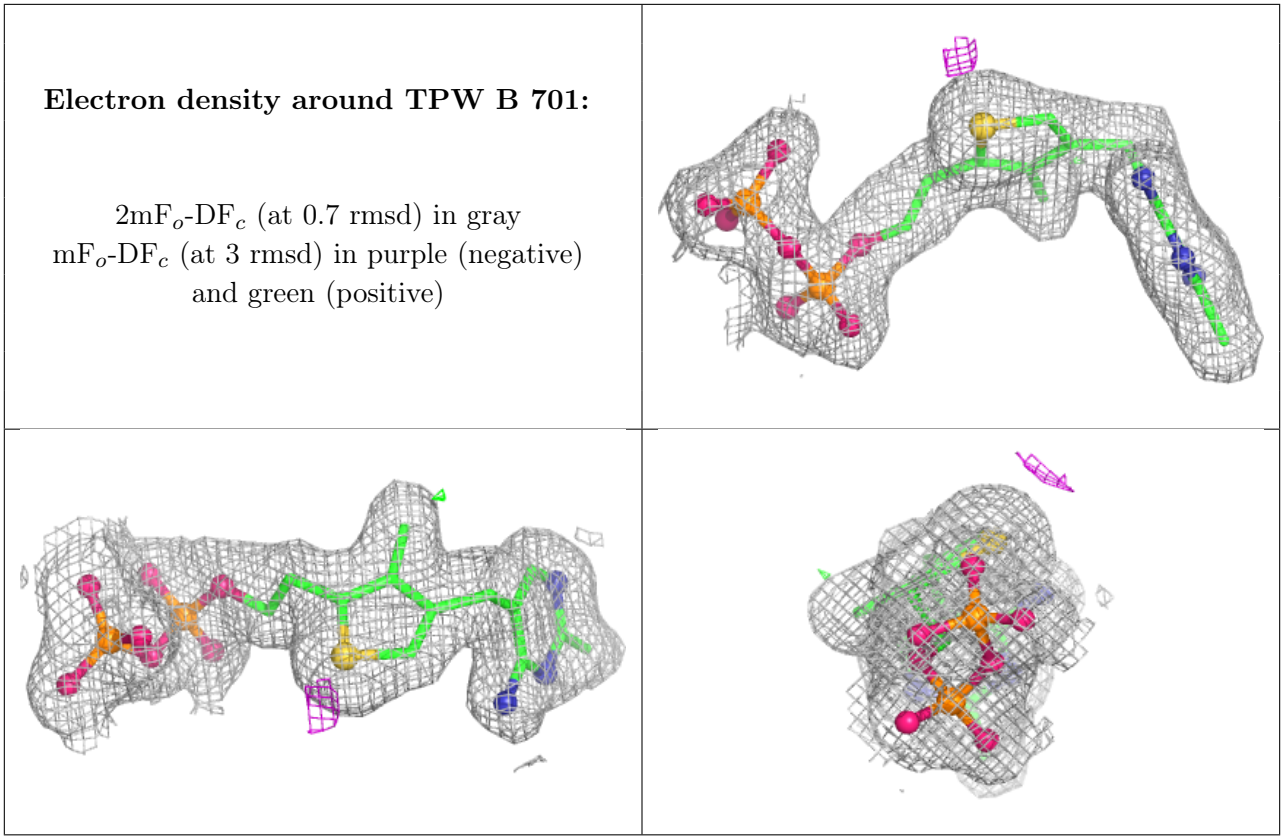






Electron density around TPW B 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.