Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 10:51 pm GMT

PDB ID	:	6QFB
Title	:	Structure of the human ATP citrate lyase holoenzyme in complex with citrate, coenzyme A and Mg.ADP
Authors	:	Verstraete, K.; Verschueren, K.
Deposited on	:	2019-01-09
Resolution	:	3.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

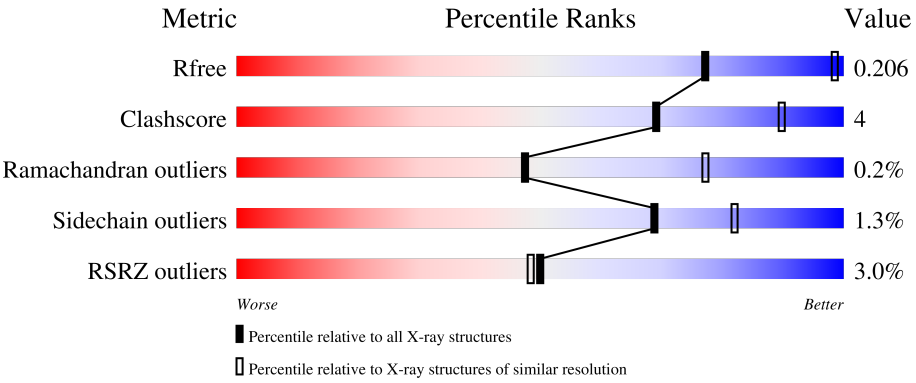
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1050	2% 91% 6%
1	B	1050	% 90% 8%
1	C	1050	4% 86% 10%
1	D	1050	4% 90% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2HP	A	1201	-	-	-	X
2	2HP	D	1201	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 32041 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 ATP-citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7907	5067	1337	1458	45			
1	B	1035	Total	C	N	O	S	0	0	0
			8019	5132	1360	1481	46			
1	C	1011	Total	C	N	O	S	0	0	0
			7841	5023	1326	1447	45			
1	D	1025	Total	C	N	O	S	0	0	0
			7954	5094	1346	1467	47			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P53396
A	?	-	GLN	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	THR	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	HIS	deletion	UNP P53396
A	?	-	THR	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	ASN	deletion	UNP P53396
A	?	-	PHE	deletion	UNP P53396
A	?	-	LEU	deletion	UNP P53396
A	?	-	LEU	deletion	UNP P53396
A	?	-	ASN	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	GLY	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	THR	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	ARG	deletion	UNP P53396
A	?	-	THR	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	PHE	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	GLU	deletion	UNP P53396
A	?	-	SER	deletion	UNP P53396
A	?	-	ARG	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	ASP	deletion	UNP P53396
A	?	-	GLU	deletion	UNP P53396
A	?	-	VAL	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	LYS	deletion	UNP P53396
A	?	-	LYS	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	LYS	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	?	-	ALA	deletion	UNP P53396
A	?	-	MET	deletion	UNP P53396
A	?	-	PRO	deletion	UNP P53396
A	486	MET	GLN	conflict	UNP P53396
A	1102	GLY	-	expression tag	UNP P53396
A	1103	GLY	-	expression tag	UNP P53396
A	1104	SER	-	expression tag	UNP P53396
A	1105	HIS	-	expression tag	UNP P53396
A	1106	HIS	-	expression tag	UNP P53396
A	1107	HIS	-	expression tag	UNP P53396
A	1108	HIS	-	expression tag	UNP P53396
A	1109	HIS	-	expression tag	UNP P53396
A	1110	HIS	-	expression tag	UNP P53396
B	?	-	ASN	deletion	UNP P53396
B	?	-	GLN	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P53396
B	?	-	THR	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	HIS	deletion	UNP P53396
B	?	-	THR	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	ASN	deletion	UNP P53396
B	?	-	PHE	deletion	UNP P53396
B	?	-	LEU	deletion	UNP P53396
B	?	-	LEU	deletion	UNP P53396
B	?	-	ASN	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	GLY	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	THR	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	THR	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	ARG	deletion	UNP P53396
B	?	-	THR	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	PHE	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	GLU	deletion	UNP P53396
B	?	-	SER	deletion	UNP P53396
B	?	-	ARG	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	ASP	deletion	UNP P53396
B	?	-	GLU	deletion	UNP P53396
B	?	-	VAL	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	LYS	deletion	UNP P53396
B	?	-	LYS	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396
B	?	-	ALA	deletion	UNP P53396
B	?	-	MET	deletion	UNP P53396
B	?	-	PRO	deletion	UNP P53396
B	486	MET	GLN	conflict	UNP P53396
B	1102	GLY	-	expression tag	UNP P53396
B	1103	GLY	-	expression tag	UNP P53396
B	1104	SER	-	expression tag	UNP P53396
B	1105	HIS	-	expression tag	UNP P53396
B	1106	HIS	-	expression tag	UNP P53396
B	1107	HIS	-	expression tag	UNP P53396
B	1108	HIS	-	expression tag	UNP P53396
B	1109	HIS	-	expression tag	UNP P53396
B	1110	HIS	-	expression tag	UNP P53396
C	?	-	ASN	deletion	UNP P53396
C	?	-	GLN	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	THR	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	HIS	deletion	UNP P53396
C	?	-	THR	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	ASN	deletion	UNP P53396
C	?	-	PHE	deletion	UNP P53396
C	?	-	LEU	deletion	UNP P53396
C	?	-	LEU	deletion	UNP P53396
C	?	-	ASN	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	GLY	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	THR	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	THR	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	ARG	deletion	UNP P53396

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	PHE	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	GLU	deletion	UNP P53396
C	?	-	SER	deletion	UNP P53396
C	?	-	ARG	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	ASP	deletion	UNP P53396
C	?	-	GLU	deletion	UNP P53396
C	?	-	VAL	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	LYS	deletion	UNP P53396
C	?	-	LYS	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	LYS	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	?	-	ALA	deletion	UNP P53396
C	?	-	MET	deletion	UNP P53396
C	?	-	PRO	deletion	UNP P53396
C	486	MET	GLN	conflict	UNP P53396
C	1102	GLY	-	expression tag	UNP P53396
C	1103	GLY	-	expression tag	UNP P53396
C	1104	SER	-	expression tag	UNP P53396
C	1105	HIS	-	expression tag	UNP P53396
C	1106	HIS	-	expression tag	UNP P53396
C	1107	HIS	-	expression tag	UNP P53396
C	1108	HIS	-	expression tag	UNP P53396
C	1109	HIS	-	expression tag	UNP P53396
C	1110	HIS	-	expression tag	UNP P53396
D	?	-	ASN	deletion	UNP P53396
D	?	-	GLN	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	THR	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	HIS	deletion	UNP P53396
D	?	-	THR	deletion	UNP P53396

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP P53396
D	?	-	ASN	deletion	UNP P53396
D	?	-	PHE	deletion	UNP P53396
D	?	-	LEU	deletion	UNP P53396
D	?	-	LEU	deletion	UNP P53396
D	?	-	ASN	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	GLY	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	THR	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	THR	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	ARG	deletion	UNP P53396
D	?	-	THR	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	PHE	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	GLU	deletion	UNP P53396
D	?	-	SER	deletion	UNP P53396
D	?	-	ARG	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	ASP	deletion	UNP P53396
D	?	-	GLU	deletion	UNP P53396
D	?	-	VAL	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	LYS	deletion	UNP P53396
D	?	-	LYS	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	LYS	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	?	-	ALA	deletion	UNP P53396
D	?	-	MET	deletion	UNP P53396
D	?	-	PRO	deletion	UNP P53396
D	486	MET	GLN	conflict	UNP P53396

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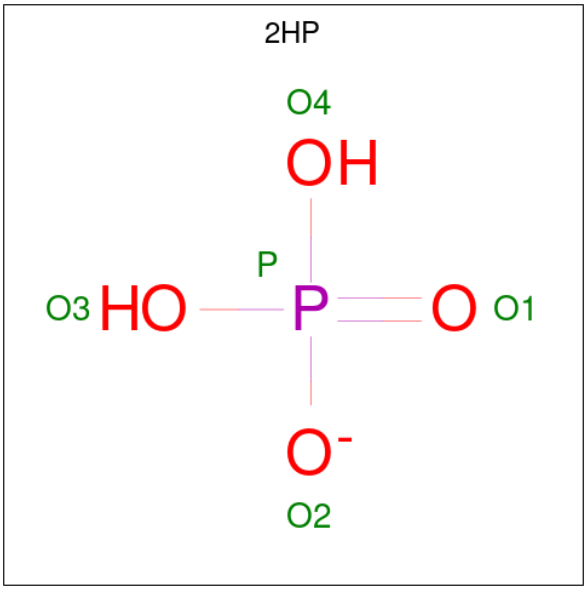
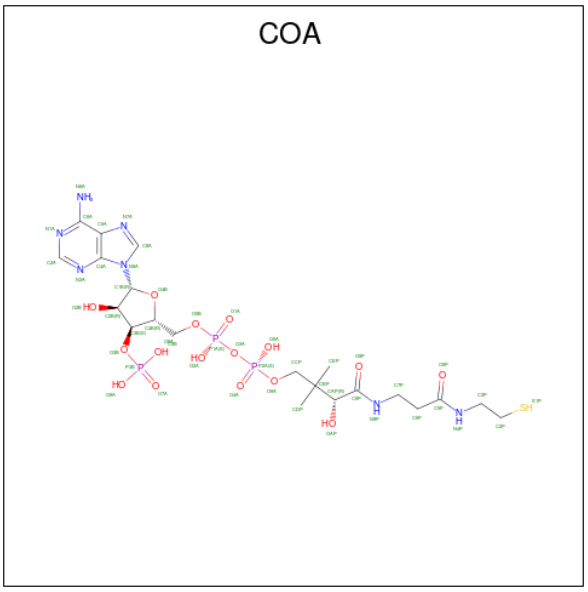
Chain	Residue	Modelled	Actual	Comment	Reference
D	1102	GLY	-	expression tag	UNP P53396
D	1103	GLY	-	expression tag	UNP P53396
D	1104	SER	-	expression tag	UNP P53396
D	1105	HIS	-	expression tag	UNP P53396
D	1106	HIS	-	expression tag	UNP P53396
D	1107	HIS	-	expression tag	UNP P53396
D	1108	HIS	-	expression tag	UNP P53396
D	1109	HIS	-	expression tag	UNP P53396
D	1110	HIS	-	expression tag	UNP P53396

- Molecule 2 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H_2O_4P) (labeled as "Ligand of Interest" by depositor).



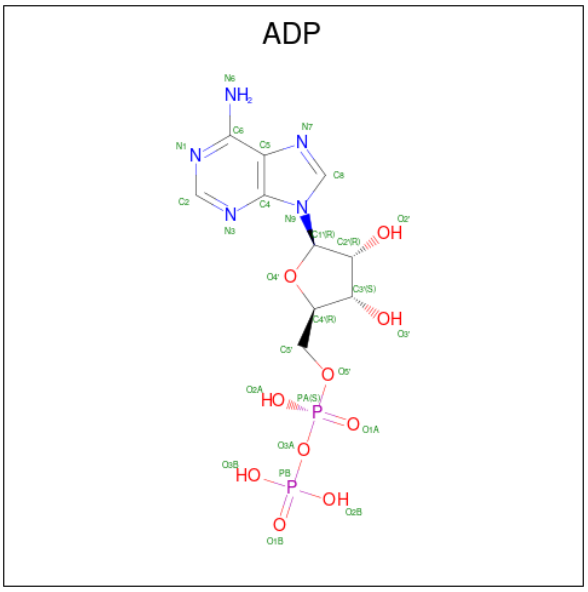
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 48 21 7 16 3 1	0	0
3	B	1	Total C N O P 41 17 6 15 3	0	0
3	C	1	Total C N O P S 48 21 7 16 3 1	0	0
3	D	1	Total C N O P 42 18 6 15 3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

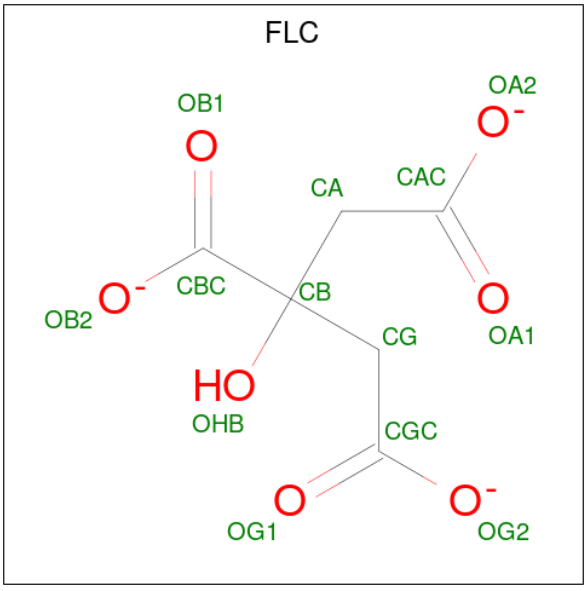


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



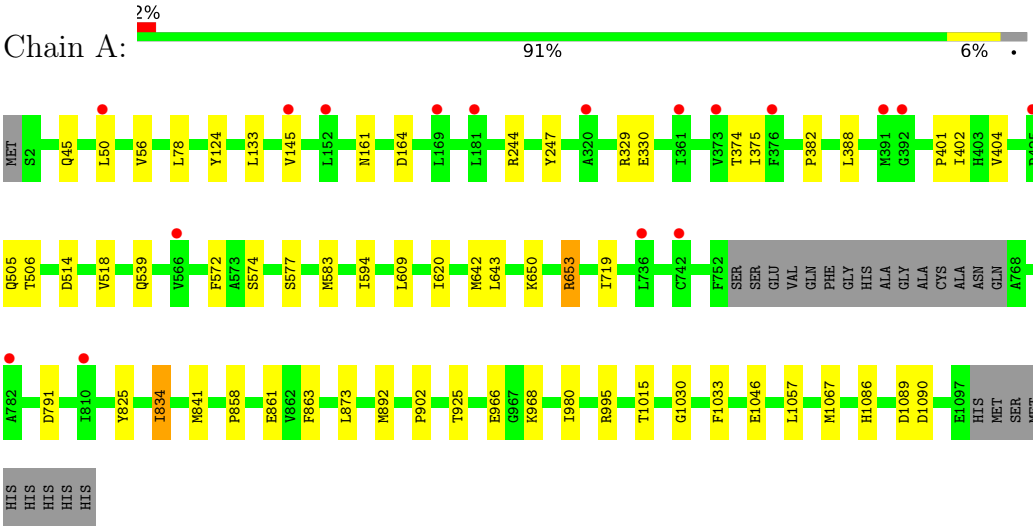
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	6	7		

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.

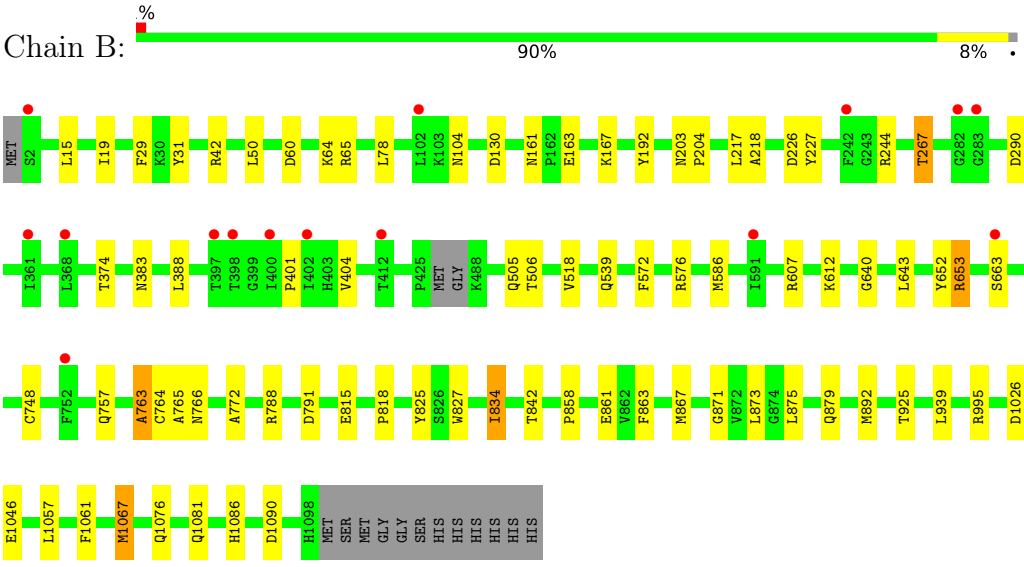
• Molecule 1: ATP-citrate synthase

Chain A:



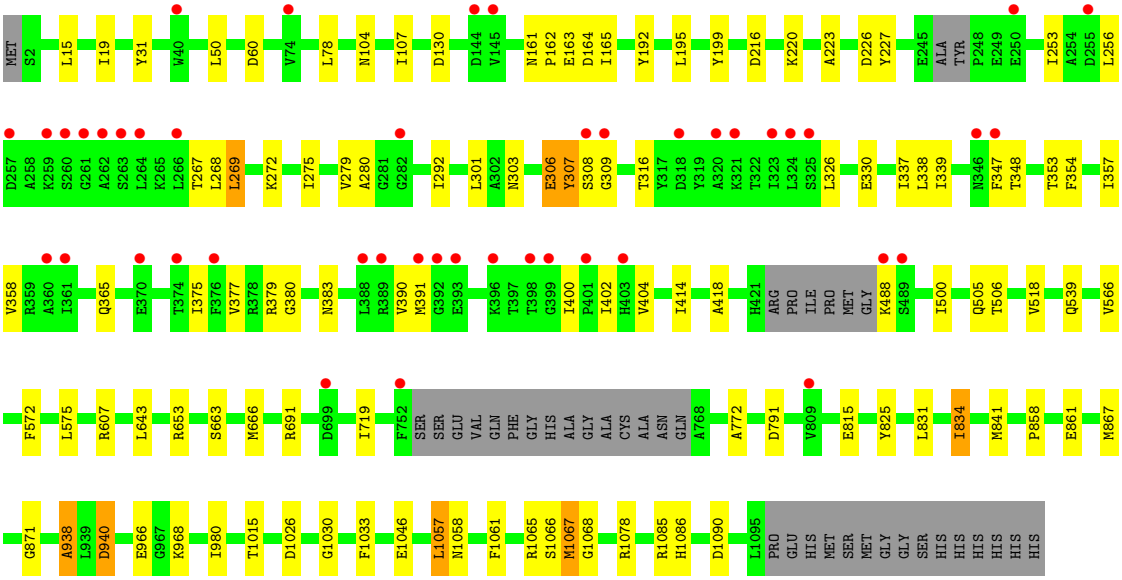
• Molecule 1: ATP-citrate synthase

Chain B:



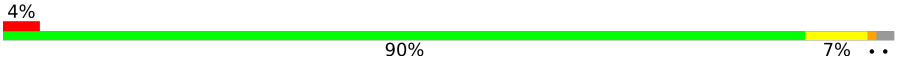
• Molecule 1: ATP-citrate synthase

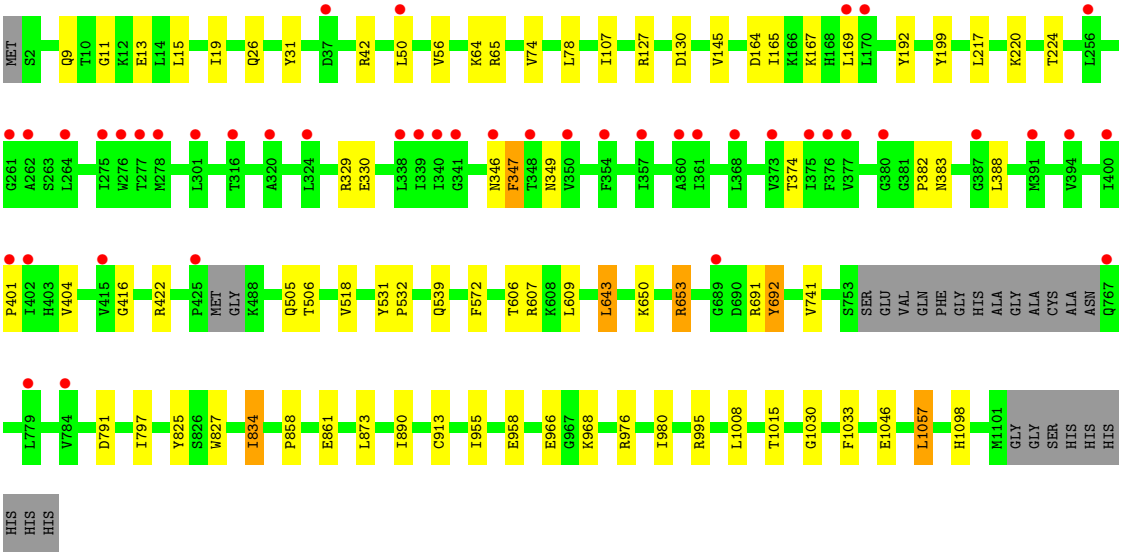
Chain C:



- Molecule 1: ATP-citrate synthase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	214.28Å 215.40Å 158.42Å 90.00° 117.27° 90.00°	Depositor
Resolution (Å)	47.83 – 3.25 49.03 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.83-3.25) 99.4 (49.03-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.162 , 0.193 0.180 , 0.206	Depositor DCC
R_{free} test set	5084 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	113.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 98.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32041	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: MG, COA, FLC, 2HP, ADP

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	0.48	0/8078	0.65	0/10931
1	B	0.55	1/8194 (0.0%)	0.71	0/11089
1	C	0.54	1/8007 (0.0%)	0.73	4/10829 (0.0%)
1	D	0.50	0/8126	0.68	0/10994
All	All	0.52	2/32405 (0.0%)	0.69	4/43843 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1067	MET	SD-CE	6.76	2.15	1.77
1	C	1067	MET	SD-CE	5.46	2.08	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	308	SER	CB-CA-C	11.12	131.23	110.10
1	C	309	GLY	N-CA-C	8.18	133.55	113.10
1	C	308	SER	N-CA-C	-7.71	90.17	111.00
1	C	488	LYS	C-N-CA	5.27	134.88	121.70

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	7907	0	7975	53	0
1	B	8019	0	8065	69	1
1	C	7841	0	7910	76	0
1	D	7954	0	8018	53	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	48	0	32	0	0
3	B	41	0	22	1	0
3	C	48	0	32	0	0
3	D	42	0	24	0	0
4	A	27	0	12	1	0
4	B	27	0	12	0	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	13	0	5	0	0
All	All	32041	0	32131	239	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (239) 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:C:1067:MET:SD	1:C:1067:MET:CE	2.08	1.41
1:B:1067:MET:SD	1:B:1067:MET:CE	2.15	1.33
1:C:383:ASN:HD22	1:C:831:LEU:CD2	1.68	1.04
1:B:244:ARG:NH2	1:B:267:THR:HG23	1.75	1.02
1:B:244:ARG:NH2	1:B:267:THR:CG2	2.30	0.94
1:A:244:ARG:NH1	1:A:247:TYR:CE1	2.37	0.93
1:C:280:ALA:HB2	1:C:307:TYR:CE1	2.08	0.89
1:A:858:PRO:HD2	1:A:861:GLU:OE1	1.73	0.86
1:A:995:ARG:HH11	1:A:995:ARG:HG2	1.39	0.86
1:C:272:LYS:HD3	1:C:330:GLU:OE2	1.75	0.85
1:D:64:LYS:HG2	1:D:65:ARG:HG3	1.59	0.84
1:A:873:LEU:HD12	1:B:1067:MET:HE2	1.58	0.84
1:B:653:ARG:NH1	1:B:815:GLU:OE2	2.12	0.82
1:B:226:ASP:OD1	1:B:227:TYR:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ASN:HD22	1:C:831:LEU:HD21	1.46	0.81
1:D:858:PRO:HD2	1:D:861:GLU:OE1	1.80	0.81
1:C:253:ILE:HA	1:C:256:LEU:HB3	1.63	0.80
1:C:858:PRO:HD2	1:C:861:GLU:OE1	1.82	0.80
1:C:130:ASP:OD2	1:C:192:TYR:HE1	1.67	0.77
1:A:995:ARG:HG2	1:A:995:ARG:NH1	1.98	0.77
1:D:995:ARG:NH1	1:D:1008:LEU:HD13	2.01	0.75
1:C:358:VAL:HG21	1:C:390:VAL:HG12	1.69	0.75
1:C:279:VAL:O	1:C:306:GLU:HA	1.87	0.73
1:B:244:ARG:HH22	1:B:267:THR:CG2	1.99	0.72
1:C:383:ASN:ND2	1:C:831:LEU:CD2	2.49	0.72
1:C:162:PRO:HA	1:C:165:ILE:HD12	1.72	0.72
1:B:244:ARG:HH22	1:B:267:THR:HG23	1.50	0.71
1:D:653:ARG:HH21	1:D:653:ARG:HG2	1.54	0.71
1:A:873:LEU:HD12	1:B:1067:MET:CE	2.21	0.71
1:B:244:ARG:HH21	1:B:267:THR:HG23	1.57	0.70
1:C:253:ILE:HG23	1:C:256:LEU:HD23	1.73	0.69
1:A:653:ARG:O	1:A:653:ARG:HD3	1.92	0.69
1:D:653:ARG:HD3	1:D:653:ARG:O	1.93	0.68
1:D:130:ASP:OD1	1:D:607:ARG:NH1	2.27	0.67
1:A:244:ARG:NH1	1:A:247:TYR:CD1	2.62	0.67
1:C:375:ILE:HB	1:C:402:ILE:HG12	1.75	0.67
1:D:995:ARG:NH1	1:D:1008:LEU:CD1	2.57	0.67
1:A:244:ARG:NH1	1:A:247:TYR:HE1	1.93	0.67
1:B:586:MET:SD	1:B:612:LYS:HD3	2.35	0.67
1:D:130:ASP:OD2	1:D:192:TYR:HE1	1.78	0.66
1:C:383:ASN:HD22	1:C:831:LEU:HD22	1.56	0.66
1:C:940:ASP:OD2	1:C:1058:ASN:ND2	2.30	0.65
1:B:858:PRO:HD2	1:B:861:GLU:OE1	1.95	0.65
1:A:244:ARG:CZ	1:A:247:TYR:HE1	2.10	0.65
1:A:653:ARG:HG2	1:A:653:ARG:HH21	1.61	0.64
1:C:280:ALA:HB2	1:C:307:TYR:HE1	1.60	0.64
1:B:1033:PHE:CD2	1:B:1057:LEU:HD11	2.33	0.63
1:C:226:ASP:OD1	1:C:227:TYR:N	2.31	0.63
1:D:650:LYS:HB3	1:D:653:ARG:HE	1.62	0.63
1:A:825:TYR:CE1	1:A:834:ILE:HD11	2.35	0.62
1:A:925:THR:CG2	1:B:925:THR:HG23	2.30	0.61
1:C:1030:GLY:HA2	1:C:1057:LEU:HD21	1.81	0.61
1:C:130:ASP:OD1	1:C:607:ARG:NH1	2.29	0.61
1:C:1085:ARG:HD2	1:D:976:ARG:HH22	1.66	0.61
1:C:506:THR:HG22	1:C:539:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:ARG:HH11	1:A:995:ARG:CG	2.13	0.60
1:A:1033:PHE:CD2	1:A:1057:LEU:HD11	2.37	0.60
1:A:518:VAL:HG21	1:A:643:LEU:HD21	1.83	0.59
1:D:653:ARG:HH21	1:D:653:ARG:CG	2.15	0.59
1:D:56:VAL:HG22	1:D:74:VAL:HA	1.85	0.59
1:C:339:ILE:HG23	1:C:414:ILE:HD11	1.85	0.58
1:D:518:VAL:HG21	1:D:643:LEU:HD21	1.86	0.58
1:C:268:LEU:HD11	1:C:326:LEU:HD13	1.87	0.57
1:A:244:ARG:CZ	1:A:247:TYR:CE1	2.87	0.57
1:C:506:THR:HG22	1:C:539:GLN:NE2	2.19	0.57
1:C:15:LEU:HD12	1:C:19:ILE:HB	1.87	0.56
1:C:825:TYR:CE1	1:C:834:ILE:HD11	2.40	0.56
1:A:858:PRO:CD	1:A:861:GLU:OE1	2.52	0.56
1:B:653:ARG:O	1:B:653:ARG:HD3	2.06	0.56
1:B:1033:PHE:CD2	1:B:1057:LEU:CD1	2.89	0.56
1:C:280:ALA:CB	1:C:307:TYR:CE1	2.88	0.55
1:B:506:THR:HG22	1:B:539:GLN:NE2	2.21	0.55
1:C:518:VAL:HG21	1:C:643:LEU:HD21	1.89	0.55
1:A:124:TYR:HE1	1:A:133:LEU:HD11	1.72	0.55
1:D:349:ASN:HA	1:D:382:PRO:HG2	1.89	0.55
1:C:216:ASP:HB2	4:C:1202:ADP:O1A	2.07	0.54
1:B:161:ASN:HD21	1:B:163:GLU:HG2	1.73	0.54
1:C:292:ILE:HG21	1:C:301:LEU:HD13	1.89	0.54
1:C:506:THR:CG2	1:C:539:GLN:HE22	2.20	0.54
1:B:825:TYR:CE1	1:B:834:ILE:HD11	2.42	0.54
1:D:995:ARG:HH12	1:D:1008:LEU:HD13	1.70	0.53
1:D:383:ASN:HB3	1:D:827:TRP:CH2	2.44	0.53
1:A:1030:GLY:HA2	1:A:1057:LEU:HD21	1.90	0.53
1:B:290:ASP:HA	1:B:748:CYS:SG	2.49	0.53
1:D:825:TYR:CE1	1:D:834:ILE:HD11	2.43	0.53
1:C:347:PHE:HD2	1:C:348:THR:HG23	1.72	0.52
1:D:199:TYR:HB3	1:D:220:LYS:HB2	1.92	0.52
1:D:506:THR:HG22	1:D:539:GLN:NE2	2.25	0.52
1:B:130:ASP:OD2	1:B:192:TYR:HE1	1.93	0.52
1:D:1033:PHE:CD2	1:D:1057:LEU:CD1	2.93	0.52
1:C:130:ASP:OD2	1:C:192:TYR:CE1	2.56	0.51
1:B:217:LEU:HD23	1:B:218:ALA:N	2.24	0.51
1:C:354:PHE:HA	1:C:357:ILE:HD12	1.91	0.51
1:C:1085:ARG:CD	1:D:976:ARG:HH22	2.23	0.51
1:C:1061:PHE:CE1	1:C:1065:ARG:NH2	2.79	0.51
1:B:939:LEU:HD22	1:B:1061:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ILE:HD12	1:B:772:ALA:H	1.76	0.51
1:B:60:ASP:HB3	1:B:104:ASN:HD22	1.74	0.51
1:D:1033:PHE:CD2	1:D:1057:LEU:HD11	2.46	0.50
1:A:825:TYR:HE1	1:A:834:ILE:HD11	1.76	0.50
1:C:377:VAL:HG11	1:C:391:MET:HG3	1.93	0.50
1:B:383:ASN:HA	1:B:827:TRP:CH2	2.46	0.50
1:C:292:ILE:HD13	1:C:301:LEU:HD13	1.94	0.50
1:D:653:ARG:CG	1:D:653:ARG:NH2	2.73	0.50
1:A:382:PRO:HB3	1:A:642:MET:CE	2.41	0.49
1:B:518:VAL:HG12	1:B:652:TYR:HB3	1.94	0.49
1:B:506:THR:HG22	1:B:539:GLN:HE22	1.76	0.49
1:D:416:GLY:HA3	1:D:422:ARG:HE	1.77	0.49
1:B:163:GLU:O	1:B:167:LYS:HB2	2.13	0.49
1:C:337:ILE:HG21	1:C:418:ALA:HB1	1.93	0.49
1:C:383:ASN:ND2	1:C:831:LEU:HD22	2.22	0.49
1:C:1065:ARG:O	1:C:1068:GLY:N	2.45	0.49
1:C:1033:PHE:CD2	1:C:1057:LEU:CD1	2.95	0.49
1:C:269:LEU:HD21	1:C:301:LEU:HG	1.93	0.49
1:A:594:ILE:HB	1:A:620:ILE:HD13	1.95	0.48
1:B:653:ARG:NH2	1:B:679:ASP:O	2.45	0.48
1:D:966:GLU:HB3	1:D:968:LYS:HD3	1.94	0.48
1:B:374:THR:HG23	1:B:401:PRO:HB2	1.95	0.48
1:A:388:LEU:HB3	1:A:404:VAL:CG1	2.43	0.48
1:B:346:ASN:HD22	1:B:640:GLY:H	1.60	0.48
1:D:1033:PHE:CG	1:D:1057:LEU:HD11	2.48	0.48
1:A:56:VAL:HG21	4:A:1203:ADP:C6	2.48	0.48
1:B:244:ARG:HH22	1:B:267:THR:HG21	1.78	0.48
1:C:268:LEU:HD23	1:C:303:ASN:HB3	1.96	0.48
1:C:966:GLU:HB3	1:C:968:LYS:HD3	1.94	0.48
1:A:966:GLU:HB3	1:A:968:LYS:HD3	1.95	0.48
1:A:1033:PHE:CD2	1:A:1057:LEU:CD1	2.97	0.48
1:D:873:LEU:HD22	1:D:890:ILE:HG21	1.96	0.48
1:B:50:LEU:HB3	1:B:78:LEU:HD13	1.96	0.48
1:B:29:PHE:HA	1:B:31:TYR:CE2	2.50	0.47
1:D:506:THR:HG22	1:D:539:GLN:HE22	1.79	0.47
1:D:858:PRO:CD	1:D:861:GLU:OE1	2.59	0.47
1:A:388:LEU:HB3	1:A:404:VAL:HG11	1.97	0.47
1:D:346:ASN:HB3	1:D:347:PHE:CD2	2.50	0.47
1:A:583:MET:SD	1:A:609:LEU:HD23	2.55	0.47
1:A:1086:HIS:HE2	1:A:1090:ASP:HB3	1.80	0.47
1:B:1033:PHE:CG	1:B:1057:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ARG:HG3	1:D:692:TYR:HB3	1.96	0.47
1:B:226:ASP:OD1	1:B:226:ASP:C	2.53	0.47
1:B:329:ARG:HB2	1:B:330:GLU:OE1	2.15	0.47
1:B:130:ASP:OD1	1:B:607:ARG:NH1	2.43	0.47
1:C:719:ILE:HD12	1:C:772:ALA:H	1.81	0.46
1:A:1046:GLU:H	1:A:1046:GLU:CD	2.18	0.46
1:A:161:ASN:HB3	1:A:164:ASP:OD2	2.15	0.46
1:C:275:ILE:HG12	1:C:337:ILE:HD12	1.96	0.46
1:C:663:SER:HB3	1:C:666:MET:HB2	1.97	0.46
1:B:506:THR:CG2	1:B:539:GLN:HE22	2.29	0.46
1:A:50:LEU:HB3	1:A:78:LEU:HD13	1.98	0.46
1:C:15:LEU:O	1:C:19:ILE:HG22	2.16	0.46
1:C:1033:PHE:CG	1:C:1057:LEU:HD11	2.51	0.45
1:B:388:LEU:HD22	1:B:404:VAL:HG13	1.98	0.45
1:A:892:MET:HG3	1:B:863:PHE:HE1	1.82	0.45
1:A:925:THR:HG22	1:B:925:THR:HG23	1.96	0.45
1:A:1067:MET:HE2	1:B:873:LEU:HD12	1.98	0.45
1:C:199:TYR:HB3	1:C:220:LYS:HB2	1.98	0.45
1:B:244:ARG:NH2	1:B:267:THR:HG21	2.27	0.45
1:C:50:LEU:HB3	1:C:78:LEU:HD13	1.99	0.45
1:D:329:ARG:HB2	1:D:330:GLU:OE1	2.16	0.45
1:D:506:THR:CG2	1:D:539:GLN:HE22	2.29	0.45
1:A:329:ARG:HB2	1:A:330:GLU:OE1	2.17	0.45
1:C:867:MET:HB3	1:C:871:GLY:HA3	2.00	0.44
1:A:505:GLN:HG3	1:A:572:PHE:CG	2.53	0.44
1:D:15:LEU:O	1:D:19:ILE:HG22	2.17	0.44
1:D:50:LEU:HB3	1:D:78:LEU:HD13	1.99	0.44
1:A:382:PRO:HB3	1:A:642:MET:HE1	1.99	0.44
1:C:1065:ARG:O	1:C:1066:SER:C	2.55	0.44
1:A:1067:MET:CE	1:B:873:LEU:HD12	2.47	0.44
1:B:15:LEU:HD12	1:B:19:ILE:HB	2.00	0.44
1:B:875:LEU:O	1:B:879:GLN:HA	2.17	0.44
1:C:1086:HIS:HE2	1:C:1090:ASP:HB3	1.83	0.44
1:D:1030:GLY:HA2	1:D:1057:LEU:HD21	1.98	0.44
1:C:379:ARG:HG3	1:C:380:GLY:H	1.82	0.44
1:A:902:PRO:HG3	1:B:842:THR:HG21	1.99	0.43
1:C:338:LEU:HD23	1:C:375:ILE:HG12	2.00	0.43
1:C:379:ARG:HG3	1:C:380:GLY:N	2.32	0.43
1:D:383:ASN:HB3	1:D:827:TRP:CZ2	2.53	0.43
1:B:203:ASN:HA	1:B:204:PRO:HA	1.84	0.43
1:A:863:PHE:HE1	1:B:892:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.54	0.43
1:C:980:ILE:HD13	1:C:1015:THR:HG21	2.00	0.43
1:C:1046:GLU:CD	1:C:1046:GLU:H	2.22	0.43
1:D:9:GLN:O	1:D:13:GLU:HB2	2.19	0.43
1:D:374:THR:HG23	1:D:401:PRO:HB2	1.99	0.43
1:A:1067:MET:HE1	1:B:873:LEU:HB2	1.98	0.43
1:B:518:VAL:HG13	1:B:818:PRO:HB2	2.00	0.43
1:B:1046:GLU:CD	1:B:1046:GLU:H	2.22	0.43
1:C:347:PHE:CD2	1:C:348:THR:HG23	2.52	0.43
1:A:719:ILE:HD12	1:A:772:ALA:H	1.84	0.43
1:B:161:ASN:ND2	1:B:163:GLU:HG2	2.34	0.43
1:D:1046:GLU:H	1:D:1046:GLU:CD	2.22	0.43
1:A:574:SER:HA	3:B:1203:COA:H133	2.01	0.43
1:B:825:TYR:HE1	1:B:834:ILE:HD11	1.84	0.43
1:C:316:THR:HG21	1:C:353:THR:O	2.18	0.43
1:D:11:GLY:HA3	1:D:217:LEU:HD22	2.01	0.43
1:D:31:TYR:HA	1:D:107:ILE:O	2.19	0.43
1:C:339:ILE:HG23	1:C:414:ILE:CD1	2.48	0.43
1:C:161:ASN:HB3	1:C:164:ASP:OD2	2.18	0.42
1:C:938:ALA:HB1	1:C:1026:ASP:HB3	2.01	0.42
1:D:741:VAL:HG11	1:D:797:ILE:HG13	2.00	0.42
1:C:825:TYR:HE1	1:C:834:ILE:HD11	1.82	0.42
1:C:505:GLN:HG3	1:C:572:PHE:CG	2.54	0.42
1:D:64:LYS:HE3	1:D:65:ARG:NE	2.34	0.42
1:B:1030:GLY:HA2	1:B:1057:LEU:HD21	2.02	0.42
1:B:1076:GLN:OE1	1:B:1081:GLN:HG3	2.20	0.42
1:C:365:GLN:HA	1:C:400:ILE:HD11	2.02	0.42
1:B:506:THR:CG2	1:B:539:GLN:NE2	2.83	0.42
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.55	0.42
1:C:60:ASP:HB3	1:C:104:ASN:HD22	1.84	0.42
1:D:388:LEU:HD22	1:D:404:VAL:HG13	2.02	0.41
1:D:980:ILE:HD13	1:D:1015:THR:HG21	2.02	0.41
1:A:514:ASP:O	1:A:518:VAL:HG23	2.20	0.41
1:B:757:GLN:HB3	1:B:763:ALA:HB2	2.02	0.41
1:C:1065:ARG:O	1:C:1067:MET:N	2.53	0.41
1:C:1033:PHE:CD2	1:C:1057:LEU:HD11	2.55	0.41
1:A:980:ILE:HD13	1:A:1015:THR:HG21	2.02	0.41
1:D:164:ASP:OD1	1:D:167:LYS:NZ	2.28	0.41
1:B:64:LYS:HG2	1:B:65:ARG:HG3	2.02	0.41
1:B:15:LEU:HD11	1:B:19:ILE:CD1	2.50	0.41
1:B:227:TYR:CD2	1:B:576:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:HG13	1:C:566:VAL:HG11	2.03	0.41
1:D:531:TYR:HA	1:D:532:PRO:HD2	1.95	0.41
1:C:31:TYR:HA	1:C:107:ILE:O	2.21	0.41
1:A:375:ILE:HB	1:A:402:ILE:HG12	2.03	0.41
1:D:606:THR:HA	1:D:609:LEU:HD12	2.03	0.41
1:D:955:ILE:HG13	1:D:958:GLU:CD	2.41	0.41
1:A:374:THR:HG23	1:A:401:PRO:HB2	2.02	0.41
1:B:15:LEU:HD11	1:B:19:ILE:HD12	2.03	0.41
1:C:506:THR:CG2	1:C:539:GLN:NE2	2.81	0.40
1:A:124:TYR:CE1	1:A:133:LEU:HD11	2.54	0.40
1:B:663:SER:HB3	1:B:666:MET:HB2	2.03	0.40
1:B:867:MET:HB3	1:B:871:GLY:HA3	2.03	0.40
1:B:939:LEU:HD12	1:B:1026:ASP:OD2	2.21	0.40
1:B:1086:HIS:HE2	1:B:1090:ASP:HB3	1.85	0.40
1:C:858:PRO:CD	1:C:861:GLU:OE1	2.61	0.40
1:D:506:THR:CG2	1:D:539:GLN:NE2	2.85	0.40
1:A:653:ARG:HH21	1:A:653:ARG:CG	2.29	0.40
1:D:165:ILE:O	1:D:169:LEU:HB2	2.22	0.40
1:A:506:THR:HG22	1:A:539:GLN:NE2	2.36	0.40
1:A:650:LYS:HB3	1:A:653:ARG:HE	1.87	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ARG:CZ	1:D:26:GLN:OE1[3_545]	2.19	0.01

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	1013/1050 (96%)	988 (98%)	25 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1031/1050 (98%)	989 (96%)	38 (4%)	4 (0%)	34 67
1	C	1003/1050 (96%)	956 (95%)	45 (4%)	2 (0%)	47 77
1	D	1019/1050 (97%)	984 (97%)	34 (3%)	1 (0%)	51 82
All	All	4066/4200 (97%)	3917 (96%)	142 (4%)	7 (0%)	47 77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	764	CYS
1	B	766	ASN
1	D	1098	HIS
1	C	938	ALA
1	B	763	ALA
1	B	765	ALA
1	C	223	ALA

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	845/868 (97%)	837 (99%)	8 (1%)	78 87
1	B	855/868 (98%)	848 (99%)	7 (1%)	81 89
1	C	838/868 (96%)	821 (98%)	17 (2%)	55 76
1	D	851/868 (98%)	839 (99%)	12 (1%)	67 81
All	All	3389/3472 (98%)	3345 (99%)	44 (1%)	69 82

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	145	VAL
1	A	577	SER
1	A	653	ARG

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Mol	Chain	Res	Type
1	A	791	ASP
1	A	834	ILE
1	A	841	MET
1	A	1089	ASP
1	B	42	ARG
1	B	267	THR
1	B	643	LEU
1	B	653	ARG
1	B	791	ASP
1	B	834	ILE
1	B	995	ARG
1	C	163	GLU
1	C	195	LEU
1	C	267	THR
1	C	269	LEU
1	C	306	GLU
1	C	307	TYR
1	C	404	VAL
1	C	575	LEU
1	C	653	ARG
1	C	691	ARG
1	C	791	ASP
1	C	815	GLU
1	C	834	ILE
1	C	841	MET
1	C	940	ASP
1	C	1057	LEU
1	C	1078	ARG
1	D	42	ARG
1	D	145	VAL
1	D	224	THR
1	D	347	PHE
1	D	643	LEU
1	D	653	ARG
1	D	691	ARG
1	D	692	TYR
1	D	791	ASP
1	D	834	ILE
1	D	913	CYS
1	D	1057	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	HIS
1	A	961	ASN
1	B	346	ASN
1	B	757	GLN
1	B	767	GLN
1	B	900	HIS
1	C	383	ASN
1	C	539	GLN
1	D	346	ASN
1	D	383	ASN
1	D	539	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	2HP	A	1201	-	4,4,4	0.77	0	6,6,6	0.79	0
2	2HP	B	1201	5	4,4,4	0.89	0	6,6,6	0.86	0
4	ADP	C	1202	5	24,29,29	0.65	0	29,45,45	0.72	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FLC	B	1202	5	12,12,12	1.06	0	17,17,17	1.30	2 (11%)
3	COA	D	1202	-	36,44,50	0.53	0	45,68,75	0.85	2 (4%)
4	ADP	D	1203	5	24,29,29	0.81	1 (4%)	29,45,45	0.79	1 (3%)
3	COA	B	1203	-	35,43,50	0.62	0	45,67,75	0.84	2 (4%)
3	COA	C	1201	-	41,50,50	0.58	0	52,75,75	0.83	2 (3%)
2	2HP	D	1201	-	4,4,4	0.86	0	6,6,6	0.44	0
3	COA	A	1202	-	41,50,50	0.58	0	52,75,75	0.87	2 (3%)
4	ADP	A	1203	5	24,29,29	0.66	0	29,45,45	0.80	1 (3%)
4	ADP	B	1204	5	24,29,29	0.71	0	29,45,45	0.86	1 (3%)

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
4	ADP	C	1202	5	-	4/12/32/32	0/3/3/3
6	FLC	B	1202	5	-	2/16/16/16	-
3	COA	D	1202	-	-	2/37/57/64	0/3/3/3
4	ADP	D	1203	5	-	3/12/32/32	0/3/3/3
3	COA	B	1203	-	-	4/36/56/64	0/3/3/3
3	COA	C	1201	-	-	3/44/64/64	0/3/3/3
3	COA	A	1202	-	-	2/44/64/64	0/3/3/3
4	ADP	A	1203	5	-	4/12/32/32	0/3/3/3
4	ADP	B	1204	5	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1203	ADP	PB-O1B	2.20	1.57	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1203	COA	O6A-P2A-O4A	3.35	122.15	109.07
6	B	1202	FLC	OB1-CBC-CB	-2.97	118.05	122.25
3	D	1202	COA	O6A-P2A-O4A	2.94	120.55	109.07
3	A	1202	COA	O6A-P2A-O4A	2.86	120.25	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1201	COA	O6A-P2A-O4A	2.62	119.30	109.07
6	B	1202	FLC	OB2-CBC-CB	2.38	117.19	113.05
4	D	1203	ADP	C5-C6-N6	2.33	123.90	120.35
3	D	1202	COA	C5A-C6A-N6A	2.33	123.89	120.35
4	C	1202	ADP	C5-C6-N6	2.31	123.86	120.35
4	A	1203	ADP	C5-C6-N6	2.25	123.77	120.35
4	B	1204	ADP	C5-C6-N6	2.22	123.73	120.35
3	C	1201	COA	C5A-C6A-N6A	2.21	123.71	120.35
3	A	1202	COA	C5A-C6A-N6A	2.18	123.67	120.35
3	B	1203	COA	C5A-C6A-N6A	2.11	123.56	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	COA	S1P-C2P-C3P-N4P
3	C	1201	COA	S1P-C2P-C3P-N4P
4	A	1203	ADP	PA-O3A-PB-O2B
4	A	1203	ADP	PA-O3A-PB-O3B
4	C	1202	ADP	PA-O3A-PB-O1B
4	B	1204	ADP	PA-O3A-PB-O2B
4	C	1202	ADP	PA-O3A-PB-O2B
3	A	1202	COA	C5B-O5B-P1A-O3A
3	B	1203	COA	C5B-O5B-P1A-O3A
3	C	1201	COA	C5B-O5B-P1A-O3A
3	D	1202	COA	C5B-O5B-P1A-O3A
6	B	1202	FLC	CBC-CB-CG-CGC
4	B	1204	ADP	PB-O3A-PA-O2A
4	C	1202	ADP	PB-O3A-PA-O2A
4	D	1203	ADP	PB-O3A-PA-O2A
6	B	1202	FLC	CA-CB-CG-CGC
4	B	1204	ADP	C4'-C5'-O5'-PA
3	B	1203	COA	CDP-CBP-CCP-O6A
4	D	1203	ADP	PB-O3A-PA-O1A
3	B	1203	COA	O9P-C9P-CAP-OAP
3	C	1201	COA	O9P-C9P-CAP-OAP
3	D	1202	COA	O9P-C9P-CAP-OAP
4	A	1203	ADP	C4'-C5'-O5'-PA
4	C	1202	ADP	C4'-C5'-O5'-PA
4	D	1203	ADP	C4'-C5'-O5'-PA
3	B	1203	COA	CCP-O6A-P2A-O3A
4	A	1203	ADP	PB-O3A-PA-O2A

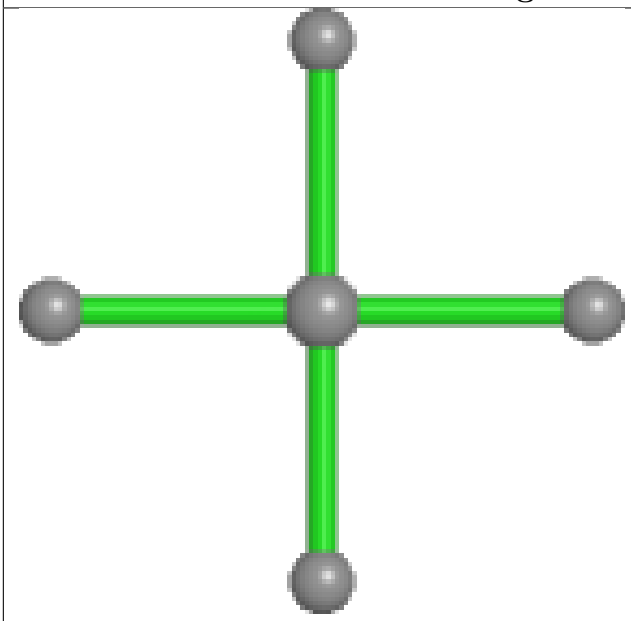
There are no ring outliers.

3 monomers are involved in 3 short contacts:

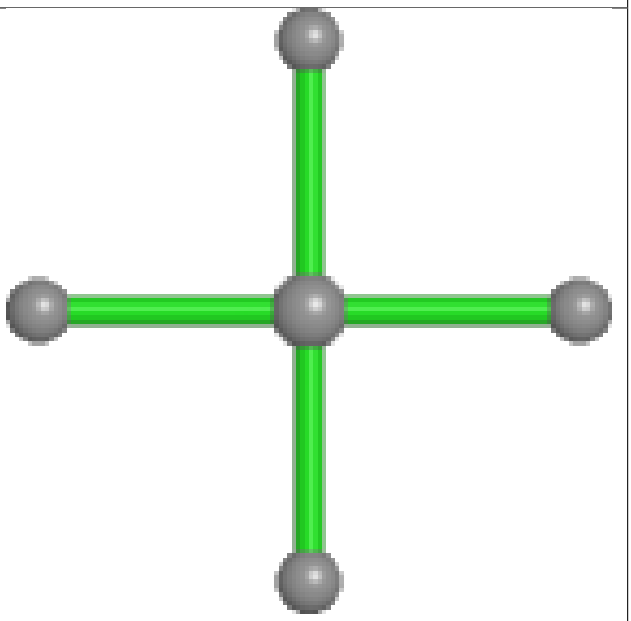
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1202	ADP	1	0
3	B	1203	COA	1	0
4	A	1203	ADP	1	0

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

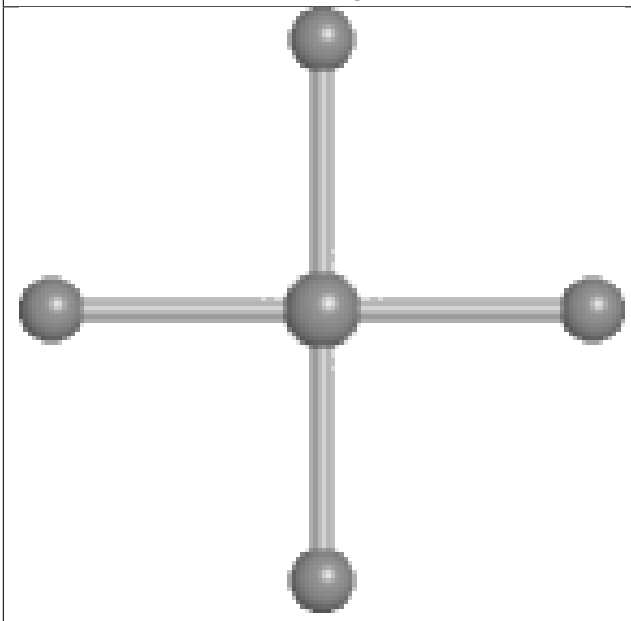
Ligand 2HP A 1201



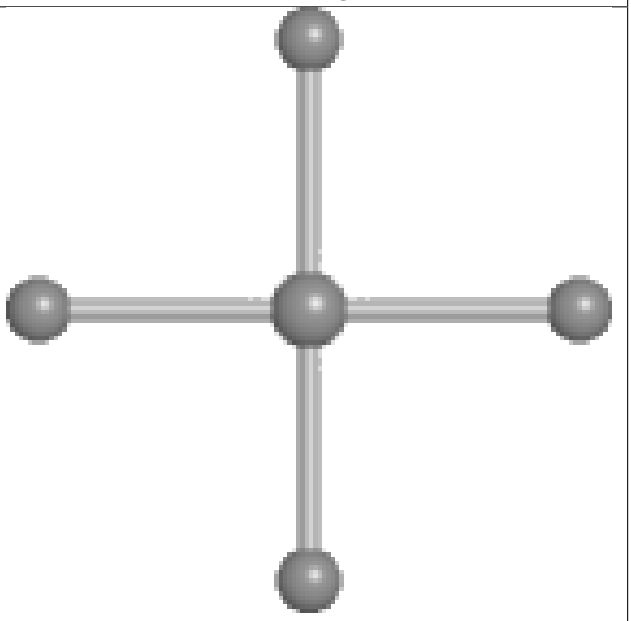
Bond lengths



Bond angles

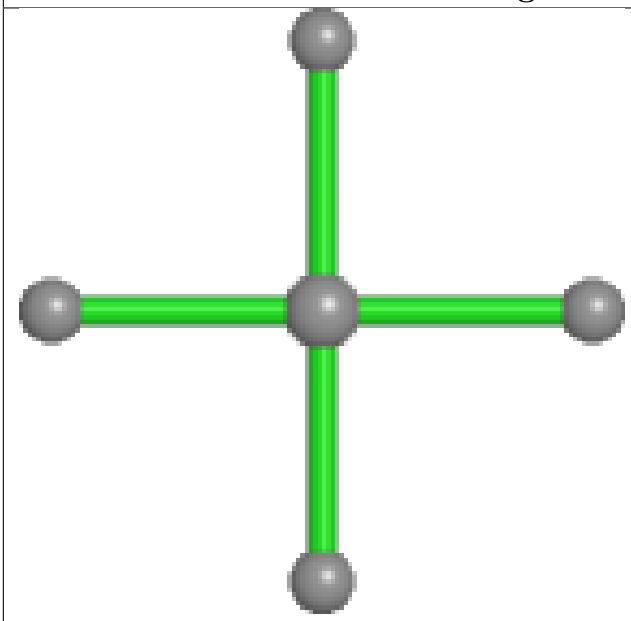


Torsions

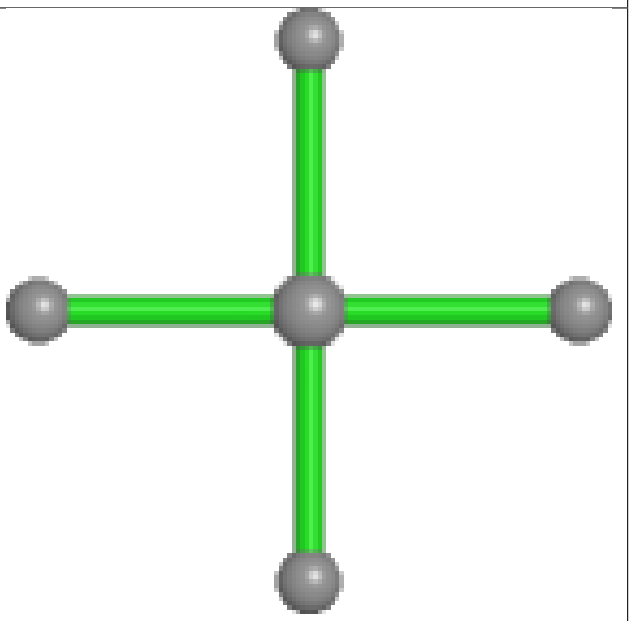


Rings

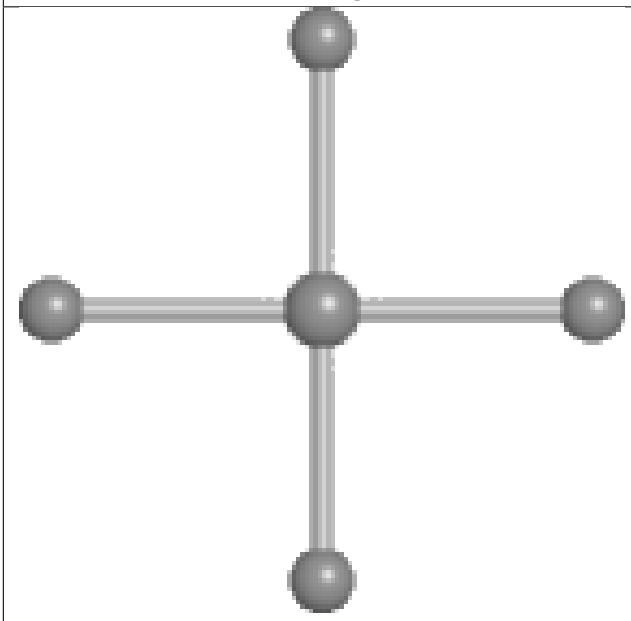
Ligand 2HP B 1201



Bond lengths



Bond angles



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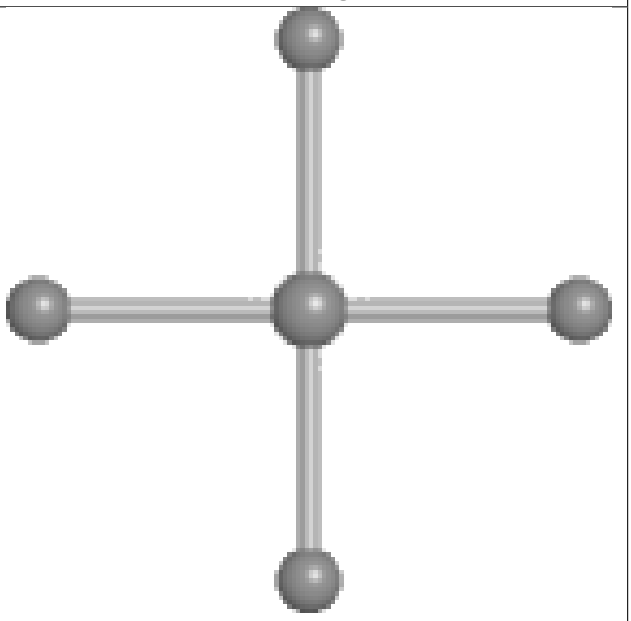
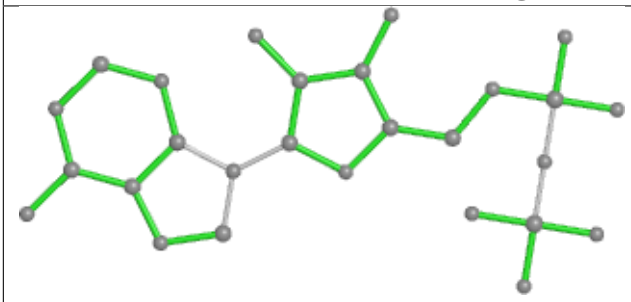
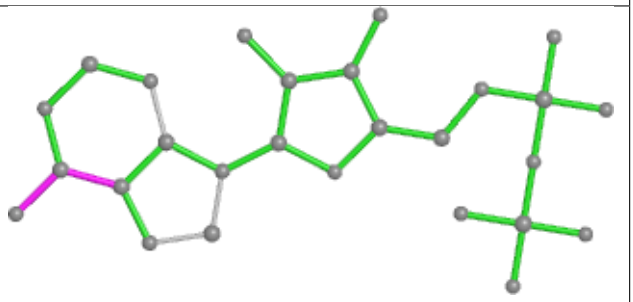


Rings

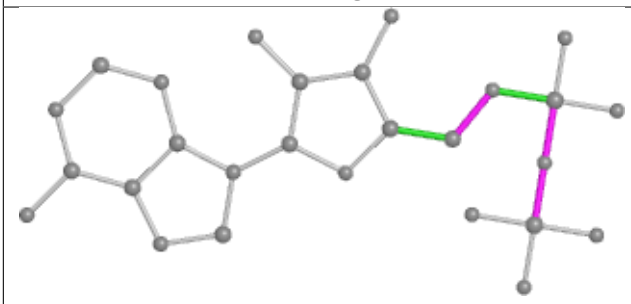
Ligand ADP C 1202



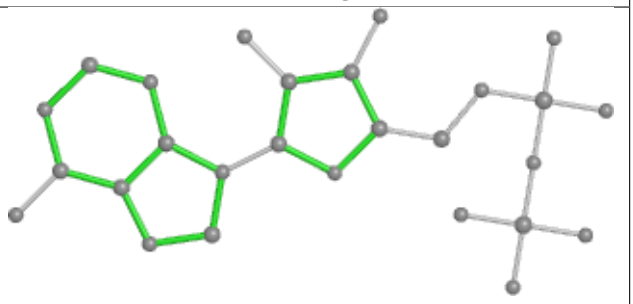
Bond lengths



Bond angles

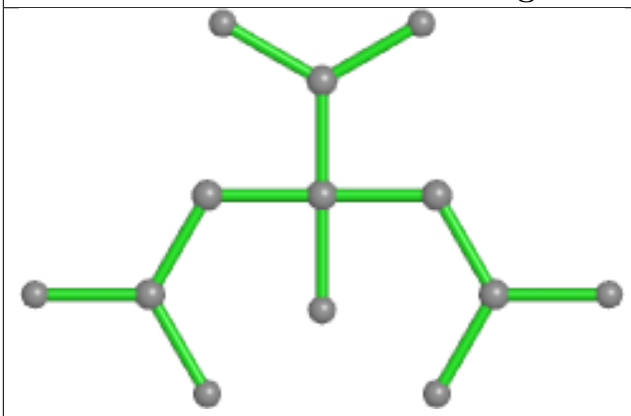


Torsions

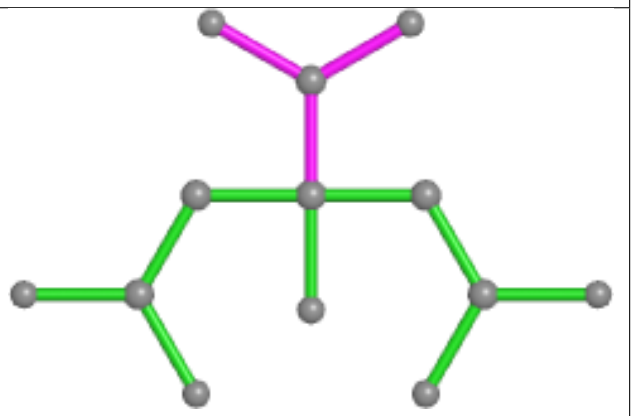


Rings

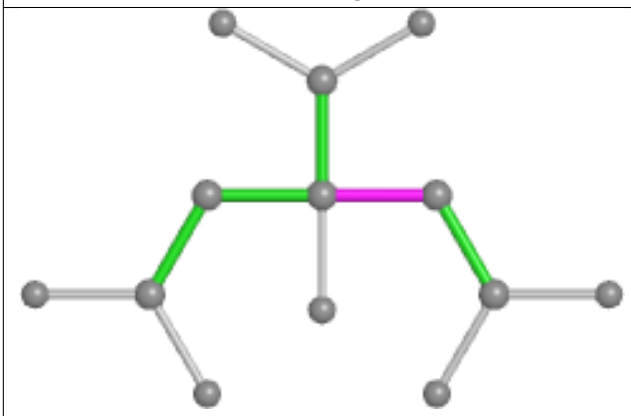
Ligand FLC B 1202



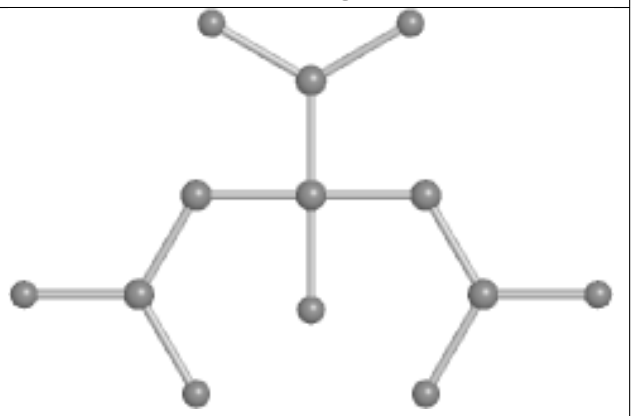
Bond lengths



Bond angles

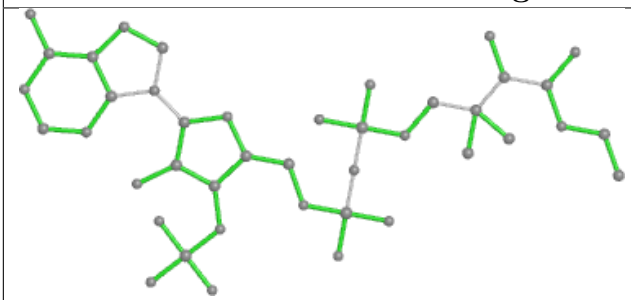


Torsions

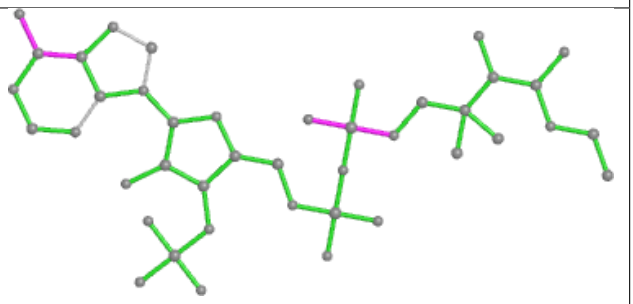


Rings

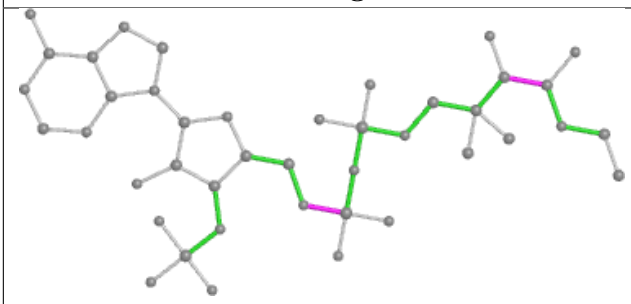
Ligand COA D 1202



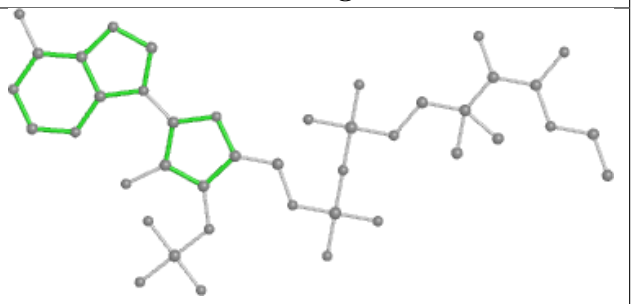
Bond lengths



Bond angles

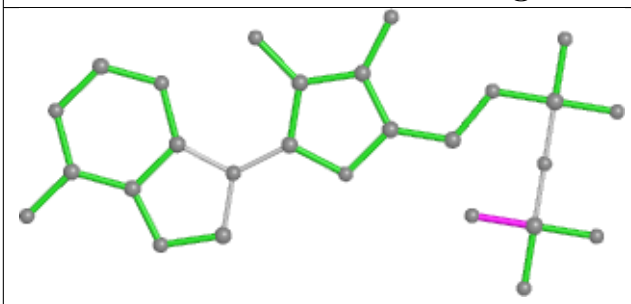


Torsions

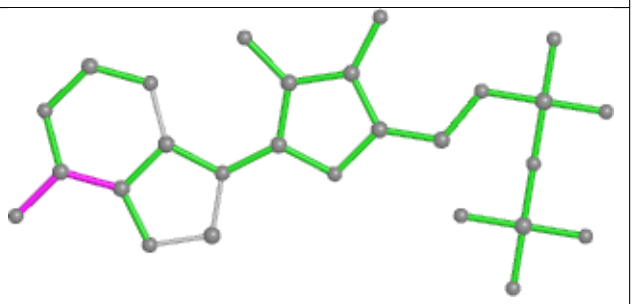


Rings

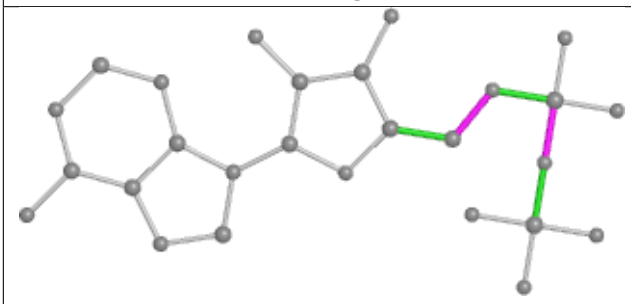
Ligand ADP D 1203



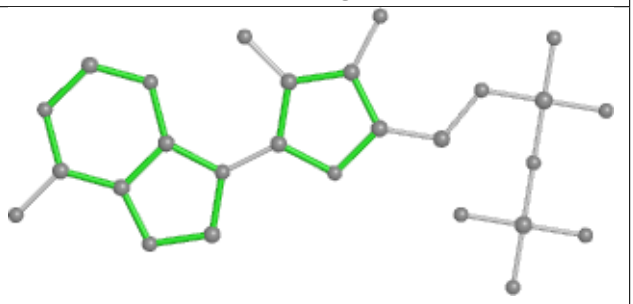
Bond lengths



Bond angles

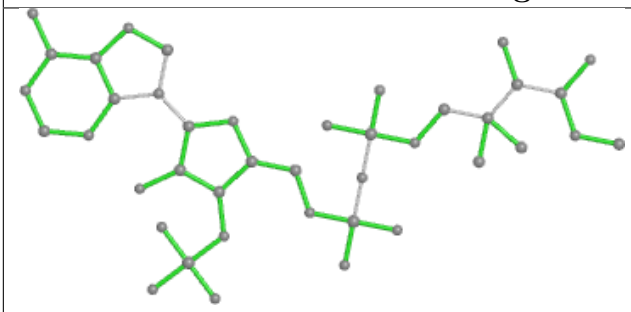


Torsions

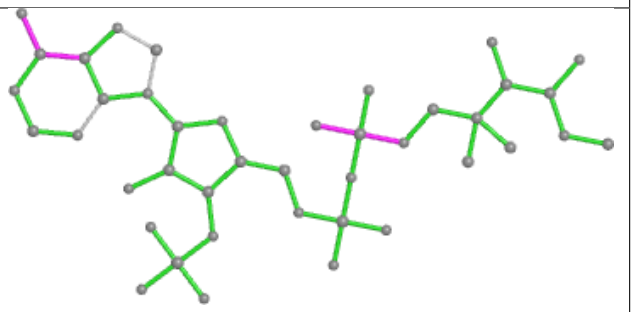


Rings

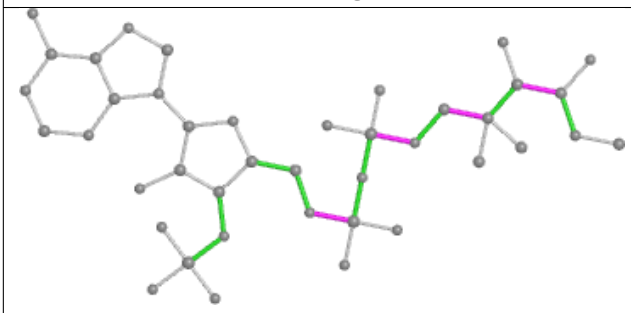
Ligand COA B 1203



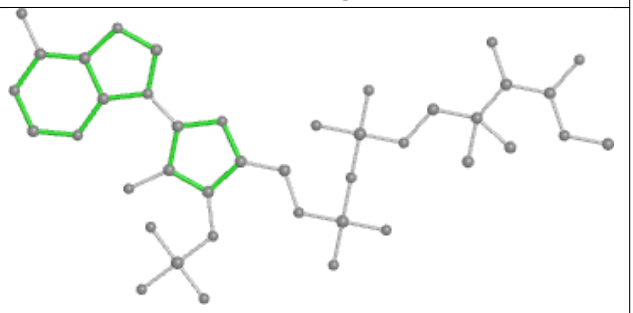
Bond lengths



Bond angles

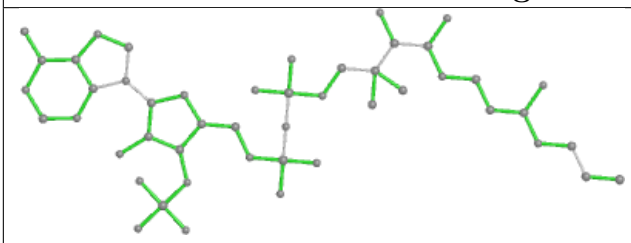


Torsions

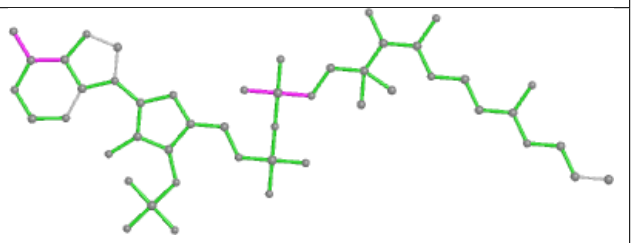


Rings

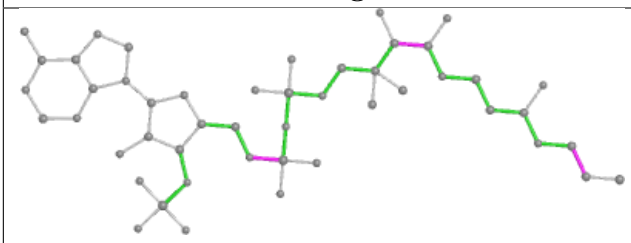
Ligand COA C 1201



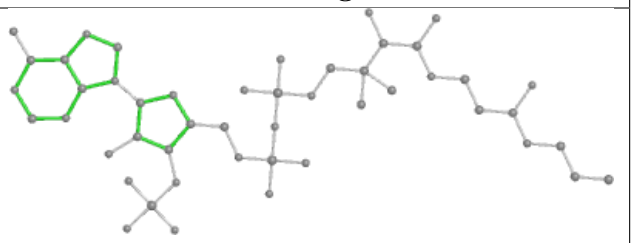
Bond lengths



Bond angles

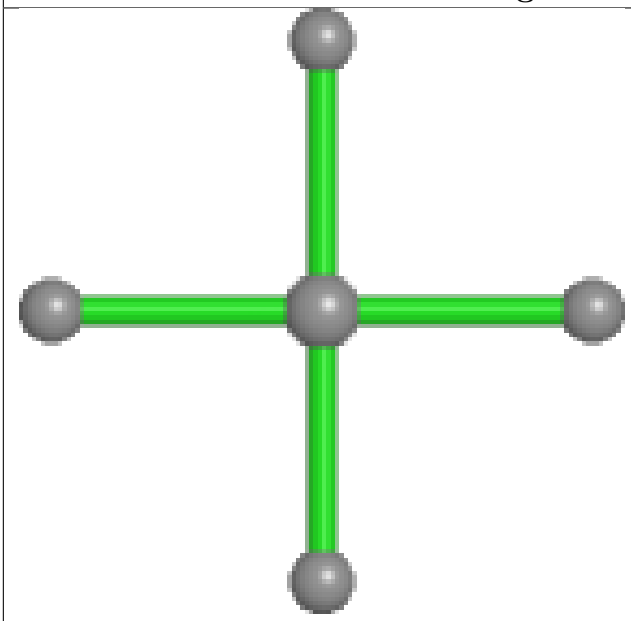


Torsions

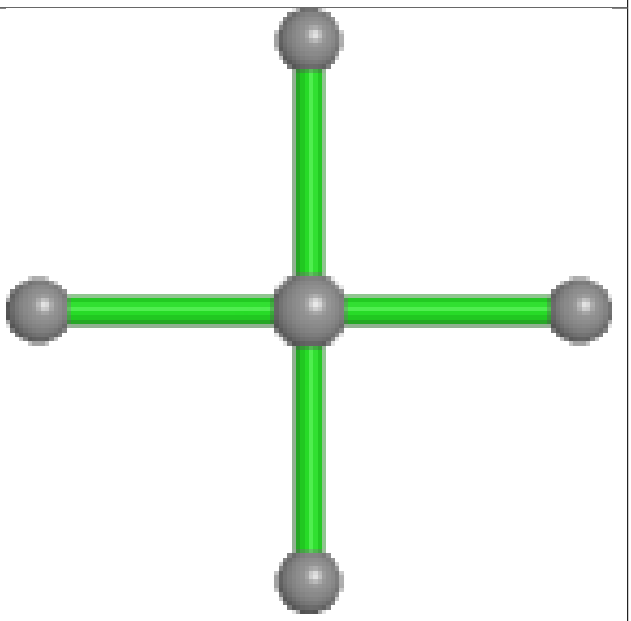


Rings

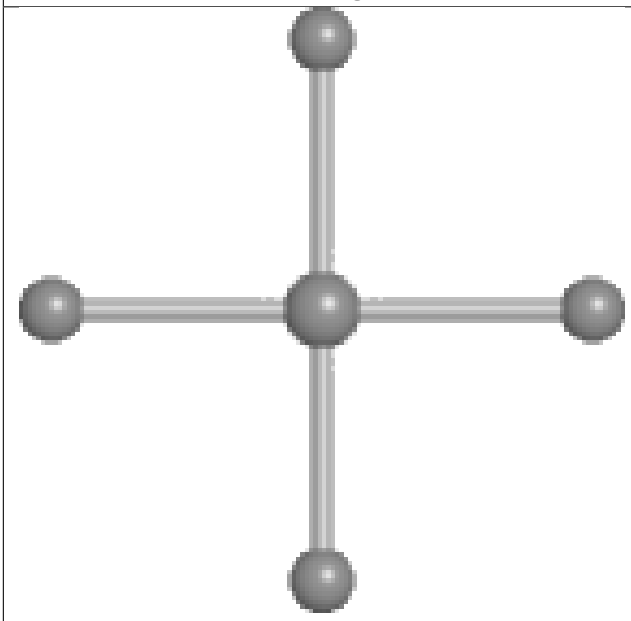
Ligand 2HP D 1201



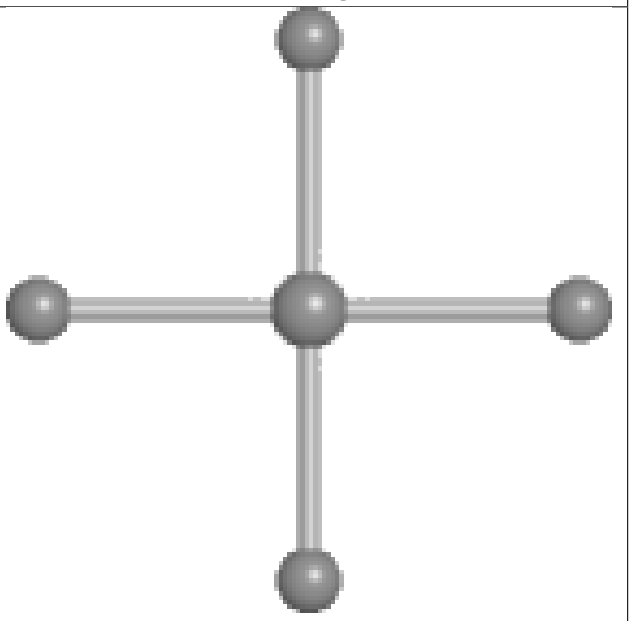
Bond lengths



Bond angles

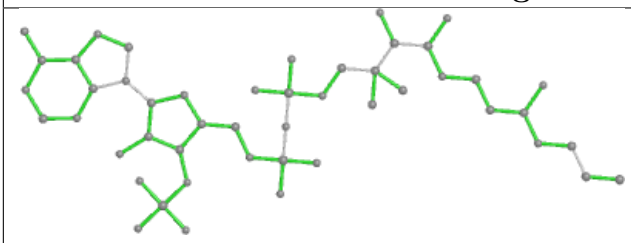


Torsions

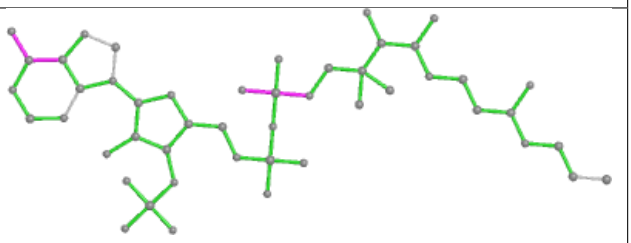


Rings

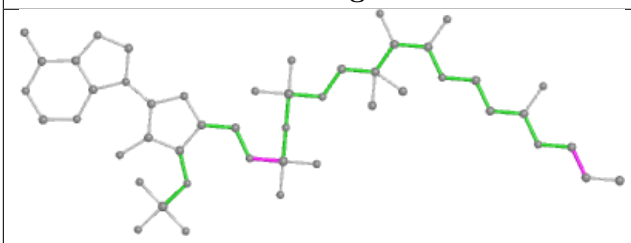
Ligand COA A 1202



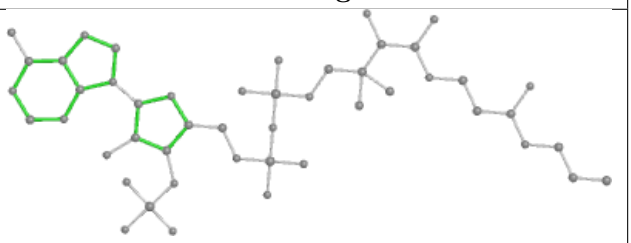
Bond lengths



Bond angles

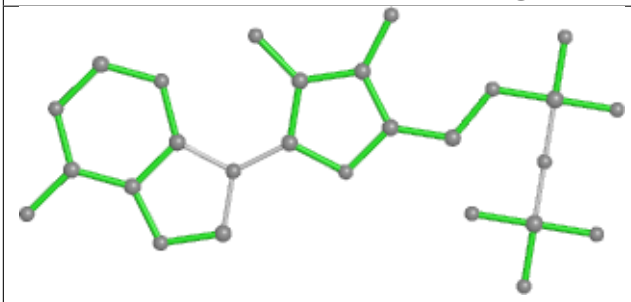


Torsions

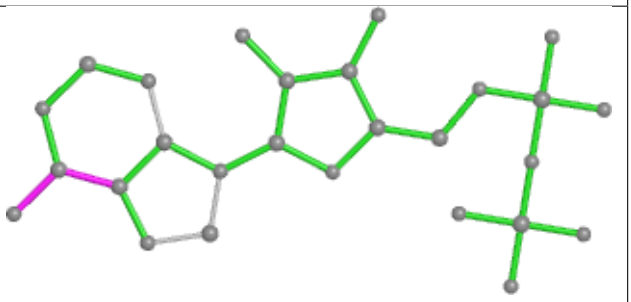


Rings

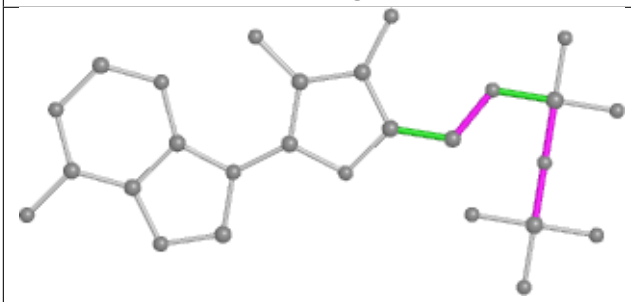
Ligand ADP A 1203



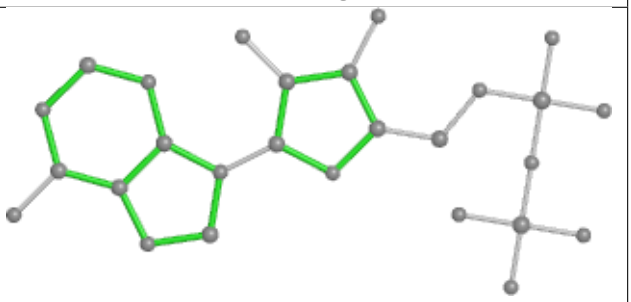
Bond lengths



Bond angles

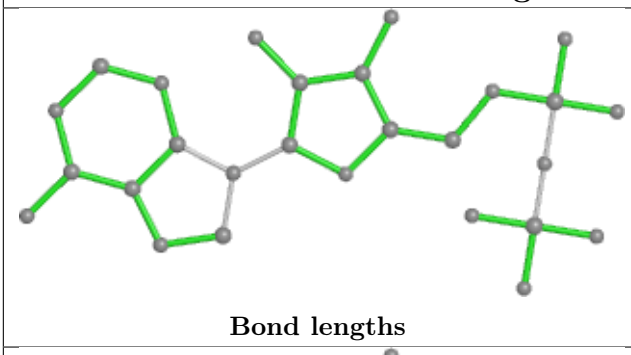


Torsions

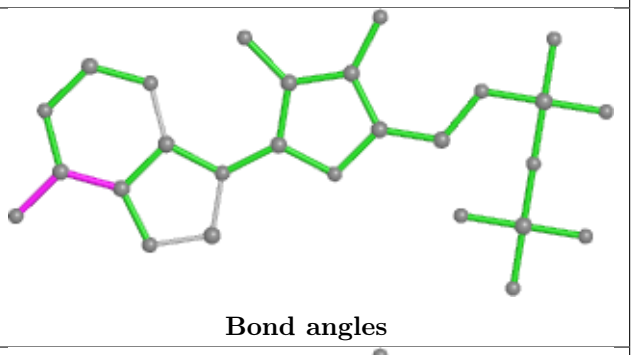


Rings

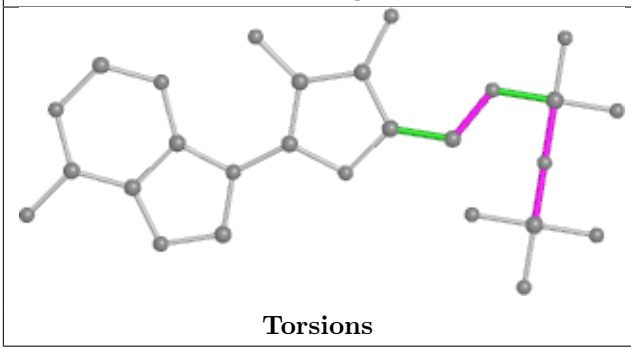
Ligand ADP B 1204



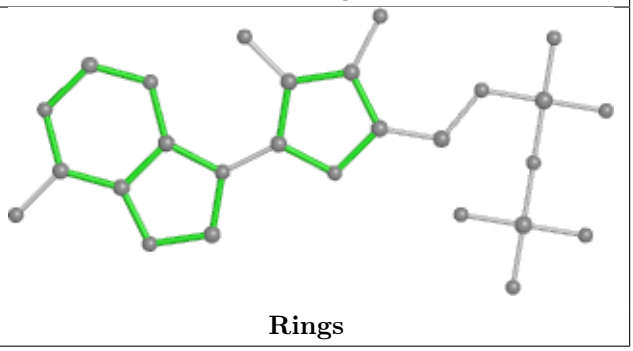
Bond lengths



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	1019/1050 (97%)	0.09	18 (1%)	68	65	63, 142, 196, 217	0
1	B	1035/1050 (98%)	0.05	15 (1%)	75	74	63, 119, 163, 209	0
1	C	1011/1050 (96%)	0.26	45 (4%)	33	31	68, 127, 213, 241	0
1	D	1025/1050 (97%)	0.21	45 (4%)	34	32	86, 141, 213, 236	0
All	All	4090/4200 (97%)	0.15	123 (3%)	50	48	63, 131, 202, 241	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	ALA	9.4
1	C	260	SER	8.0
1	C	261	GLY	7.5
1	D	425	PRO	6.6
1	C	259	LYS	5.9
1	D	357	ILE	5.5
1	C	324	LEU	5.3
1	D	341	GLY	5.2
1	C	401	PRO	4.8
1	D	348	THR	4.7
1	D	361	ILE	4.7
1	C	374	THR	4.7
1	D	262	ALA	4.7
1	C	320	ALA	4.6
1	C	144	ASP	4.4
1	D	360	ALA	4.3
1	C	250	GLU	4.3
1	C	376	PHE	4.2
1	D	320	ALA	4.1
1	C	257	ASP	4.0
1	D	324	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	275	ILE	3.7
1	C	308	SER	3.7
1	D	278	MET	3.6
1	A	391	MET	3.6
1	D	277	THR	3.6
1	C	399	GLY	3.6
1	D	354	PHE	3.6
1	C	360	ALA	3.5
1	A	779	LEU	3.5
1	D	340	ILE	3.4
1	D	276	TRP	3.4
1	D	380	GLY	3.3
1	D	400	ILE	3.3
1	D	391	MET	3.3
1	D	376	PHE	3.2
1	D	316	THR	3.1
1	A	425	PRO	3.1
1	D	338	LEU	3.1
1	D	779	LEU	3.0
1	D	350	VAL	3.0
1	A	376	PHE	3.0
1	C	393	GLU	3.0
1	C	361	ILE	3.0
1	A	181	LEU	2.9
1	C	347	PHE	2.9
1	A	320	ALA	2.9
1	C	318	ASP	2.9
1	C	489	SER	2.8
1	A	50	LEU	2.8
1	C	398	THR	2.8
1	A	782	ALA	2.8
1	D	339	ILE	2.8
1	D	394	VAL	2.8
1	C	145	VAL	2.8
1	D	373	VAL	2.7
1	D	375	ILE	2.7
1	B	102	LEU	2.7
1	C	370	GLU	2.7
1	D	301	LEU	2.7
1	D	346	ASN	2.7
1	B	400	ILE	2.7
1	C	40	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	50	LEU	2.6
1	C	282	GLY	2.6
1	C	346	ASN	2.6
1	B	398	THR	2.6
1	A	152	LEU	2.5
1	A	566	VAL	2.5
1	C	388	LEU	2.5
1	B	2	SER	2.5
1	C	488	LYS	2.5
1	C	309	GLY	2.5
1	D	37	ASP	2.5
1	D	387	GLY	2.5
1	D	261	GLY	2.5
1	C	752	PHE	2.4
1	D	170	LEU	2.4
1	B	282	GLY	2.4
1	C	264	LEU	2.4
1	D	689	GLY	2.4
1	C	323	ILE	2.4
1	A	742	CYS	2.4
1	B	242	PHE	2.3
1	D	415	VAL	2.3
1	C	263	SER	2.3
1	A	392	GLY	2.3
1	A	810	ILE	2.3
1	B	368	LEU	2.3
1	A	169	LEU	2.2
1	C	74	VAL	2.2
1	C	255	ASP	2.2
1	D	377	VAL	2.2
1	D	784	VAL	2.2
1	C	392	GLY	2.2
1	C	389	ARG	2.2
1	C	325	SER	2.2
1	D	767	GLN	2.2
1	B	412	THR	2.2
1	B	752	PHE	2.2
1	D	368	LEU	2.2
1	C	391	MET	2.2
1	B	591	ILE	2.1
1	C	699	ASP	2.1
1	D	169	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	2.1
1	B	663	SER	2.1
1	A	373	VAL	2.1
1	C	321	LYS	2.1
1	C	266	LEU	2.1
1	D	264	LEU	2.1
1	C	809	VAL	2.1
1	D	256	LEU	2.1
1	B	361	ILE	2.1
1	B	397	THR	2.1
1	A	361	ILE	2.1
1	D	402	ILE	2.0
1	A	736	LEU	2.0
1	B	402	ILE	2.0
1	C	396	LYS	2.0
1	B	283	GLY	2.0
1	C	403	HIS	2.0
1	D	401	PRO	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
2	2HP	D	1201	5/5	0.73	0.80	204,205,205,207	0
2	2HP	A	1201	5/5	0.77	0.59	196,197,197,197	0
3	COA	C	1201	48/48	0.89	0.21	115,131,144,156	0
3	COA	B	1203	41/48	0.91	0.20	106,132,185,187	0
4	ADP	D	1203	27/27	0.91	0.21	119,131,142,143	0

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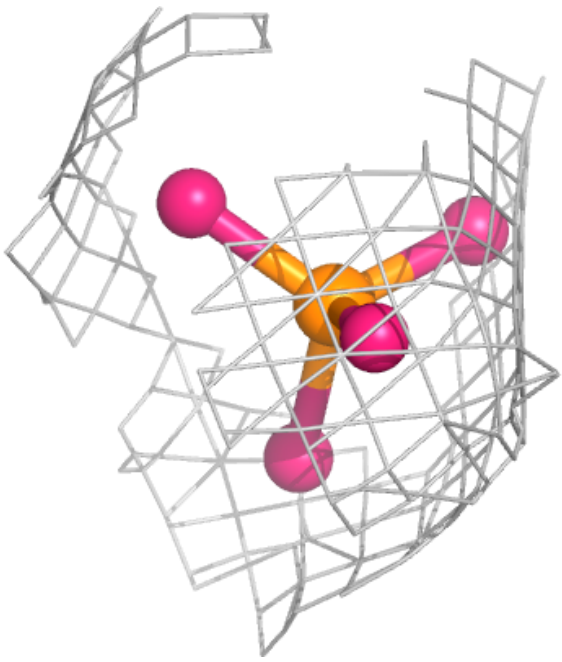
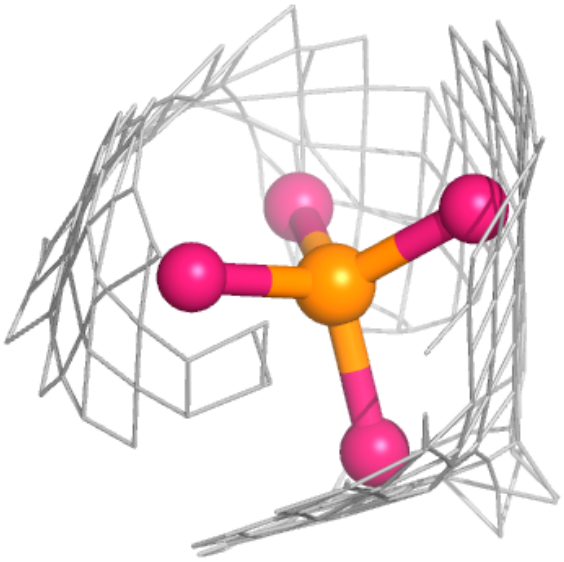
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	C	1202	27/27	0.92	0.22	142,149,151,152	0
3	COA	D	1202	42/48	0.92	0.21	129,137,160,163	0
5	MG	B	1206	1/1	0.92	0.59	91,91,91,91	0
6	FLC	B	1202	13/13	0.92	0.32	123,132,137,139	0
3	COA	A	1202	48/48	0.93	0.21	107,128,148,151	0
5	MG	D	1204	1/1	0.95	0.32	93,93,93,93	0
4	ADP	B	1204	27/27	0.97	0.18	112,120,133,134	0
2	2HP	B	1201	5/5	0.97	0.55	126,126,128,128	0
4	ADP	A	1203	27/27	0.97	0.16	124,139,150,153	0
5	MG	A	1204	1/1	0.98	0.21	89,89,89,89	0
5	MG	C	1203	1/1	0.98	0.21	123,123,123,123	0
5	MG	B	1205	1/1	0.99	0.21	84,84,84,84	0

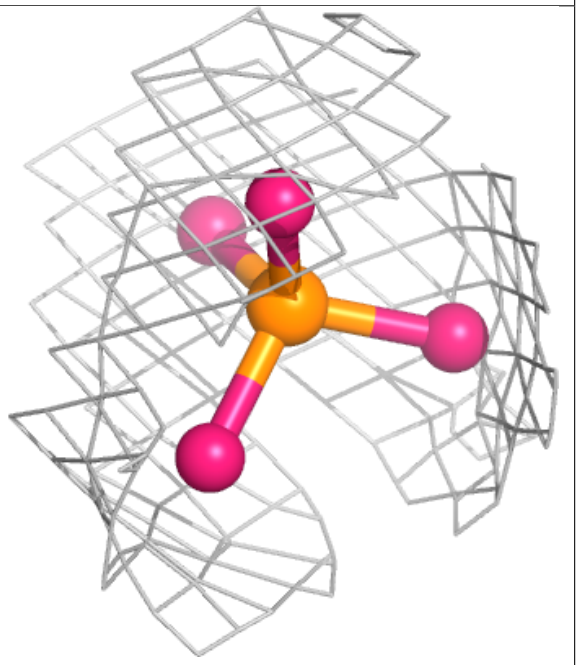
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2HP D 1201:

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

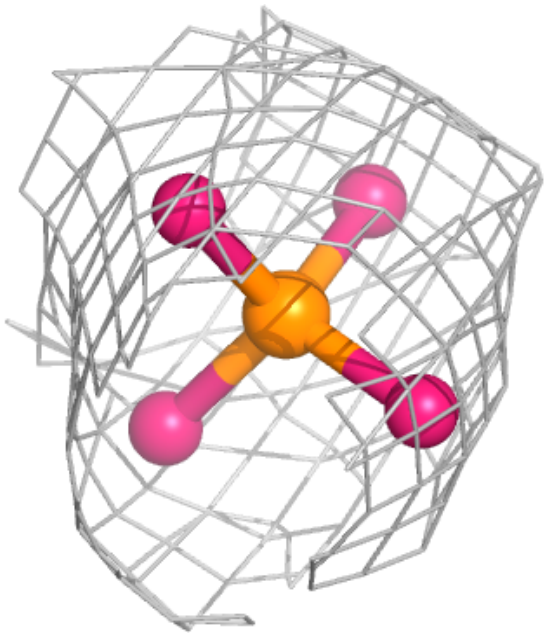


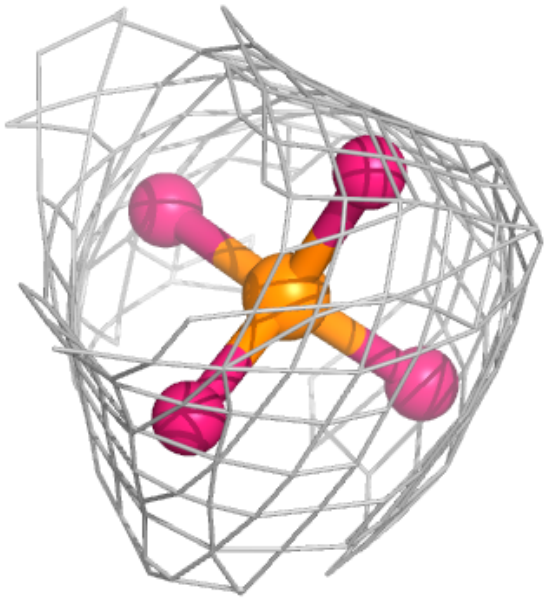


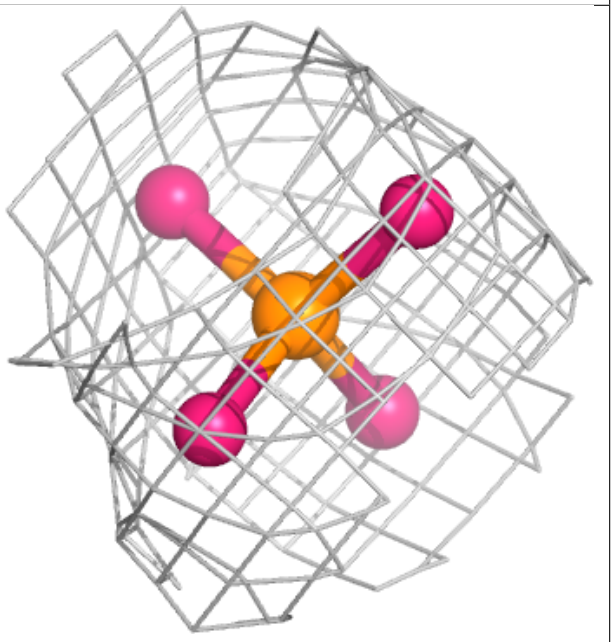


Electron density around 2HP A 1201:

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

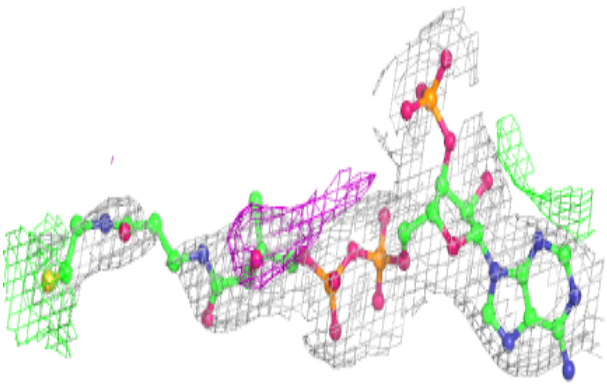


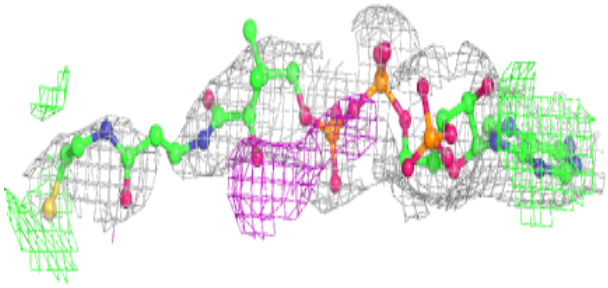


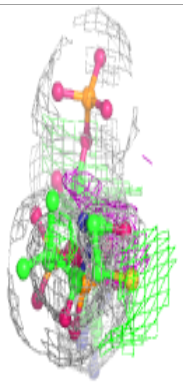


Electron density around COA C 1201:

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

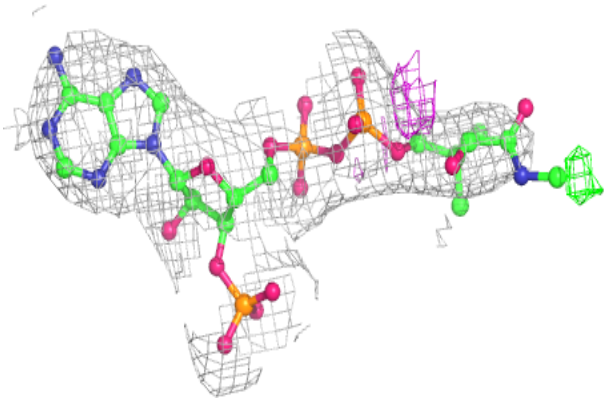


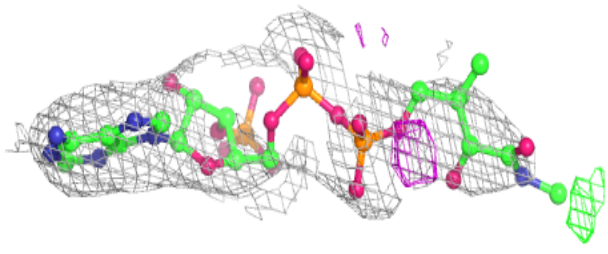


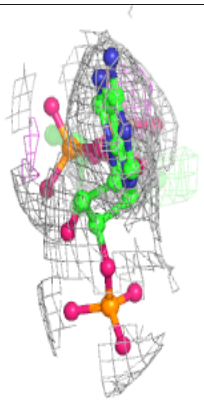


Electron density around COA B 1203:

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

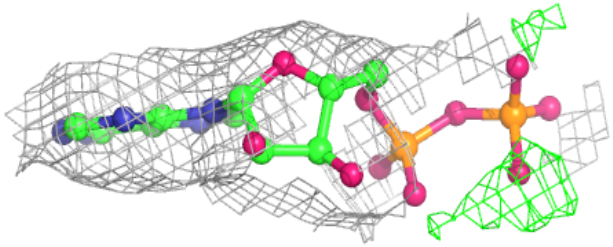


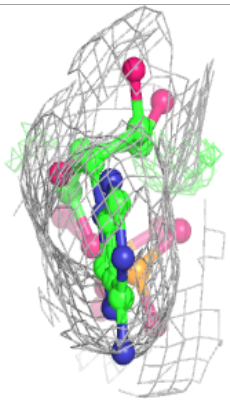




Electron density around ADP D 1203:

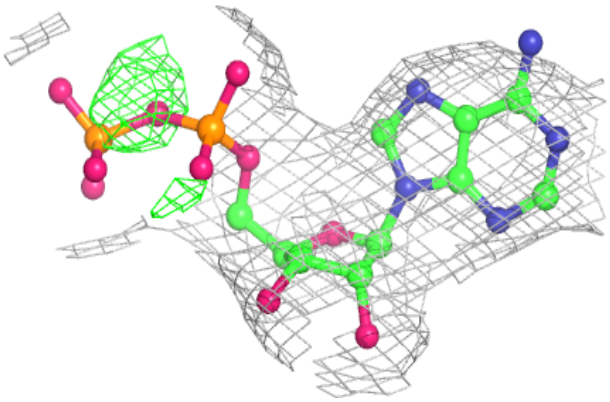
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

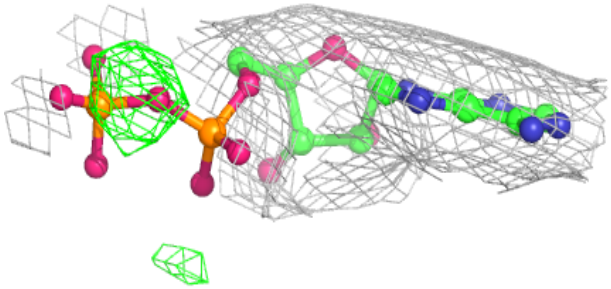


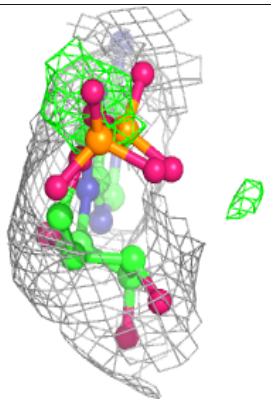


Electron density around ADP C 1202:

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

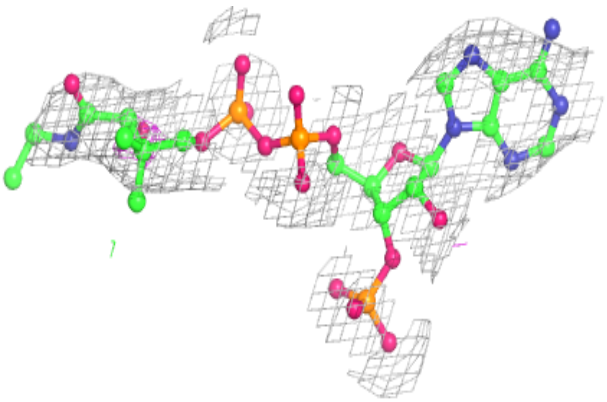


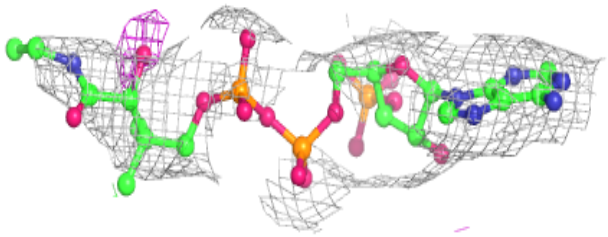


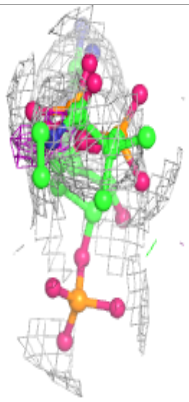


Electron density around COA D 1202:

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

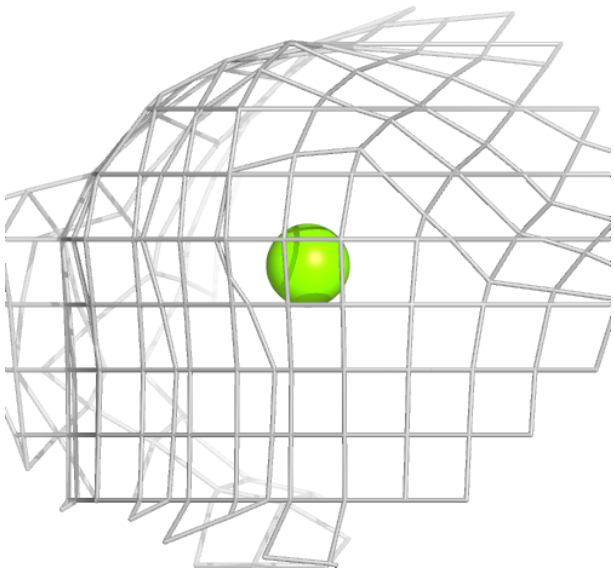


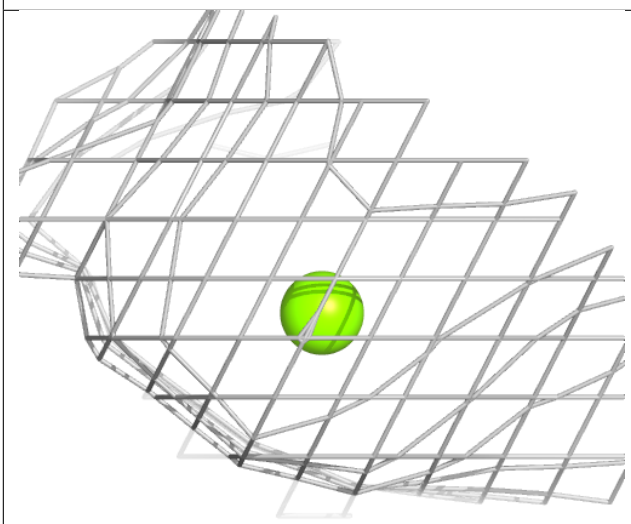


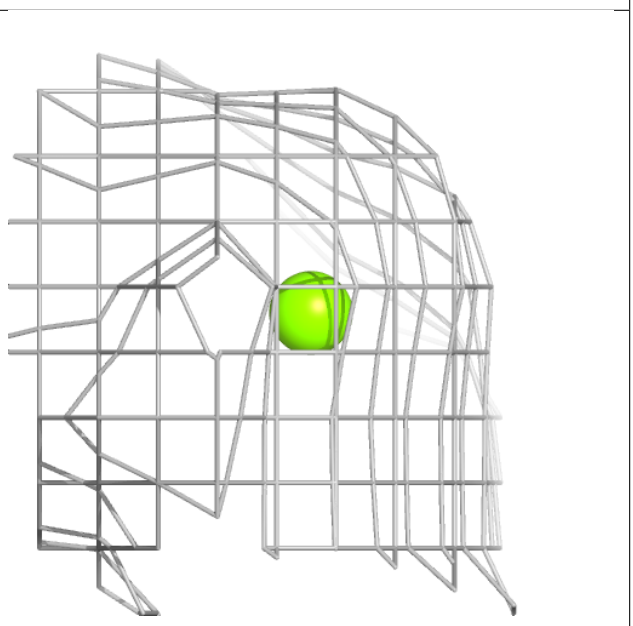


Electron density around MG B 1206:

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

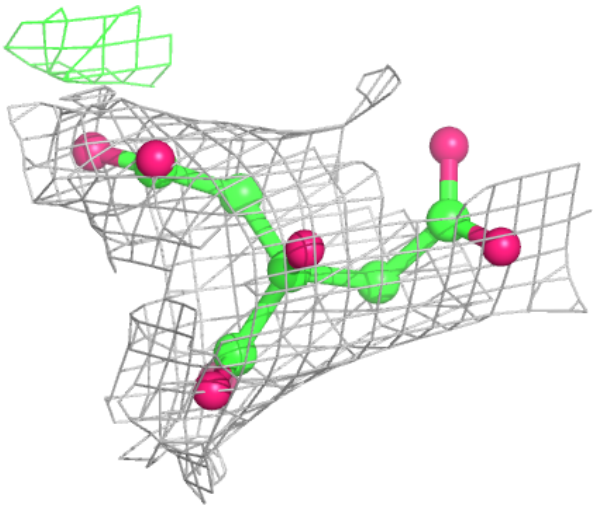


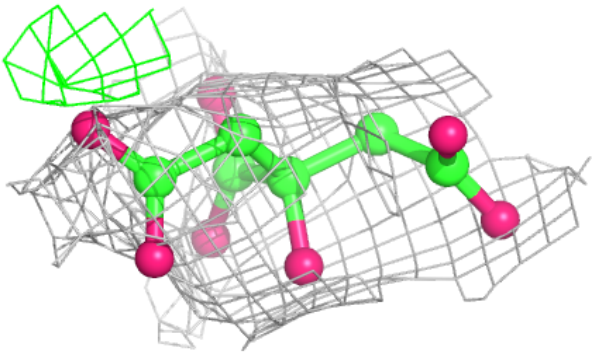


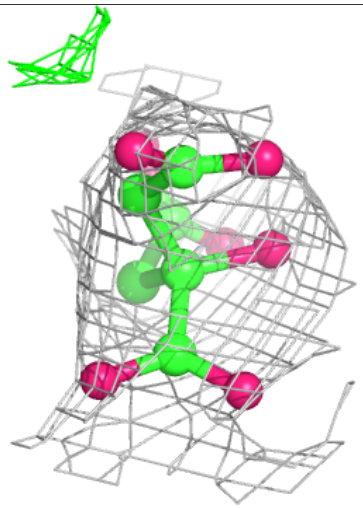


Electron density around FLC B 1202:

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

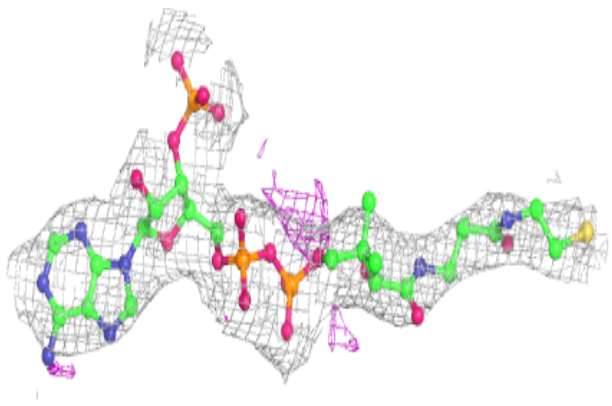


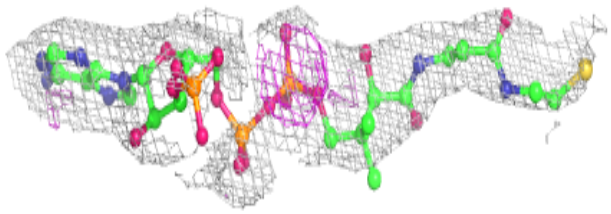


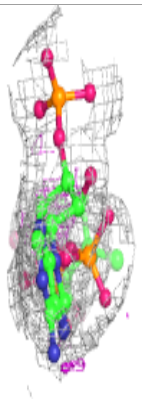


Electron density around COA A 1202:

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

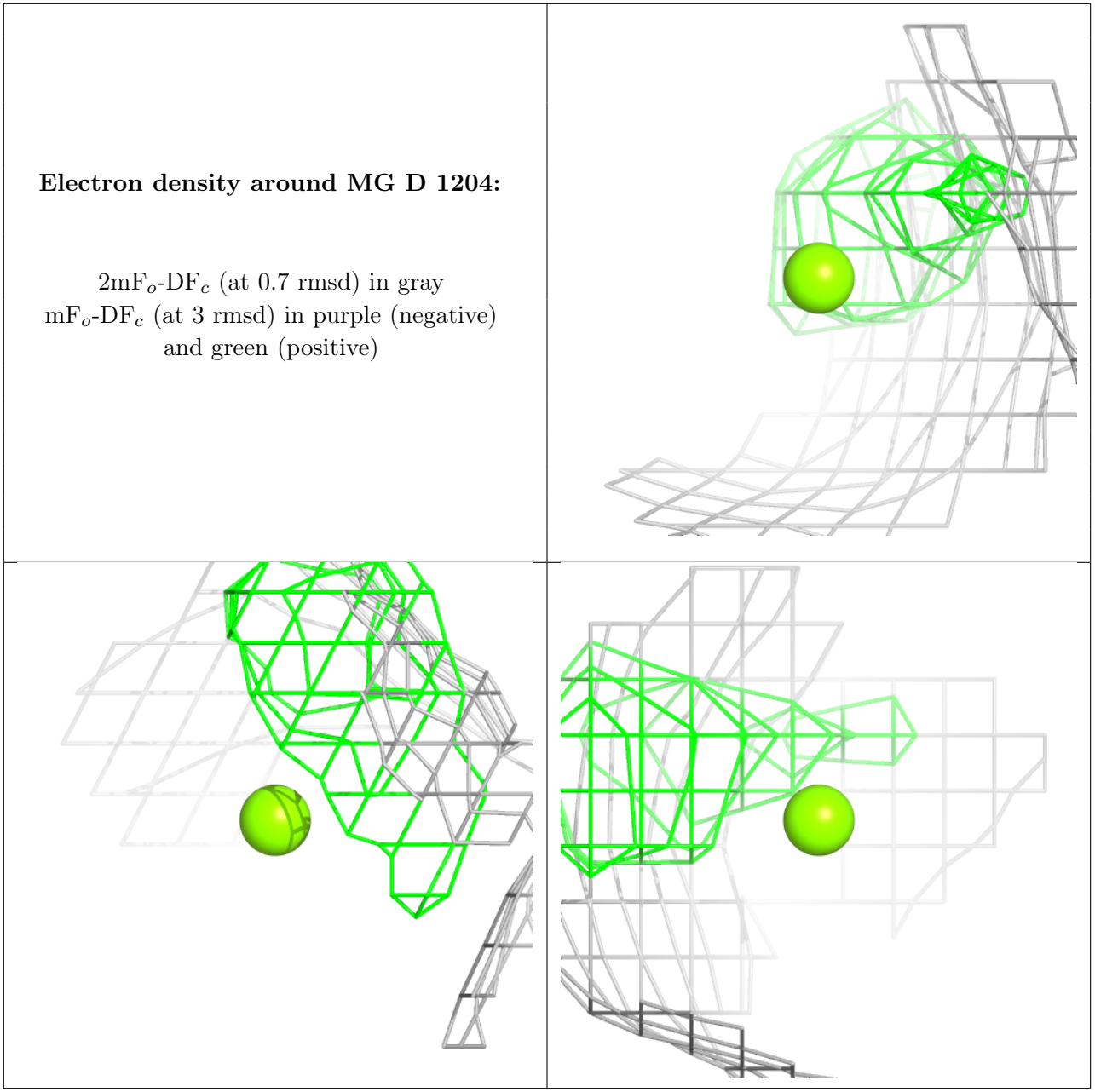






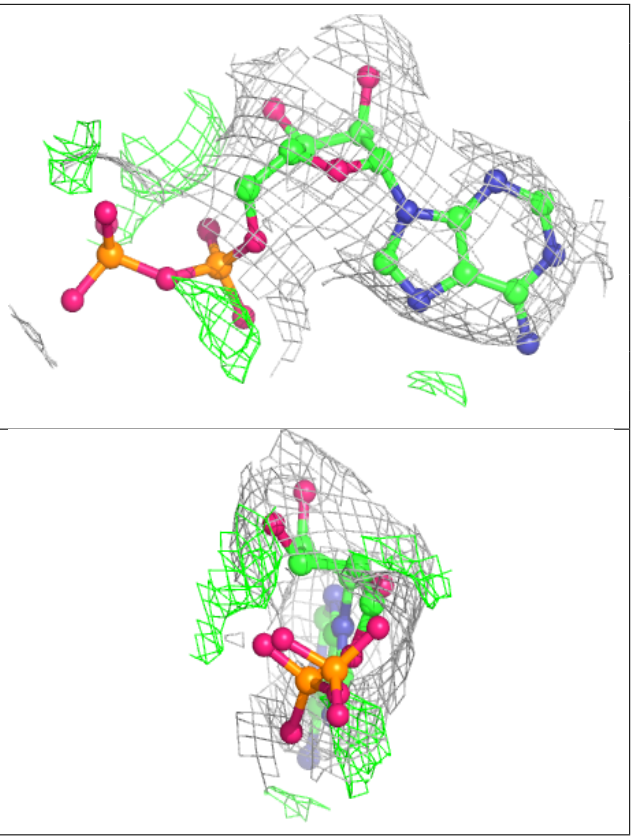
Electron density around MG D 1204:

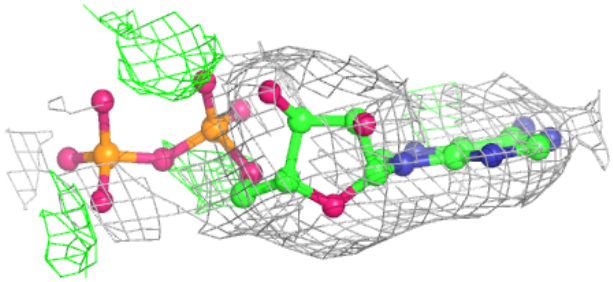
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP B 1204:

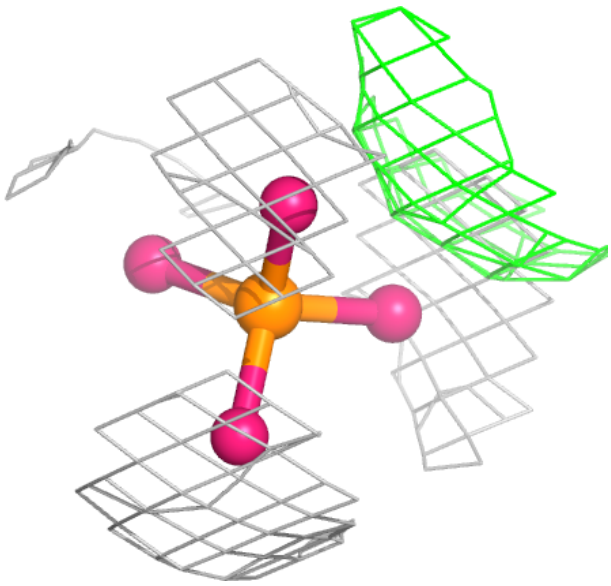
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

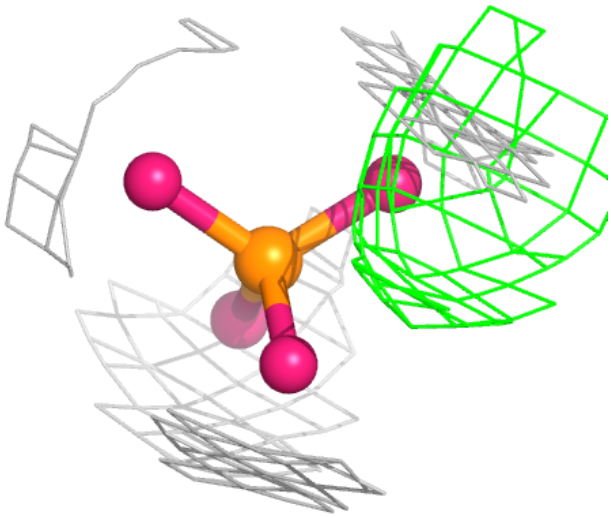


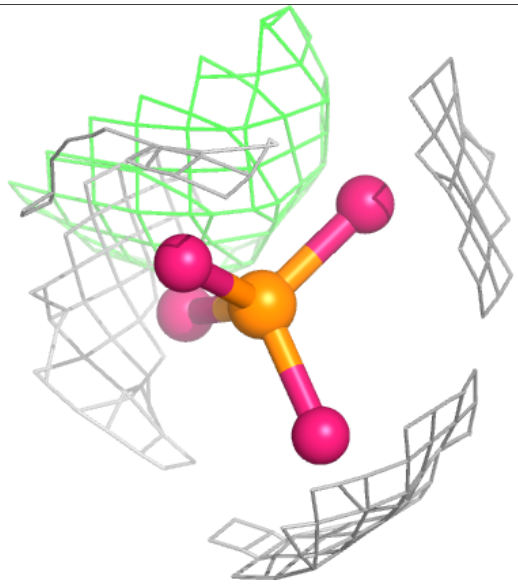


Electron density around 2HP B 1201:

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

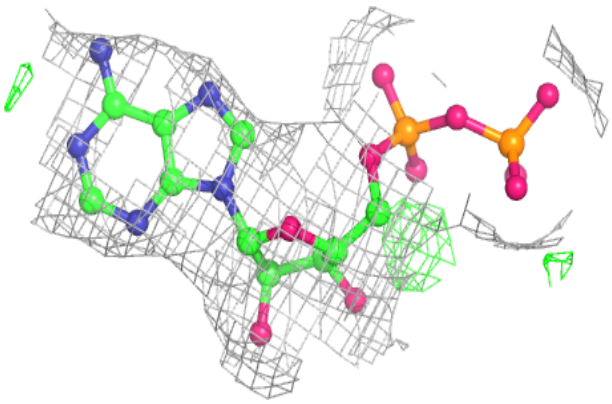


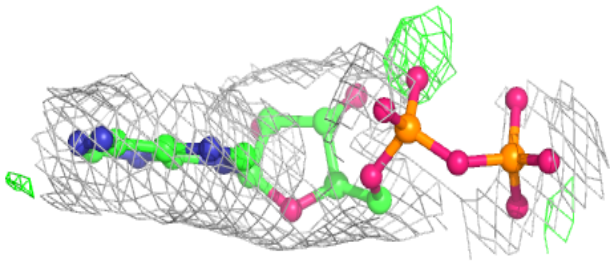


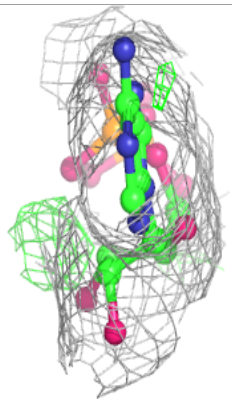


Electron density around ADP A 1203:

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

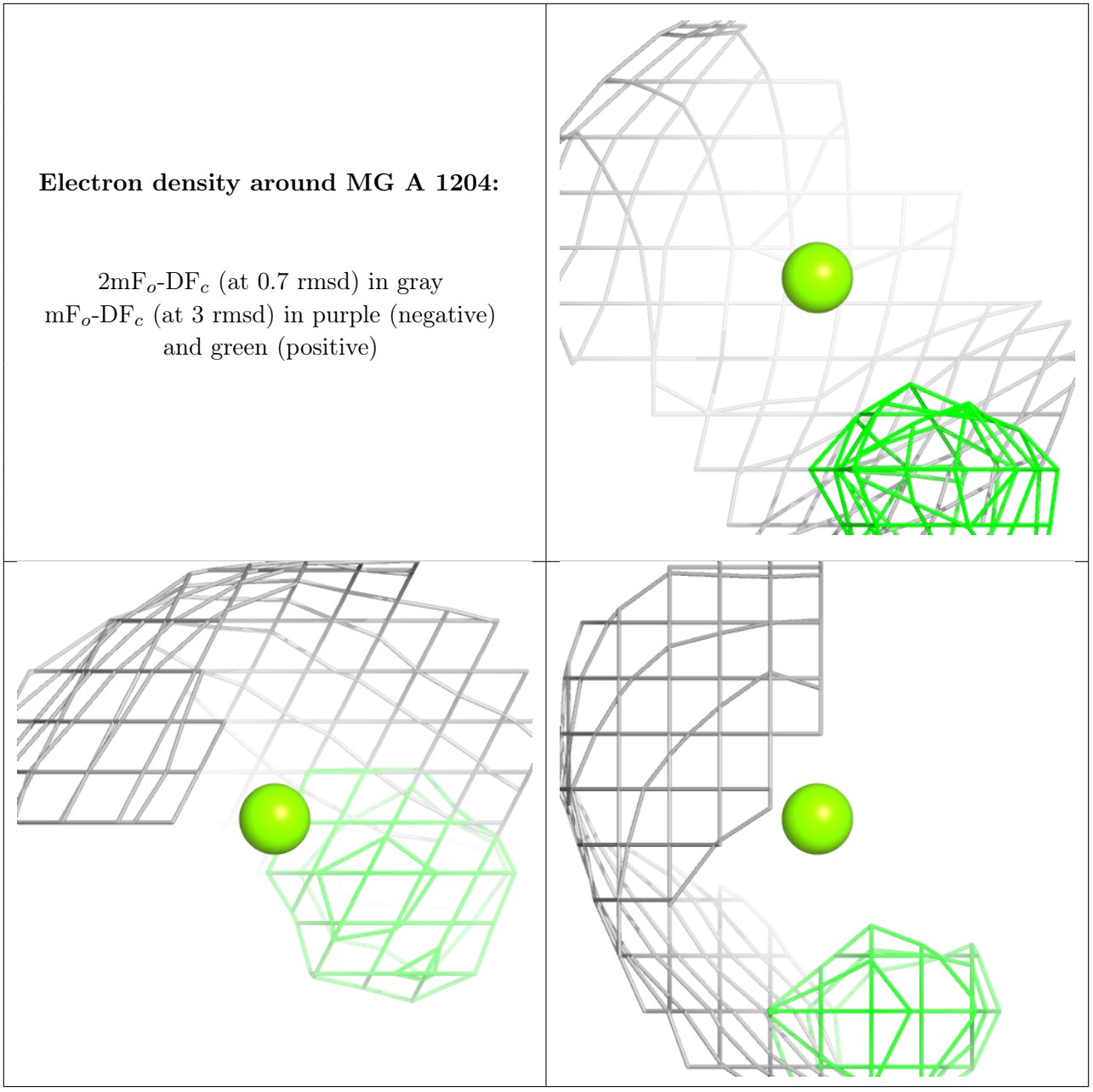






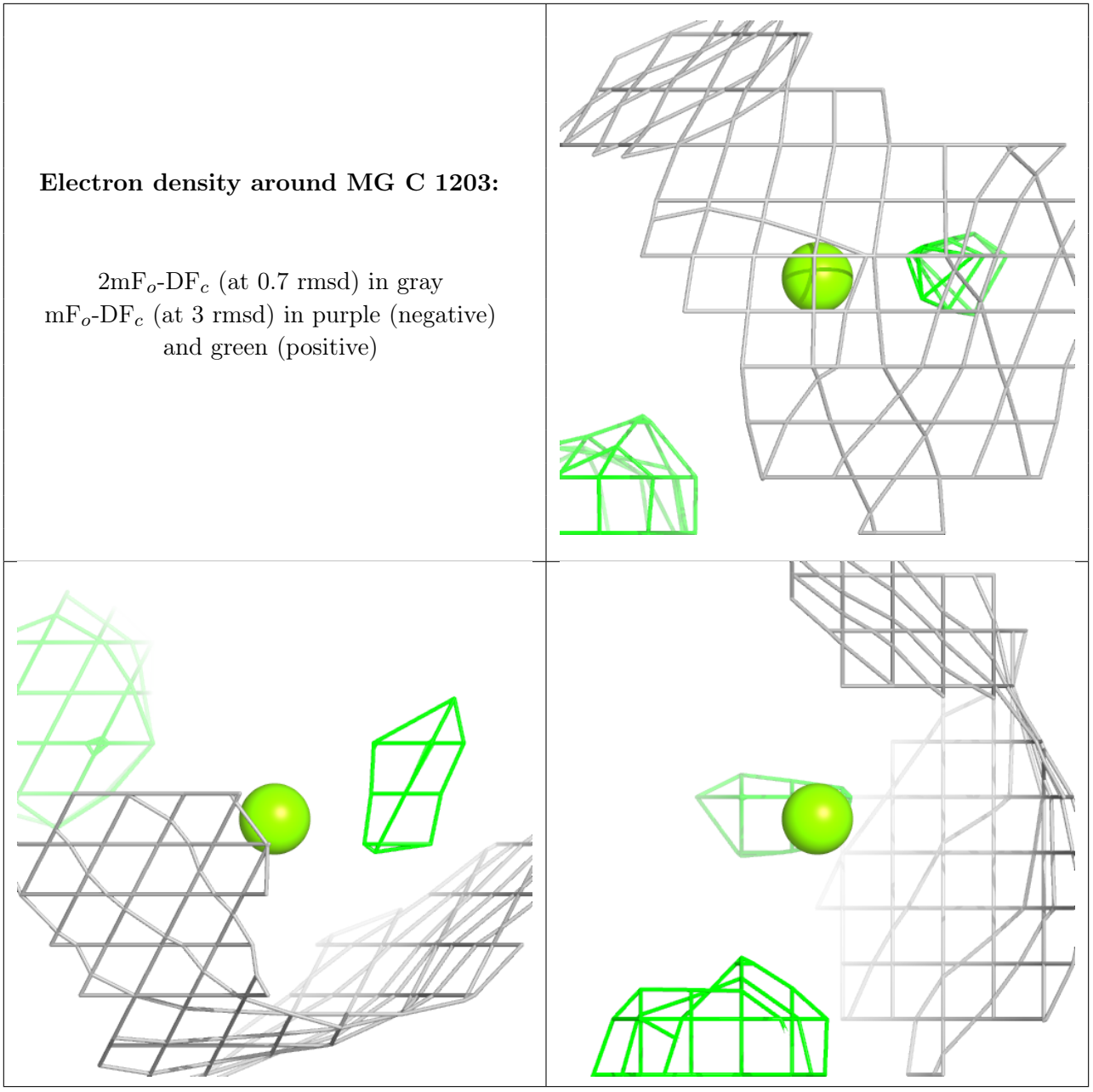
Electron density around MG A 1204:

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



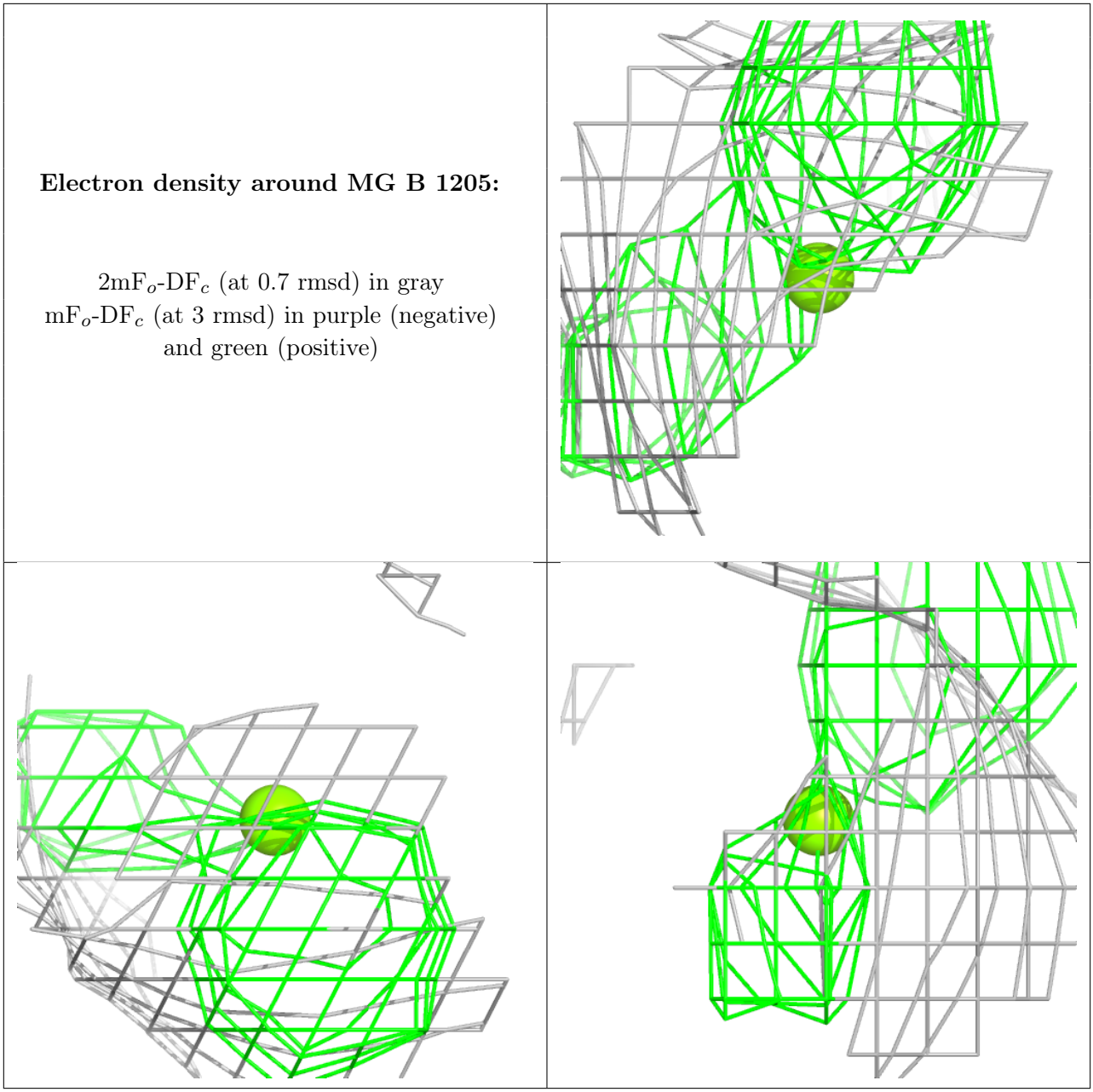
Electron density around MG C 1203:

$2mF_o$-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 1205:

$2mF_o$-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.