wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 06:29 PM EST

PDB ID	:	2D3A
Title	:	Crystal Structure of the Maize Glutamine Synthetase complexed with ADP and Methionine sulfoximine Phosphate
Authors	:	Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.
Deposited on	:	2005-09-26
Resolution	:	2.63 Å(reported)

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

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

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

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

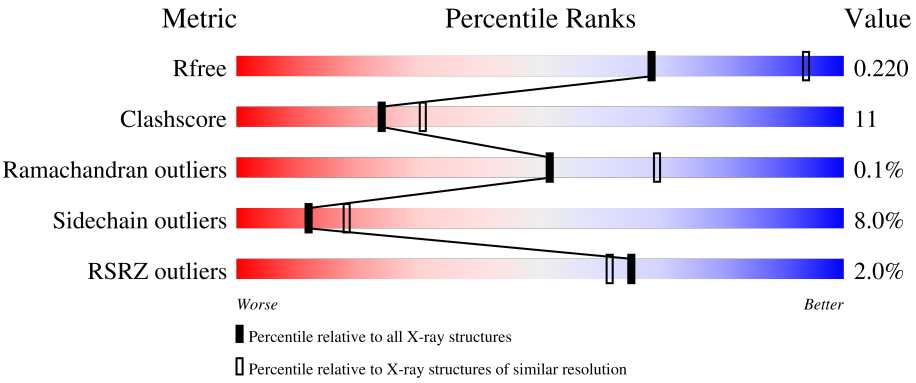
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	356	2% 76% 20%
1	B	356	76% 19%
1	C	356	2% 75% 20%
1	D	356	3% 70% 24%

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Mol	Chain	Length	Quality of chain
1	E	356	4% 74% 22%
1	F	356	3% 73% 23%
1	G	356	3% 78% 18%
1	H	356	% 77% 20%
1	I	356	% 73% 22%
1	J	356	% 78% 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28621 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		

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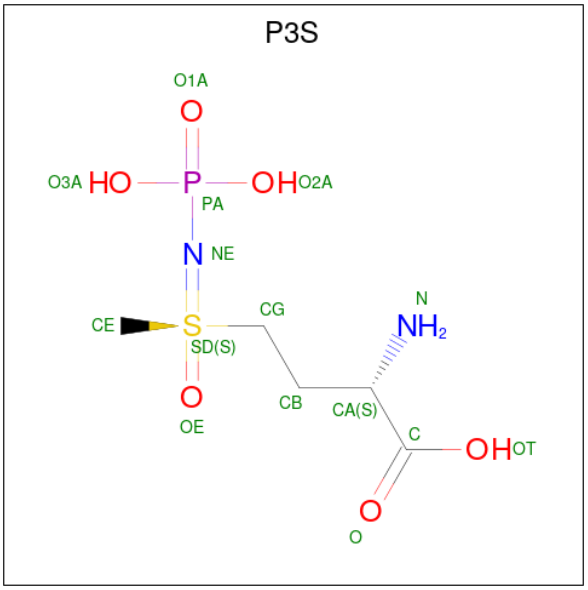
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	3	Total Mn 3 3	0	0
2	F	3	Total Mn 3 3	0	0
2	G	3	Total Mn 3 3	0	0
2	H	3	Total Mn 3 3	0	0
2	I	3	Total Mn 3 3	0	0
2	J	3	Total Mn 3 3	0	0

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 15 5 2 6 1 1	0	0
3	B	1	Total C N O P S 15 5 2 6 1 1	0	0
3	C	1	Total C N O P S 15 5 2 6 1 1	0	0
3	D	1	Total C N O P S 15 5 2 6 1 1	0	0
3	E	1	Total C N O P S 15 5 2 6 1 1	0	0

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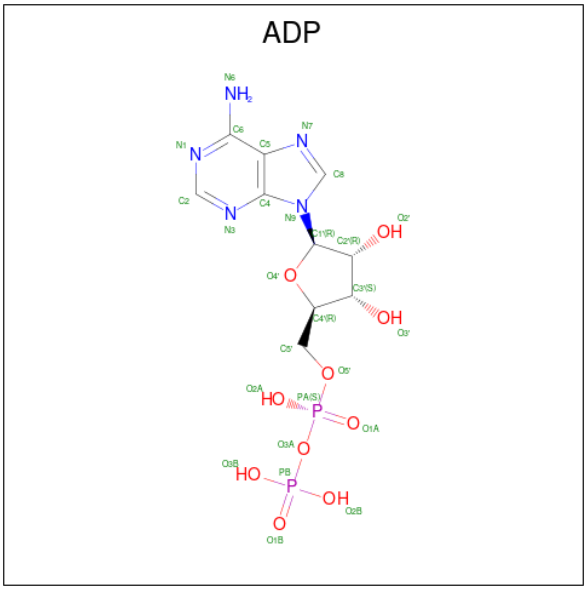
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	G	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	I	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	J	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

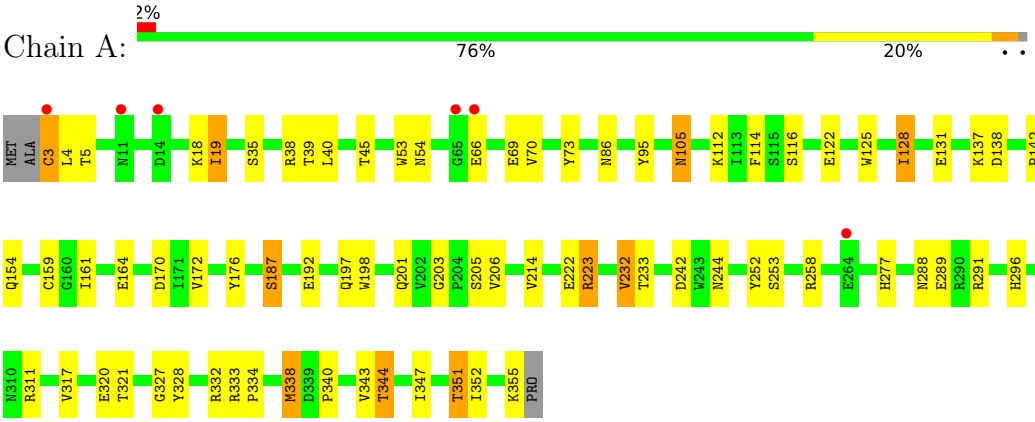
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	100	Total	O	0	0
			100	100		
5	C	63	Total	O	0	0
			63	63		
5	D	63	Total	O	0	0
			63	63		
5	E	57	Total	O	0	0
			57	57		
5	F	58	Total	O	0	0
			58	58		
5	G	54	Total	O	0	0
			54	54		
5	H	88	Total	O	0	0
			88	88		
5	I	76	Total	O	0	0
			76	76		
5	J	92	Total	O	0	0
			92	92		

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.

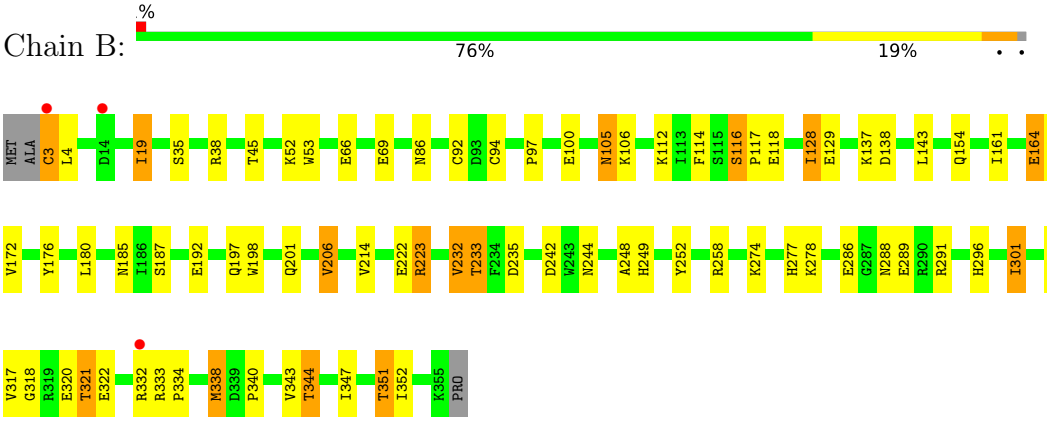
• Molecule 1: glutamine synthetase

Chain A:



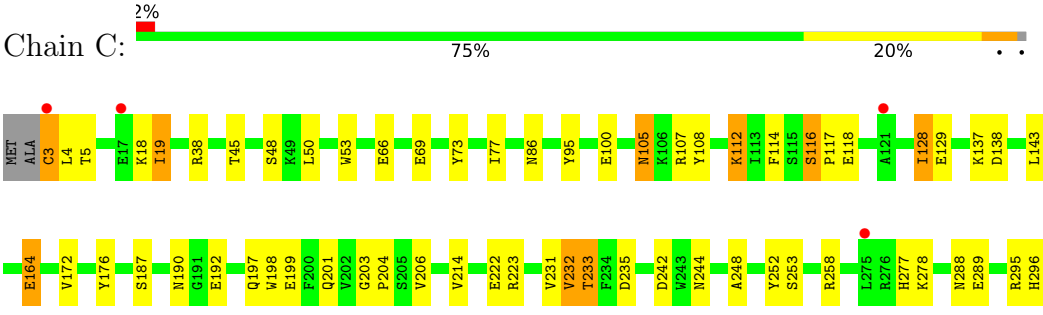
• Molecule 1: glutamine synthetase

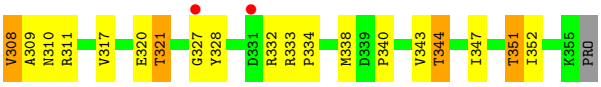
Chain B:



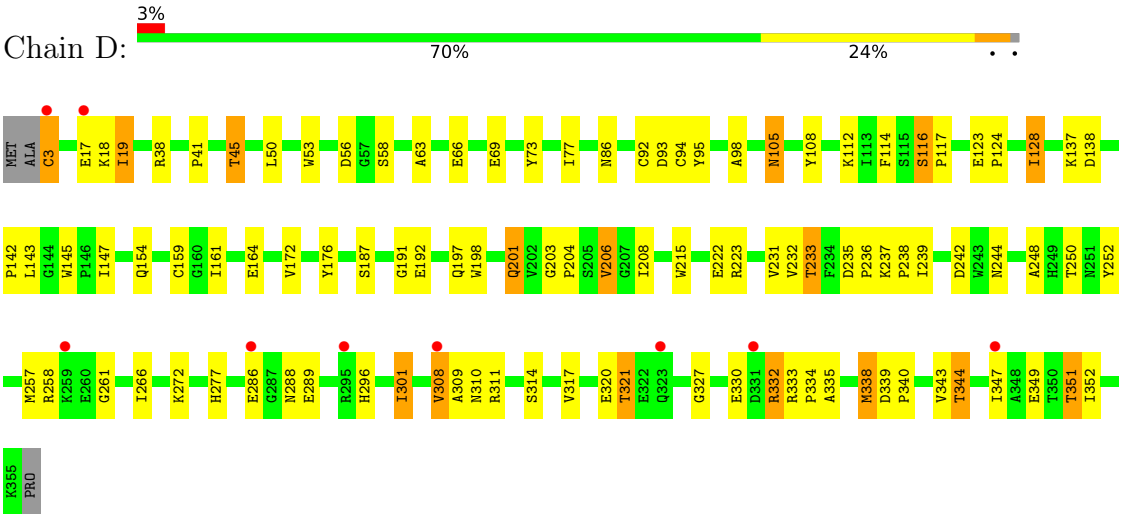
• Molecule 1: glutamine synthetase

Chain C:

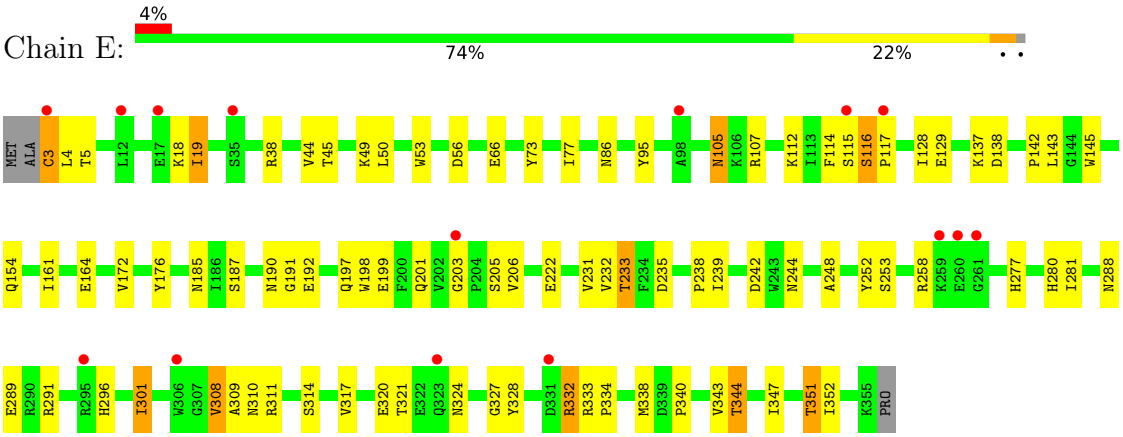




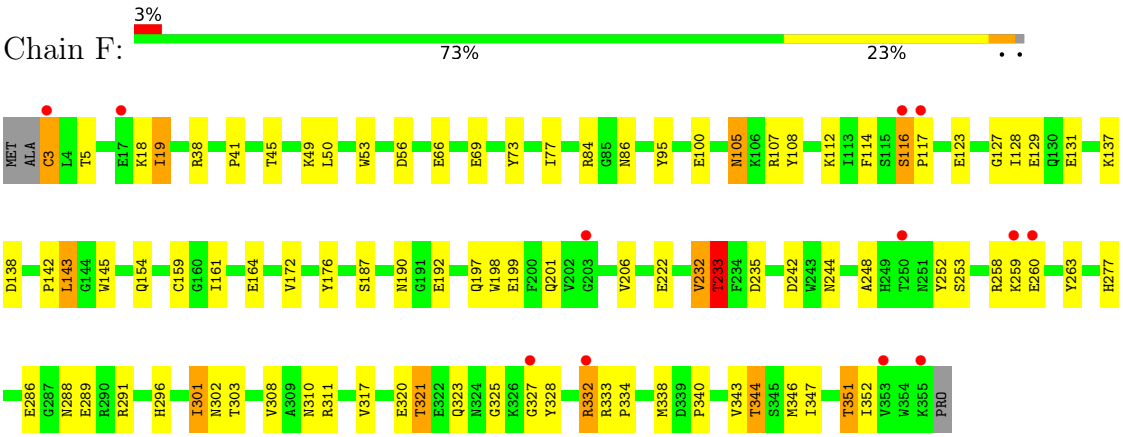
• Molecule 1: glutamine synthetase



• Molecule 1: glutamine synthetase

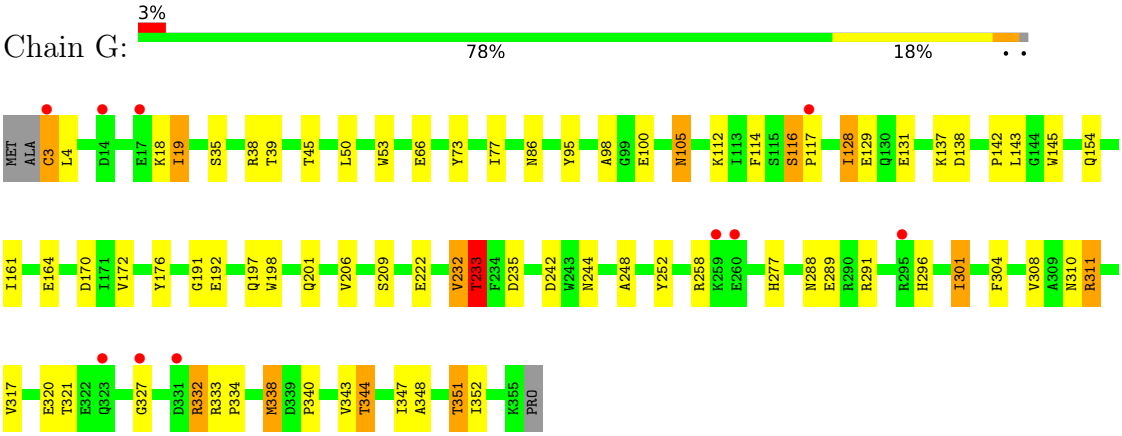


• Molecule 1: glutamine synthetase



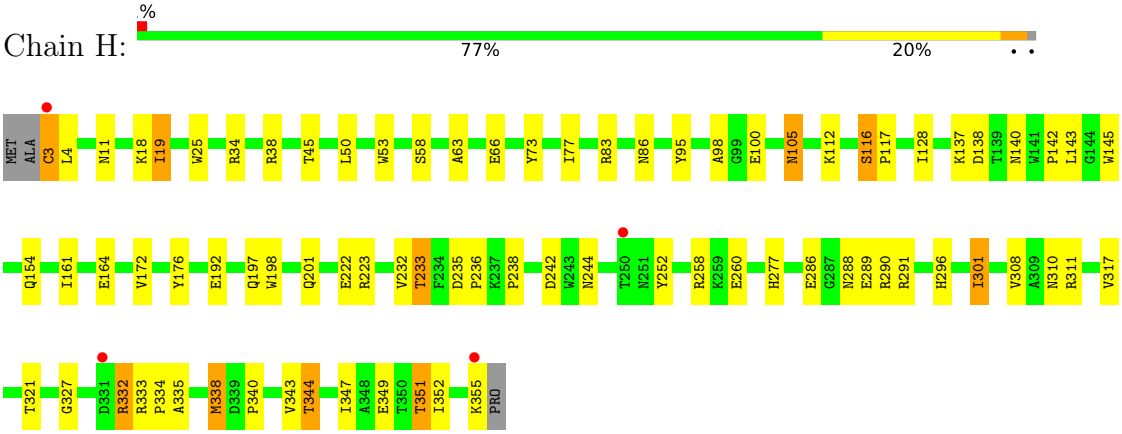
• Molecule 1: glutamine synthetase

Chain G:



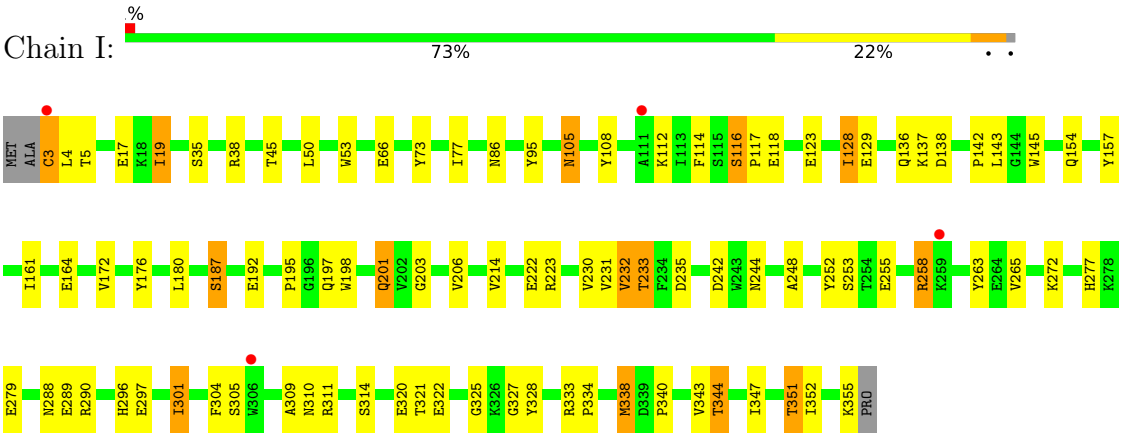
• Molecule 1: glutamine synthetase

Chain H:



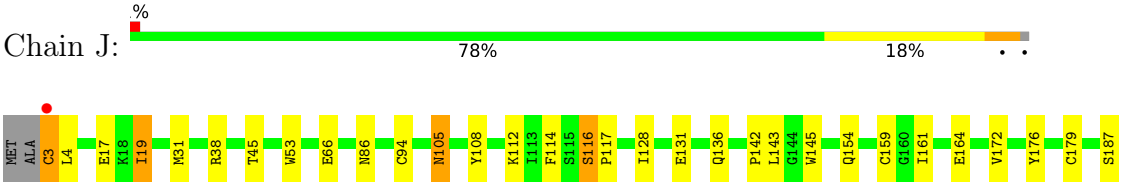
• Molecule 1: glutamine synthetase

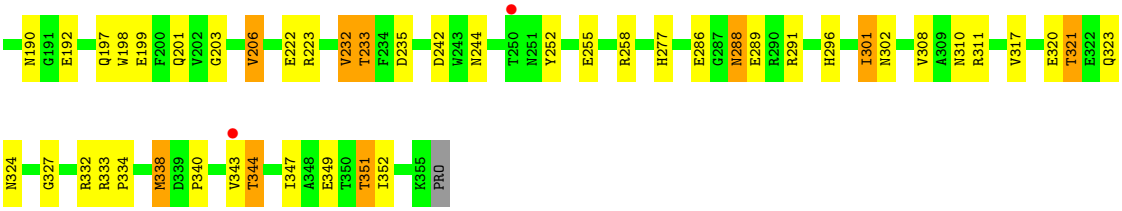
Chain I:



• Molecule 1: glutamine synthetase

Chain J:




N190
G191
E192
Q197
W198
E199
F200
Q201
V202
G203
V206
E222
R223
V232
T233
F234
D235
D242
W243
N244
T250
N251
Y252
E255
R258
H277
E286
G287
N288
E289
R290
R291
H296
I301
N302
V308
A309
N310
R311
V317
E320
T321
E322
Q323

N324
G327
R332
R333
P334
M338
D339
P340
V343
T344
I347
A348
E349
T350
T351
I352
K355
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.80Å 191.04Å 118.10Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	26.13 – 2.63 26.13 – 2.63	Depositor EDS
% Data completeness (in resolution range)	86.8 (26.13-2.63) 86.8 (26.13-2.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.220 0.184 , 0.220	Depositor DCC
R_{free} test set	5400 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28621	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P3S, ADP, MN

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	0.79	0/2819	0.79	5/3834 (0.1%)
1	B	0.79	2/2819 (0.1%)	0.78	3/3834 (0.1%)
1	C	0.76	0/2819	0.76	1/3834 (0.0%)
1	D	0.88	1/2819 (0.0%)	0.80	2/3834 (0.1%)
1	E	0.86	0/2819	0.79	3/3834 (0.1%)
1	F	0.80	0/2819	0.78	6/3834 (0.2%)
1	G	0.82	0/2819	0.79	6/3834 (0.2%)
1	H	0.78	0/2819	0.79	2/3834 (0.1%)
1	I	0.77	0/2819	0.76	2/3834 (0.1%)
1	J	0.80	2/2819 (0.1%)	0.79	3/3834 (0.1%)
All	All	0.80	5/28190 (0.0%)	0.78	33/38340 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	179	CYS	CB-SG	-7.34	1.69	1.82
1	D	92	CYS	CB-SG	-6.80	1.70	1.82
1	B	94	CYS	CB-SG	-6.15	1.71	1.82
1	B	92	CYS	CB-SG	-5.60	1.72	1.81
1	J	94	CYS	CB-SG	-5.47	1.72	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	291	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	332	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	J	291	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	H	332	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	291	ARG	NE-CZ-NH1	6.69	123.64	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2653	56	0
1	B	2745	0	2653	57	0
1	C	2745	0	2653	60	0
1	D	2745	0	2653	86	0
1	E	2745	0	2653	62	0
1	F	2745	0	2653	66	0
1	G	2745	0	2653	64	0
1	H	2745	0	2653	60	0
1	I	2745	0	2653	70	0
1	J	2745	0	2653	57	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	15	0	10	2	0
3	B	15	0	10	2	0
3	C	15	0	10	1	0
3	D	15	0	10	2	0
3	E	15	0	10	1	0
3	F	15	0	10	2	0
3	G	15	0	10	4	0
3	H	15	0	10	2	0
3	I	15	0	10	1	0
3	J	15	0	10	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	0	0
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	1	0
5	A	70	0	0	11	0
5	B	100	0	0	18	0
5	C	63	0	0	16	0
5	D	63	0	0	31	0
5	E	57	0	0	16	0
5	F	58	0	0	22	0
5	G	54	0	0	17	0
5	H	88	0	0	20	0
5	I	76	0	0	20	0
5	J	92	0	0	17	0
All	All	28621	0	26750	605	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 11.

The worst 5 of 605 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:J:206:VAL:HB	5:J:6073:HOH:O	1.37	1.23
1:C:203:GLY:HA3	5:C:6039:HOH:O	1.39	1.20
1:H:321:THR:HG23	5:H:6097:HOH:O	1.47	1.13
1:H:344:THR:HG21	5:H:6011:HOH:O	1.51	1.09
1:G:321:THR:HG23	5:G:6024:HOH:O	1.53	1.09

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	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	B	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	C	351/356 (99%)	333 (95%)	17 (5%)	1 (0%)	41	56
1	D	351/356 (99%)	332 (95%)	18 (5%)	1 (0%)	41	56
1	E	351/356 (99%)	330 (94%)	19 (5%)	2 (1%)	25	37
1	F	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	G	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	H	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	I	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	J	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
All	All	3510/3560 (99%)	3323 (95%)	183 (5%)	4 (0%)	51	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	308	VAL
1	C	308	VAL
1	D	308	VAL
1	E	281	ILE

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	288/290 (99%)	265 (92%)	23 (8%)	12	18
1	B	288/290 (99%)	264 (92%)	24 (8%)	11	16
1	C	288/290 (99%)	265 (92%)	23 (8%)	12	18
1	D	288/290 (99%)	263 (91%)	25 (9%)	10	14
1	E	288/290 (99%)	266 (92%)	22 (8%)	13	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	288/290 (99%)	265 (92%)	23 (8%)	12 18
1	G	288/290 (99%)	266 (92%)	22 (8%)	13 20
1	H	288/290 (99%)	267 (93%)	21 (7%)	14 21
1	I	288/290 (99%)	264 (92%)	24 (8%)	11 16
1	J	288/290 (99%)	264 (92%)	24 (8%)	11 16
All	All	2880/2900 (99%)	2649 (92%)	231 (8%)	12 18

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	344	THR
1	J	258	ARG
1	G	105	ASN
1	J	232	VAL
1	I	288	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	190	ASN
1	H	296	HIS
1	G	201	GLN
1	H	154	GLN
1	I	190	ASN

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 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	E	6004	2	24,29,29	0.96	1 (4%)	29,45,45	1.95	6 (20%)
3	P3S	A	5001	2	11,14,14	2.22	3 (27%)	12,21,21	2.17	3 (25%)
3	P3S	B	5002	2	11,14,14	1.81	3 (27%)	12,21,21	2.82	4 (33%)
4	ADP	H	6010	2	24,29,29	0.97	0	29,45,45	1.94	8 (27%)
3	P3S	C	5003	2	11,14,14	1.65	1 (9%)	12,21,21	1.69	2 (16%)
3	P3S	G	5006	2	11,14,14	1.79	2 (18%)	12,21,21	0.90	0
3	P3S	D	5004	2	11,14,14	2.23	2 (18%)	12,21,21	1.50	1 (8%)
3	P3S	E	5005	2	11,14,14	1.91	2 (18%)	12,21,21	1.66	2 (16%)
3	P3S	H	5010	2	11,14,14	1.98	2 (18%)	12,21,21	2.21	3 (25%)
4	ADP	G	6006	2	24,29,29	0.85	1 (4%)	29,45,45	1.42	2 (6%)
3	P3S	I	5008	2	11,14,14	1.84	1 (9%)	12,21,21	2.18	5 (41%)
4	ADP	A	6001	2	24,29,29	0.82	0	29,45,45	1.89	6 (20%)
3	P3S	J	5009	2	11,14,14	1.70	1 (9%)	12,21,21	2.07	4 (33%)
4	ADP	J	6009	2	24,29,29	1.40	3 (12%)	29,45,45	1.88	6 (20%)
4	ADP	F	6007	2	24,29,29	0.95	1 (4%)	29,45,45	1.48	2 (6%)
3	P3S	F	5007	2	11,14,14	1.69	2 (18%)	12,21,21	1.96	4 (33%)
4	ADP	C	6003	2	24,29,29	0.96	2 (8%)	29,45,45	1.55	2 (6%)
4	ADP	B	6002	2	24,29,29	1.01	2 (8%)	29,45,45	1.89	4 (13%)
4	ADP	D	6005	2	24,29,29	0.93	1 (4%)	29,45,45	1.55	5 (17%)
4	ADP	I	6008	2	24,29,29	0.98	1 (4%)	29,45,45	1.58	3 (10%)

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	E	6004	2	-	4/12/32/32	0/3/3/3
3	P3S	A	5001	2	-	6/9/16/16	-
3	P3S	B	5002	2	-	4/9/16/16	-
4	ADP	H	6010	2	-	2/12/32/32	0/3/3/3
3	P3S	C	5003	2	-	4/9/16/16	-
3	P3S	G	5006	2	-	7/9/16/16	-
3	P3S	D	5004	2	-	7/9/16/16	-
3	P3S	E	5005	2	-	4/9/16/16	-
3	P3S	H	5010	2	-	4/9/16/16	-
4	ADP	G	6006	2	-	6/12/32/32	0/3/3/3
3	P3S	I	5008	2	-	4/9/16/16	-
4	ADP	A	6001	2	-	1/12/32/32	0/3/3/3
3	P3S	J	5009	2	-	8/9/16/16	-
4	ADP	J	6009	2	-	2/12/32/32	0/3/3/3
4	ADP	F	6007	2	-	6/12/32/32	0/3/3/3
3	P3S	F	5007	2	-	4/9/16/16	-
4	ADP	C	6003	2	-	5/12/32/32	0/3/3/3
4	ADP	B	6002	2	-	4/12/32/32	0/3/3/3
4	ADP	D	6005	2	-	7/12/32/32	0/3/3/3
4	ADP	I	6008	2	-	3/12/32/32	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5004	P3S	PA-NE	4.95	1.77	1.59
3	I	5008	P3S	PA-NE	4.88	1.77	1.59
3	E	5005	P3S	PA-NE	4.53	1.76	1.59
3	J	5009	P3S	PA-NE	4.47	1.76	1.59
3	G	5006	P3S	PA-NE	4.46	1.75	1.59

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5002	P3S	OE-SD-CG	7.47	114.22	108.37
4	B	6002	ADP	N3-C2-N1	-7.10	117.59	128.68
4	J	6009	ADP	N3-C2-N1	-6.52	118.48	128.68
3	H	5010	P3S	OE-SD-CG	6.28	113.28	108.37
4	A	6001	ADP	N3-C2-N1	-6.21	118.97	128.68

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	P3S	CB-CG-SD-OE
3	A	5001	P3S	CB-CG-SD-CE
3	A	5001	P3S	O-C-CA-N
3	C	5003	P3S	O-C-CA-N
3	D	5004	P3S	CB-CG-SD-OE

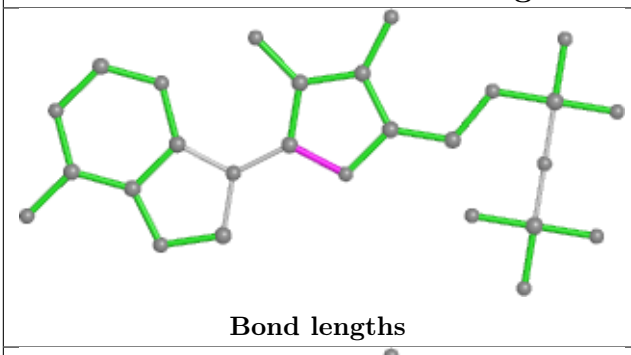
There are no ring outliers.

14 monomers are involved in 26 short contacts:

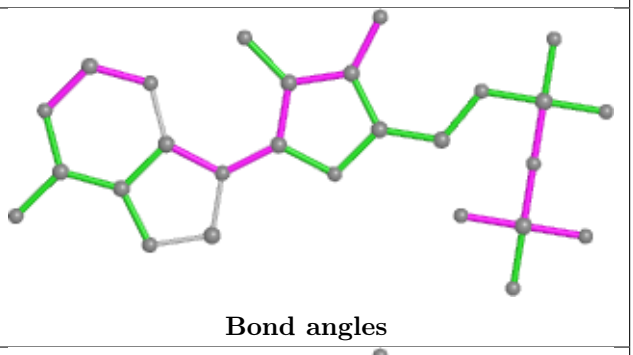
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	6004	ADP	1	0
3	A	5001	P3S	2	0
3	B	5002	P3S	2	0
3	C	5003	P3S	1	0
3	G	5006	P3S	4	0
3	D	5004	P3S	2	0
3	E	5005	P3S	1	0
3	H	5010	P3S	2	0
3	I	5008	P3S	1	0
3	J	5009	P3S	3	0
4	J	6009	ADP	1	0
4	F	6007	ADP	1	0
3	F	5007	P3S	2	0
4	D	6005	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

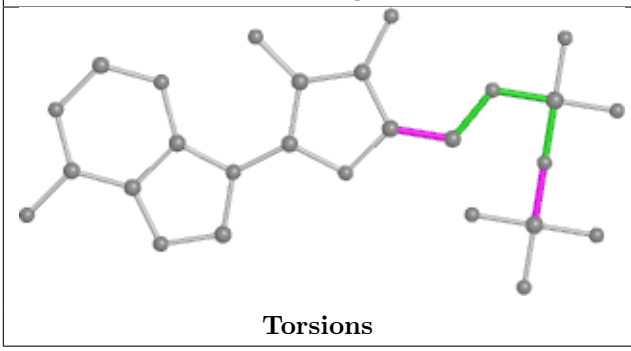
Ligand ADP E 6004



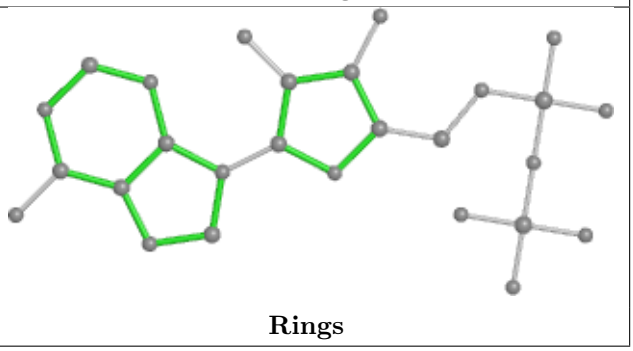
Bond lengths



Bond angles

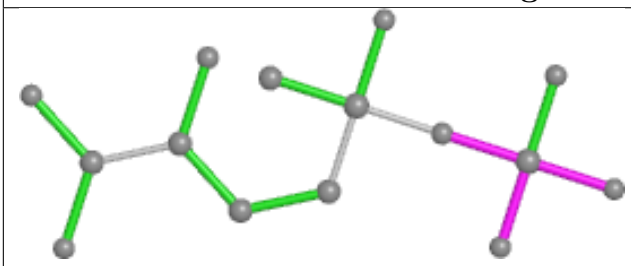


Torsions



Rings

Ligand P3S A 5001



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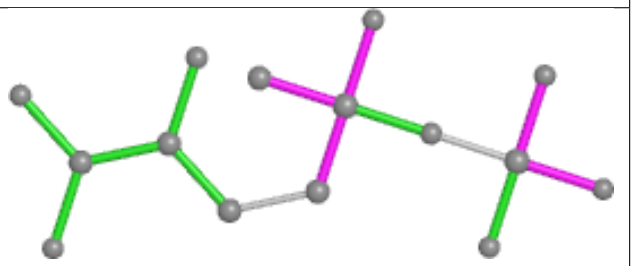

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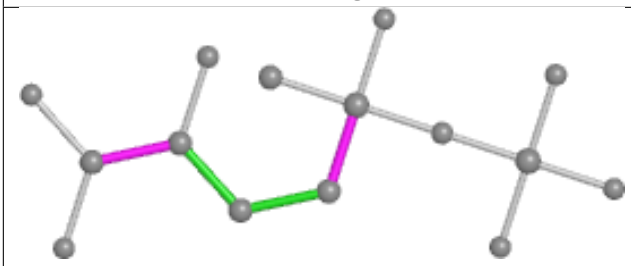

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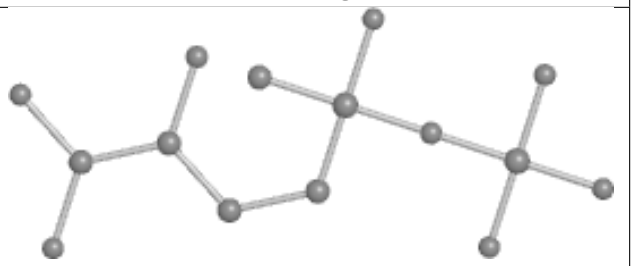
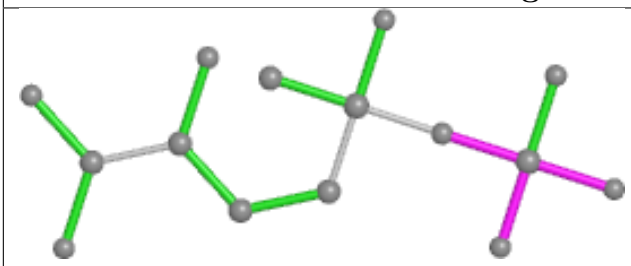


Rings

Ligand P3S B 5002



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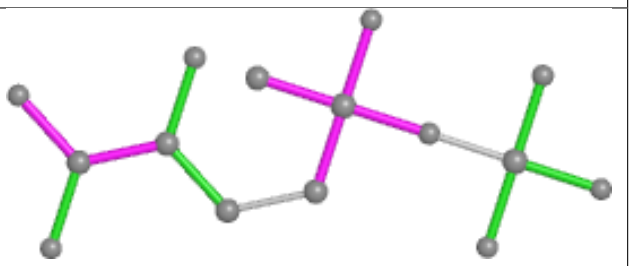

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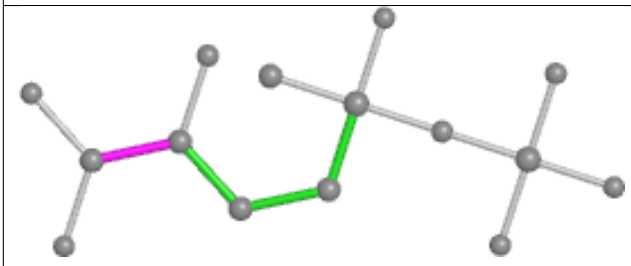

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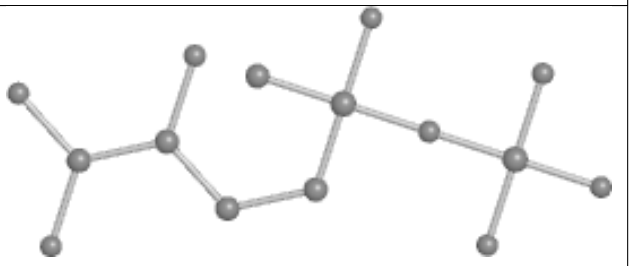
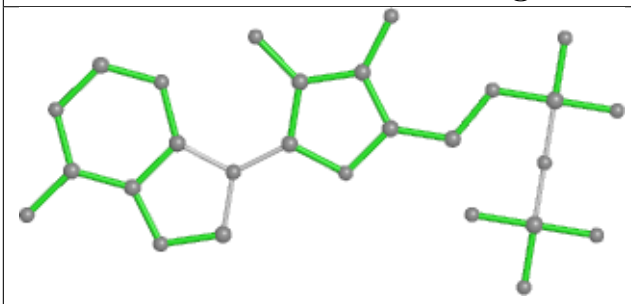
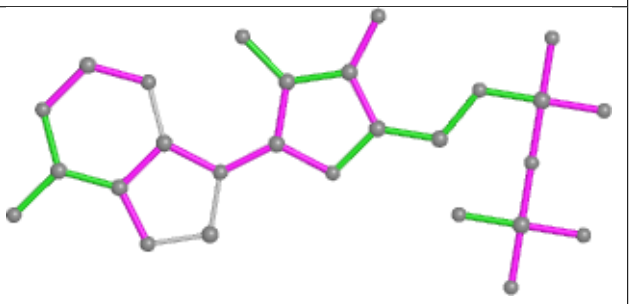


Rings

Ligand ADP H 6010



Bond lengths



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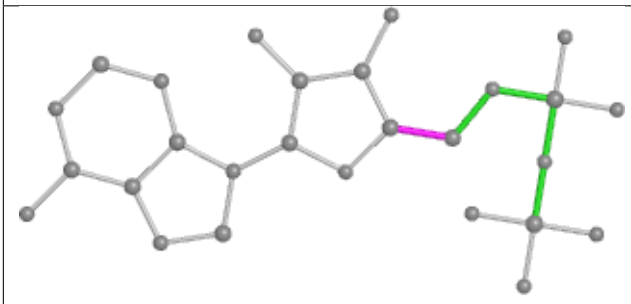

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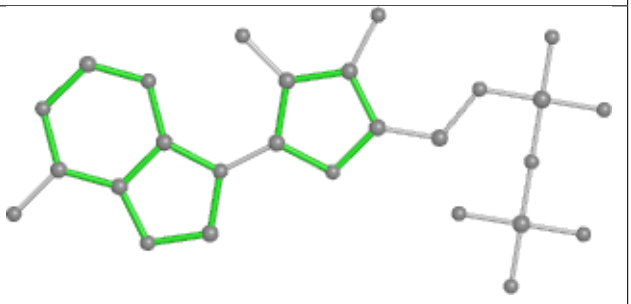
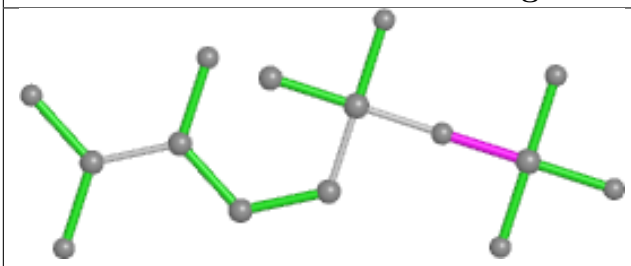


Rings

Ligand P3S C 5003



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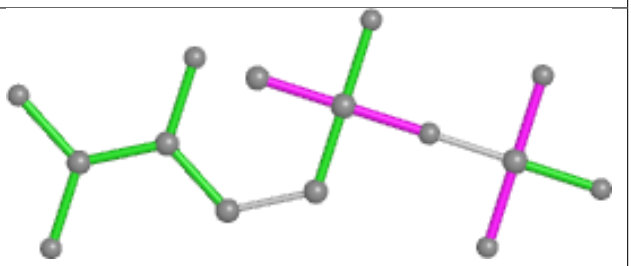

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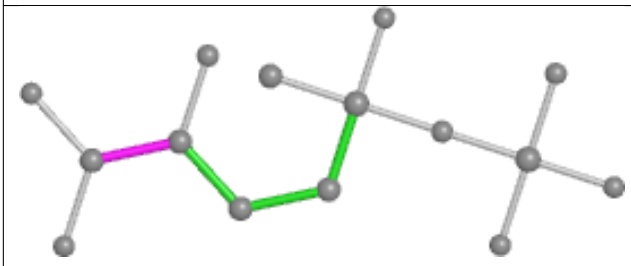

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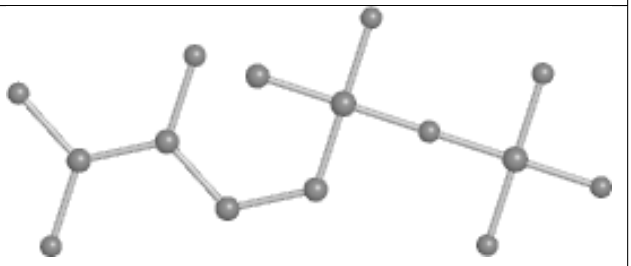
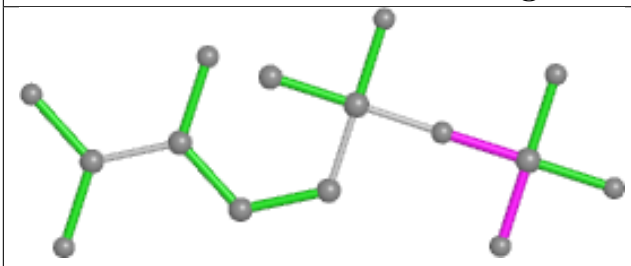
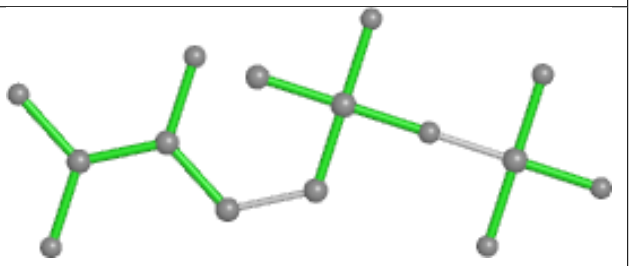


Rings

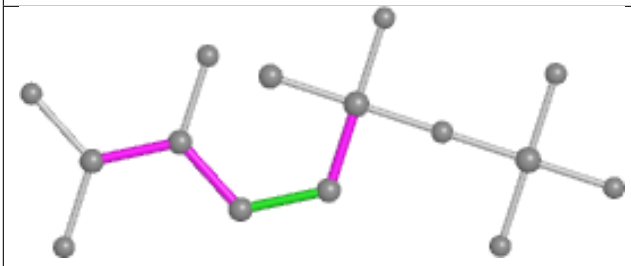
Ligand P3S G 5006



Bond lengths



Bond angles



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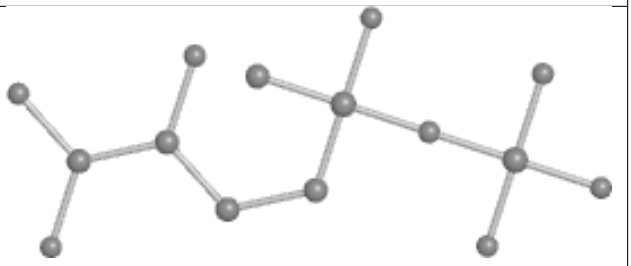
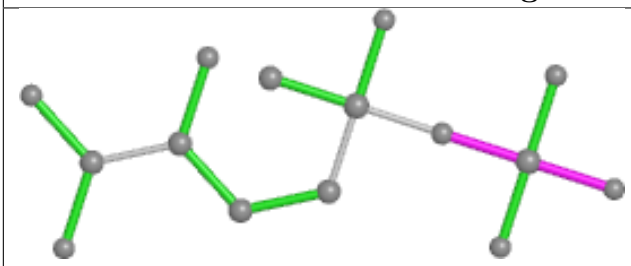
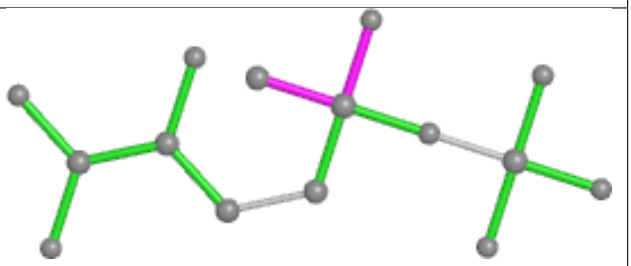


Rings

Ligand P3S D 5004



Bond lengths



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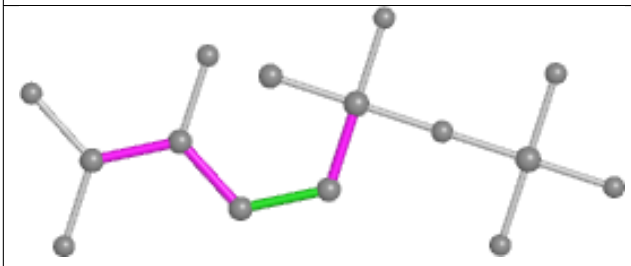

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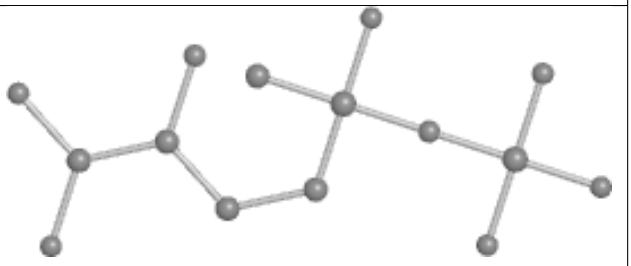
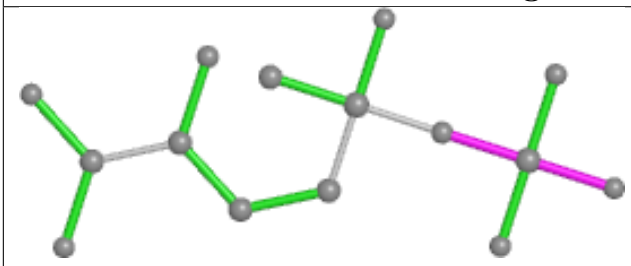


Rings

Ligand P3S E 5005



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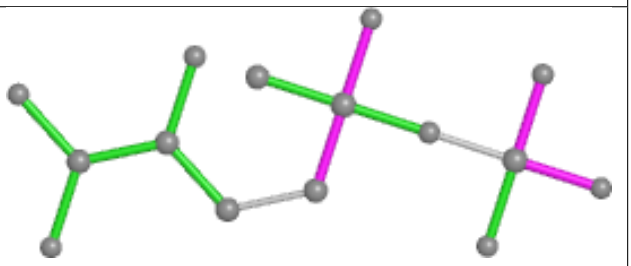
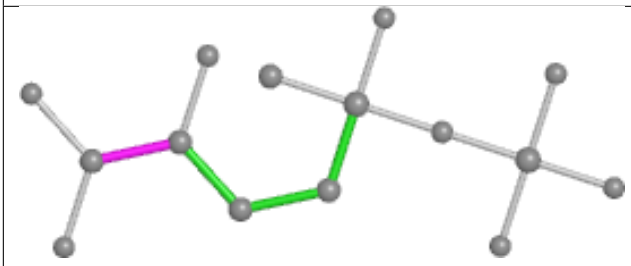
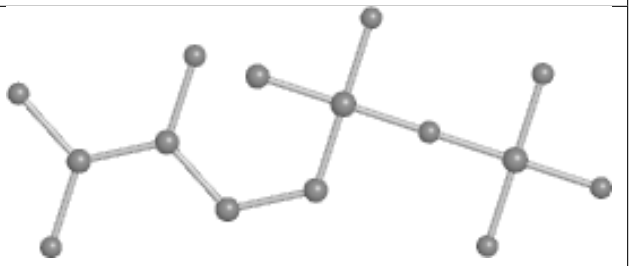


Bond angles

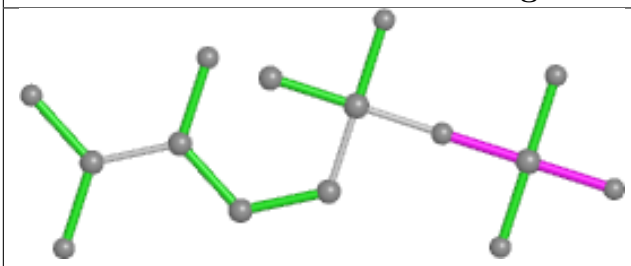


Torsions

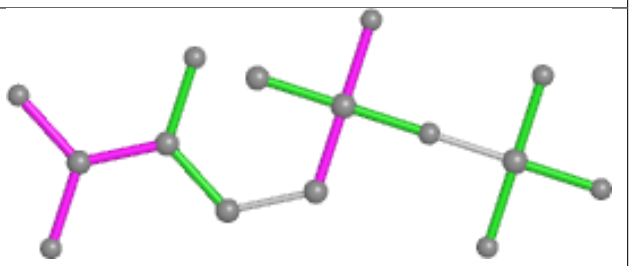


Rings

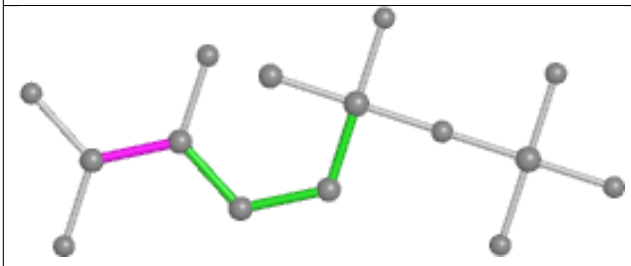
Ligand P3S H 5010



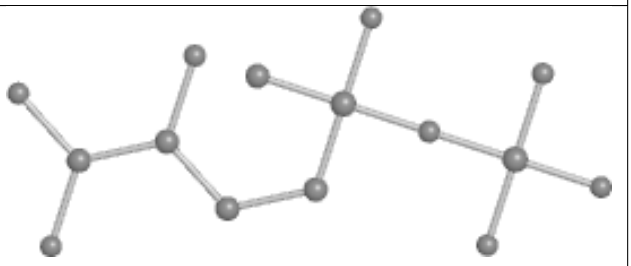
Bond lengths



Bond angles

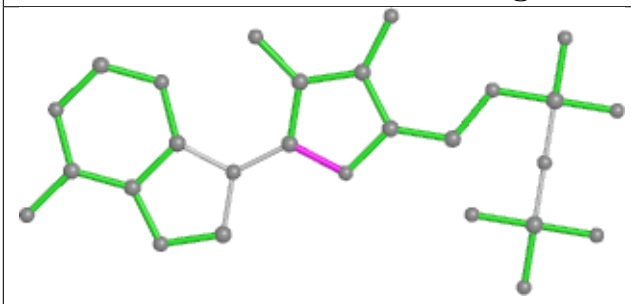


Torsions

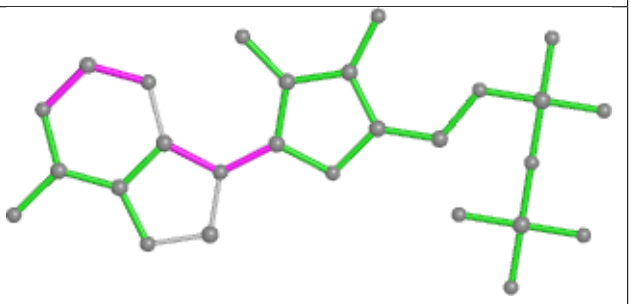


Rings

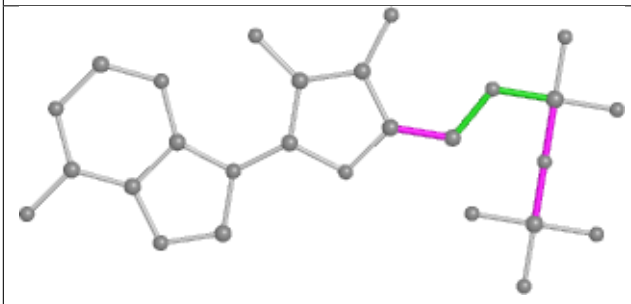
Ligand ADP G 6006



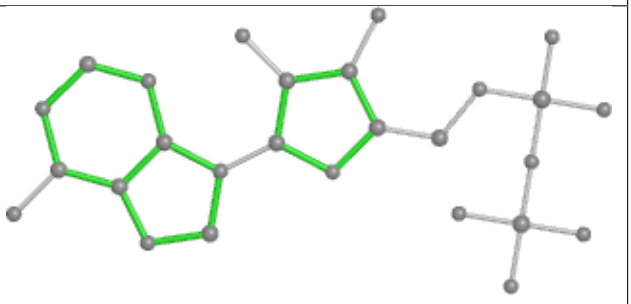
Bond lengths



Bond angles

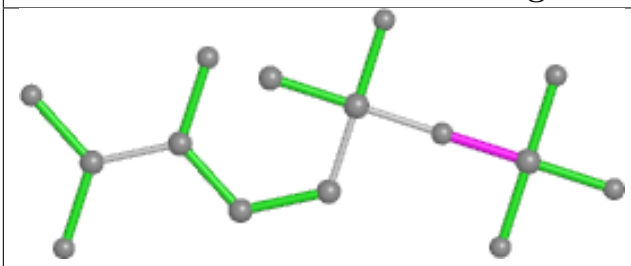


Torsions

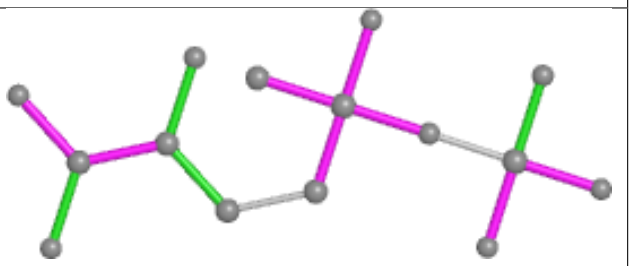


Rings

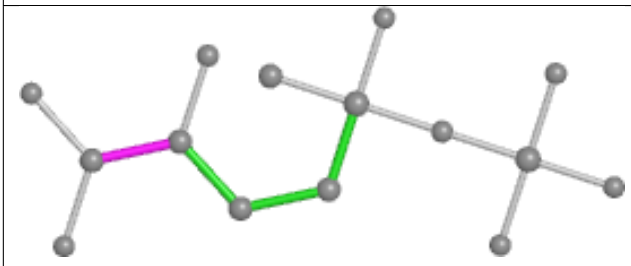
Ligand P3S I 5008



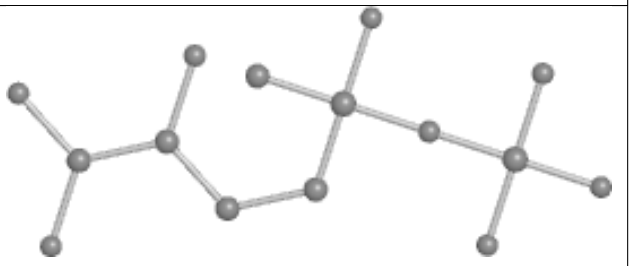
Bond lengths



Bond angles

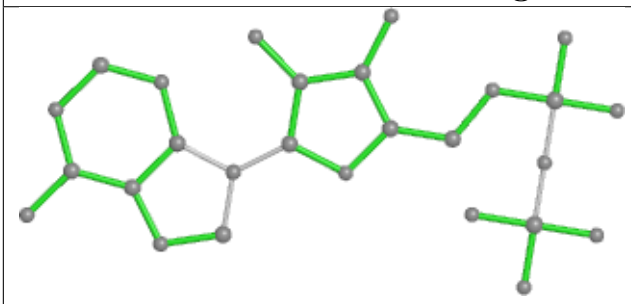


Torsions

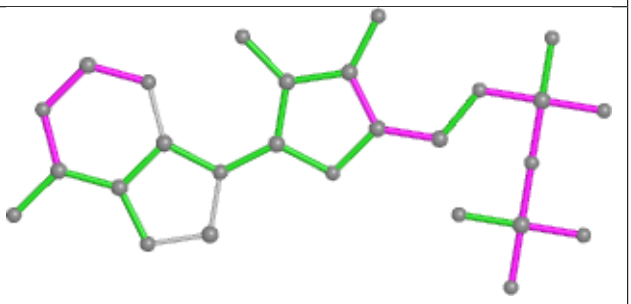


Rings

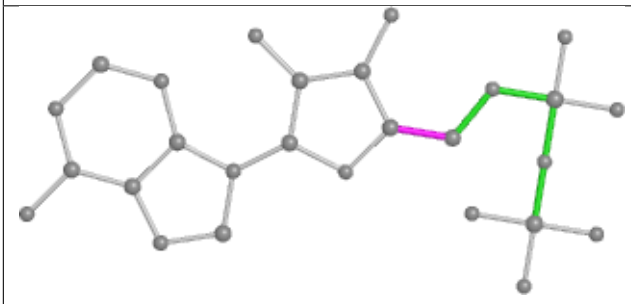
Ligand ADP A 6001



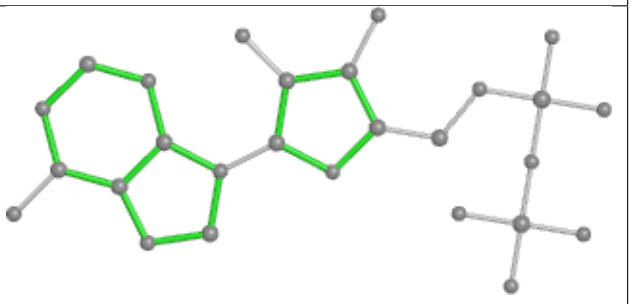
Bond lengths



Bond angles

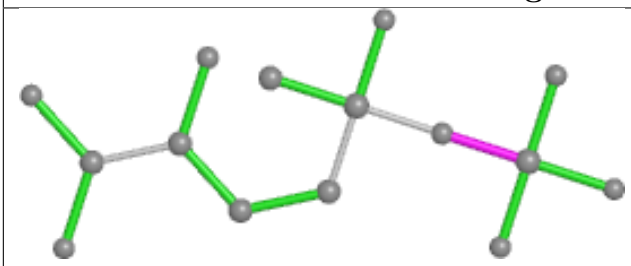


Torsions

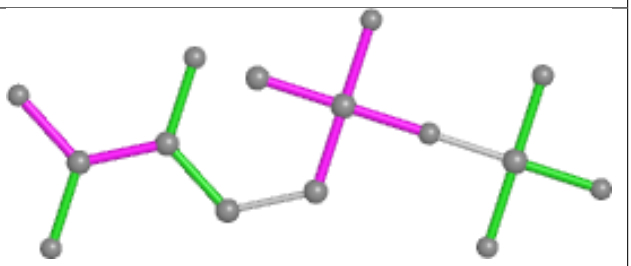


Rings

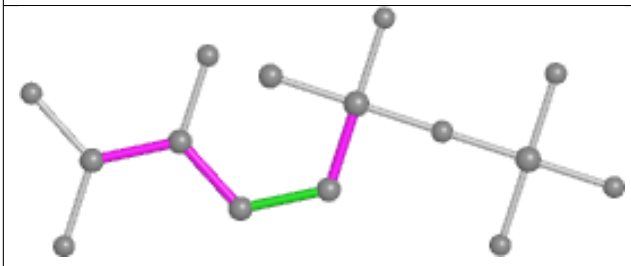
Ligand P3S J 5009



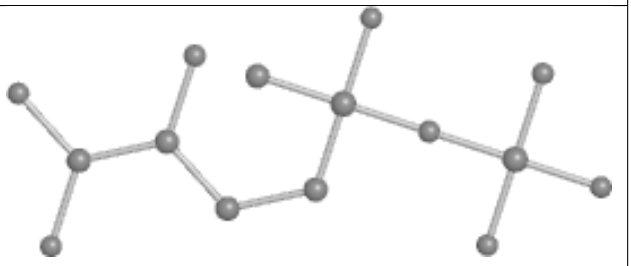
Bond lengths



Bond angles

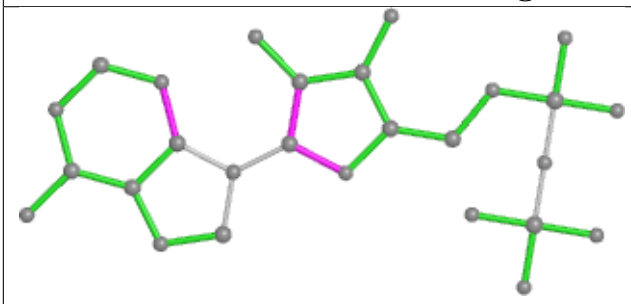


Torsions

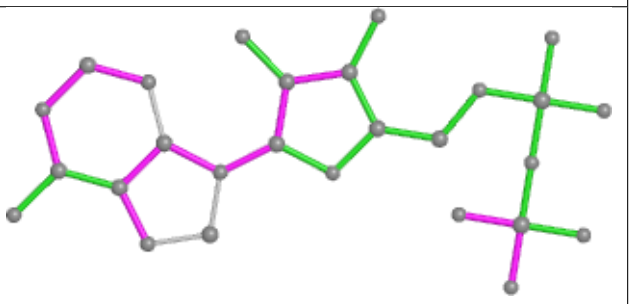


Rings

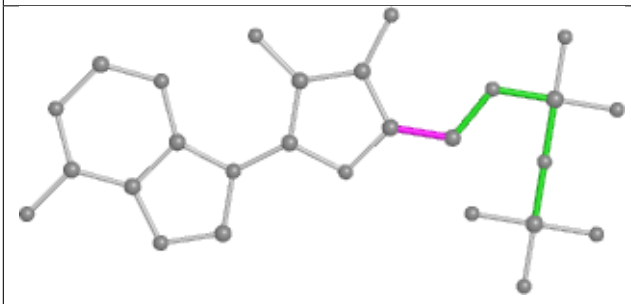
Ligand ADP J 6009



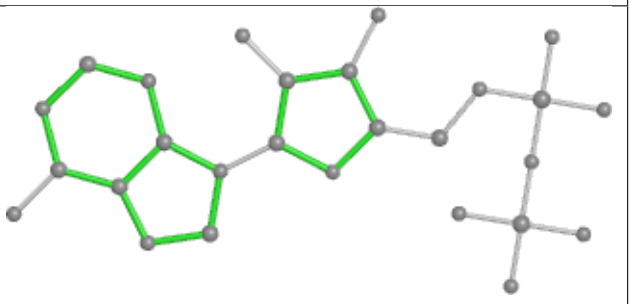
Bond lengths



Bond angles

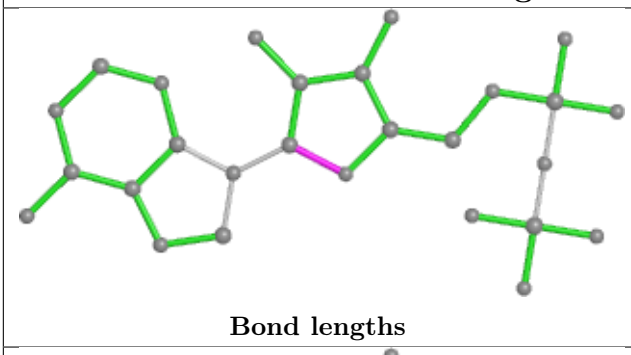


Torsions

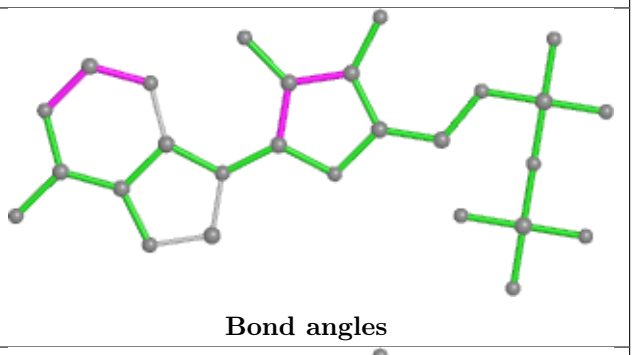


Rings

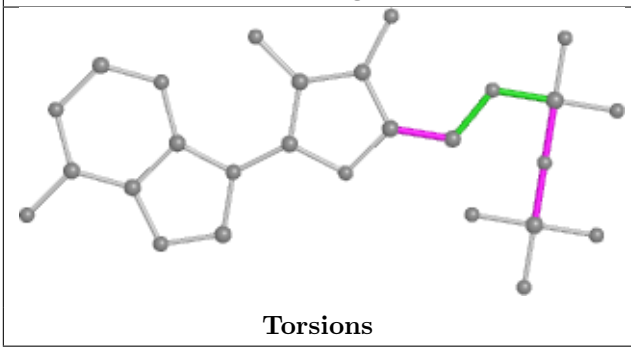
Ligand ADP F 6007



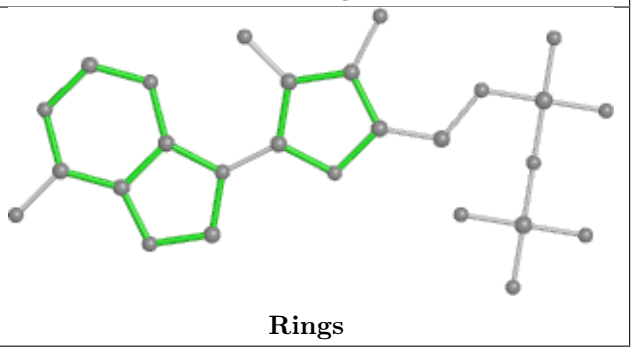
Bond lengths



Bond angles

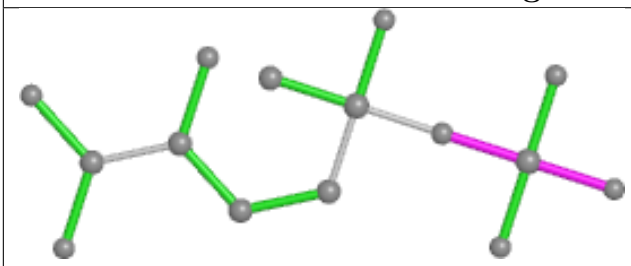


Torsions

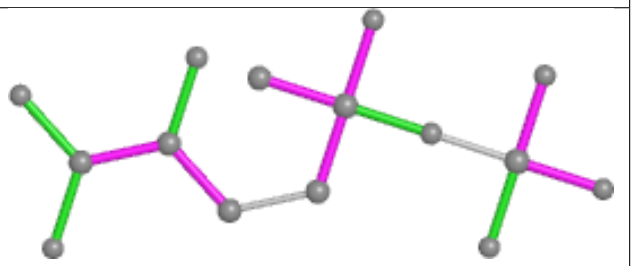


Rings

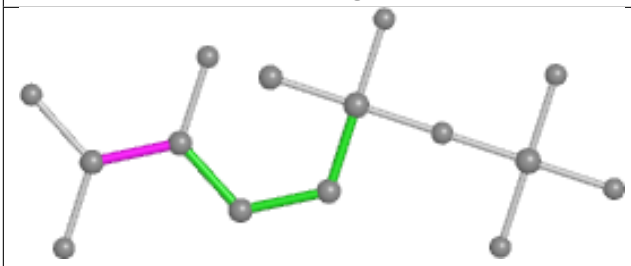
Ligand P3S F 5007



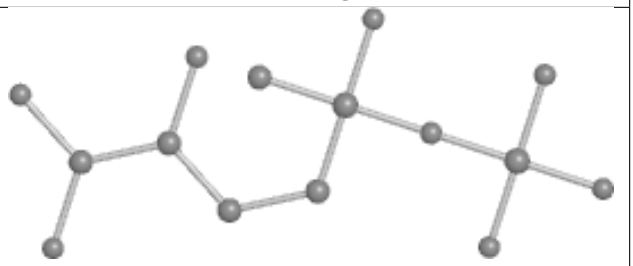
Bond lengths



Bond angles

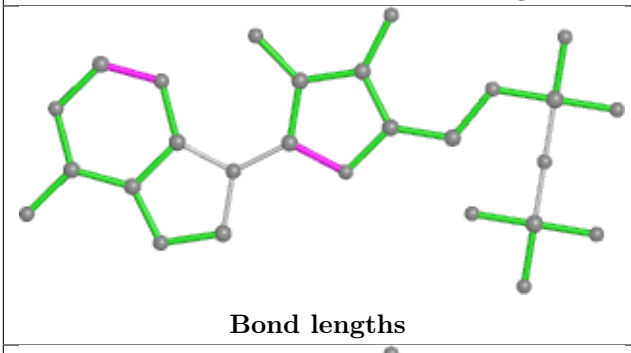


Torsions

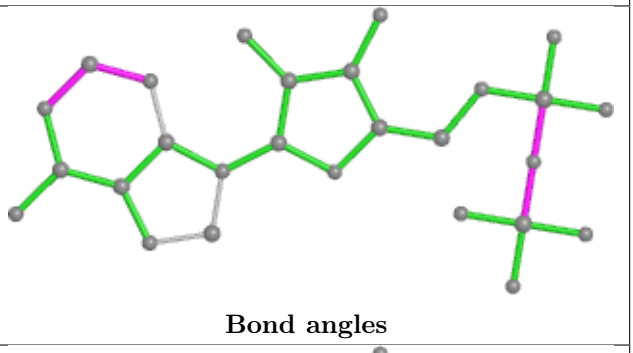


Rings

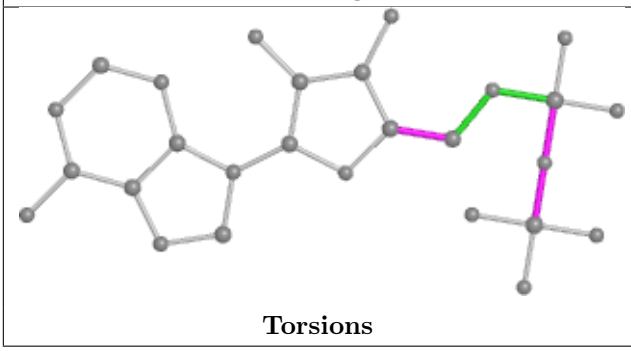
Ligand ADP C 6003



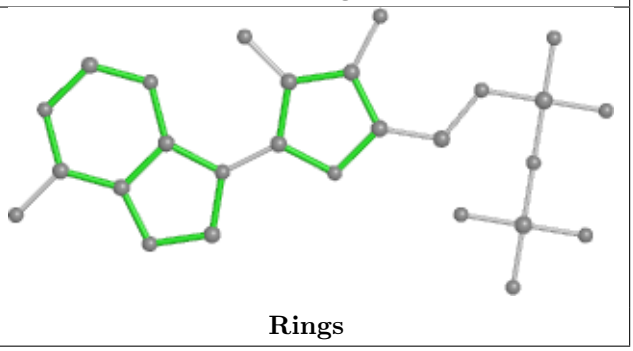
Bond lengths



Bond angles

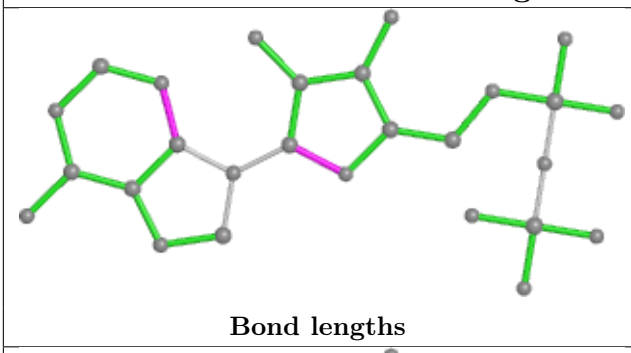


Torsions

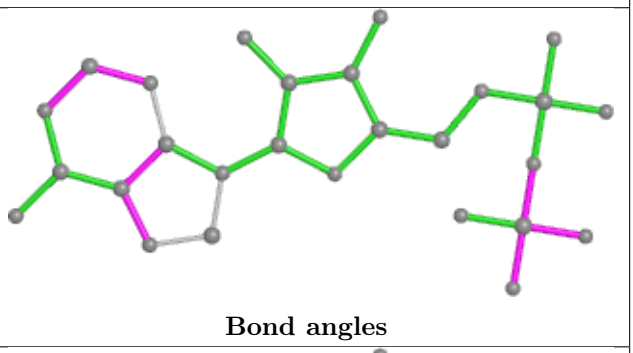


Rings

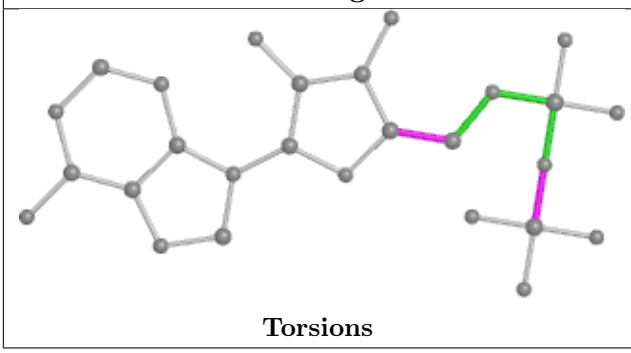
Ligand ADP B 6002



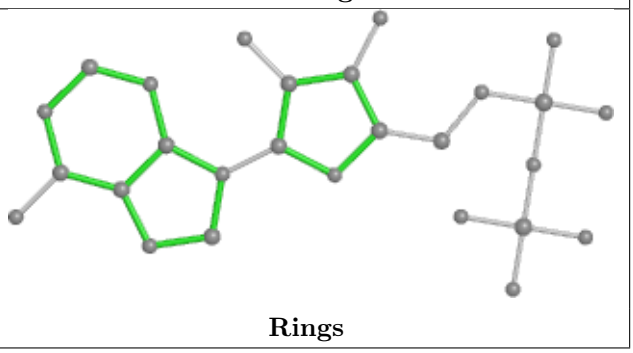
Bond lengths



Bond angles

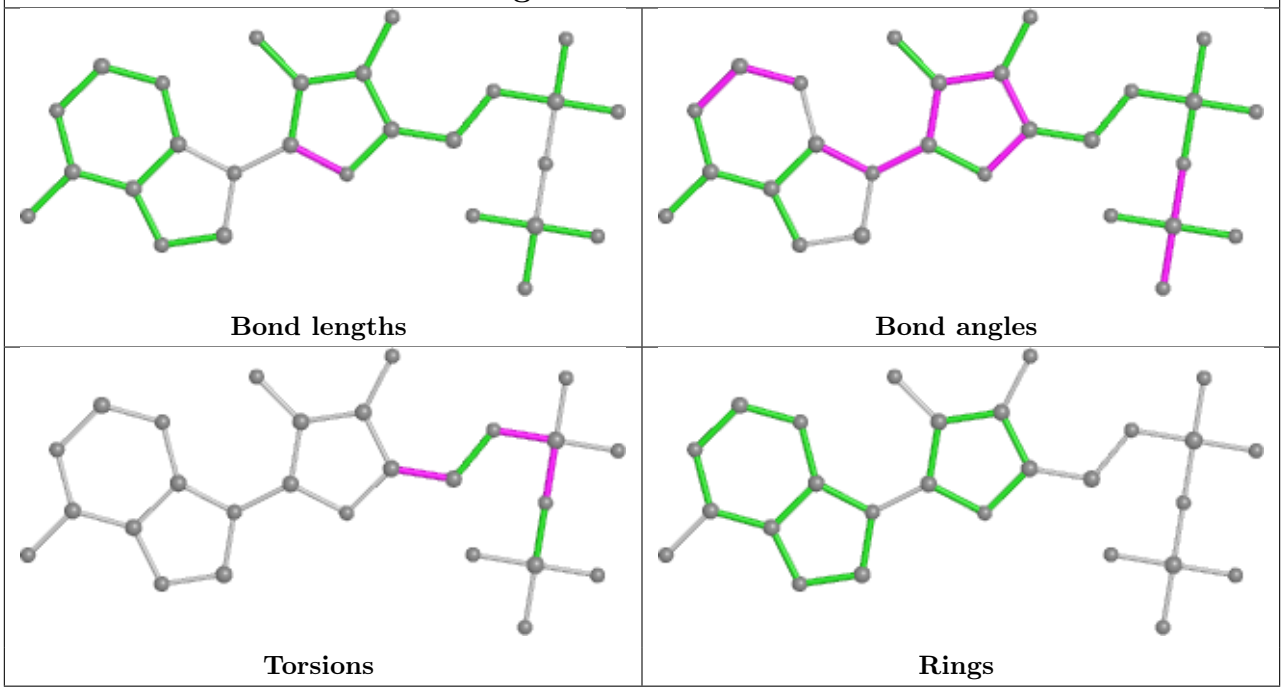


Torsions

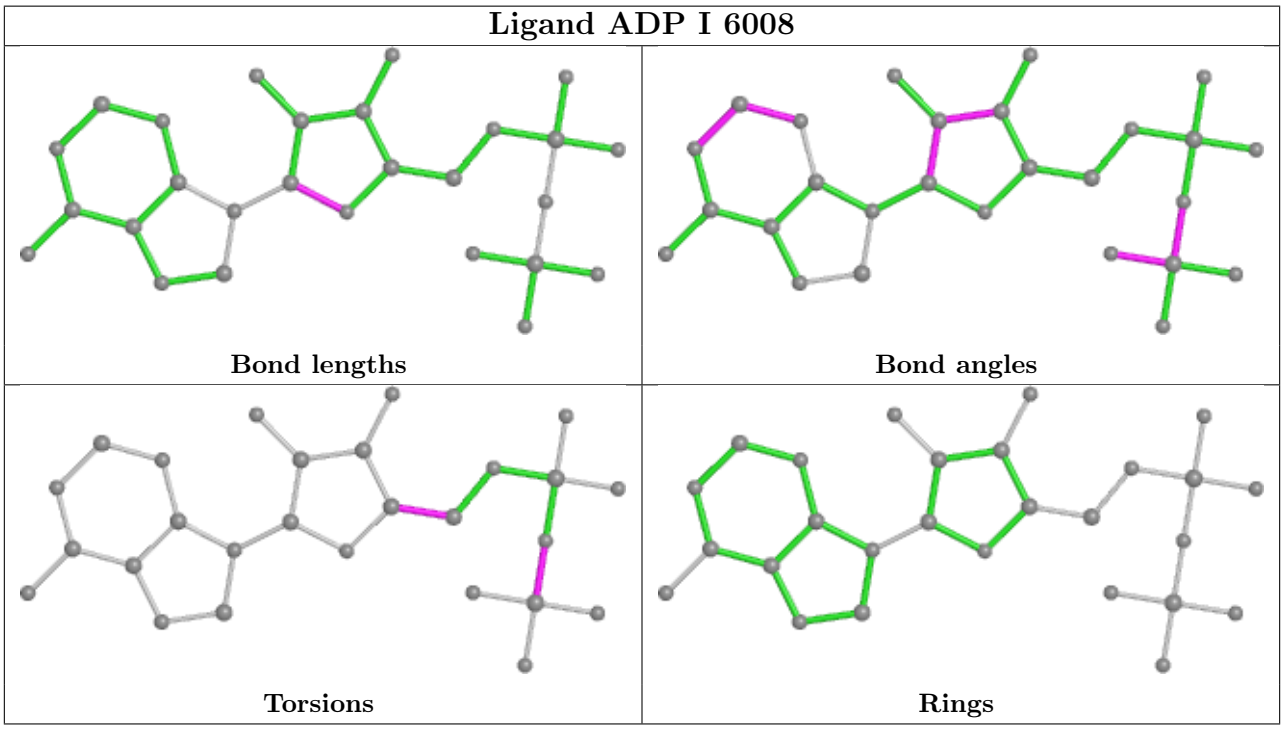


Rings

Ligand ADP D 6005



Ligand ADP I 6008



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	353/356 (99%)	-0.26	6 (1%)	70	67	46, 64, 86, 99	0
1	B	353/356 (99%)	-0.20	3 (0%)	86	85	46, 64, 86, 99	0
1	C	353/356 (99%)	-0.24	6 (1%)	70	67	46, 64, 86, 99	0
1	D	353/356 (99%)	-0.11	9 (2%)	57	53	46, 64, 86, 99	0
1	E	353/356 (99%)	-0.15	15 (4%)	36	33	46, 64, 86, 99	0
1	F	353/356 (99%)	-0.18	12 (3%)	45	41	46, 64, 86, 99	0
1	G	353/356 (99%)	-0.18	10 (2%)	53	49	46, 64, 86, 99	0
1	H	353/356 (99%)	-0.10	4 (1%)	80	78	46, 64, 86, 99	0
1	I	353/356 (99%)	-0.30	4 (1%)	80	78	46, 64, 86, 99	0
1	J	353/356 (99%)	-0.19	3 (0%)	86	85	46, 64, 86, 99	0
All	All	3530/3560 (99%)	-0.19	72 (2%)	65	61	46, 64, 87, 99	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	GLY	6.5
1	F	3	CYS	5.8
1	C	3	CYS	5.5
1	A	3	CYS	5.5
1	I	3	CYS	5.4

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

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	MN	E	1041	1/1	0.94	0.14	66,66,66,66	0
4	ADP	E	6004	27/27	0.94	0.16	67,86,94,95	0
2	MN	J	1091	1/1	0.95	0.16	47,47,47,47	0
4	ADP	C	6003	27/27	0.95	0.15	62,75,80,81	0
2	MN	F	1051	1/1	0.95	0.12	66,66,66,66	0
2	MN	C	1021	1/1	0.96	0.22	73,73,73,73	0
4	ADP	B	6002	27/27	0.96	0.14	39,50,52,53	0
2	MN	G	1061	1/1	0.96	0.11	57,57,57,57	0
4	ADP	D	6005	27/27	0.96	0.12	55,78,85,86	0
2	MN	I	1081	1/1	0.96	0.13	56,56,56,56	0
4	ADP	F	6007	27/27	0.96	0.12	61,78,84,84	0
3	P3S	E	5005	15/15	0.97	0.16	65,68,70,70	0
2	MN	B	1011	1/1	0.97	0.15	49,49,49,49	0
2	MN	H	1071	1/1	0.97	0.14	49,49,49,49	0
2	MN	D	1033	1/1	0.97	0.20	68,68,68,68	0
2	MN	I	1083	1/1	0.97	0.12	54,54,54,54	0
2	MN	F	1052	1/1	0.97	0.13	66,66,66,66	0
4	ADP	G	6006	27/27	0.97	0.12	47,68,76,77	0
4	ADP	I	6008	27/27	0.97	0.14	54,68,70,70	0
3	P3S	F	5007	15/15	0.98	0.13	59,64,69,71	0
3	P3S	I	5008	15/15	0.98	0.15	43,48,53,54	0
4	ADP	A	6001	27/27	0.98	0.13	48,62,73,74	0
2	MN	H	1073	1/1	0.98	0.17	47,47,47,47	0
2	MN	F	1053	1/1	0.98	0.07	67,67,67,67	0
2	MN	D	1031	1/1	0.98	0.08	58,58,58,58	0
2	MN	G	1062	1/1	0.98	0.09	60,60,60,60	0
3	P3S	A	5001	15/15	0.98	0.16	41,51,59,62	0
3	P3S	D	5004	15/15	0.98	0.15	55,63,71,72	0
4	ADP	H	6010	27/27	0.98	0.12	38,44,47,48	0
2	MN	E	1042	1/1	0.98	0.11	70,70,70,70	0
4	ADP	J	6009	27/27	0.98	0.11	42,54,60,61	0
2	MN	A	1003	1/1	0.99	0.18	53,53,53,53	0

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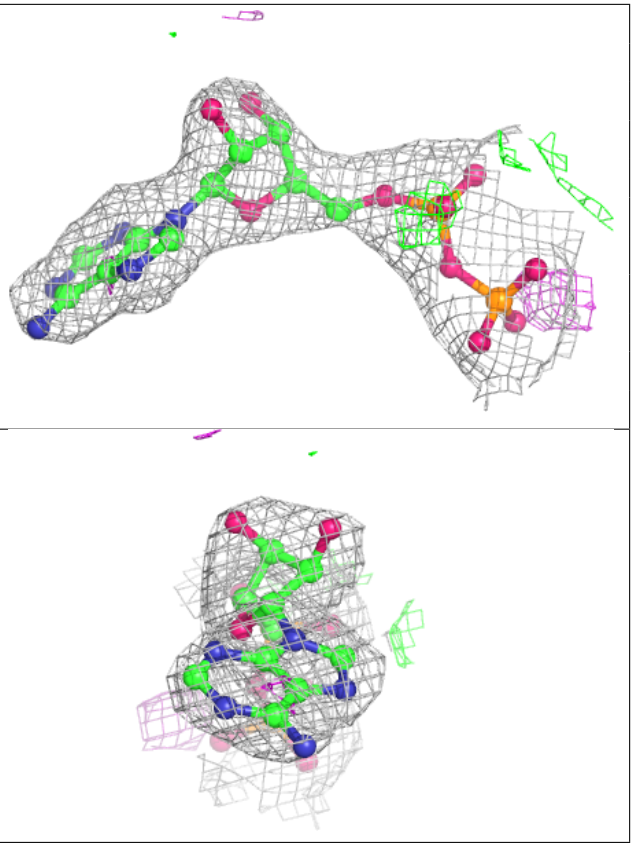
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P3S	G	5006	15/15	0.99	0.10	52,59,63,63	0
3	P3S	H	5010	15/15	0.99	0.11	33,40,52,53	0
2	MN	D	1032	1/1	0.99	0.10	63,63,63,63	0
3	P3S	J	5009	15/15	0.99	0.14	40,47,49,49	0
2	MN	I	1082	1/1	0.99	0.12	56,56,56,56	0
2	MN	A	1001	1/1	0.99	0.12	47,47,47,47	0
2	MN	A	1002	1/1	0.99	0.13	56,56,56,56	0
2	MN	J	1092	1/1	0.99	0.11	53,53,53,53	0
2	MN	J	1093	1/1	0.99	0.14	45,45,45,45	0
2	MN	C	1023	1/1	0.99	0.10	62,62,62,62	0
3	P3S	B	5002	15/15	0.99	0.13	32,41,45,51	0
3	P3S	C	5003	15/15	0.99	0.13	53,57,61,61	0
2	MN	E	1043	1/1	0.99	0.09	58,58,58,58	0
2	MN	H	1072	1/1	0.99	0.12	44,44,44,44	0
2	MN	B	1012	1/1	1.00	0.14	51,51,51,51	0
2	MN	C	1022	1/1	1.00	0.12	59,59,59,59	0
2	MN	G	1063	1/1	1.00	0.10	53,53,53,53	0
2	MN	B	1013	1/1	1.00	0.10	46,46,46,46	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.

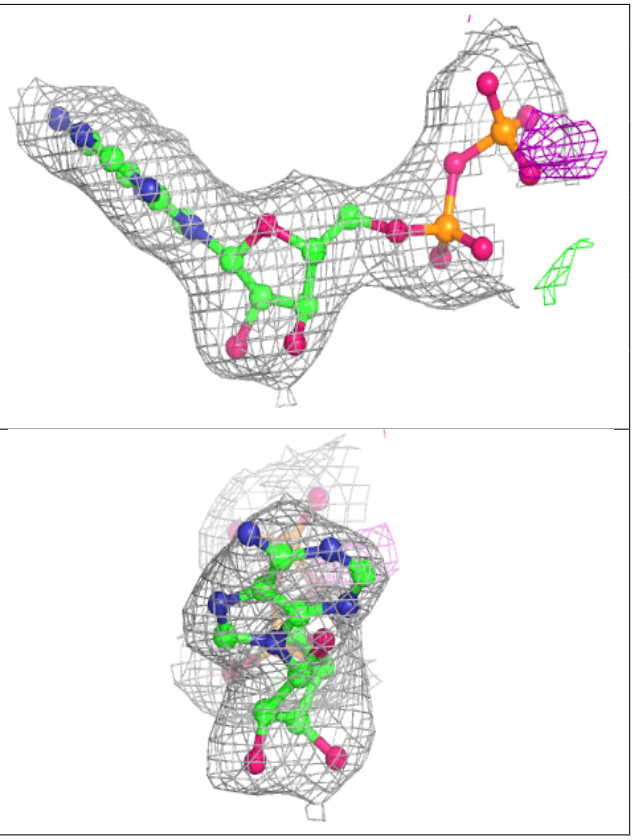
Electron density around ADP E 6004:

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



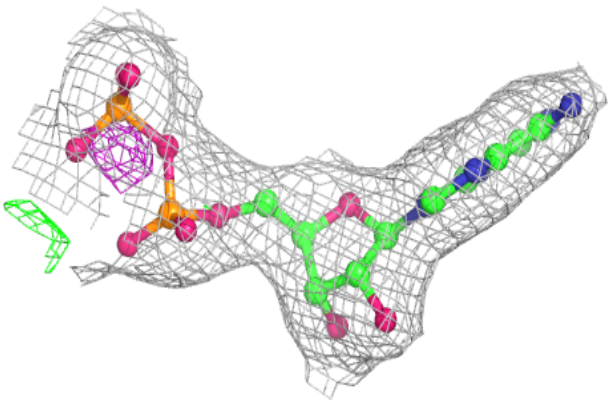
Electron density around ADP C 6003:

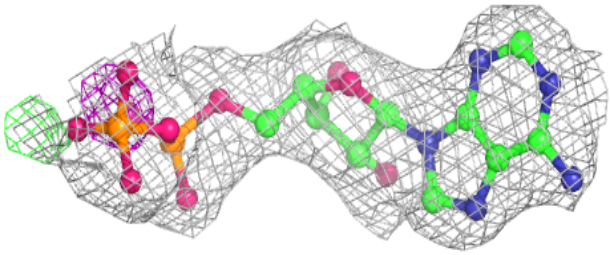
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

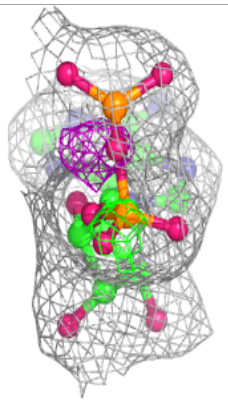


Electron density around ADP B 6002:

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

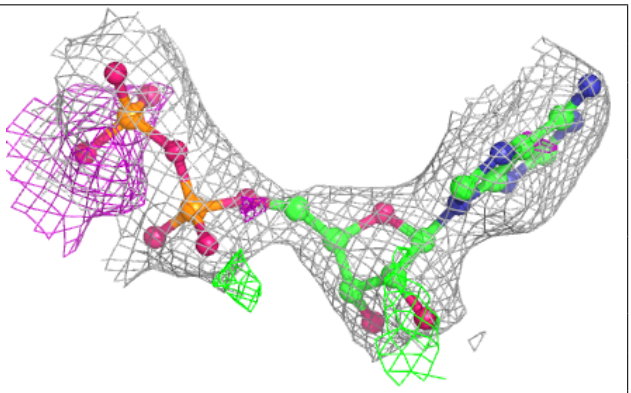


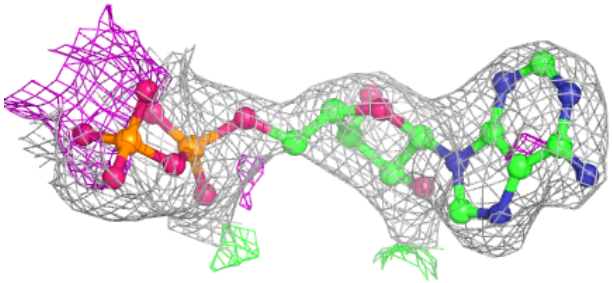


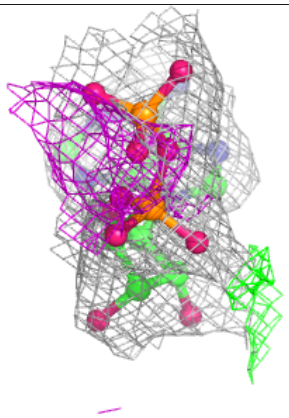


Electron density around ADP D 6005:

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

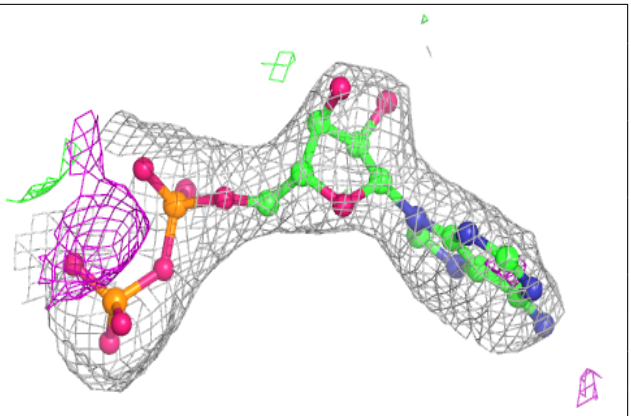


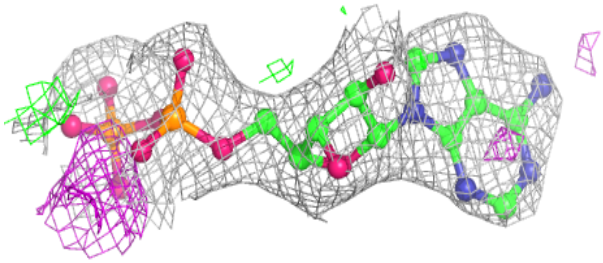


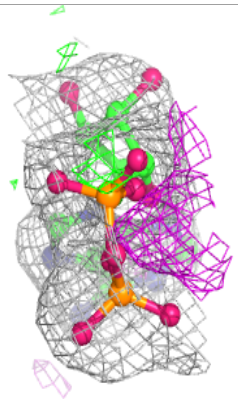


Electron density around ADP F 6007:

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

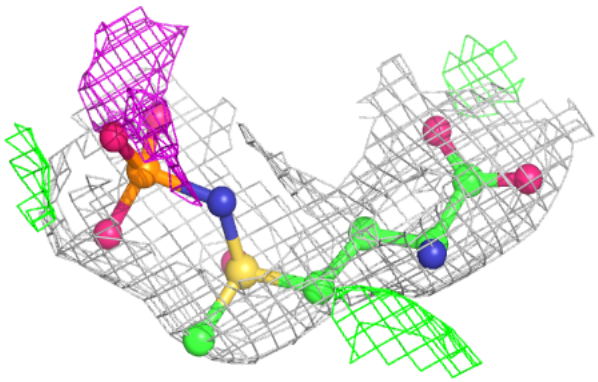


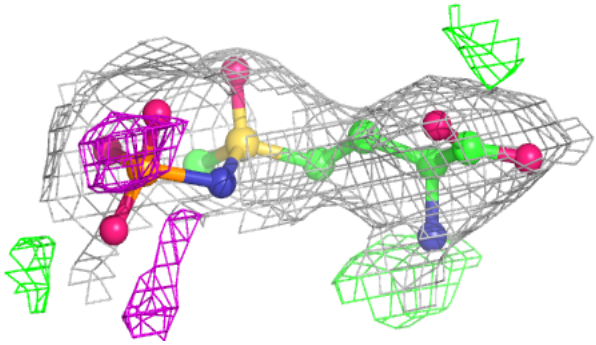


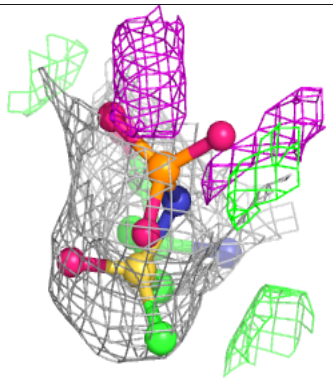


Electron density around P3S E 5005:

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

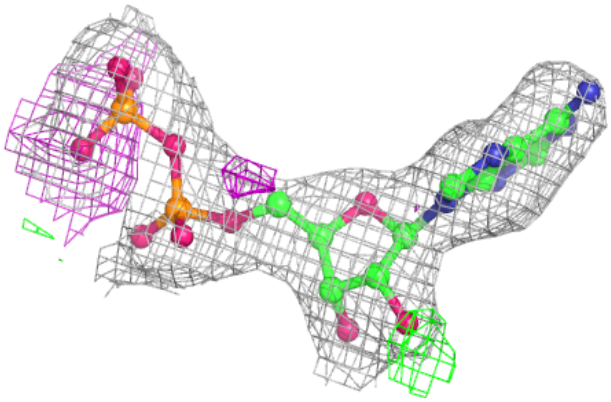


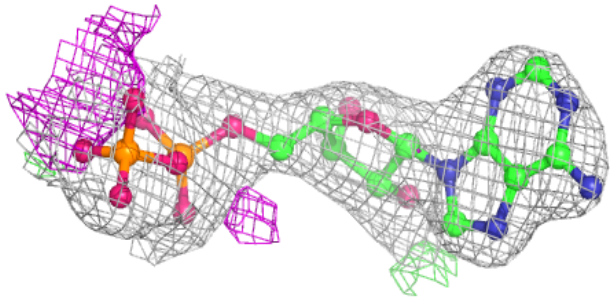


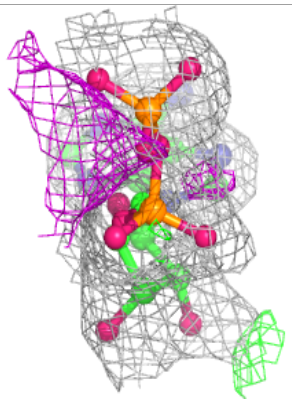


Electron density around ADP G 6006:

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

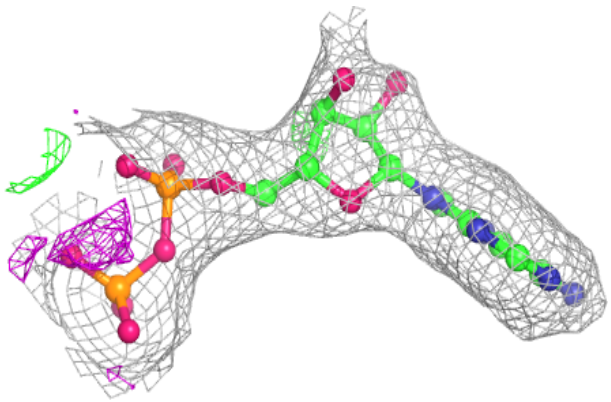


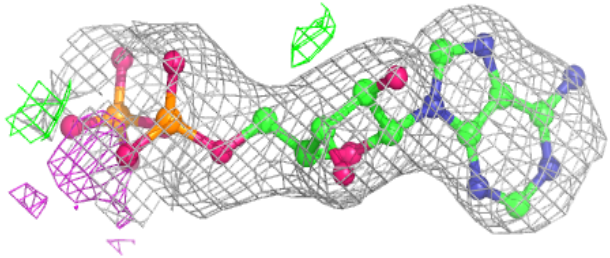


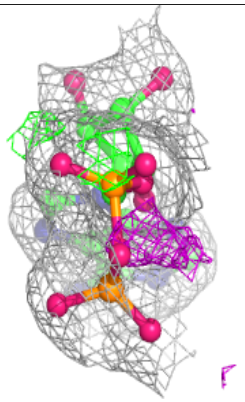


Electron density around ADP I 6008:

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

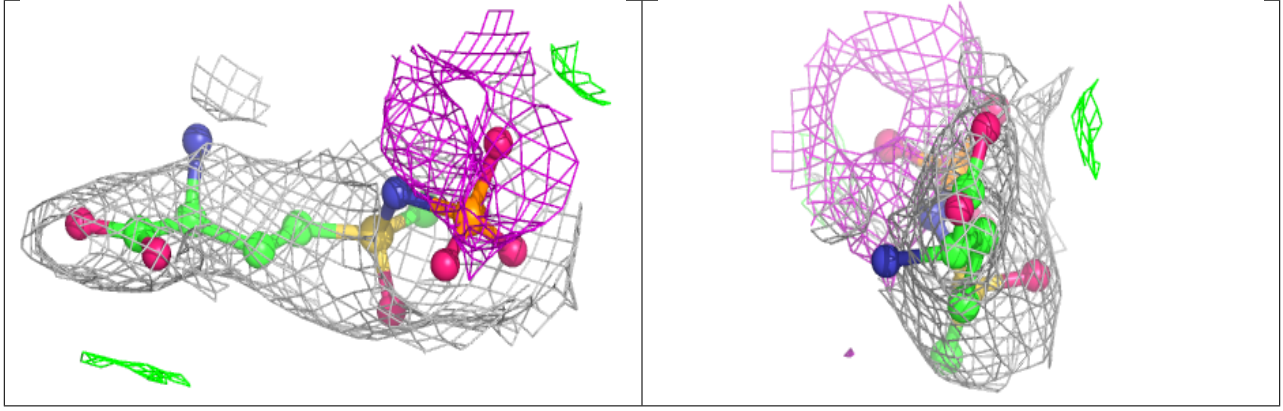






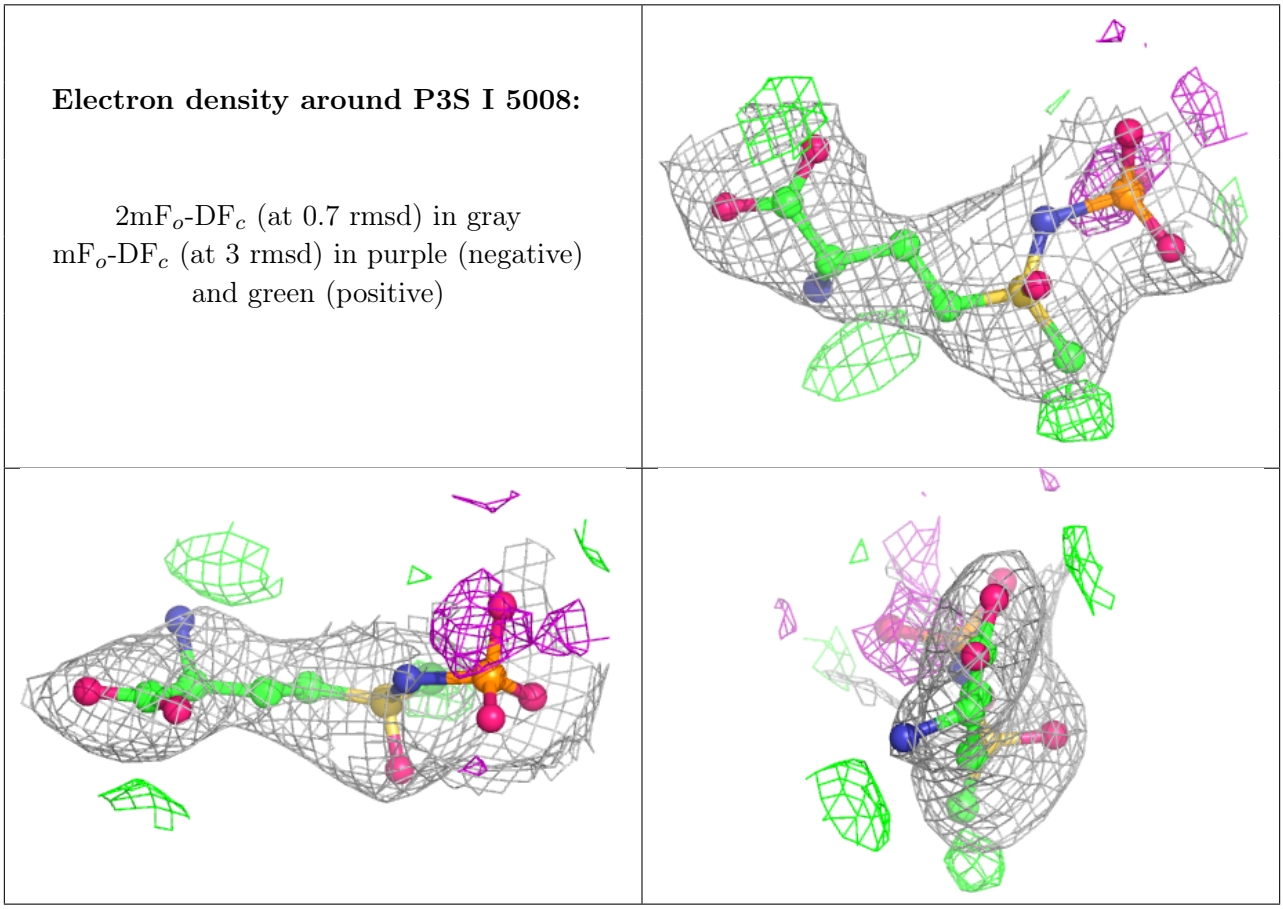
Electron density around P3S F 5007:

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



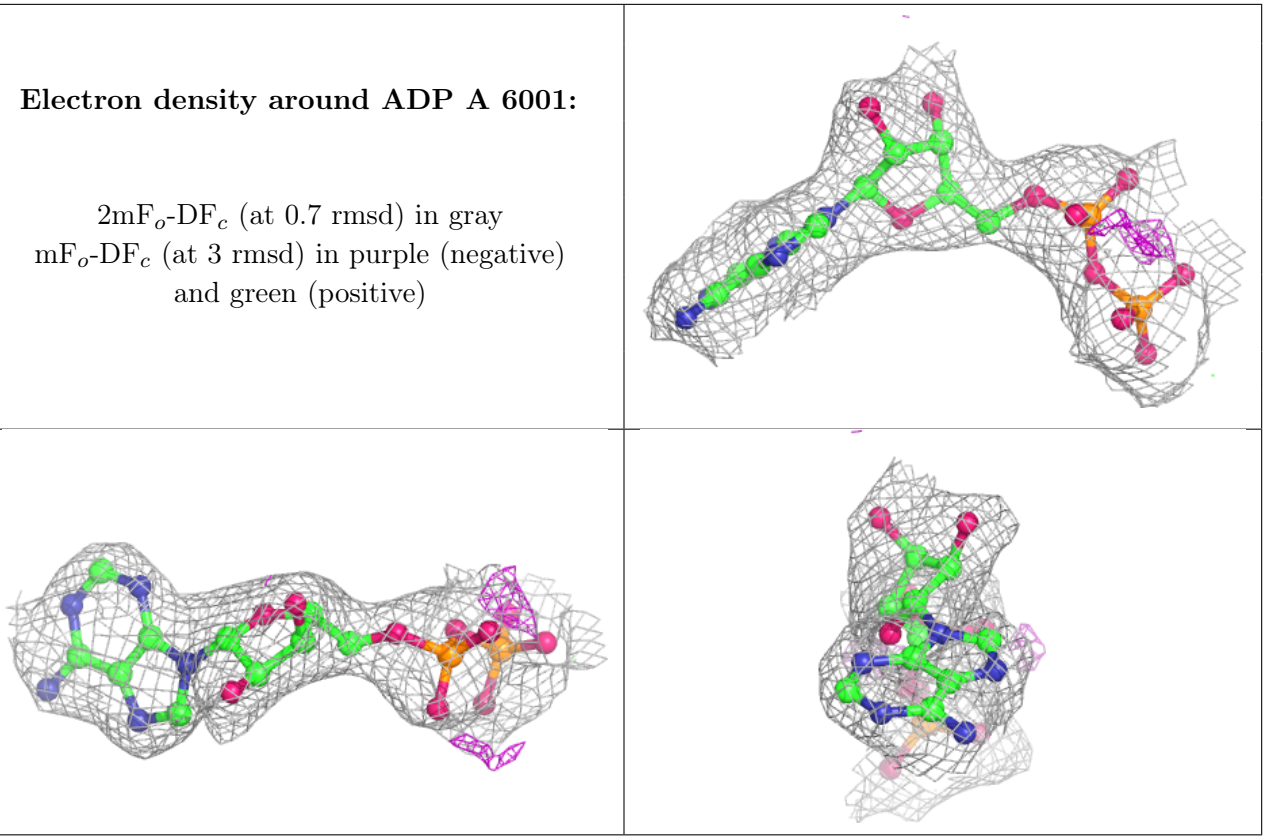
Electron density around P3S I 5008:

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



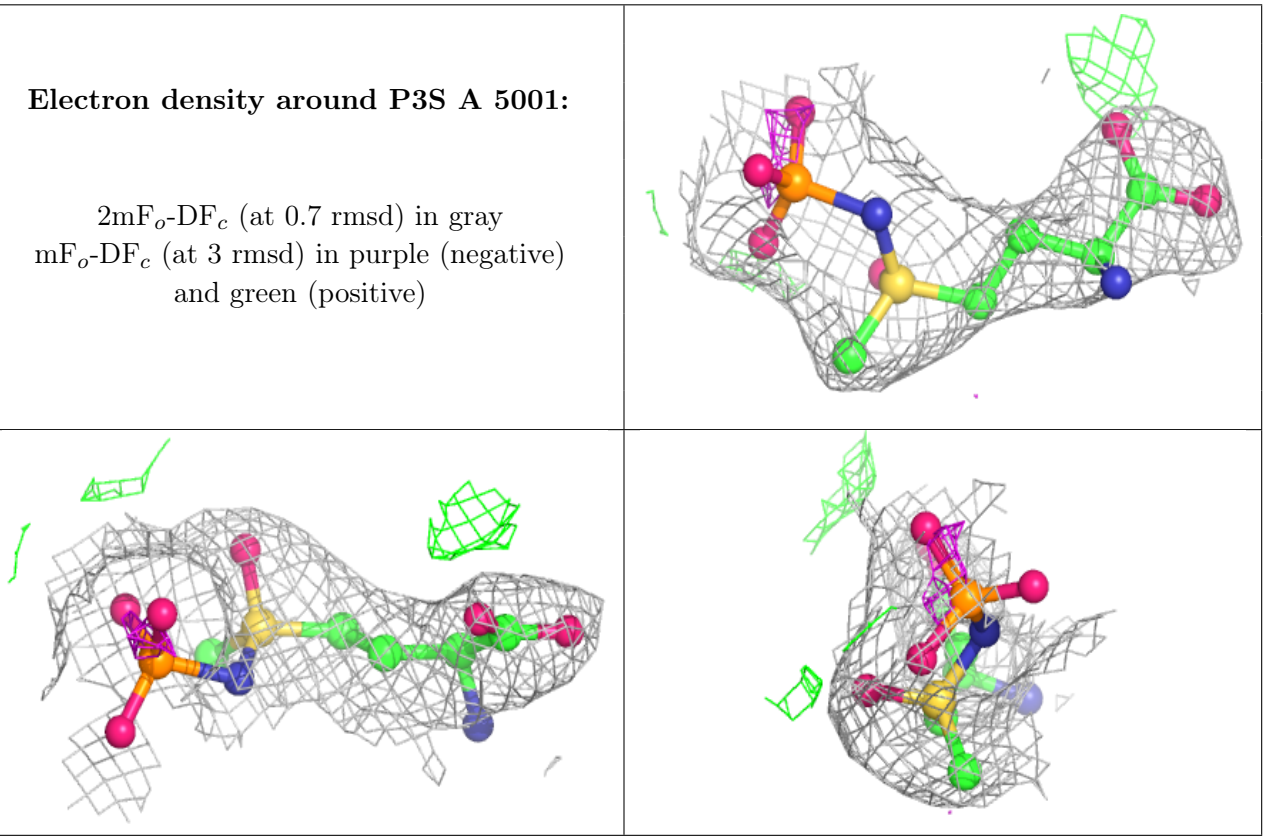
Electron density around ADP A 6001:

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



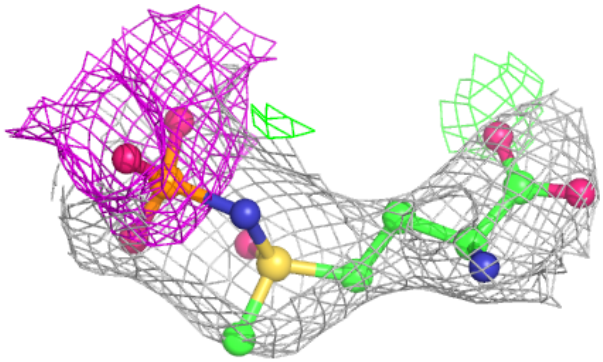
Electron density around P3S A 5001:

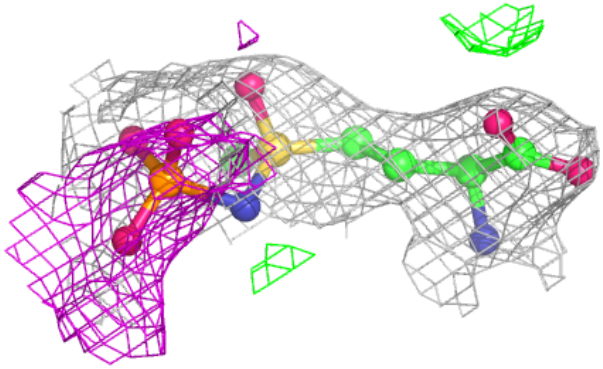
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

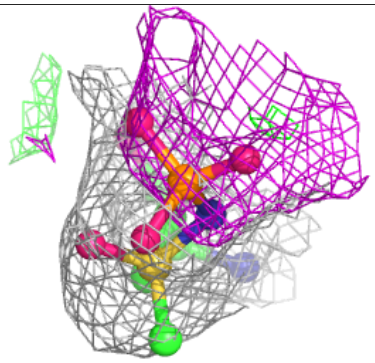


Electron density around P3S D 5004:

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

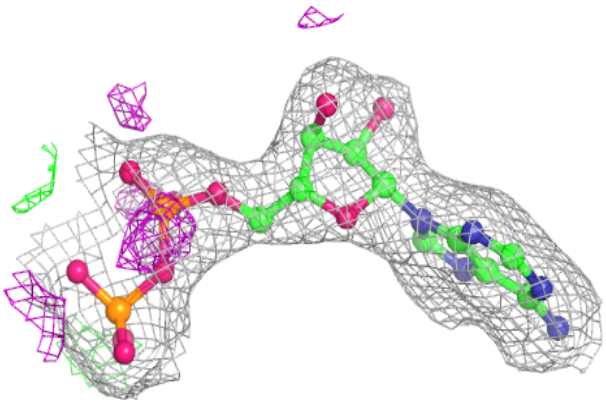


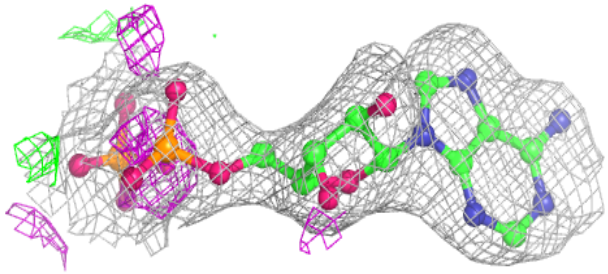


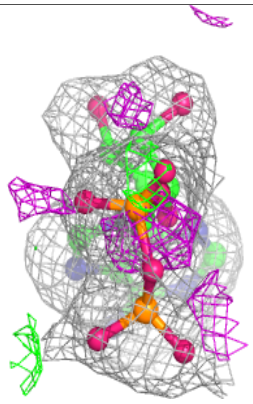


Electron density around ADP H 6010:

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

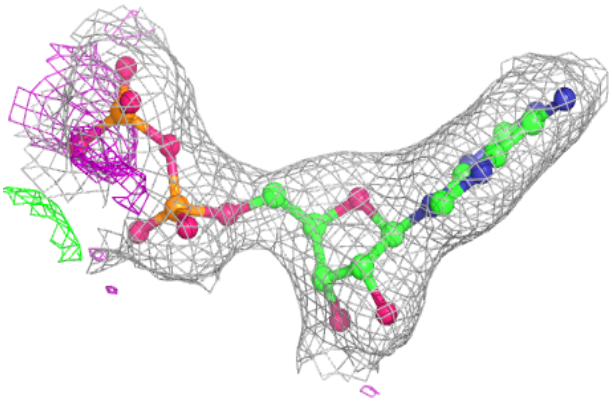


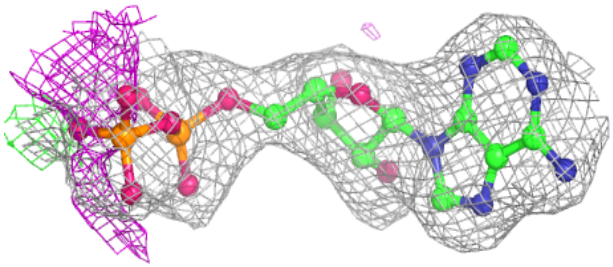


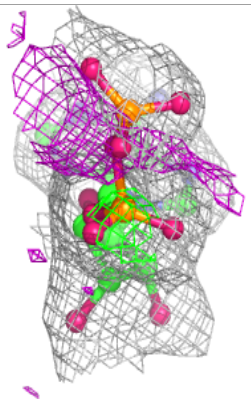


Electron density around ADP J 6009:

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

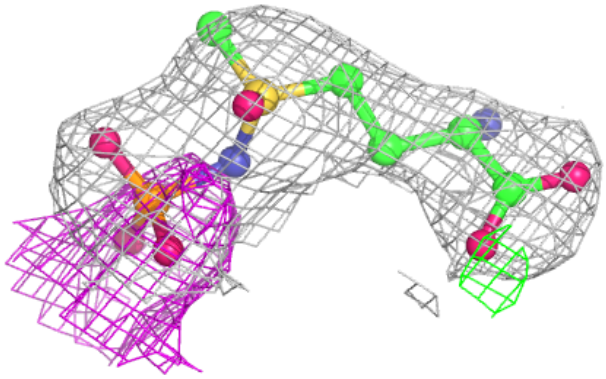


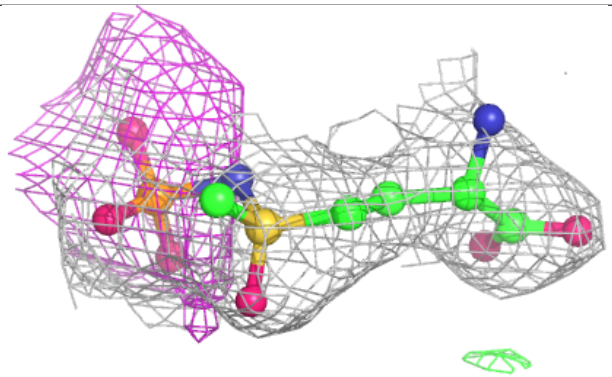


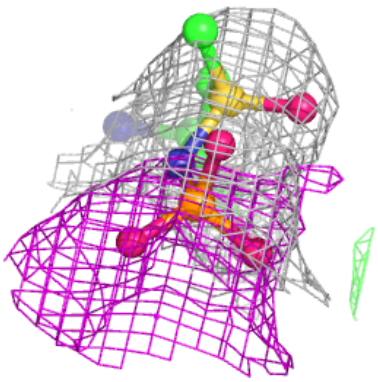


Electron density around P3S G 5006:

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

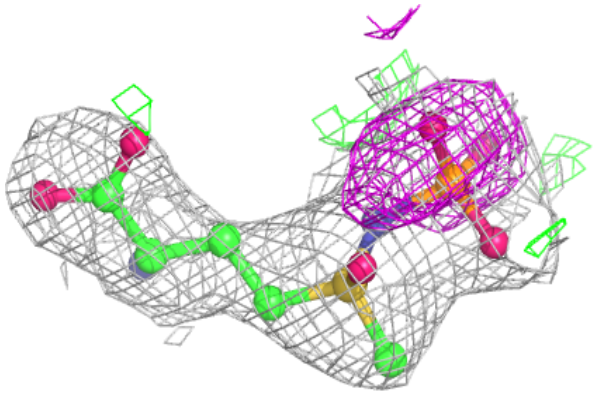


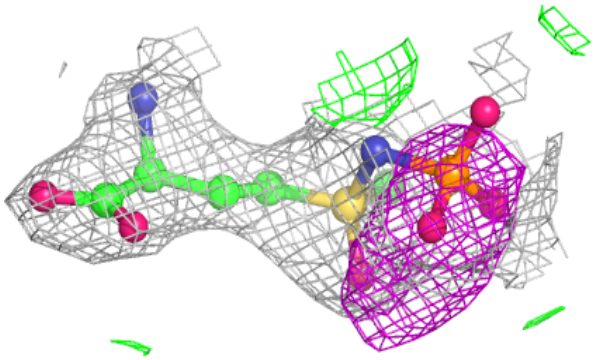


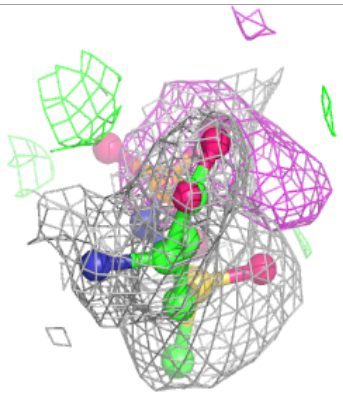


Electron density around P3S H 5010:

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

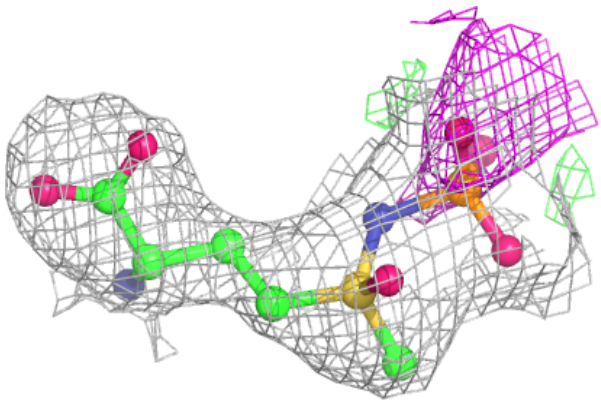


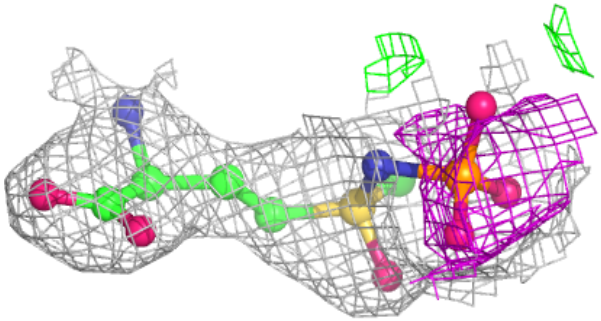


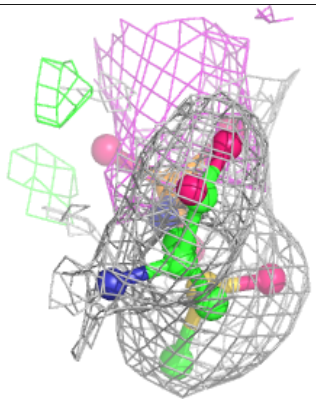


Electron density around P3S J 5009:

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

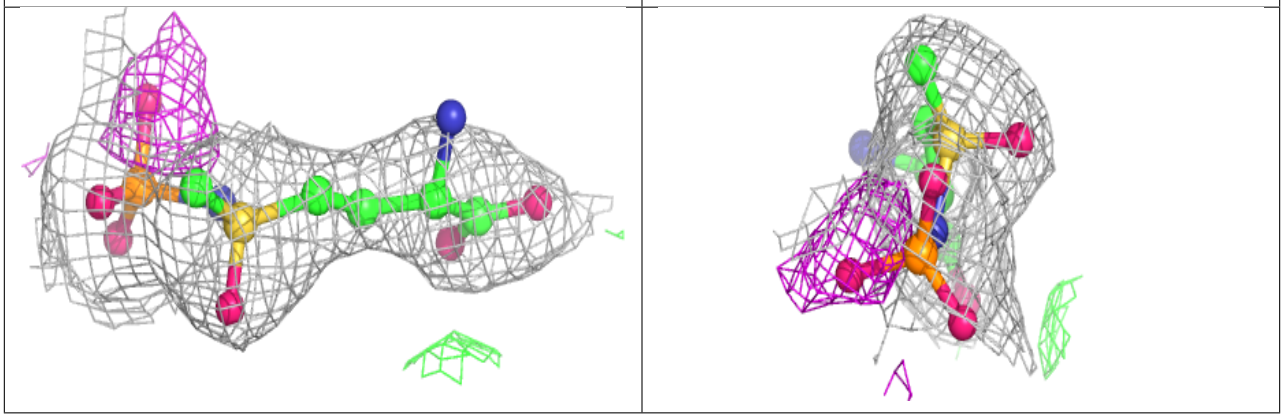






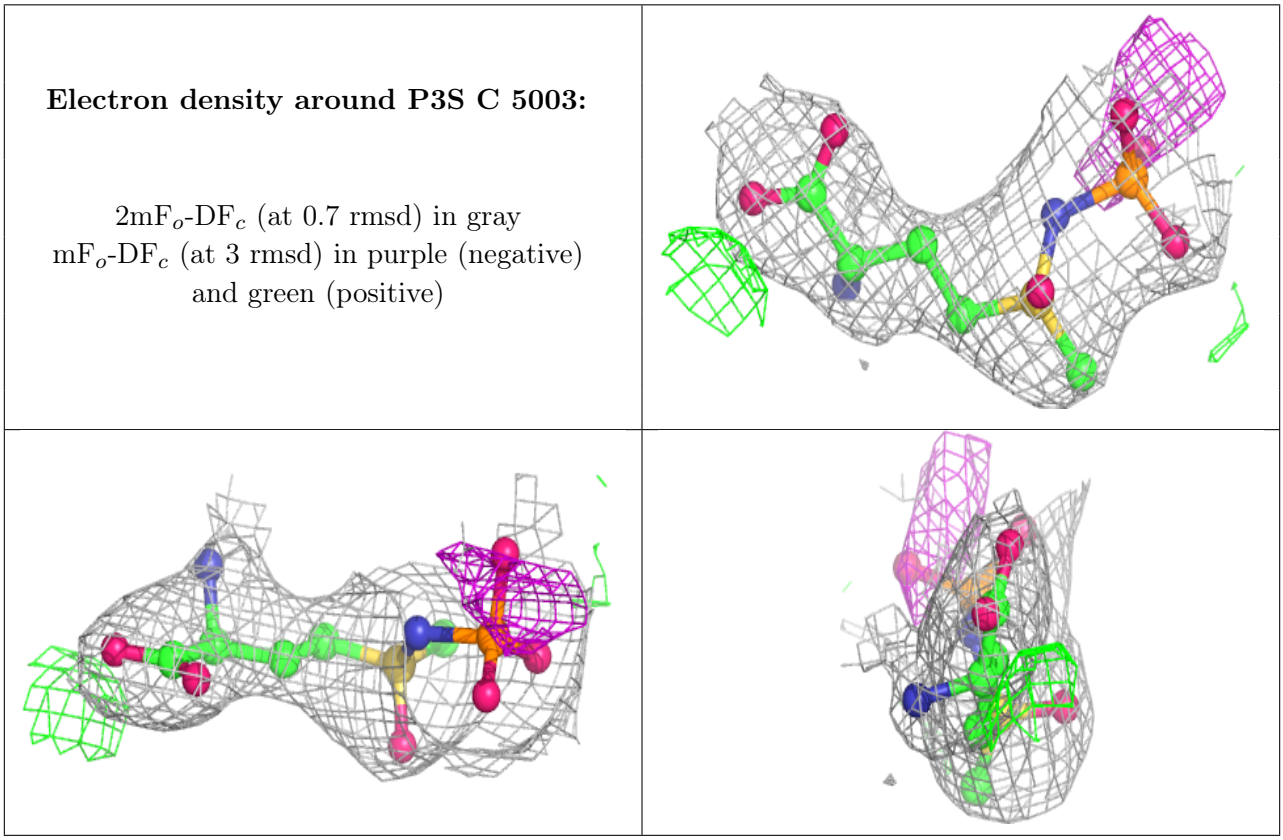
Electron density around P3S B 5002:

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



Electron density around P3S C 5003:

$2mF_o$-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.