Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 12:34 PM EDT

PDB ID	:	6UKO
Title	:	Structure analysis of full-length mouse bcs1 complex
Authors	:	Xia, D.; Esser, L.
Deposited on	:	2019-10-05
Resolution	:	4.40 Å(reported)

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

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

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

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

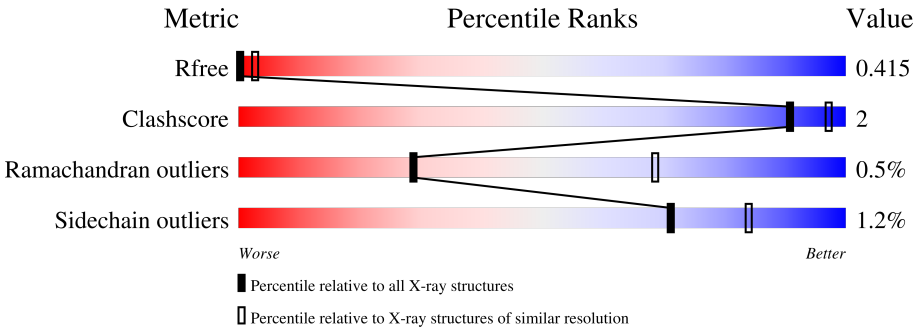
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	424	83% · 12%
1	B	424	83% 5% 12%
1	C	424	81% 6% 12%
1	D	424	82% 6% 12%
1	E	424	83% · · 12%
1	F	424	82% 6% 12%
1	G	424	82% 5% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41825 atoms, of which 20699 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 Mitochondrial chaperone BCS1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	B	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	C	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	D	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	E	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	F	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			
1	G	371	Total	C	H	N	O	S	0	0	0
			5935	1906	2945	528	544	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1419	HIS	-	expression tag	UNP Q9CZP5
A	1420	HIS	-	expression tag	UNP Q9CZP5
A	1421	HIS	-	expression tag	UNP Q9CZP5
A	1422	HIS	-	expression tag	UNP Q9CZP5
A	1423	HIS	-	expression tag	UNP Q9CZP5
A	1424	HIS	-	expression tag	UNP Q9CZP5
B	1419	HIS	-	expression tag	UNP Q9CZP5
B	1420	HIS	-	expression tag	UNP Q9CZP5
B	1421	HIS	-	expression tag	UNP Q9CZP5
B	1422	HIS	-	expression tag	UNP Q9CZP5
B	1423	HIS	-	expression tag	UNP Q9CZP5
B	1424	HIS	-	expression tag	UNP Q9CZP5
C	1419	HIS	-	expression tag	UNP Q9CZP5
C	1420	HIS	-	expression tag	UNP Q9CZP5
C	1421	HIS	-	expression tag	UNP Q9CZP5

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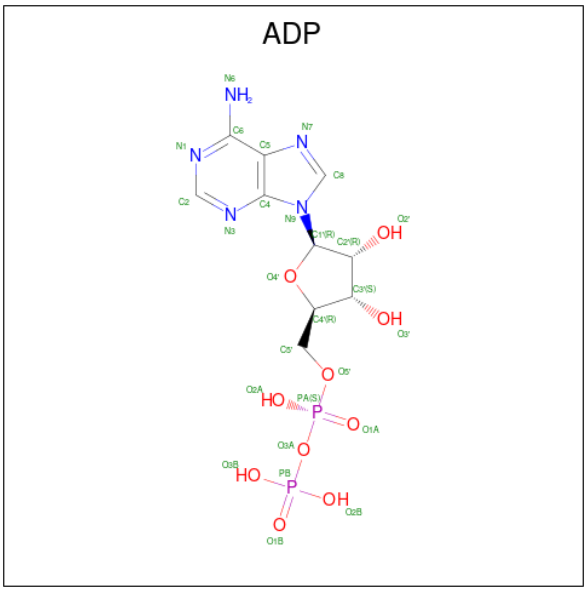
Chain	Residue	Modelled	Actual	Comment	Reference
C	1422	HIS	-	expression tag	UNP Q9CZP5
C	1423	HIS	-	expression tag	UNP Q9CZP5
C	1424	HIS	-	expression tag	UNP Q9CZP5
D	1419	HIS	-	expression tag	UNP Q9CZP5
D	1420	HIS	-	expression tag	UNP Q9CZP5
D	1421	HIS	-	expression tag	UNP Q9CZP5
D	1422	HIS	-	expression tag	UNP Q9CZP5
D	1423	HIS	-	expression tag	UNP Q9CZP5
D	1424	HIS	-	expression tag	UNP Q9CZP5
E	1419	HIS	-	expression tag	UNP Q9CZP5
E	1420	HIS	-	expression tag	UNP Q9CZP5
E	1421	HIS	-	expression tag	UNP Q9CZP5
E	1422	HIS	-	expression tag	UNP Q9CZP5
E	1423	HIS	-	expression tag	UNP Q9CZP5
E	1424	HIS	-	expression tag	UNP Q9CZP5
F	1419	HIS	-	expression tag	UNP Q9CZP5
F	1420	HIS	-	expression tag	UNP Q9CZP5
F	1421	HIS	-	expression tag	UNP Q9CZP5
F	1422	HIS	-	expression tag	UNP Q9CZP5
F	1423	HIS	-	expression tag	UNP Q9CZP5
F	1424	HIS	-	expression tag	UNP Q9CZP5
G	1419	HIS	-	expression tag	UNP Q9CZP5
G	1420	HIS	-	expression tag	UNP Q9CZP5
G	1421	HIS	-	expression tag	UNP Q9CZP5
G	1422	HIS	-	expression tag	UNP Q9CZP5
G	1423	HIS	-	expression tag	UNP Q9CZP5
G	1424	HIS	-	expression tag	UNP Q9CZP5

- Molecule 2 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
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	F	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	G	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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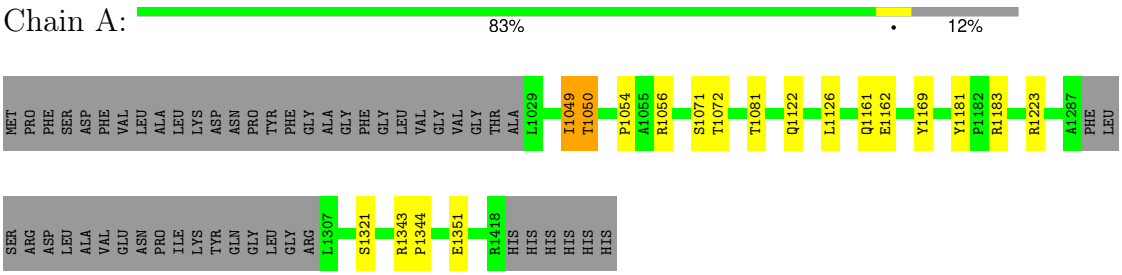
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

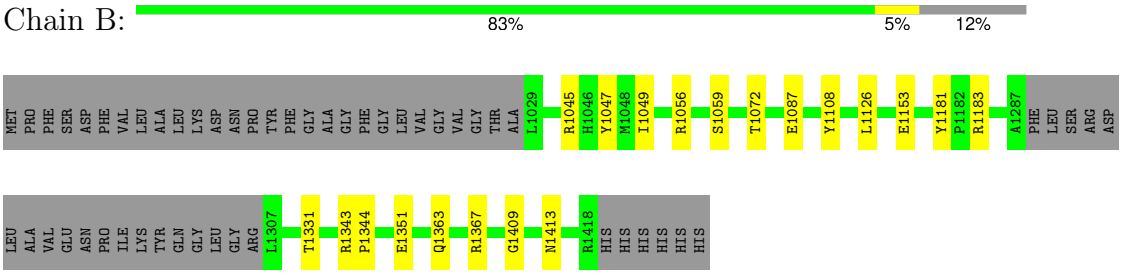
• Molecule 1: Mitochondrial chaperone BCS1

Chain A:



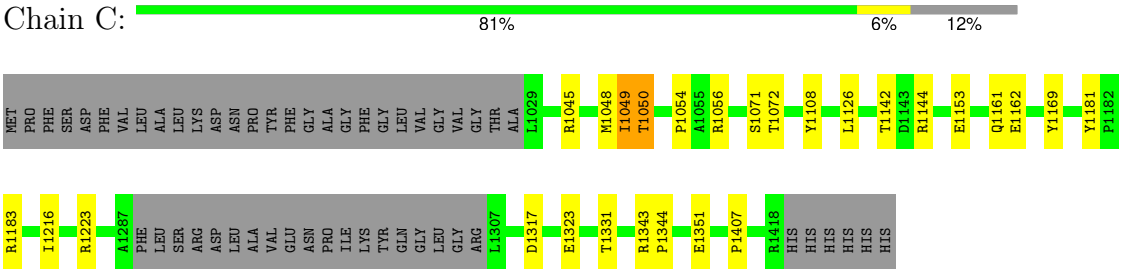
• Molecule 1: Mitochondrial chaperone BCS1

Chain B:



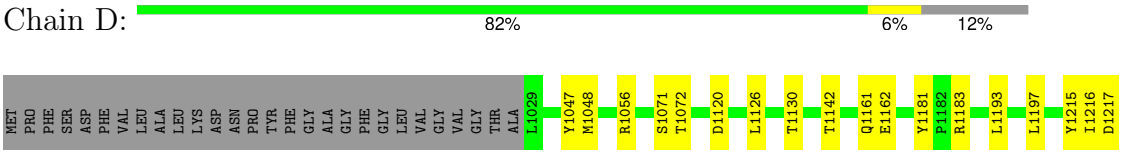
• Molecule 1: Mitochondrial chaperone BCS1

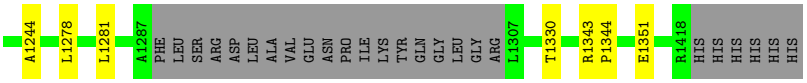
Chain C:



• Molecule 1: Mitochondrial chaperone BCS1

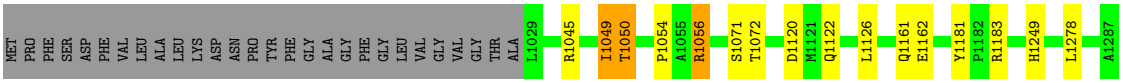
Chain D:





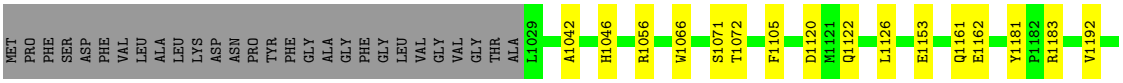
• Molecule 1: Mitochondrial chaperone BCS1

Chain E:



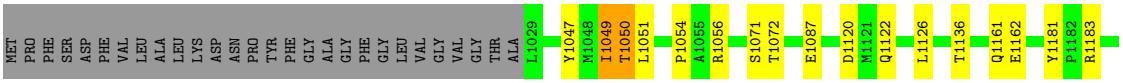
• Molecule 1: Mitochondrial chaperone BCS1

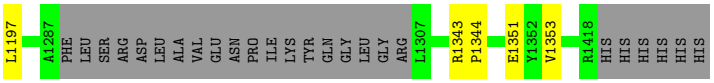
Chain F:



• Molecule 1: Mitochondrial chaperone BCS1

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	254.06Å 161.13Å 132.59Å 90.00° 107.27° 90.00°	Depositor
Resolution (Å)	24.91 – 4.40 49.78 – 4.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.91-4.40) 90.0 (49.78-4.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.357 , 0.407 0.374 , 0.415	Depositor DCC
R_{free} test set	1066 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å^2)	171.0	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	41825	wwPDB-VP
Average B, all atoms (Å^2)	284.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/3063	0.55	0/4154
1	B	0.25	0/3063	0.49	0/4154
1	C	0.27	0/3063	0.55	0/4154
1	D	0.26	0/3063	0.50	0/4154
1	E	0.26	0/3063	0.54	0/4154
1	F	0.25	0/3063	0.49	0/4154
1	G	0.26	0/3063	0.54	0/4154
All	All	0.26	0/21441	0.52	0/29078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2990	2945	2955	10	0
1	B	2990	2945	2955	9	1
1	C	2990	2945	2955	13	0
1	D	2990	2945	2955	11	0
1	E	2990	2945	2955	12	0
1	F	2990	2945	2955	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2990	2945	2955	13	1
2	A	27	12	12	0	0
2	B	27	12	12	0	0
2	C	27	12	12	0	0
2	D	27	12	12	0	0
2	E	27	12	12	0	0
2	F	27	12	12	0	0
2	G	27	12	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
All	All	21126	20699	20769	70	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 2.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1049:ILE:HG22	1:E:1050:THR:H	1.46	0.78
1:A:1049:ILE:HG22	1:A:1050:THR:H	1.49	0.78
1:C:1049:ILE:HG22	1:C:1050:THR:H	1.48	0.78
1:G:1049:ILE:HG22	1:G:1050:THR:H	1.48	0.78
1:A:1181:TYR:O	1:A:1183:ARG:NH1	2.30	0.64
1:F:1120:ASP:O	1:G:1122:GLN:NE2	2.34	0.61
1:C:1108:TYR:OH	1:C:1153:GLU:OE2	2.19	0.60
1:C:1181:TYR:O	1:C:1183:ARG:NH1	2.35	0.59
1:B:1363:GLN:OE1	1:B:1367:ARG:NH1	2.35	0.59
1:B:1072:THR:O	1:C:1144:ARG:NH2	2.36	0.58
1:A:1122:GLN:NE2	1:G:1120:ASP:O	2.37	0.58
1:B:1087:GLU:O	1:C:1169:TYR:OH	2.21	0.58
1:B:1409:GLY:O	1:B:1413:ASN:ND2	2.36	0.56
1:D:1215:TYR:O	1:D:1217:ASP:N	2.38	0.56
1:C:1343:ARG:NH1	1:C:1344:PRO:O	2.40	0.55
1:C:1071:SER:O	1:C:1072:THR:OG1	2.23	0.55
1:D:1181:TYR:O	1:D:1183:ARG:NH1	2.37	0.55
1:E:1045:ARG:HB3	1:E:1049:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1071:SER:O	1:F:1072:THR:OG1	2.23	0.54
1:G:1181:TYR:O	1:G:1183:ARG:NH1	2.41	0.54
1:F:1181:TYR:O	1:F:1183:ARG:NH1	2.42	0.53
1:A:1223:ARG:NH1	1:A:1321:SER:OG	2.43	0.52
1:E:1181:TYR:O	1:E:1183:ARG:NH1	2.42	0.51
1:C:1223:ARG:NH2	1:C:1317:ASP:OD1	2.45	0.50
1:E:1071:SER:O	1:E:1072:THR:OG1	2.24	0.50
1:D:1071:SER:O	1:D:1072:THR:OG1	2.24	0.50
1:F:1363:GLN:OE1	1:F:1367:ARG:NH1	2.43	0.50
1:F:1192:VAL:O	1:F:1360:GLN:NE2	2.44	0.50
1:B:1181:TYR:O	1:B:1183:ARG:NH1	2.44	0.49
1:A:1071:SER:O	1:A:1072:THR:OG1	2.24	0.49
1:B:1343:ARG:NH1	1:B:1344:PRO:O	2.46	0.49
1:F:1343:ARG:NH1	1:F:1344:PRO:O	2.46	0.48
1:E:1343:ARG:NH1	1:E:1344:PRO:O	2.46	0.48
1:D:1048:MET:HA	1:D:1142:THR:HG22	1.95	0.48
1:C:1049:ILE:HG22	1:C:1050:THR:N	2.25	0.46
1:D:1343:ARG:NH1	1:D:1344:PRO:O	2.48	0.46
1:F:1042:ALA:O	1:F:1046:HIS:N	2.46	0.46
1:F:1256:LEU:HD12	1:F:1284:VAL:HG22	1.97	0.46
1:G:1049:ILE:HG22	1:G:1050:THR:N	2.25	0.46
1:F:1161:GLN:OE1	1:F:1162:GLU:N	2.50	0.45
1:G:1161:GLN:OE1	1:G:1162:GLU:N	2.49	0.45
1:G:1071:SER:O	1:G:1072:THR:OG1	2.28	0.45
1:A:1161:GLN:OE1	1:A:1162:GLU:N	2.50	0.45
1:D:1161:GLN:OE1	1:D:1162:GLU:N	2.49	0.45
1:E:1161:GLN:OE1	1:E:1162:GLU:N	2.49	0.45
1:C:1161:GLN:OE1	1:C:1162:GLU:N	2.50	0.44
1:D:1244:ALA:HB2	1:D:1278:LEU:HD12	1.98	0.44
1:B:1045:ARG:HB3	1:B:1049:ILE:HD12	2.00	0.44
1:D:1281:LEU:O	1:D:1330:THR:OG1	2.32	0.44
1:A:1169:TYR:OH	1:G:1087:GLU:O	2.27	0.44
1:G:1197:LEU:HD21	1:G:1353:VAL:HG22	1.99	0.44
1:D:1130:THR:HG22	1:E:1056:ARG:HH12	1.82	0.44
1:A:1081:THR:HG21	1:B:1059:SER:HB3	2.00	0.44
1:E:1249:HIS:HD2	1:E:1278:LEU:HD21	1.83	0.43
1:A:1049:ILE:HG22	1:A:1050:THR:N	2.25	0.43
1:E:1278:LEU:HD22	1:E:1326:ILE:HB	2.01	0.43
1:C:1045:ARG:HB3	1:C:1049:ILE:HD12	2.01	0.43
1:G:1049:ILE:O	1:G:1050:THR:HG23	2.19	0.43
1:A:1343:ARG:NH1	1:A:1344:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1120:ASP:O	1:F:1122:GLN:NE2	2.51	0.43
1:C:1216:ILE:HD11	1:C:1323:GLU:OE1	2.18	0.42
1:D:1193:LEU:HB3	1:D:1197:LEU:HD23	2.01	0.42
1:C:1048:MET:HA	1:C:1142:THR:HG22	2.02	0.41
1:B:1108:TYR:OH	1:B:1153:GLU:OE2	2.35	0.41
1:D:1120:ASP:O	1:E:1122:GLN:NE2	2.54	0.41
1:F:1105:PHE:O	1:G:1047:TYR:OH	2.39	0.41
1:G:1343:ARG:NH1	1:G:1344:PRO:O	2.54	0.41
1:F:1066:TRP:NE1	1:F:1153:GLU:OE1	2.51	0.41
1:G:1051:LEU:HD11	1:G:1136:THR:OG1	2.22	0.40
1:E:1049:ILE:O	1:E:1050:THR:HG23	2.21	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:1413:ASN:OD1	1:G:1072:THR:OG1[4_445]	2.14	0.06

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	367/424 (87%)	348 (95%)	16 (4%)	3 (1%)	19 60
1	B	367/424 (87%)	348 (95%)	19 (5%)	0	100 100
1	C	367/424 (87%)	347 (95%)	16 (4%)	4 (1%)	14 52
1	D	367/424 (87%)	348 (95%)	18 (5%)	1 (0%)	41 76
1	E	367/424 (87%)	345 (94%)	19 (5%)	3 (1%)	19 60
1	F	367/424 (87%)	349 (95%)	18 (5%)	0	100 100
1	G	367/424 (87%)	344 (94%)	20 (5%)	3 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2569/2968 (87%)	2429 (95%)	126 (5%)	14 (0%)	29 68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1216	ILE
1	E	1050	THR
1	G	1050	THR
1	A	1050	THR
1	C	1050	THR
1	A	1049	ILE
1	A	1054	PRO
1	C	1049	ILE
1	C	1054	PRO
1	E	1049	ILE
1	G	1049	ILE
1	C	1407	PRO
1	E	1054	PRO
1	G	1054	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	320/362 (88%)	317 (99%)	3 (1%)	78 88
1	B	320/362 (88%)	315 (98%)	5 (2%)	62 79
1	C	320/362 (88%)	316 (99%)	4 (1%)	69 82
1	D	320/362 (88%)	316 (99%)	4 (1%)	69 82
1	E	320/362 (88%)	316 (99%)	4 (1%)	69 82
1	F	320/362 (88%)	317 (99%)	3 (1%)	78 88
1	G	320/362 (88%)	317 (99%)	3 (1%)	78 88
All	All	2240/2534 (88%)	2214 (99%)	26 (1%)	71 84

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

Mol	Chain	Res	Type
1	A	1056	ARG
1	A	1126	LEU
1	A	1351	GLU
1	B	1047	TYR
1	B	1056	ARG
1	B	1126	LEU
1	B	1331	THR
1	B	1351	GLU
1	C	1056	ARG
1	C	1126	LEU
1	C	1331	THR
1	C	1351	GLU
1	D	1047	TYR
1	D	1056	ARG
1	D	1126	LEU
1	D	1351	GLU
1	E	1056	ARG
1	E	1126	LEU
1	E	1331	THR
1	E	1351	GLU
1	F	1056	ARG
1	F	1126	LEU
1	F	1351	GLU
1	G	1056	ARG
1	G	1126	LEU
1	G	1351	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1397	GLN
1	C	1397	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	ADP	D	1800	3	24,29,29	0.98	3 (12%)	29,45,45	1.23	3 (10%)
2	ADP	G	1800	3	24,29,29	0.97	2 (8%)	29,45,45	1.27	3 (10%)
2	ADP	E	1800	3	24,29,29	1.05	3 (12%)	29,45,45	1.28	2 (6%)
2	ADP	F	1800	3	24,29,29	1.00	3 (12%)	29,45,45	1.22	2 (6%)
2	ADP	B	1800	3	24,29,29	1.02	3 (12%)	29,45,45	1.31	2 (6%)
2	ADP	A	1800	3	24,29,29	0.94	1 (4%)	29,45,45	1.26	4 (13%)
2	ADP	C	1800	3	24,29,29	1.01	2 (8%)	29,45,45	1.27	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	1800	3	-	4/12/32/32	0/3/3/3
2	ADP	G	1800	3	-	5/12/32/32	0/3/3/3
2	ADP	E	1800	3	-	5/12/32/32	0/3/3/3
2	ADP	F	1800	3	-	5/12/32/32	0/3/3/3
2	ADP	B	1800	3	-	5/12/32/32	0/3/3/3
2	ADP	A	1800	3	-	5/12/32/32	0/3/3/3
2	ADP	C	1800	3	-	5/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1800	ADP	PA-O3A	2.35	1.62	1.59
2	C	1800	ADP	O4'-C1'	2.29	1.43	1.40
2	C	1800	ADP	C2-N3	2.29	1.35	1.32
2	G	1800	ADP	C2-N3	2.28	1.35	1.32
2	E	1800	ADP	C2-N3	2.25	1.35	1.32
2	B	1800	ADP	C2-N3	2.24	1.35	1.32
2	E	1800	ADP	O4'-C1'	2.21	1.43	1.40
2	B	1800	ADP	O4'-C1'	2.19	1.43	1.40
2	A	1800	ADP	C2-N3	2.19	1.35	1.32
2	D	1800	ADP	PA-O3A	2.18	1.61	1.59
2	F	1800	ADP	C2-N3	2.18	1.35	1.32
2	D	1800	ADP	C2-N3	2.16	1.35	1.32
2	B	1800	ADP	PA-O3A	2.15	1.61	1.59
2	F	1800	ADP	PA-O3A	2.13	1.61	1.59
2	F	1800	ADP	O4'-C1'	2.06	1.43	1.40
2	D	1800	ADP	O4'-C1'	2.04	1.43	1.40
2	G	1800	ADP	O4'-C1'	2.00	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1800	ADP	N3-C2-N1	-3.83	123.47	128.67
2	D	1800	ADP	N3-C2-N1	-3.79	123.53	128.67
2	G	1800	ADP	N3-C2-N1	-3.72	123.62	128.67
2	E	1800	ADP	N3-C2-N1	-3.71	123.64	128.67
2	A	1800	ADP	N3-C2-N1	-3.66	123.70	128.67
2	B	1800	ADP	N3-C2-N1	-3.60	123.79	128.67
2	C	1800	ADP	N3-C2-N1	-3.56	123.85	128.67
2	B	1800	ADP	C4-C5-N7	-2.77	106.41	109.34
2	E	1800	ADP	C4-C5-N7	-2.63	106.55	109.34
2	C	1800	ADP	C4-C5-N7	-2.61	106.58	109.34
2	A	1800	ADP	C4-C5-N7	-2.46	106.73	109.34
2	F	1800	ADP	C4-C5-N7	-2.42	106.78	109.34
2	G	1800	ADP	C4-C5-N7	-2.23	106.98	109.34
2	D	1800	ADP	C4-C5-N7	-2.19	107.02	109.34
2	A	1800	ADP	O3B-PB-O2B	2.19	116.01	107.80
2	G	1800	ADP	N6-C6-N1	2.18	122.99	118.33
2	D	1800	ADP	N6-C6-N1	2.14	122.91	118.33
2	A	1800	ADP	N6-C6-N1	2.08	122.78	118.33

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1800	ADP	C5'-O5'-PA-O3A
2	B	1800	ADP	C5'-O5'-PA-O3A
2	C	1800	ADP	C5'-O5'-PA-O3A
2	D	1800	ADP	C5'-O5'-PA-O3A
2	E	1800	ADP	C5'-O5'-PA-O3A
2	F	1800	ADP	C5'-O5'-PA-O3A
2	G	1800	ADP	C5'-O5'-PA-O3A
2	A	1800	ADP	O4'-C4'-C5'-O5'
2	B	1800	ADP	O4'-C4'-C5'-O5'
2	C	1800	ADP	O4'-C4'-C5'-O5'
2	D	1800	ADP	O4'-C4'-C5'-O5'
2	E	1800	ADP	O4'-C4'-C5'-O5'
2	F	1800	ADP	O4'-C4'-C5'-O5'
2	G	1800	ADP	O4'-C4'-C5'-O5'
2	B	1800	ADP	C3'-C4'-C5'-O5'
2	C	1800	ADP	C3'-C4'-C5'-O5'
2	E	1800	ADP	C3'-C4'-C5'-O5'
2	A	1800	ADP	C3'-C4'-C5'-O5'
2	D	1800	ADP	C3'-C4'-C5'-O5'
2	F	1800	ADP	C3'-C4'-C5'-O5'
2	G	1800	ADP	C3'-C4'-C5'-O5'
2	E	1800	ADP	PA-O3A-PB-O1B
2	F	1800	ADP	PA-O3A-PB-O1B
2	C	1800	ADP	PA-O3A-PB-O2B
2	A	1800	ADP	C5'-O5'-PA-O1A
2	B	1800	ADP	C5'-O5'-PA-O1A
2	C	1800	ADP	C5'-O5'-PA-O1A
2	D	1800	ADP	C5'-O5'-PA-O1A
2	E	1800	ADP	C5'-O5'-PA-O1A
2	F	1800	ADP	C5'-O5'-PA-O1A
2	G	1800	ADP	C5'-O5'-PA-O1A
2	A	1800	ADP	PA-O3A-PB-O2B
2	B	1800	ADP	PA-O3A-PB-O2B
2	G	1800	ADP	PA-O3A-PB-O2B

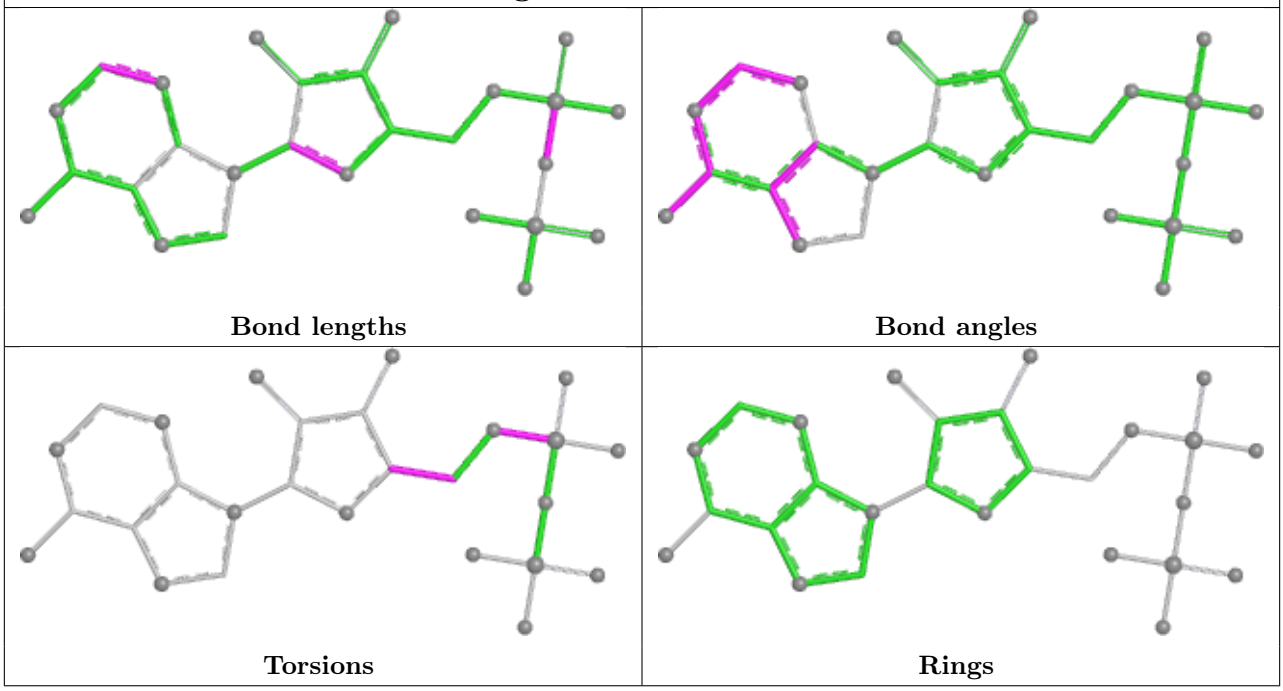
There are no ring outliers.

No monomer is involved in short contacts.

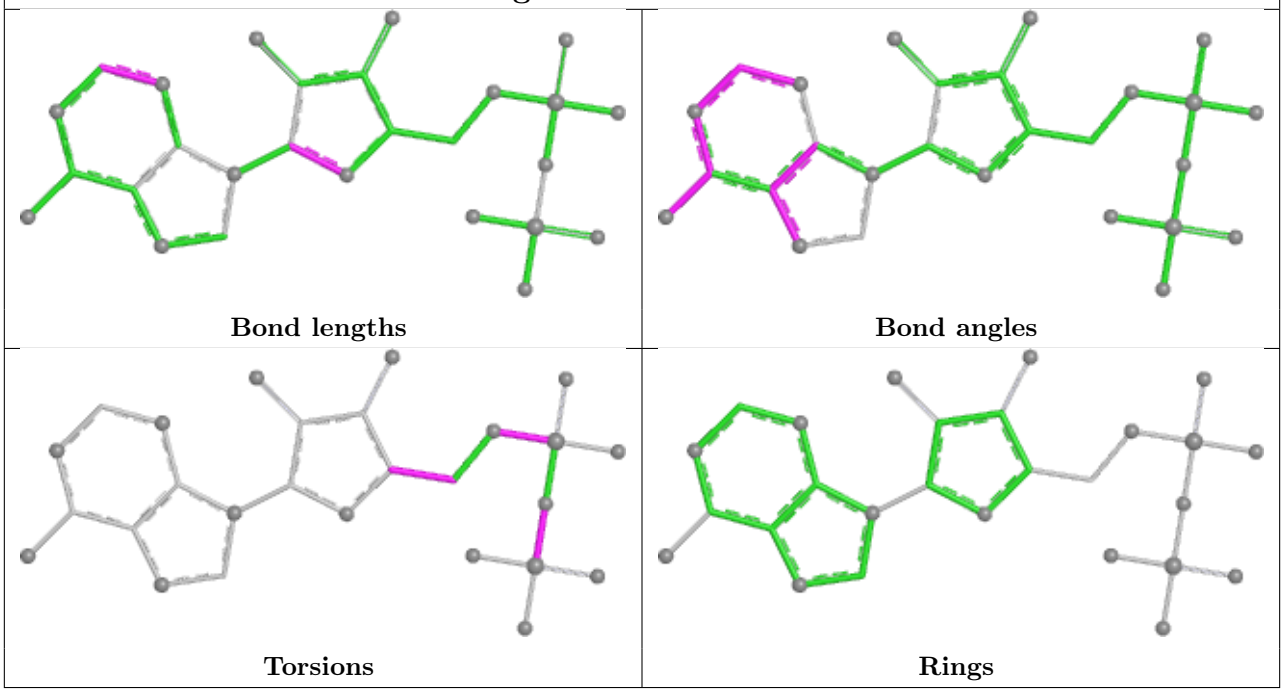
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

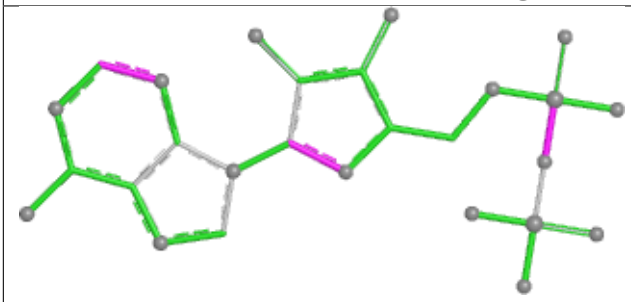
Ligand ADP D 1800



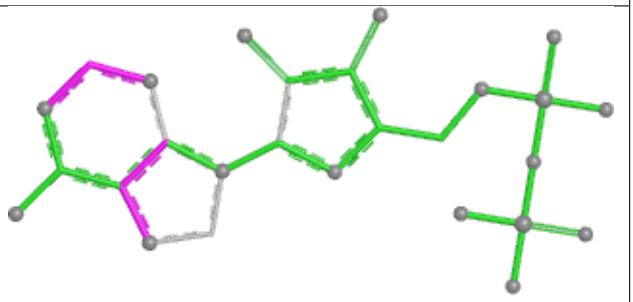
Ligand ADP G 1800



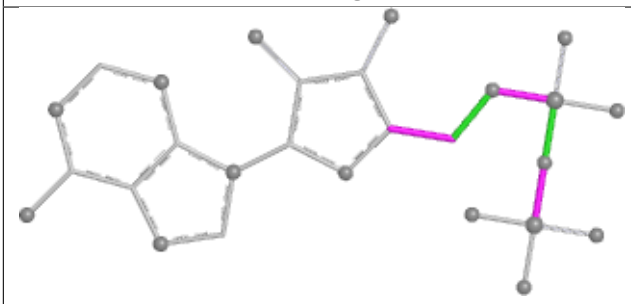
Ligand ADP E 1800



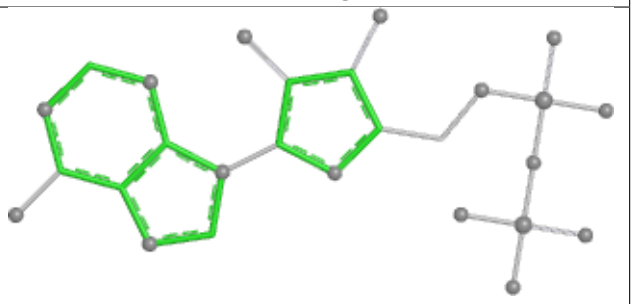
Bond lengths



Bond angles

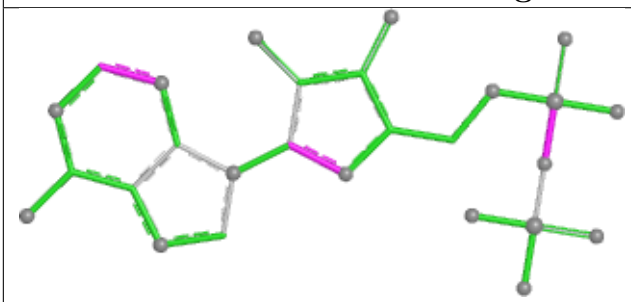


Torsions

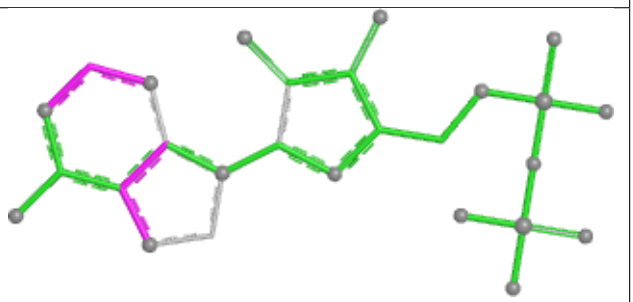


Rings

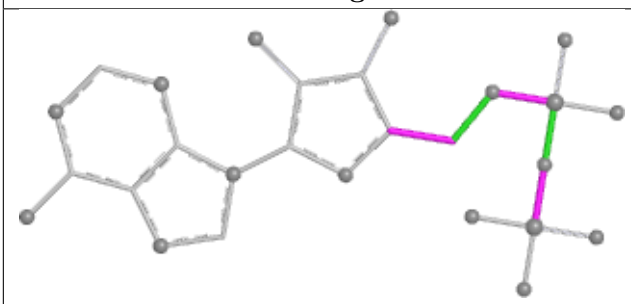
Ligand ADP F 1800



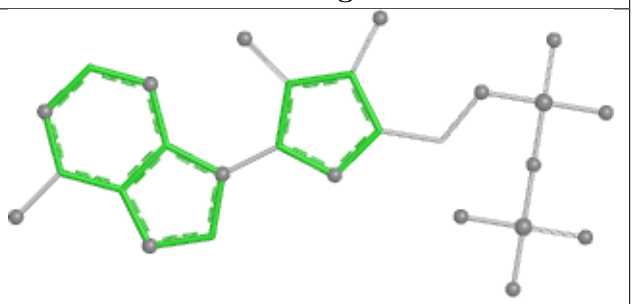
Bond lengths



Bond angles

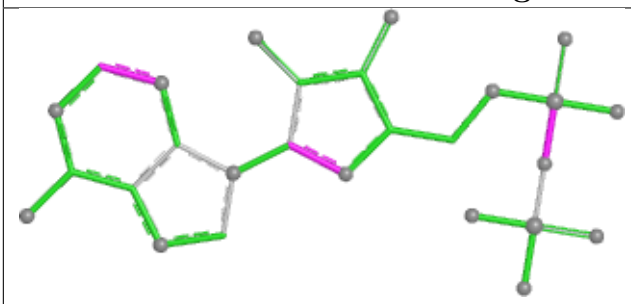


Torsions

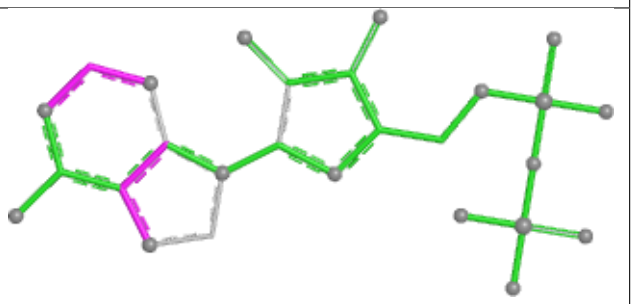


Rings

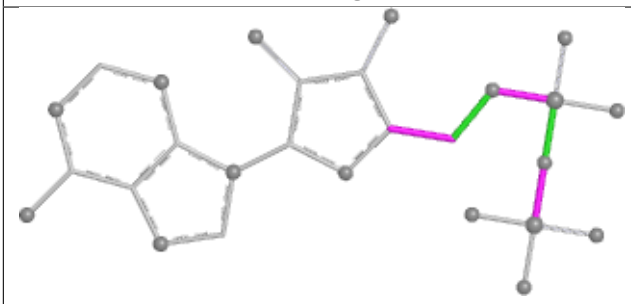
Ligand ADP B 1800



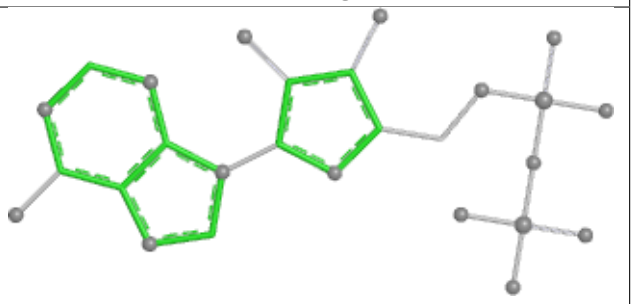
Bond lengths



Bond angles

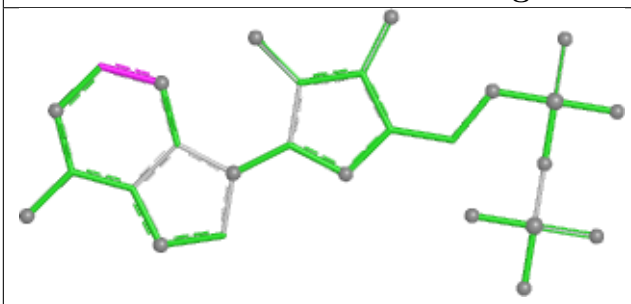


Torsions

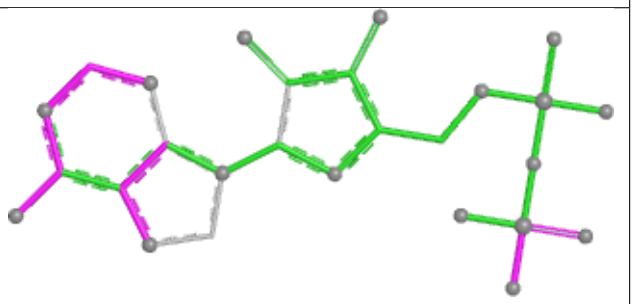


Rings

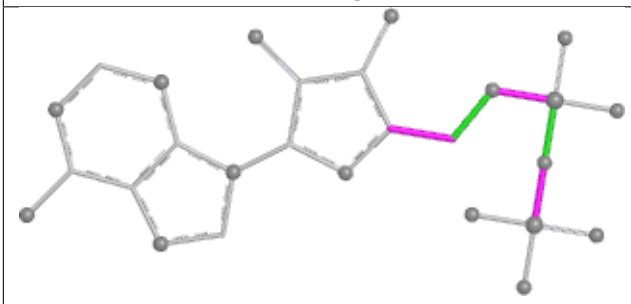
Ligand ADP A 1800



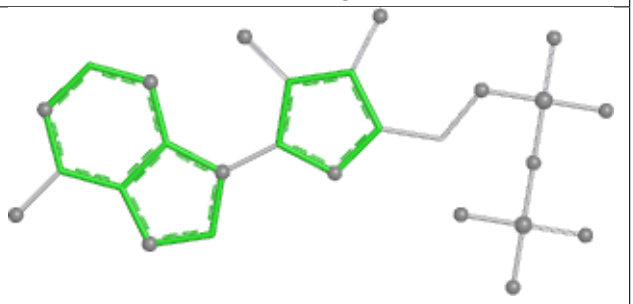
Bond lengths



Bond angles

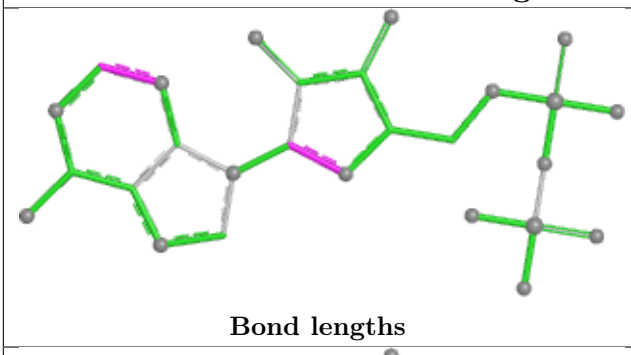


Torsions

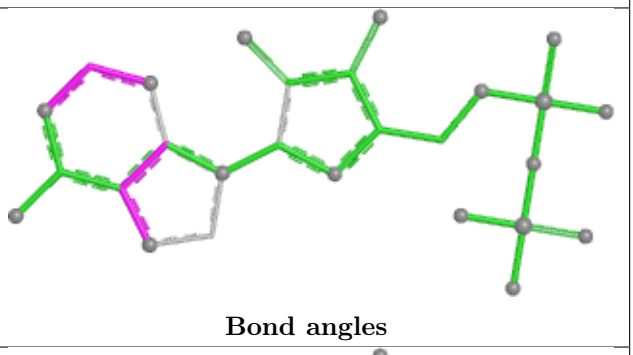


Rings

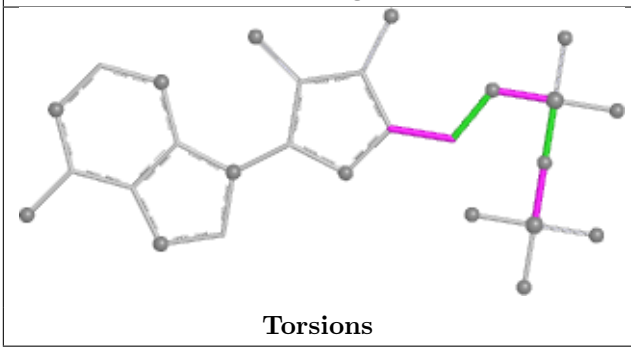
Ligand ADP C 1800



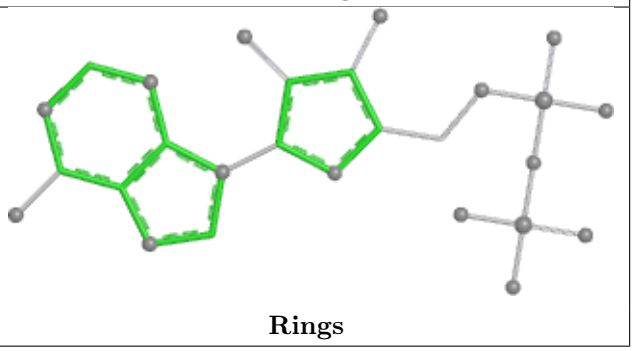
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

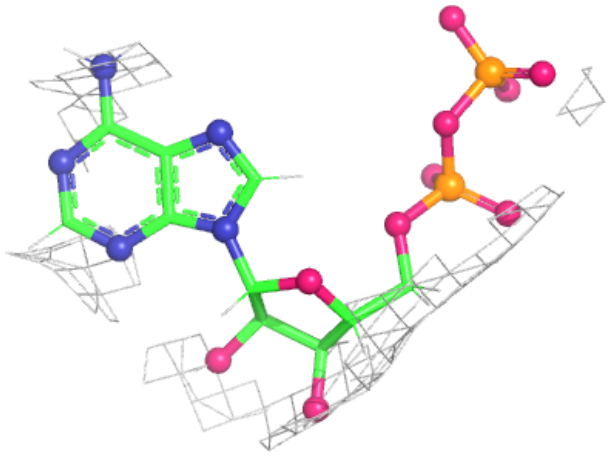
6.4 Ligands

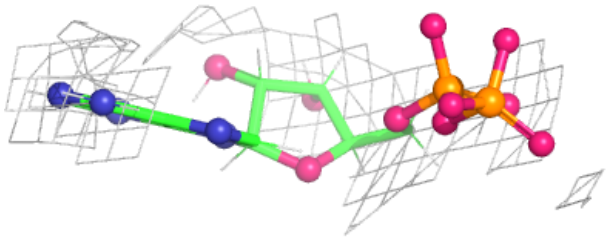
Unable to reproduce the depositors R factor - this section is therefore empty.

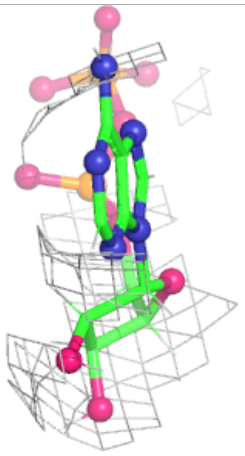
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1800:

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

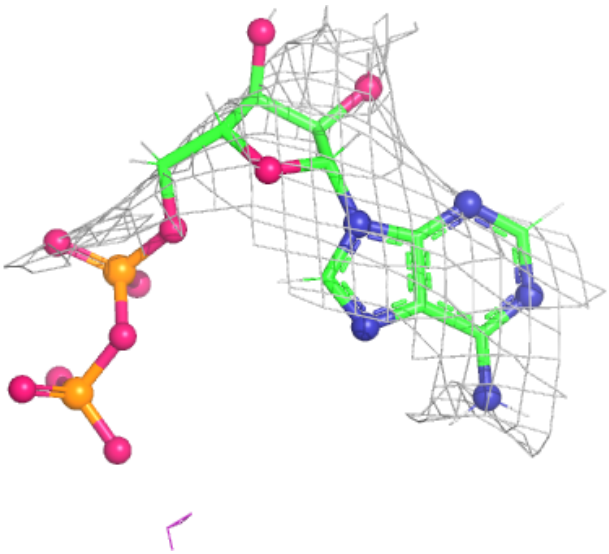


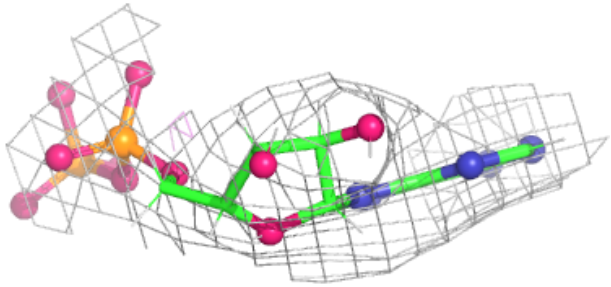


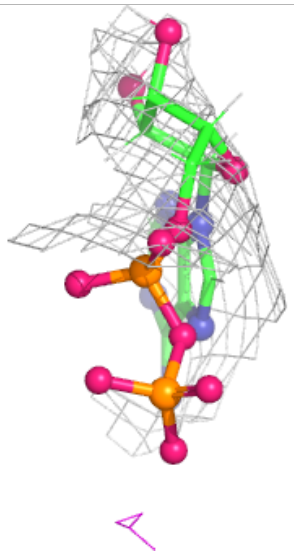


Electron density around ADP B 1800:

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

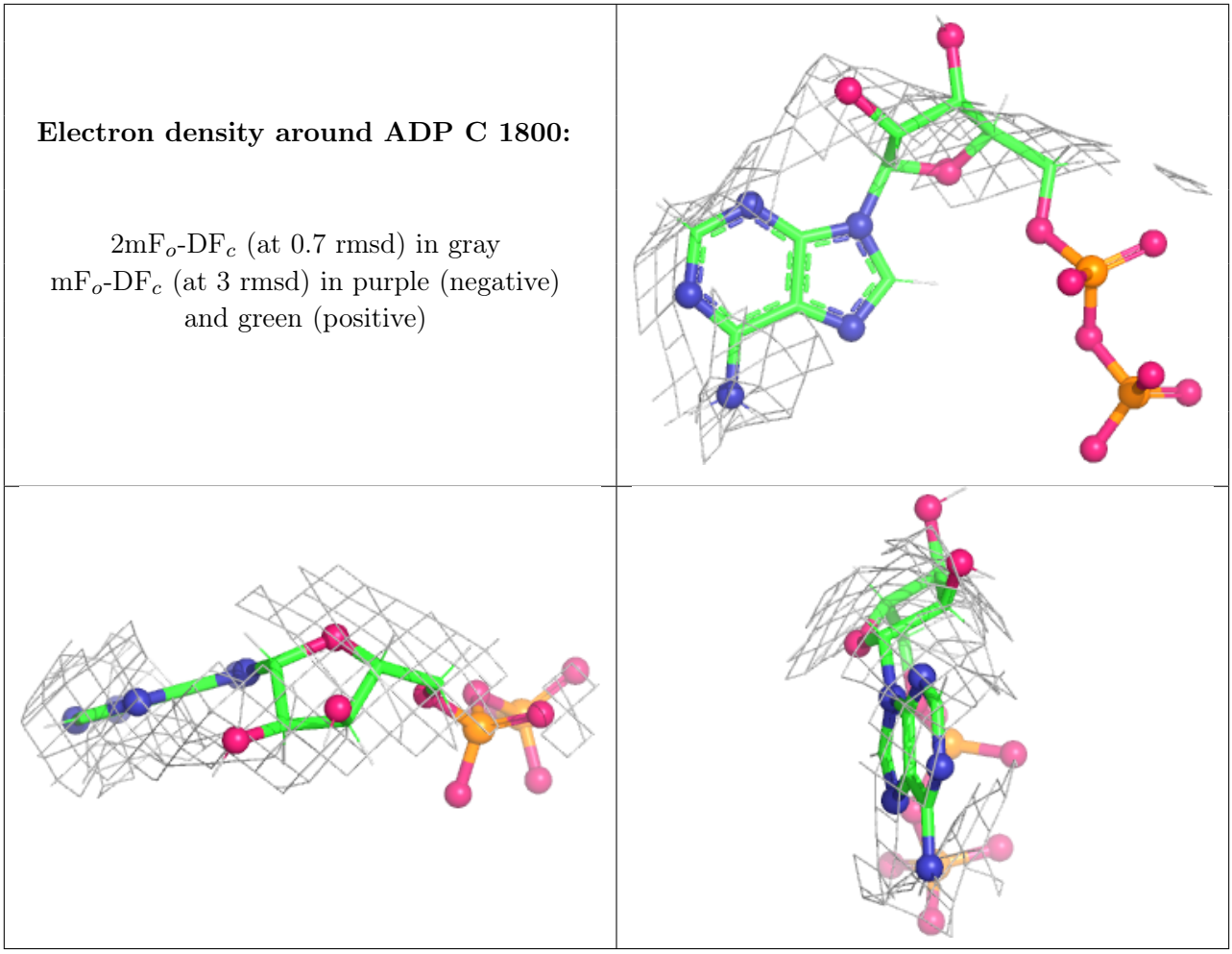






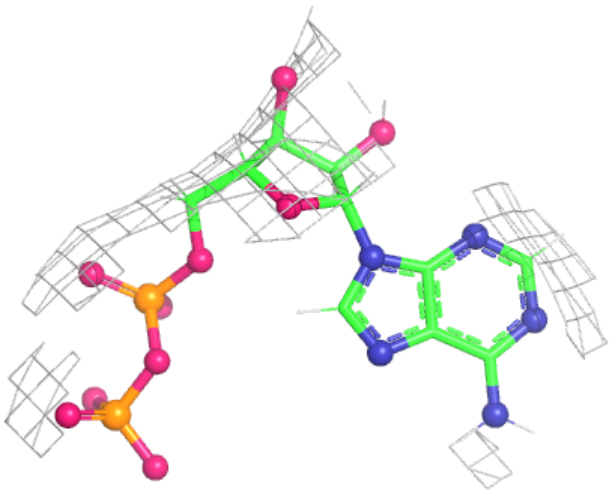
Electron density around ADP C 1800:

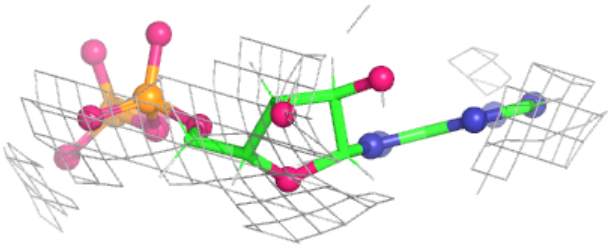
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

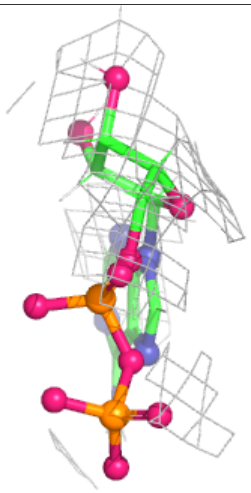


Electron density around ADP D 1800:

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

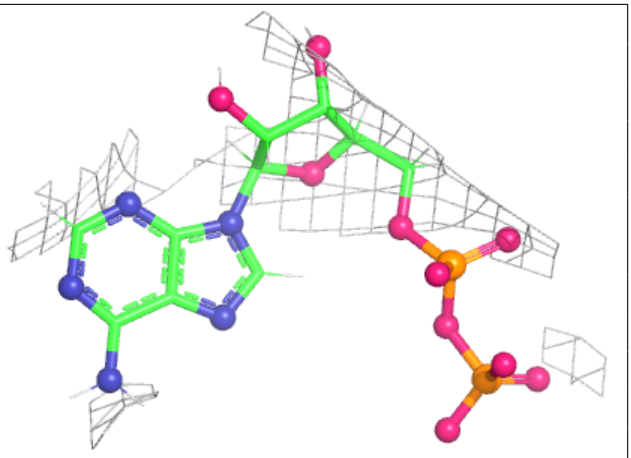


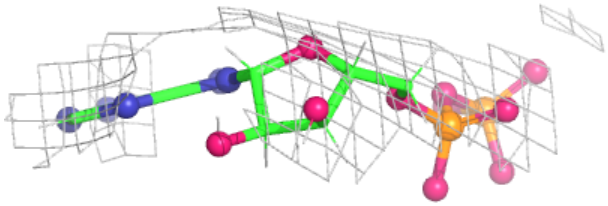


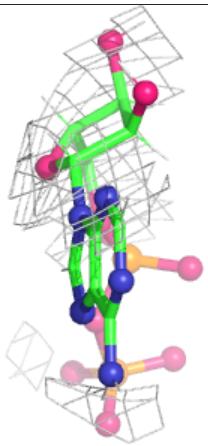


Electron density around ADP E 1800:

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

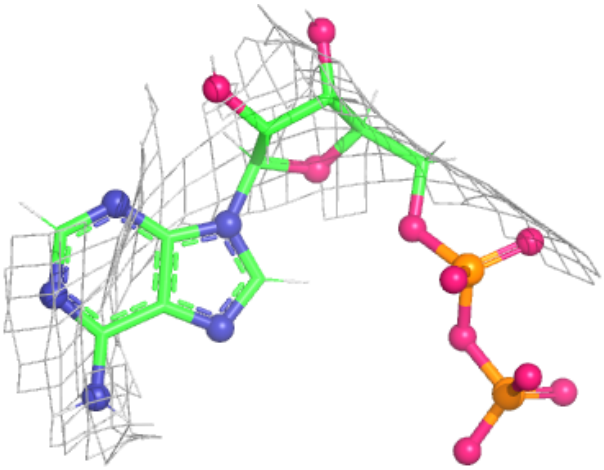


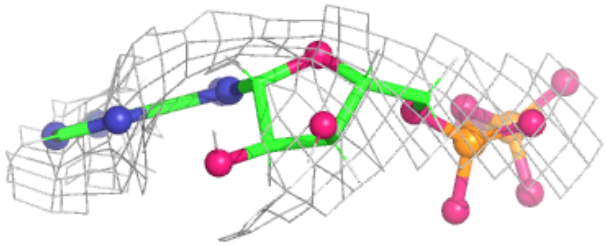


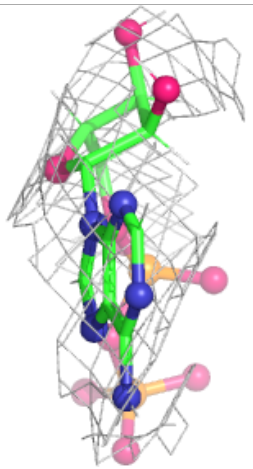


Electron density around ADP F 1800:

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

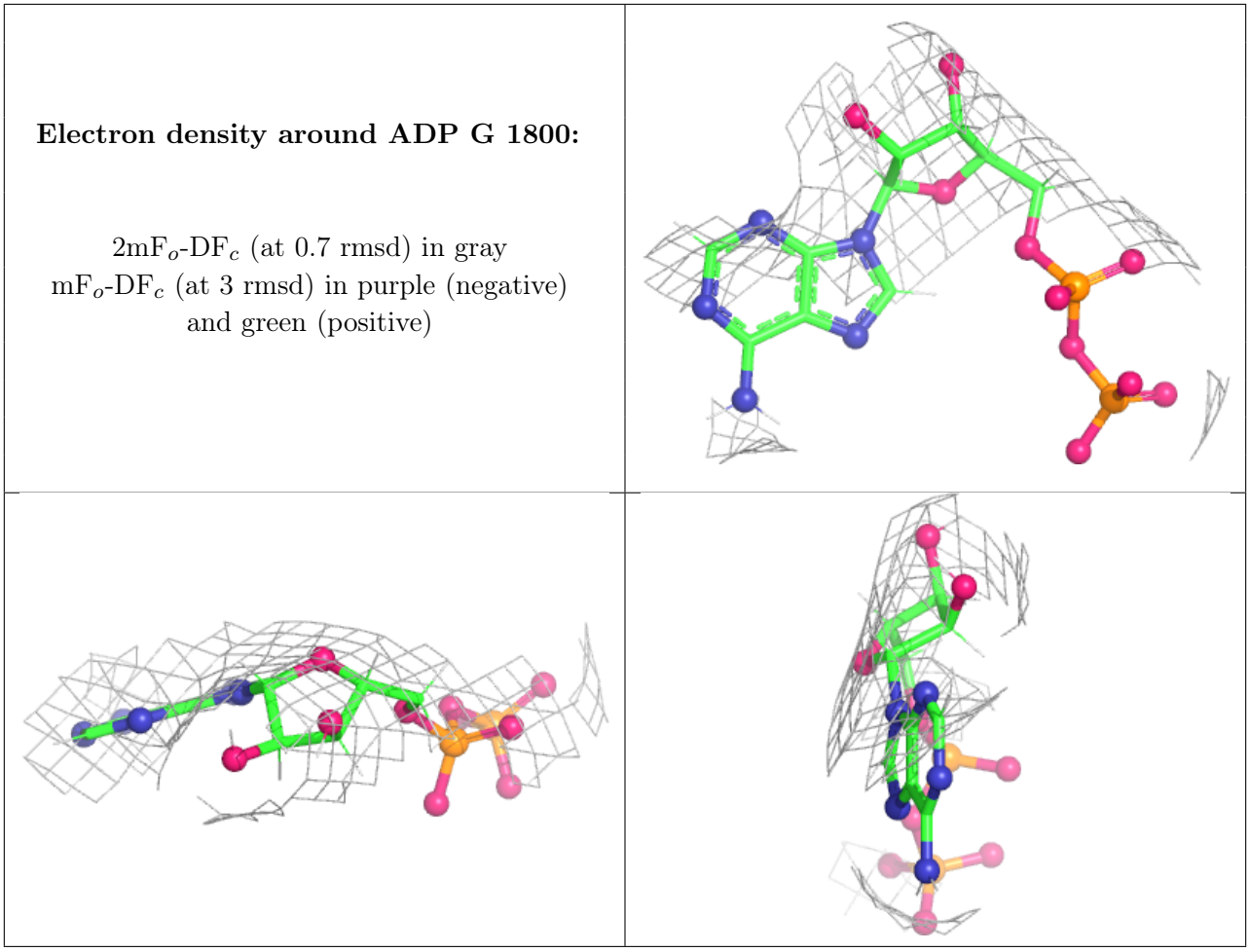






Electron density around ADP G 1800:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.