Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 01:11 AM EDT

PDB ID	:	3ROJ
Title	:	D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase of Synechocystis sp. PCC 6803
Authors	:	Hu, X.; Hui, D.; Lingling, F.; Jian, W.
Deposited on	:	2011-04-26
Resolution	:	2.30 Å(reported)

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

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

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

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

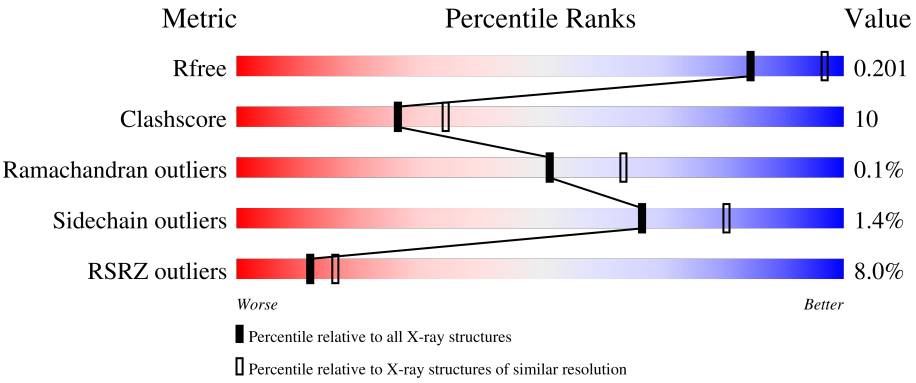
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	379	7% 75% 16% 8%
1	B	379	8% 72% 18% 9%
1	C	379	7% 75% 16% • 8%
1	D	379	7% 73% 18% • 9%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	355	-	-	X	-
5	CL	A	361	-	-	X	-
5	CL	B	351	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11412 atoms, of which 8 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 D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	4	0
			2591	1607	455	507	22			
1	B	345	Total	C	N	O	S	0	4	0
			2576	1599	454	501	22			
1	C	347	Total	C	N	O	S	0	2	0
			2563	1590	452	499	22			
1	D	346	Total	C	N	O	S	0	2	0
			2579	1602	453	502	22			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP P73922
A	-32	GLY	-	expression tag	UNP P73922
A	-31	SER	-	expression tag	UNP P73922
A	-30	SER	-	expression tag	UNP P73922
A	-29	HIS	-	expression tag	UNP P73922
A	-28	HIS	-	expression tag	UNP P73922
A	-27	HIS	-	expression tag	UNP P73922
A	-26	HIS	-	expression tag	UNP P73922
A	-25	HIS	-	expression tag	UNP P73922
A	-24	HIS	-	expression tag	UNP P73922
A	-23	SER	-	expression tag	UNP P73922
A	-22	SER	-	expression tag	UNP P73922
A	-21	GLY	-	expression tag	UNP P73922
A	-20	LEU	-	expression tag	UNP P73922
A	-19	VAL	-	expression tag	UNP P73922
A	-18	PRO	-	expression tag	UNP P73922
A	-17	ARG	-	expression tag	UNP P73922
A	-16	GLY	-	expression tag	UNP P73922
A	-15	SER	-	expression tag	UNP P73922
A	-14	HIS	-	expression tag	UNP P73922
A	-13	MET	-	expression tag	UNP P73922

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP P73922
A	-11	SER	-	expression tag	UNP P73922
A	-10	MET	-	expression tag	UNP P73922
A	-9	THR	-	expression tag	UNP P73922
A	-8	GLY	-	expression tag	UNP P73922
A	-7	GLY	-	expression tag	UNP P73922
A	-6	GLN	-	expression tag	UNP P73922
A	-5	GLN	-	expression tag	UNP P73922
A	-4	MET	-	expression tag	UNP P73922
A	-3	GLY	-	expression tag	UNP P73922
A	-2	ARG	-	expression tag	UNP P73922
A	-1	GLY	-	expression tag	UNP P73922
A	0	SER	-	expression tag	UNP P73922
A	1	VAL	-	expression tag	UNP P73922
B	-33	MET	-	expression tag	UNP P73922
B	-32	GLY	-	expression tag	UNP P73922
B	-31	SER	-	expression tag	UNP P73922
B	-30	SER	-	expression tag	UNP P73922
B	-29	HIS	-	expression tag	UNP P73922
B	-28	HIS	-	expression tag	UNP P73922
B	-27	HIS	-	expression tag	UNP P73922
B	-26	HIS	-	expression tag	UNP P73922
B	-25	HIS	-	expression tag	UNP P73922
B	-24	HIS	-	expression tag	UNP P73922
B	-23	SER	-	expression tag	UNP P73922
B	-22	SER	-	expression tag	UNP P73922
B	-21	GLY	-	expression tag	UNP P73922
B	-20	LEU	-	expression tag	UNP P73922
B	-19	VAL	-	expression tag	UNP P73922
B	-18	PRO	-	expression tag	UNP P73922
B	-17	ARG	-	expression tag	UNP P73922
B	-16	GLY	-	expression tag	UNP P73922
B	-15	SER	-	expression tag	UNP P73922
B	-14	HIS	-	expression tag	UNP P73922
B	-13	MET	-	expression tag	UNP P73922
B	-12	ALA	-	expression tag	UNP P73922
B	-11	SER	-	expression tag	UNP P73922
B	-10	MET	-	expression tag	UNP P73922
B	-9	THR	-	expression tag	UNP P73922
B	-8	GLY	-	expression tag	UNP P73922
B	-7	GLY	-	expression tag	UNP P73922
B	-6	GLN	-	expression tag	UNP P73922

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLN	-	expression tag	UNP P73922
B	-4	MET	-	expression tag	UNP P73922
B	-3	GLY	-	expression tag	UNP P73922
B	-2	ARG	-	expression tag	UNP P73922
B	-1	GLY	-	expression tag	UNP P73922
B	0	SER	-	expression tag	UNP P73922
B	1	VAL	-	expression tag	UNP P73922
C	-33	MET	-	expression tag	UNP P73922
C	-32	GLY	-	expression tag	UNP P73922
C	-31	SER	-	expression tag	UNP P73922
C	-30	SER	-	expression tag	UNP P73922
C	-29	HIS	-	expression tag	UNP P73922
C	-28	HIS	-	expression tag	UNP P73922
C	-27	HIS	-	expression tag	UNP P73922
C	-26	HIS	-	expression tag	UNP P73922
C	-25	HIS	-	expression tag	UNP P73922
C	-24	HIS	-	expression tag	UNP P73922
C	-23	SER	-	expression tag	UNP P73922
C	-22	SER	-	expression tag	UNP P73922
C	-21	GLY	-	expression tag	UNP P73922
C	-20	LEU	-	expression tag	UNP P73922
C	-19	VAL	-	expression tag	UNP P73922
C	-18	PRO	-	expression tag	UNP P73922
C	-17	ARG	-	expression tag	UNP P73922
C	-16	GLY	-	expression tag	UNP P73922
C	-15	SER	-	expression tag	UNP P73922
C	-14	HIS	-	expression tag	UNP P73922
C	-13	MET	-	expression tag	UNP P73922
C	-12	ALA	-	expression tag	UNP P73922
C	-11	SER	-	expression tag	UNP P73922
C	-10	MET	-	expression tag	UNP P73922
C	-9	THR	-	expression tag	UNP P73922
C	-8	GLY	-	expression tag	UNP P73922
C	-7	GLY	-	expression tag	UNP P73922
C	-6	GLN	-	expression tag	UNP P73922
C	-5	GLN	-	expression tag	UNP P73922
C	-4	MET	-	expression tag	UNP P73922
C	-3	GLY	-	expression tag	UNP P73922
C	-2	ARG	-	expression tag	UNP P73922
C	-1	GLY	-	expression tag	UNP P73922
C	0	SER	-	expression tag	UNP P73922
C	1	VAL	-	expression tag	UNP P73922

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-33	MET	-	expression tag	UNP P73922
D	-32	GLY	-	expression tag	UNP P73922
D	-31	SER	-	expression tag	UNP P73922
D	-30	SER	-	expression tag	UNP P73922
D	-29	HIS	-	expression tag	UNP P73922
D	-28	HIS	-	expression tag	UNP P73922
D	-27	HIS	-	expression tag	UNP P73922
D	-26	HIS	-	expression tag	UNP P73922
D	-25	HIS	-	expression tag	UNP P73922
D	-24	HIS	-	expression tag	UNP P73922
D	-23	SER	-	expression tag	UNP P73922
D	-22	SER	-	expression tag	UNP P73922
D	-21	GLY	-	expression tag	UNP P73922
D	-20	LEU	-	expression tag	UNP P73922
D	-19	VAL	-	expression tag	UNP P73922
D	-18	PRO	-	expression tag	UNP P73922
D	-17	ARG	-	expression tag	UNP P73922
D	-16	GLY	-	expression tag	UNP P73922
D	-15	SER	-	expression tag	UNP P73922
D	-14	HIS	-	expression tag	UNP P73922
D	-13	MET	-	expression tag	UNP P73922
D	-12	ALA	-	expression tag	UNP P73922
D	-11	SER	-	expression tag	UNP P73922
D	-10	MET	-	expression tag	UNP P73922
D	-9	THR	-	expression tag	UNP P73922
D	-8	GLY	-	expression tag	UNP P73922
D	-7	GLY	-	expression tag	UNP P73922
D	-6	GLN	-	expression tag	UNP P73922
D	-5	GLN	-	expression tag	UNP P73922
D	-4	MET	-	expression tag	UNP P73922
D	-3	GLY	-	expression tag	UNP P73922
D	-2	ARG	-	expression tag	UNP P73922
D	-1	GLY	-	expression tag	UNP P73922
D	0	SER	-	expression tag	UNP P73922
D	1	VAL	-	expression tag	UNP P73922

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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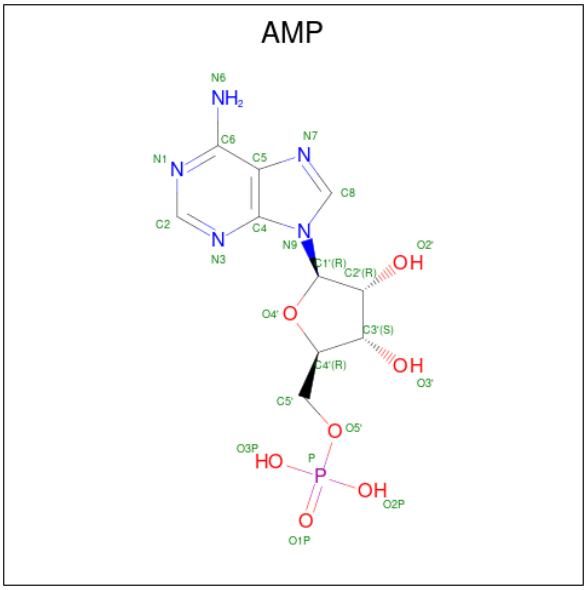
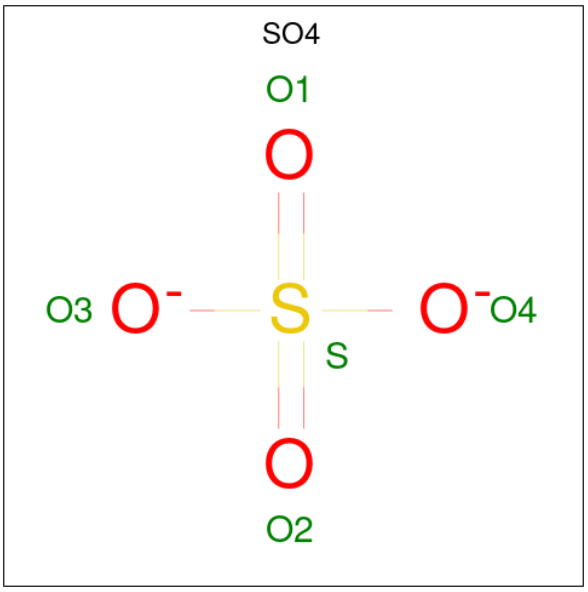
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0
3	B	1	Total C N O P 23 10 5 7 1	0	0
3	C	1	Total C N O P 23 10 5 7 1	0	0
3	C	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

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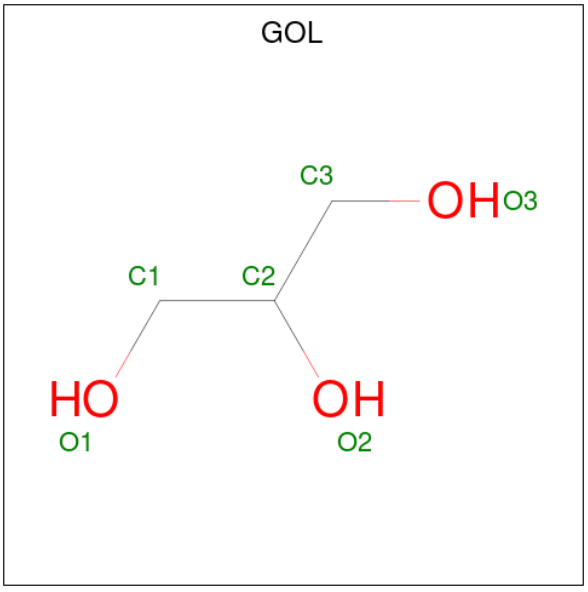
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total Cl 10 10	0	0
5	B	5	Total Cl 5 5	0	0
5	C	6	Total Cl 6 6	0	0
5	D	2	Total Cl 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is water.

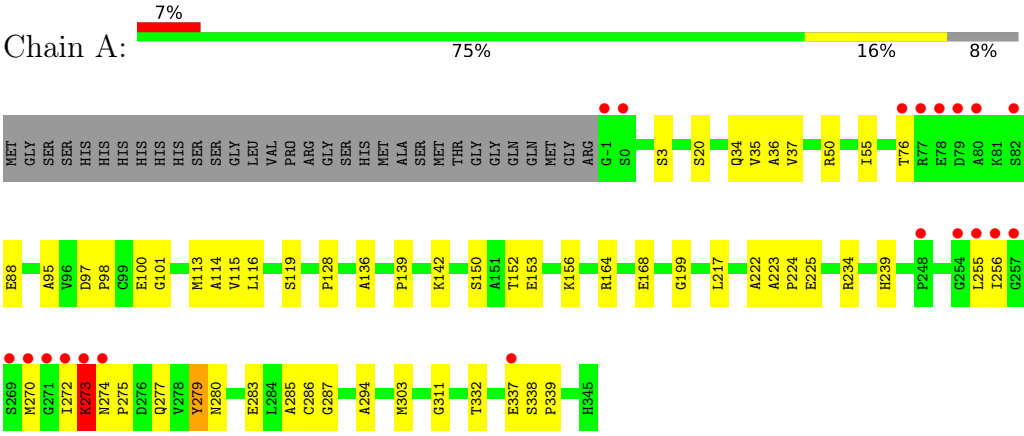
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	239	Total O 239 239	0	0
7	B	209	Total O 209 209	0	0
7	C	237	Total O 237 237	0	0
7	D	196	Total O 196 196	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

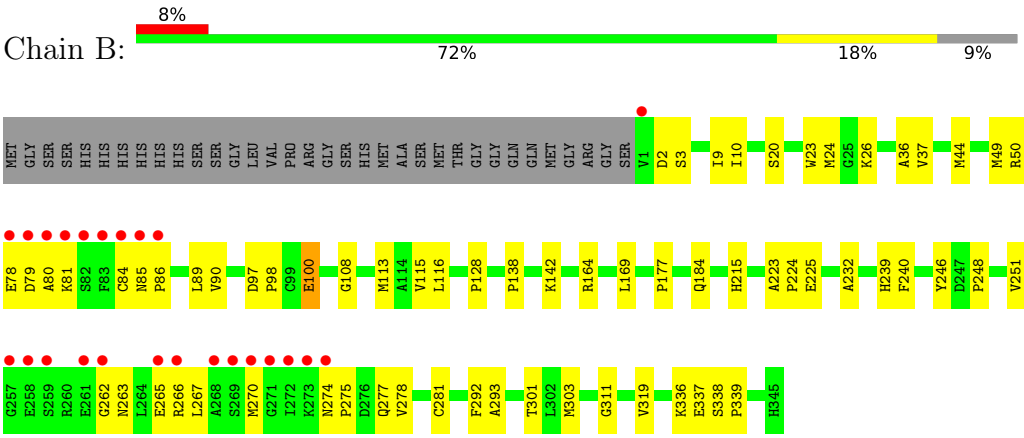
• Molecule 1: D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase

Chain A:



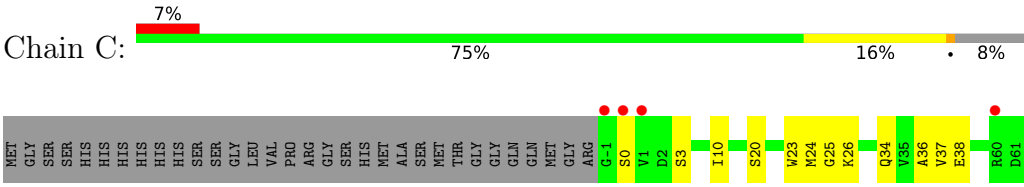
• Molecule 1: D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase

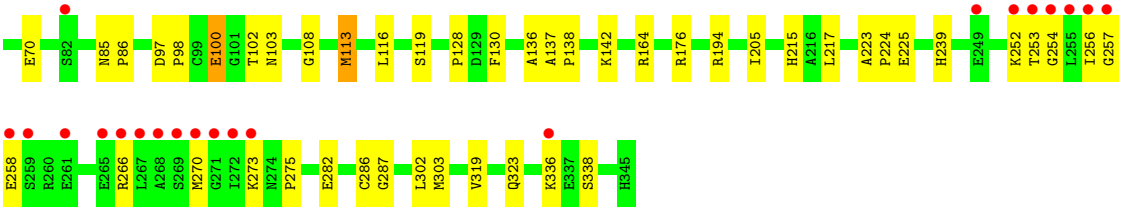
Chain B:



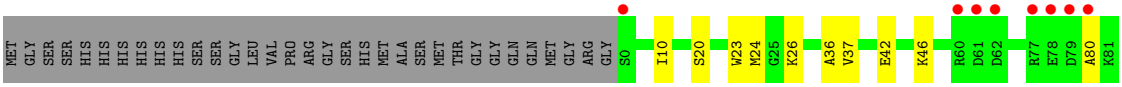
• Molecule 1: D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase

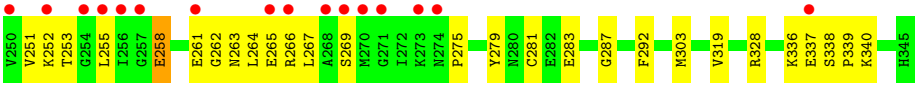
Chain C:





• Molecule 1: D-fructose 1,6-bisphosphatase class 2/sedoheptulose 1,7-bisphosphatase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	144.28Å 144.28Å 168.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.54 – 2.30 25.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.54-2.30) 99.3 (25.54-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.183 , 0.204 0.176 , 0.201	Depositor DCC
R_{free} test set	4396 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: GOL, MG, CL, SO4, CSO, AMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/2630	0.45	0/3550
1	B	0.25	0/2615	0.43	0/3532
1	C	0.26	0/2596	0.44	0/3507
1	D	0.24	0/2612	0.42	0/3525
All	All	0.25	0/10453	0.43	0/14114

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	2591	0	2564	54	0
1	B	2576	0	2552	64	0
1	C	2563	0	2525	46	0
1	D	2579	0	2563	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	12	0	0
3	C	46	0	24	1	0
4	A	30	0	0	0	0
4	B	10	0	0	0	0
4	C	20	0	0	2	0
4	D	25	0	0	1	0
5	A	10	0	0	7	0
5	B	5	0	0	3	0
5	C	6	0	0	0	0
5	D	2	0	0	1	0
6	A	6	8	8	2	0
7	A	239	0	0	4	0
7	B	209	0	0	5	0
7	C	237	0	0	5	0
7	D	196	0	0	0	0
All	All	11404	8	10260	213	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 10.

All (213) 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:D:263:ASN:HA	1:D:266:ARG:HD2	1.37	1.07
1:B:301:THR:O	7:B:707:HOH:O	1.92	0.85
1:A:150:SER:OG	1:A:153[A]:GLU:HG3	1.78	0.84
1:D:253:THR:HG22	1:D:258:GLU:CD	2.00	0.82
1:B:277[B]:GLN:HE21	1:B:277[B]:GLN:HA	1.49	0.78
1:B:113:MET:HE2	1:B:303:MET:CE	2.13	0.77
1:A:113:MET:HE2	1:A:303:MET:CE	2.15	0.76
1:A:280:ASN:HB2	6:A:365:GOL:H2	1.68	0.76
1:A:273:LYS:HG2	1:A:274:ASN:H	1.50	0.76
1:D:150:SER:OG	1:D:153[B]:GLU:HG2	1.84	0.75
1:A:273:LYS:H	1:A:273:LYS:CD	1.99	0.75
1:C:266:ARG:O	1:C:270:MET:HG3	1.87	0.74
1:B:81:LYS:HA	1:B:89:LEU:HD11	1.70	0.74
1:A:234:ARG:NE	5:A:355:CL:CL	2.56	0.73
1:A:273:LYS:H	1:A:273:LYS:HD3	1.53	0.73
1:A:273:LYS:HD3	1:A:273:LYS:N	2.03	0.73
1:D:262:GLY:O	1:D:266:ARG:HG3	1.90	0.72
1:D:85:ASN:HB2	1:D:86:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:CE	1:B:303:MET:CE	2.68	0.71
1:C:113:MET:HE2	1:C:303:MET:CE	2.20	0.71
1:B:113:MET:CE	1:B:303:MET:HE1	2.22	0.70
1:B:277[B]:GLN:HA	1:B:277[B]:GLN:NE2	2.05	0.70
5:B:351:CL:CL	7:B:600:HOH:O	2.47	0.70
1:D:253:THR:HG22	1:D:258:GLU:OE2	1.90	0.69
1:B:90:VAL:O	7:B:683:HOH:O	2.09	0.69
1:D:85:ASN:HB2	1:D:86:PRO:HD2	1.75	0.69
1:A:113:MET:HE2	1:A:303:MET:HE3	1.75	0.69
1:B:85:ASN:HB2	1:B:86:PRO:HD2	1.75	0.68
1:B:277[B]:GLN:NE2	1:B:278:VAL:H	1.91	0.68
1:C:194:ARG:NE	7:C:732:HOH:O	2.28	0.66
1:B:262:GLY:O	1:B:266:ARG:HG3	1.95	0.66
1:D:138:PRO:HD3	1:D:215:HIS:O	1.96	0.66
1:A:274:ASN:ND2	1:A:277[B]:GLN:HG2	2.10	0.65
1:A:113:MET:CE	1:A:303:MET:CE	2.74	0.65
1:A:136:ALA:HB3	1:A:217:LEU:HB3	1.79	0.64
1:C:136:ALA:HB3	1:C:217:LEU:HB3	1.79	0.64
5:B:351:CL:CL	7:B:538:HOH:O	2.52	0.64
1:B:80:ALA:CB	1:B:89:LEU:HD21	2.28	0.64
1:C:113:MET:CE	1:C:303:MET:CE	2.77	0.63
1:B:113:MET:HE2	1:B:303:MET:HE1	1.78	0.63
1:C:336:LYS:HA	7:C:781:HOH:O	1.99	0.63
1:B:23:TRP:CE3	1:B:26:LYS:HD3	2.33	0.62
1:B:128:PRO:HB3	1:B:270:MET:HE3	1.81	0.62
1:D:97:ASP:OD1	1:D:100:GLU:HG2	2.00	0.62
1:A:273:LYS:O	1:A:275:PRO:HD3	2.00	0.62
1:D:136:ALA:HB3	1:D:217:LEU:HB3	1.83	0.60
1:A:311:GLY:O	1:A:339:PRO:HG3	2.01	0.60
1:B:97:ASP:HB3	1:B:115:VAL:HG13	1.84	0.60
1:B:263:ASN:HA	1:B:266:ARG:HD2	1.84	0.60
1:D:253:THR:HG23	1:D:255:LEU:H	1.67	0.60
1:B:164:ARG:HD2	1:B:169:LEU:HD23	1.85	0.59
5:A:358:CL:CL	7:A:577:HOH:O	2.54	0.59
1:B:338:SER:N	1:B:339:PRO:CD	2.65	0.59
1:C:97:ASP:OD1	1:C:100:GLU:HG2	2.02	0.59
1:B:248:PRO:HA	1:B:251:VAL:O	2.03	0.59
1:A:280:ASN:CB	6:A:365:GOL:H2	2.32	0.58
1:D:336:LYS:HA	1:D:337:GLU:HB2	1.86	0.58
1:A:101:GLY:N	5:A:361:CL:CL	2.72	0.58
1:C:38:GLU:HG2	1:C:65:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:CD	1:A:273:LYS:N	2.62	0.57
1:D:338:SER:N	1:D:339:PRO:CD	2.68	0.57
1:B:23:TRP:CZ3	1:B:26:LYS:HD3	2.40	0.57
1:B:142:LYS:HA	1:B:239:HIS:HB2	1.88	0.56
1:D:261:GLU:O	1:D:265:GLU:HG3	2.05	0.56
1:A:273:LYS:HG2	1:A:274:ASN:N	2.20	0.56
1:B:97:ASP:HB3	1:B:115:VAL:CG1	2.35	0.56
1:C:10:ILE:HG12	1:C:319:VAL:HG21	1.87	0.56
1:C:205:ILE:HG22	1:C:302:LEU:HD11	1.86	0.56
1:D:80:ALA:HA	1:D:83:PHE:CE1	2.41	0.56
1:A:20:SER:HB2	1:A:36:ALA:HB2	1.88	0.55
1:C:336:LYS:CA	7:C:781:HOH:O	2.54	0.55
1:B:184:GLN:NE2	7:B:694:HOH:O	2.41	0.54
1:C:142:LYS:HA	1:C:239:HIS:HB2	1.89	0.54
1:D:130:PHE:CE2	1:D:267:LEU:HD21	2.43	0.53
1:C:38:GLU:HG2	1:C:65:MET:SD	2.48	0.53
1:B:9:ILE:HD12	1:B:293:ALA:HB2	1.91	0.53
1:C:20:SER:HB2	1:C:36:ALA:HB2	1.89	0.53
1:C:85:ASN:HB2	1:C:86:PRO:HD2	1.89	0.53
1:B:80:ALA:HB1	1:B:84:CYS:SG	2.49	0.52
1:B:80:ALA:HB3	1:B:89:LEU:HD21	1.90	0.52
1:B:20:SER:HB2	1:B:36:ALA:HB2	1.92	0.52
1:B:37:VAL:HG22	1:B:98:PRO:HG2	1.91	0.52
1:D:240:PHE:HB3	1:D:281:CYS:HB3	1.92	0.52
1:C:85:ASN:HB2	1:C:86:PRO:CD	2.41	0.51
1:B:85:ASN:HB2	1:B:86:PRO:CD	2.39	0.51
1:C:37:VAL:HG22	1:C:98:PRO:HG2	1.93	0.51
1:B:113:MET:HE1	1:B:303:MET:HE1	1.93	0.51
1:B:116:LEU:HD12	1:B:116:LEU:C	2.31	0.50
1:D:37:VAL:HG22	1:D:98:PRO:HG2	1.93	0.50
1:D:42:GLU:OE2	1:D:46:LYS:HE3	2.11	0.50
1:A:277[B]:GLN:NE2	7:A:591:HOH:O	2.43	0.50
1:C:24:MET:HG3	1:C:108:GLY:HA2	1.92	0.50
1:D:119:SER:OG	1:D:287:GLY:HA3	2.12	0.50
1:B:246:TYR:CE2	1:B:275:PRO:HB2	2.47	0.50
1:C:253:THR:HB	1:C:258:GLU:OE2	2.12	0.50
1:D:113:MET:SD	1:D:303:MET:CE	3.00	0.50
1:A:332:THR:OG1	1:D:328:ARG:HG2	2.12	0.49
1:A:97:ASP:HB3	1:A:115:VAL:HG13	1.94	0.49
1:C:23:TRP:HA	1:C:26:LYS:HG3	1.95	0.49
1:A:85:ASN:HB2	1:A:86:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LYS:HA	1:D:239:HIS:HB2	1.94	0.49
1:D:177:PRO:HD2	4:D:349:SO4:O3	2.12	0.49
1:A:85:ASN:HB2	1:A:86:PRO:CD	2.42	0.49
1:A:274:ASN:HD22	1:A:277[B]:GLN:HG2	1.74	0.49
1:C:38:GLU:CG	1:C:65:MET:CE	2.91	0.49
1:B:75:CYS:O	1:B:80:ALA:HB2	2.12	0.48
1:D:225:GLU:OE2	1:D:225:GLU:N	2.44	0.48
1:A:267:LEU:HD13	1:A:275:PRO:HB3	1.96	0.48
1:D:116:LEU:HD12	1:D:116:LEU:C	2.33	0.48
1:B:113:MET:HE1	1:B:303:MET:CE	2.41	0.48
1:C:113:MET:CE	1:C:303:MET:HE2	2.43	0.48
1:B:80:ALA:HB1	1:B:89:LEU:HD21	1.94	0.48
1:A:279:TYR:HA	1:A:283:GLU:OE2	2.13	0.48
1:D:172:VAL:HG11	1:D:203:ALA:CB	2.44	0.48
1:B:240:PHE:HB3	1:B:281:CYS:HB3	1.95	0.47
1:A:337:GLU:HA	1:A:338:SER:HA	1.46	0.47
1:D:23:TRP:HA	1:D:26:LYS:HD2	1.96	0.47
1:B:50:ARG:HA	1:B:76:THR:HG23	1.97	0.47
1:C:336:LYS:CB	7:C:781:HOH:O	2.62	0.47
1:D:115:VAL:HG22	1:D:116:LEU:N	2.29	0.47
1:C:10:ILE:CG1	1:C:319:VAL:HG21	2.44	0.47
1:C:128:PRO:HB2	1:C:130:PHE:CD2	2.50	0.47
1:A:273:LYS:CG	1:A:274:ASN:H	2.23	0.47
1:B:232:ALA:HB2	1:B:292:PHE:CD2	2.49	0.47
1:C:273:LYS:O	1:C:275:PRO:HD3	2.15	0.47
1:A:142:LYS:HA	1:A:239:HIS:HB2	1.96	0.46
1:A:85:ASN:OD1	1:A:88:GLU:HG3	2.14	0.46
1:B:44:MET:HE3	1:B:116:LEU:HD22	1.97	0.46
1:C:142:LYS:HE2	7:C:698:HOH:O	2.14	0.46
1:D:253:THR:HG22	1:D:258:GLU:OE1	2.14	0.46
1:A:55:ILE:HB	1:A:95:ALA:CB	2.46	0.46
1:B:225:GLU:OE2	1:B:225:GLU:N	2.48	0.46
1:B:277[B]:GLN:NE2	1:B:277[B]:GLN:CA	2.76	0.46
1:D:20:SER:HB2	1:D:36:ALA:HB2	1.98	0.45
1:B:78:GLU:HA	1:B:79:ASP:HA	1.51	0.45
1:C:113:MET:HE1	1:C:303:MET:HE2	1.98	0.45
1:A:34[B]:GLN:HG3	1:A:35:VAL:N	2.32	0.45
1:A:100:GLU:OE2	1:A:199:GLY:HA2	2.17	0.45
1:B:128:PRO:HB3	1:B:270:MET:CE	2.47	0.45
1:D:232:ALA:HB2	1:D:292:PHE:CD2	2.51	0.45
1:C:137:ALA:HB1	1:C:138:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLY:O	5:A:355:CL:CL	2.72	0.45
1:B:2:ASP:OD1	1:B:3:SER:N	2.49	0.45
1:B:138:PRO:HD3	1:B:215:HIS:O	2.17	0.45
1:D:248:PRO:HA	1:D:251:VAL:O	2.16	0.45
1:B:270:MET:HB3	1:B:270:MET:HE2	1.55	0.45
5:A:363:CL:CL	7:A:678:HOH:O	2.58	0.44
1:B:177:PRO:O	5:B:353:CL:CL	2.72	0.44
1:C:116:LEU:C	1:C:116:LEU:HD12	2.37	0.44
1:D:10:ILE:HG12	1:D:319:VAL:HG21	1.99	0.44
1:A:274:ASN:O	1:A:277[B]:GLN:HB2	2.17	0.44
1:C:205:ILE:CG2	1:C:302:LEU:HD11	2.47	0.44
1:A:285:ALA:O	5:A:355:CL:CL	2.73	0.44
1:D:246:TYR:CE2	1:D:275:PRO:HB2	2.53	0.44
1:C:25:GLY:HA3	1:D:193:VAL:O	2.18	0.44
1:D:24:MET:HG3	1:D:108:GLY:HA2	1.99	0.44
1:A:101:GLY:CA	5:A:361:CL:CL	3.03	0.44
1:A:223:ALA:N	1:A:224:PRO:CD	2.80	0.44
1:C:128:PRO:HB2	1:C:130:PHE:HD2	1.81	0.44
1:B:10:ILE:HG12	1:B:319:VAL:HG21	2.00	0.43
1:B:77:ARG:N	1:B:77:ARG:HD3	2.32	0.43
1:C:164:ARG:NH2	3:C:348:AMP:O1P	2.47	0.43
1:A:37:VAL:HG22	1:A:98:PRO:HG2	2.00	0.43
1:A:139:PRO:HB2	1:D:340:LYS:O	2.18	0.43
1:B:50:ARG:NH1	1:B:76:THR:HA	2.34	0.43
1:A:286:CSO:SG	7:A:457:HOH:O	2.62	0.43
1:D:223:ALA:N	1:D:224:PRO:CD	2.82	0.43
1:A:255:LEU:HA	1:A:256:ILE:HA	1.63	0.43
1:C:256:ILE:HA	1:C:257:GLY:HA2	1.55	0.43
1:B:100:GLU:O	1:B:100:GLU:HG3	2.16	0.43
1:D:266:ARG:NH1	1:D:266:ARG:HG2	2.34	0.43
1:A:116:LEU:C	1:A:116:LEU:HD12	2.39	0.42
1:A:164:ARG:HD2	1:A:168:GLU:O	2.20	0.42
1:C:67:TYR:CE1	1:C:70:GLU:HB2	2.55	0.42
1:D:264:LEU:HD12	1:D:264:LEU:HA	1.87	0.42
1:C:113:MET:HE1	1:C:303:MET:CE	2.49	0.42
1:D:113:MET:SD	1:D:303:MET:HE1	2.59	0.42
1:B:24:MET:CG	1:B:108:GLY:HA2	2.49	0.42
1:C:282:GLU:O	1:C:286:CSO:HA	2.19	0.42
1:D:172:VAL:HG11	1:D:203:ALA:HB1	2.00	0.42
1:B:24:MET:HG3	1:B:108:GLY:HA2	2.01	0.42
1:B:223:ALA:HB3	1:B:224:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:N	1:B:337:GLU:HA	2.35	0.42
1:D:248:PRO:O	1:D:252:LYS:HG2	2.19	0.42
1:C:3:SER:HA	1:C:323:GLN:OE1	2.19	0.41
1:D:223:ALA:HB3	1:D:224:PRO:HD3	2.01	0.41
1:A:267:LEU:O	1:A:272:ILE:HB	2.19	0.41
1:C:119:SER:OG	1:C:287:GLY:HA3	2.19	0.41
1:D:337:GLU:OE2	5:D:353:CL:CL	2.75	0.41
1:D:131:TYR:CE2	1:D:251:VAL:HG22	2.55	0.41
1:D:279:TYR:HA	1:D:283:GLU:OE2	2.20	0.41
1:A:114:ALA:O	1:A:294:ALA:HA	2.19	0.41
1:A:267:LEU:HD23	1:A:270:MET:CE	2.50	0.41
1:B:74:ILE:O	1:B:77:ARG:HG2	2.20	0.41
1:C:176:ARG:HB3	4:C:351:SO4:O2	2.21	0.41
1:C:225:GLU:OE2	1:C:225:GLU:N	2.53	0.41
1:B:267:LEU:HD13	1:B:275:PRO:HB3	2.01	0.41
1:C:102:THR:HG23	4:C:352:SO4:O4	2.21	0.41
1:C:138:PRO:HD3	1:C:215:HIS:O	2.21	0.41
1:C:252:LYS:HG2	1:C:254:GLY:H	1.86	0.41
1:A:222:ALA:HB3	1:A:225:GLU:OE2	2.20	0.41
1:B:49:MET:C	1:B:75:CYS:HB2	2.41	0.41
1:C:223:ALA:HB3	1:C:224:PRO:HD3	2.01	0.41
1:A:97:ASP:HB3	1:A:115:VAL:CG1	2.50	0.40
1:B:274[A]:ASN:HA	1:B:275:PRO:HD2	1.88	0.40
1:A:128:PRO:HB3	1:A:270:MET:SD	2.60	0.40
1:B:223:ALA:N	1:B:224:PRO:CD	2.84	0.40
1:B:277[B]:GLN:NE2	1:B:278:VAL:N	2.65	0.40
1:A:50:ARG:HA	1:A:76:THR:HG23	2.03	0.40
1:A:152:THR:O	1:A:156:LYS:HG3	2.22	0.40
1:A:119:SER:OG	1:A:287:GLY:HA3	2.22	0.40
1:B:311:GLY:HA3	1:B:339:PRO:HB3	2.03	0.40
1:B:336:LYS:HA	1:B:337:GLU:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/379 (92%)	340 (98%)	7 (2%)	1 (0%)	41 50
1	B	346/379 (91%)	336 (97%)	10 (3%)	0	100 100
1	C	346/379 (91%)	340 (98%)	6 (2%)	0	100 100
1	D	345/379 (91%)	338 (98%)	7 (2%)	0	100 100
All	All	1385/1516 (91%)	1354 (98%)	30 (2%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	LYS

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	272/301 (90%)	269 (99%)	3 (1%)	73 86
1	B	270/301 (90%)	268 (99%)	2 (1%)	84 92
1	C	266/301 (88%)	260 (98%)	6 (2%)	50 67
1	D	271/301 (90%)	267 (98%)	4 (2%)	65 79
All	All	1079/1204 (90%)	1064 (99%)	15 (1%)	67 81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	273	LYS
1	A	279	TYR
1	B	100	GLU
1	B	265	GLU
1	C	0	SER
1	C	34	GLN

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Mol	Chain	Res	Type
1	C	100	GLU
1	C	103	ASN
1	C	113	MET
1	C	338	SER
1	D	100	GLU
1	D	234	ARG
1	D	258	GLU
1	D	269	SER

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

Mol	Chain	Res	Type
1	B	184	GLN
1	C	34	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	CSO	D	286	1	3,6,7	0.60	0	0,6,8	-	-
1	CSO	C	286	1	3,6,7	0.60	0	0,6,8	-	-
1	CSO	A	286	1	3,6,7	0.60	0	0,6,8	-	-
1	CSO	B	286	1	3,6,7	0.61	0	0,6,8	-	-

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
1	CSO	D	286	1	-	0/1/5/7	-
1	CSO	C	286	1	-	0/1/5/7	-
1	CSO	A	286	1	-	0/1/5/7	-
1	CSO	B	286	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	286	CSO	1	0
1	A	286	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 31 are monoatomic - leaving 22 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	SO4	A	353	-	4,4,4	0.14	0	6,6,6	0.06	0
3	AMP	C	349	-	22,25,25	0.86	1 (4%)	25,38,38	1.22	2 (8%)
4	SO4	C	351	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	C	352	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	350	-	4,4,4	0.15	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	350	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	350	-	4,4,4	0.14	0	6,6,6	0.06	0
3	AMP	C	348	-	22,25,25	0.84	1 (4%)	25,38,38	1.26	3 (12%)
4	SO4	D	351	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	B	349	-	4,4,4	0.15	0	6,6,6	0.04	0
3	AMP	B	348	-	22,25,25	0.84	1 (4%)	25,38,38	1.26	3 (12%)
3	AMP	A	348	-	22,25,25	0.87	1 (4%)	25,38,38	1.22	3 (12%)
4	SO4	D	348	-	4,4,4	0.12	0	6,6,6	0.21	0
6	GOL	A	365	-	5,5,5	0.35	0	5,5,5	0.75	0
4	SO4	A	351	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	354	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	D	350	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	352	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	352	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	353	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	D	349	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	A	349	-	4,4,4	0.14	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	C	349	-	-	1/6/26/26	0/3/3/3
3	AMP	B	348	-	-	0/6/26/26	0/3/3/3
3	AMP	A	348	-	-	1/6/26/26	0/3/3/3
3	AMP	C	348	-	-	0/6/26/26	0/3/3/3
6	GOL	A	365	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	348	AMP	C5-C4	2.44	1.47	1.40
3	B	348	AMP	C5-C4	2.33	1.47	1.40
3	C	349	AMP	C5-C4	2.32	1.47	1.40
3	C	348	AMP	C5-C4	2.31	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	348	AMP	N3-C2-N1	-3.39	123.37	128.68
3	C	348	AMP	N3-C2-N1	-3.36	123.43	128.68
3	C	349	AMP	N3-C2-N1	-3.18	123.72	128.68
3	A	348	AMP	N3-C2-N1	-3.10	123.83	128.68
3	C	348	AMP	C4-C5-N7	-2.70	106.58	109.40
3	A	348	AMP	C4-C5-N7	-2.68	106.61	109.40
3	C	349	AMP	C4-C5-N7	-2.50	106.79	109.40
3	B	348	AMP	C4-C5-N7	-2.44	106.85	109.40
3	C	348	AMP	O3P-P-O5'	-2.33	100.52	106.73
3	B	348	AMP	O3P-P-O5'	-2.15	101.02	106.73
3	A	348	AMP	O3P-P-O5'	-2.09	101.17	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	365	GOL	O1-C1-C2-C3
6	A	365	GOL	O1-C1-C2-O2
3	C	349	AMP	C5'-O5'-P-O2P
6	A	365	GOL	O2-C2-C3-O3
3	A	348	AMP	C5'-O5'-P-O2P
6	A	365	GOL	C1-C2-C3-O3

There are no ring outliers.

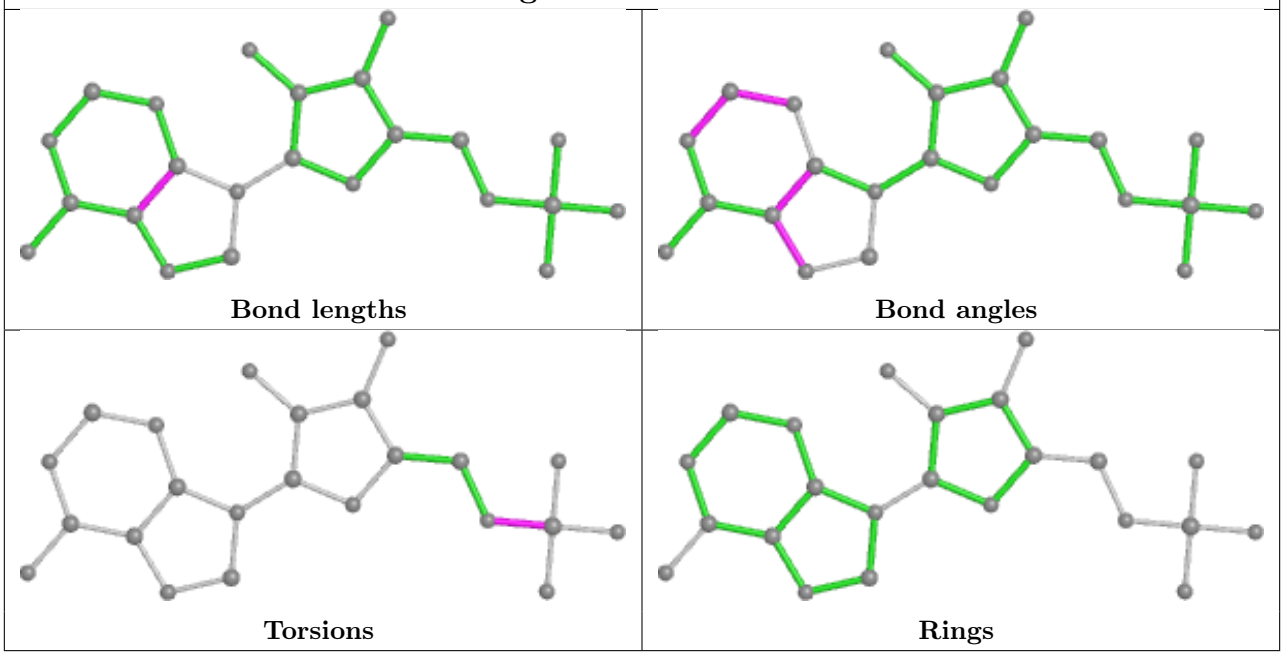
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	351	SO4	1	0
4	C	352	SO4	1	0
3	C	348	AMP	1	0
6	A	365	GOL	2	0
4	D	349	SO4	1	0

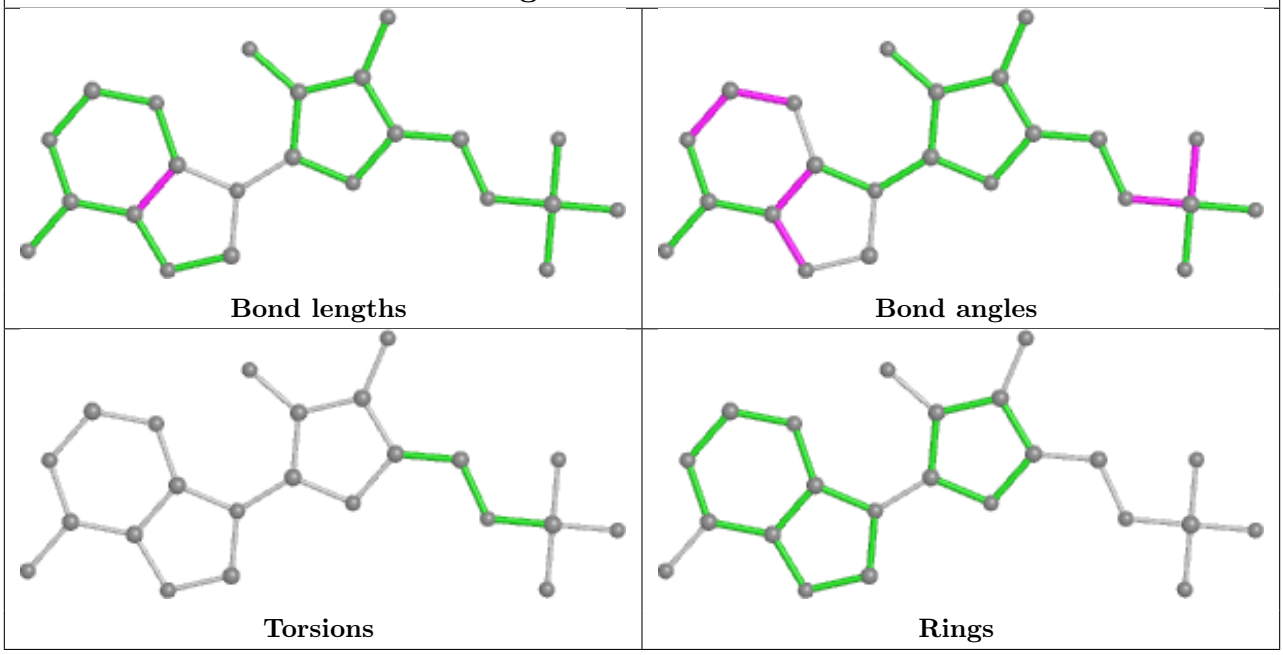
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

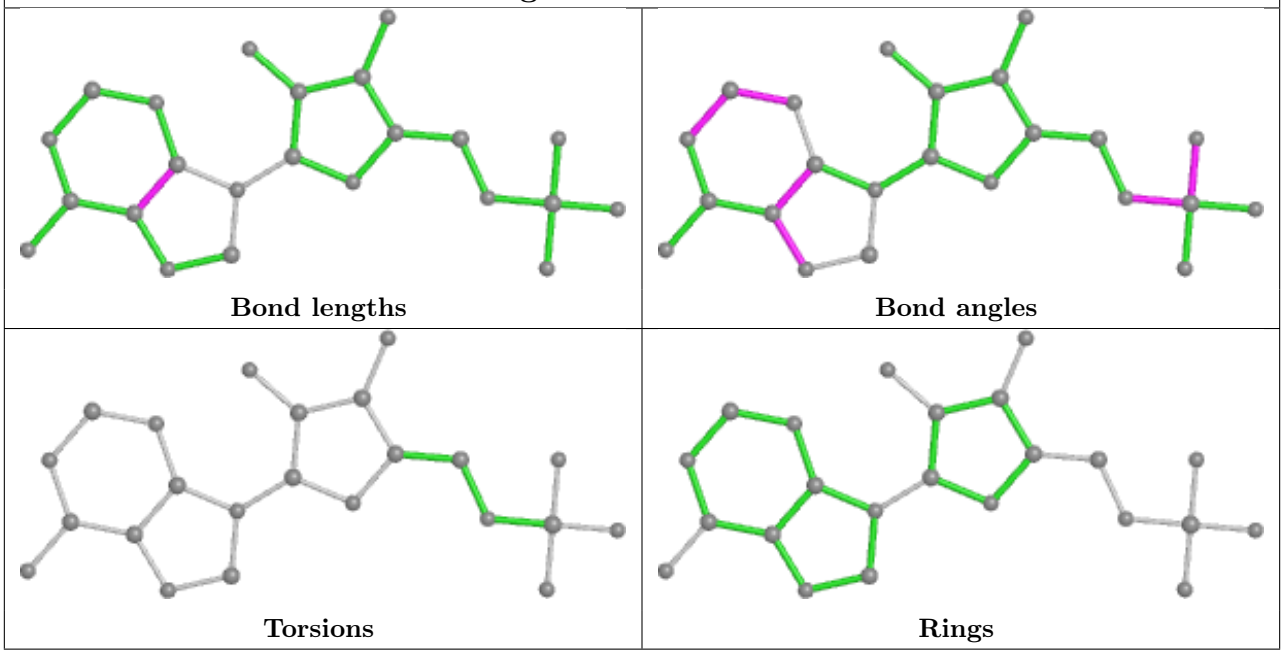
Ligand AMP C 349



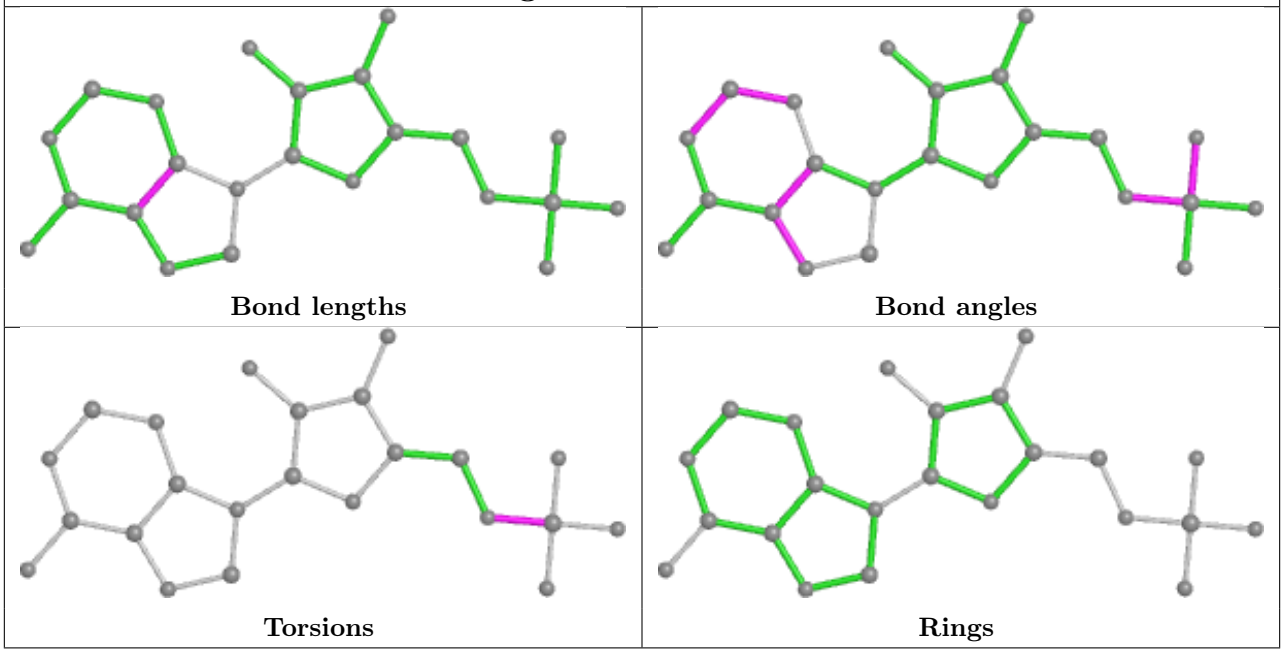
Ligand AMP C 348



Ligand AMP B 348



Ligand AMP A 348



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	346/379 (91%)	0.06	25 (7%)	15 20	17, 24, 61, 86	0
1	B	344/379 (90%)	0.14	32 (9%)	8 11	14, 25, 64, 93	0
1	C	346/379 (91%)	0.04	26 (7%)	14 19	15, 24, 71, 106	0
1	D	345/379 (91%)	0.12	28 (8%)	12 16	16, 26, 70, 90	0
All	All	1381/1516 (91%)	0.09	111 (8%)	12 16	14, 25, 67, 106	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	9.0
1	C	256	ILE	8.9
1	B	78	GLU	7.8
1	B	84	CYS	7.5
1	A	254	GLY	7.5
1	C	254	GLY	7.5
1	D	257	GLY	7.4
1	B	80	ALA	7.2
1	D	256	ILE	6.6
1	A	-1	GLY	6.5
1	C	255	LEU	6.4
1	B	256	ILE	6.3
1	D	254	GLY	6.3
1	D	255	LEU	6.1
1	B	82	SER	5.8
1	D	79	ASP	5.8
1	A	83	PHE	5.7
1	C	257	GLY	5.7
1	B	83	PHE	5.6
1	A	82	SER	5.5
1	C	269	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	269	SER	5.2
1	B	254	GLY	5.1
1	C	271	GLY	5.1
1	D	83	PHE	5.1
1	A	271	GLY	5.1
1	B	270	MET	4.8
1	B	268	ALA	4.7
1	D	82	SER	4.5
1	C	0	SER	4.4
1	D	86	PRO	4.4
1	B	257	GLY	4.3
1	A	79	ASP	4.3
1	D	78	GLU	4.2
1	D	269	SER	4.2
1	A	256	ILE	4.1
1	C	268	ALA	4.1
1	D	268	ALA	4.0
1	A	255	LEU	4.0
1	B	271	GLY	3.9
1	C	-1	GLY	3.9
1	C	261	GLU	3.9
1	D	80	ALA	3.8
1	D	85	ASN	3.8
1	B	75	CYS	3.8
1	B	76	THR	3.7
1	C	253	THR	3.7
1	A	257	GLY	3.7
1	C	249	GLU	3.6
1	A	0	SER	3.6
1	A	268	ALA	3.6
1	D	273	LYS	3.6
1	D	62	ASP	3.5
1	D	270	MET	3.5
1	A	80	ALA	3.5
1	D	77	ARG	3.5
1	A	78	GLU	3.4
1	B	266	ARG	3.3
1	B	252	LYS	3.3
1	B	261	GLU	3.3
1	D	0	SER	3.3
1	B	77	ARG	3.3
1	B	255	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	77	ARG	3.3
1	A	86	PRO	3.2
1	B	273	LYS	3.2
1	A	76	THR	3.2
1	B	258	GLU	3.2
1	D	61	ASP	3.2
1	D	261	GLU	3.1
1	B	262	GLY	3.1
1	C	266	ARG	3.1
1	C	270	MET	3.1
1	A	272	ILE	3.1
1	B	1	VAL	3.0
1	D	266	ARG	3.0
1	B	274[A]	ASN	3.0
1	A	267	LEU	2.9
1	C	258	GLU	2.9
1	B	259	SER	2.8
1	C	336	LYS	2.7
1	C	60	ARG	2.7
1	A	270	MET	2.7
1	A	274	ASN	2.7
1	A	337	GLU	2.6
1	C	267	LEU	2.6
1	B	86	PRO	2.6
1	D	252	LYS	2.6
1	D	60	ARG	2.5
1	C	259	SER	2.5
1	A	248	PRO	2.5
1	C	265	GLU	2.5
1	A	261	GLU	2.5
1	B	269	SER	2.5
1	B	265	GLU	2.5
1	B	85	ASN	2.5
1	D	271	GLY	2.4
1	D	337	GLU	2.4
1	C	62	ASP	2.4
1	B	272	ILE	2.3
1	C	252	LYS	2.3
1	D	274	ASN	2.3
1	C	273	LYS	2.2
1	B	253	THR	2.2
1	B	81	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	82	SER	2.2
1	C	272	ILE	2.2
1	D	265	GLU	2.1
1	A	273	LYS	2.1
1	C	1	VAL	2.1
1	D	250	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	D	286	7/8	0.94	0.12	29,30,34,36	0
1	CSO	C	286	7/8	0.96	0.19	26,27,32,57	0
1	CSO	A	286	7/8	0.96	0.13	25,26,29,54	0
1	CSO	B	286	7/8	0.97	0.08	25,25,30,31	0

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
5	CL	A	361	1/1	0.36	0.20	55,55,55,55	0
5	CL	B	353	1/1	0.39	0.23	57,57,57,57	0
5	CL	C	355	1/1	0.71	0.16	58,58,58,58	0
5	CL	C	359	1/1	0.72	0.14	57,57,57,57	0
5	CL	D	354	1/1	0.74	0.13	74,74,74,74	0
5	CL	C	358	1/1	0.75	0.18	67,67,67,67	0
5	CL	A	358	1/1	0.76	0.20	55,55,55,55	0
5	CL	A	363	1/1	0.78	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	356	1/1	0.78	0.25	61,61,61,61	0
5	CL	A	357	1/1	0.80	0.21	53,53,53,53	0
5	CL	A	364	1/1	0.81	0.09	57,57,57,57	0
5	CL	D	353	1/1	0.81	0.09	53,53,53,53	0
5	CL	B	355	1/1	0.81	0.59	115,115,115,115	0
6	GOL	A	365	6/6	0.83	0.21	33,40,50,52	0
2	MG	B	346	1/1	0.84	0.17	48,48,48,48	0
5	CL	A	360	1/1	0.86	0.12	65,65,65,65	0
5	CL	C	354	1/1	0.87	0.23	59,59,59,59	0
5	CL	A	362	1/1	0.89	0.33	66,66,66,66	0
2	MG	A	346	1/1	0.89	0.33	52,52,52,52	0
5	CL	C	357	1/1	0.91	0.12	61,61,61,61	0
5	CL	B	352	1/1	0.92	0.08	71,71,71,71	0
4	SO4	D	352	5/5	0.92	0.31	47,61,71,78	0
5	CL	B	354	1/1	0.92	0.06	53,53,53,53	0
4	SO4	A	354	5/5	0.93	0.30	54,58,69,72	0
5	CL	A	359	1/1	0.94	0.12	55,55,55,55	0
4	SO4	C	353	5/5	0.94	0.30	52,55,63,67	0
5	CL	A	355	1/1	0.95	0.23	45,45,45,45	0
4	SO4	A	353	5/5	0.95	0.29	55,55,69,72	0
2	MG	C	346	1/1	0.95	0.26	42,42,42,42	0
2	MG	C	347	1/1	0.95	0.19	39,39,39,39	0
4	SO4	A	351	5/5	0.95	0.22	42,52,54,62	0
5	CL	B	351	1/1	0.95	0.09	49,49,49,49	0
4	SO4	D	351	5/5	0.96	0.30	42,52,54,60	0
2	MG	D	347	1/1	0.96	0.11	36,36,36,36	0
2	MG	D	346	1/1	0.96	0.29	44,44,44,44	0
4	SO4	A	352	5/5	0.96	0.25	56,57,63,67	0
4	SO4	D	350	5/5	0.96	0.22	37,44,52,54	0
2	MG	A	347	1/1	0.97	0.22	36,36,36,36	0
4	SO4	C	350	5/5	0.97	0.11	37,39,43,47	0
2	MG	B	347	1/1	0.97	0.23	36,36,36,36	0
4	SO4	D	349	5/5	0.97	0.25	37,42,46,50	0
4	SO4	A	350	5/5	0.97	0.28	44,50,54,57	0
3	AMP	C	349	23/23	0.98	0.10	16,18,19,20	0
3	AMP	A	348	23/23	0.98	0.10	16,18,19,22	0
4	SO4	B	349	5/5	0.98	0.08	35,36,42,43	0
4	SO4	B	350	5/5	0.98	0.23	37,51,52,52	0
3	AMP	B	348	23/23	0.98	0.11	15,17,18,19	0
4	SO4	C	351	5/5	0.98	0.32	40,46,49,53	0
4	SO4	C	352	5/5	0.98	0.25	44,45,54,60	0
3	AMP	C	348	23/23	0.98	0.10	15,16,17,18	0

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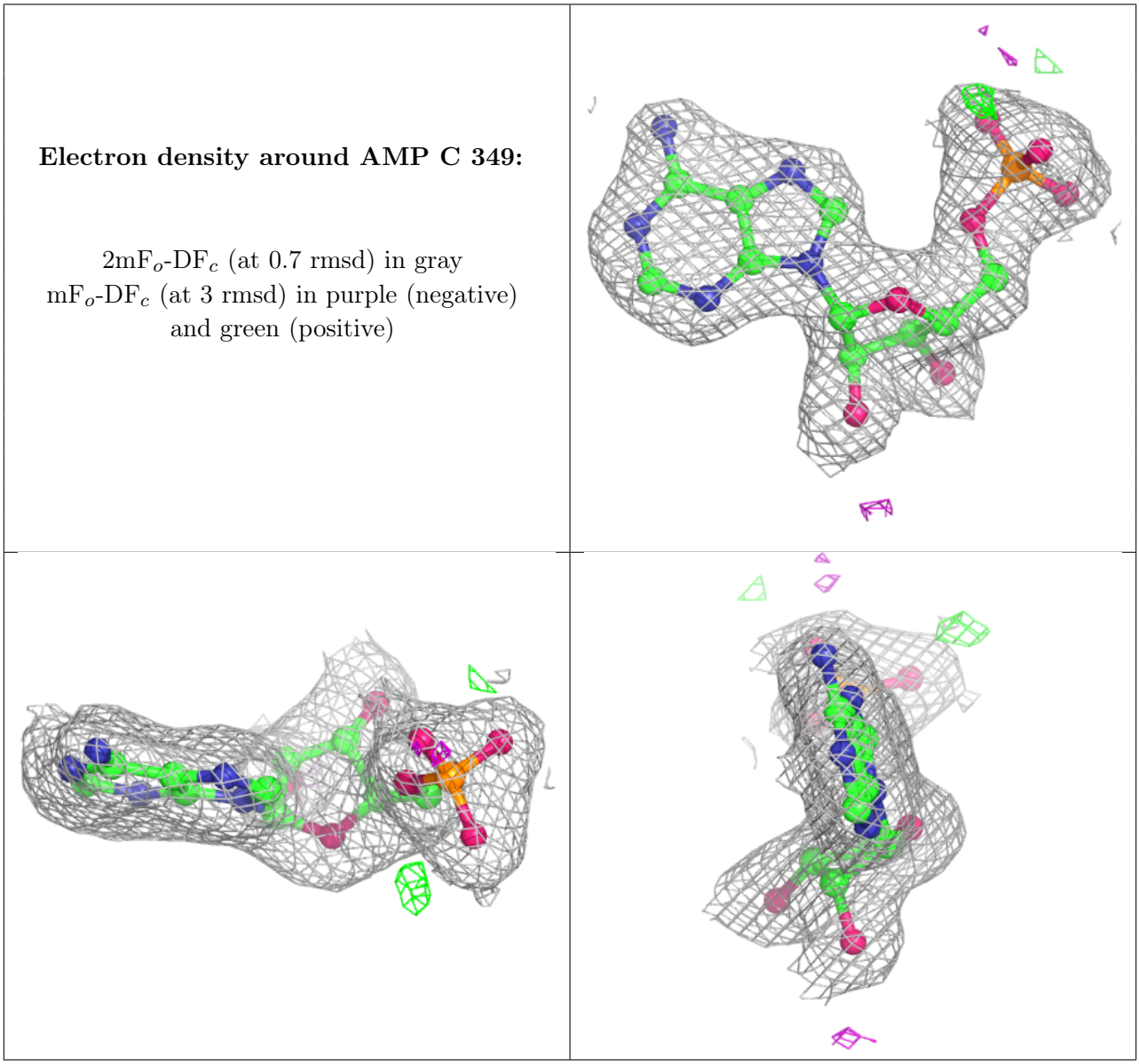
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	348	5/5	0.98	0.09	37,39,42,43	0
4	SO4	A	349	5/5	0.99	0.14	34,37,39,43	0
5	CL	C	356	1/1	0.99	0.06	38,38,38,38	0

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.

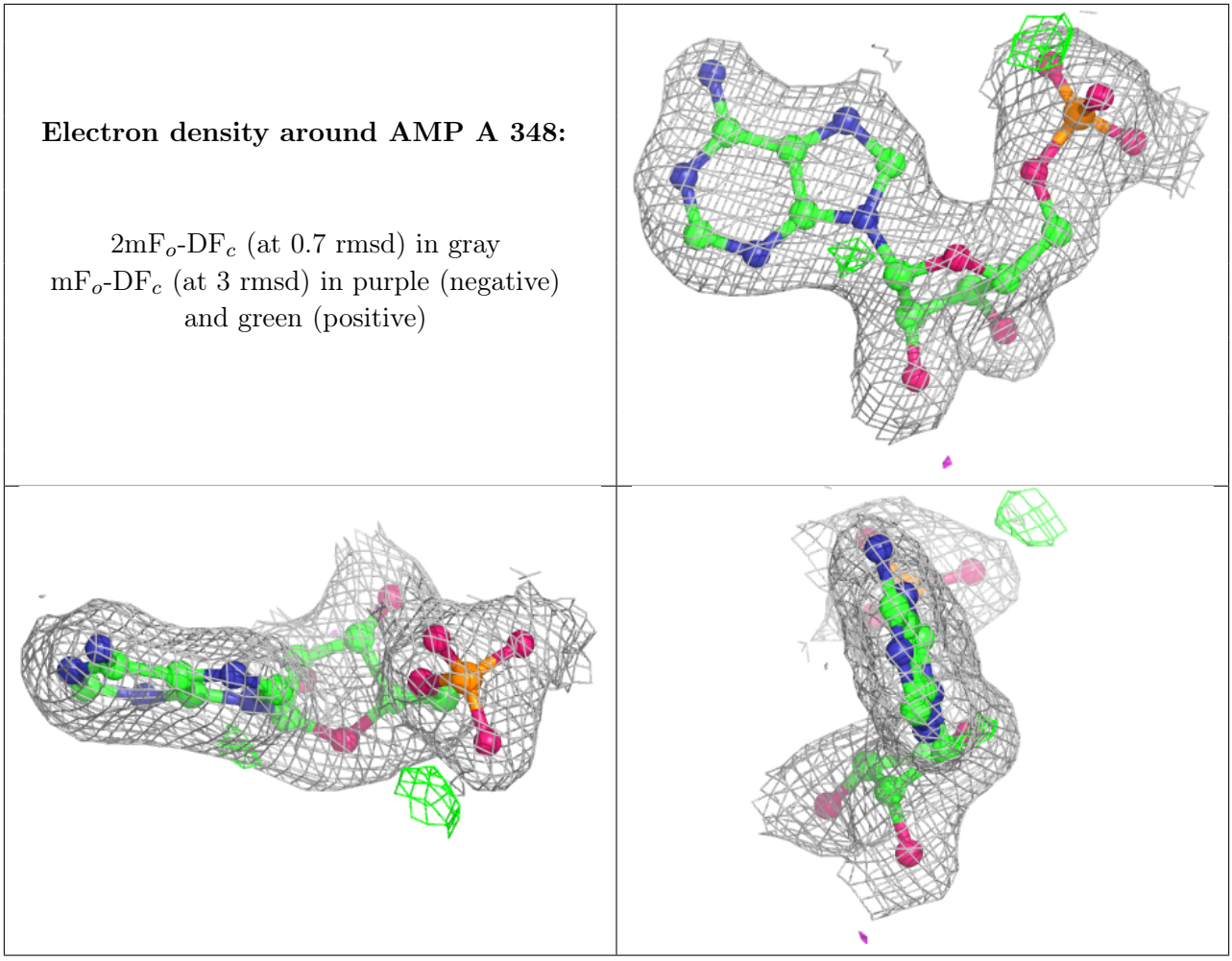
Electron density around AMP C 349:

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



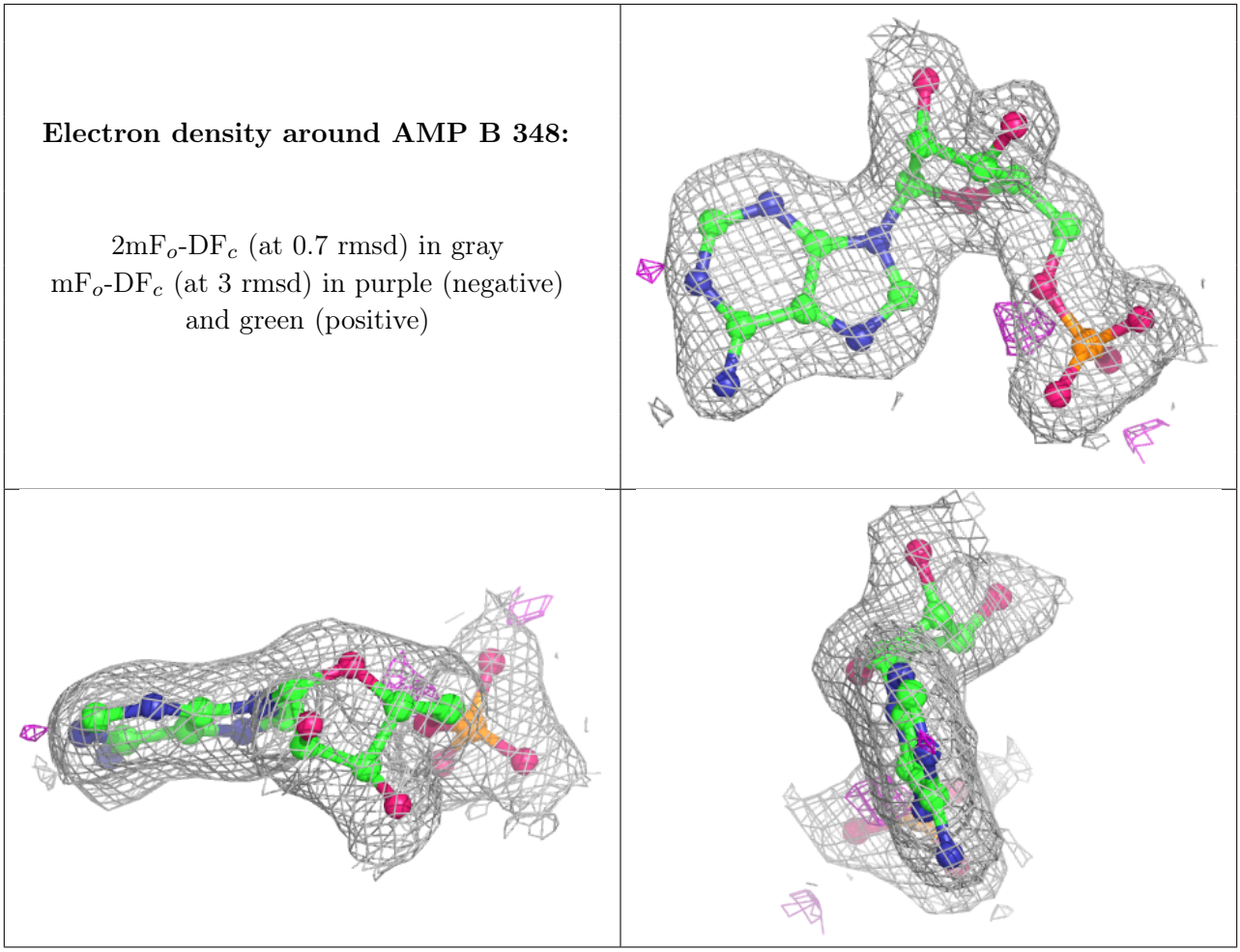
Electron density around AMP A 348:

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



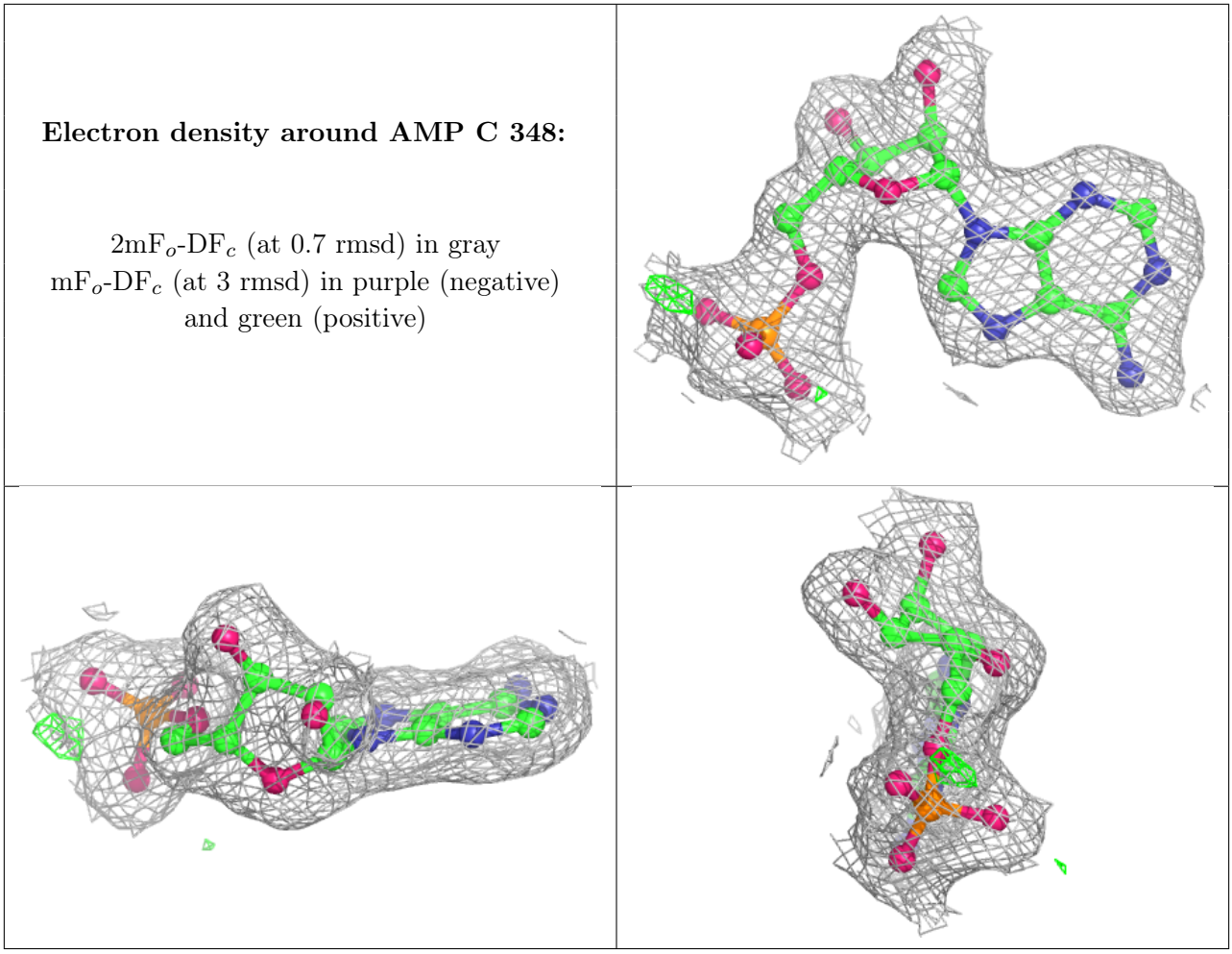
Electron density around AMP B 348:

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



Electron density around AMP C 348:

$2mF_o$-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.