



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:32 am BST

PDB ID : 6JRQ  
Title : Crystal structure of adenylosuccinate synthetase, PurA, from *Thermus thermophilus*  
Authors : Sampei, G.; Kawai, G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2019-04-05  
Resolution : 2.10 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](mailto: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.

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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 : 2.11  
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) : 2.11

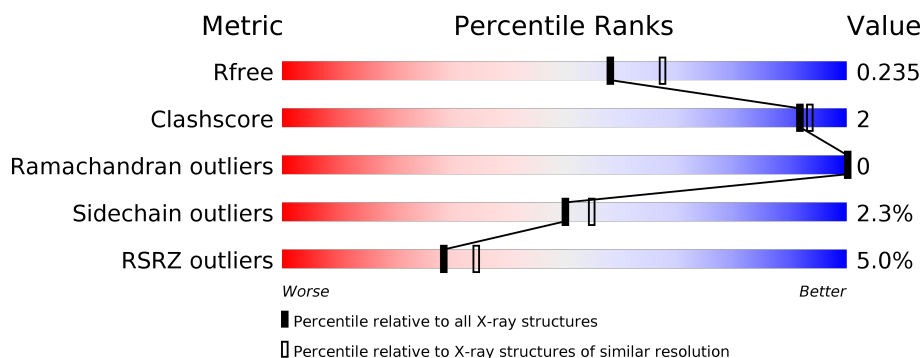
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	408	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	B	408	<div> <div>7%</div> <div>92%</div> <div>7%</div> </div>
1	C	408	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	D	408	<div> <div>6%</div> <div>89%</div> <div>10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	504	-	-	X	-

## 2 Entry composition [i](#)

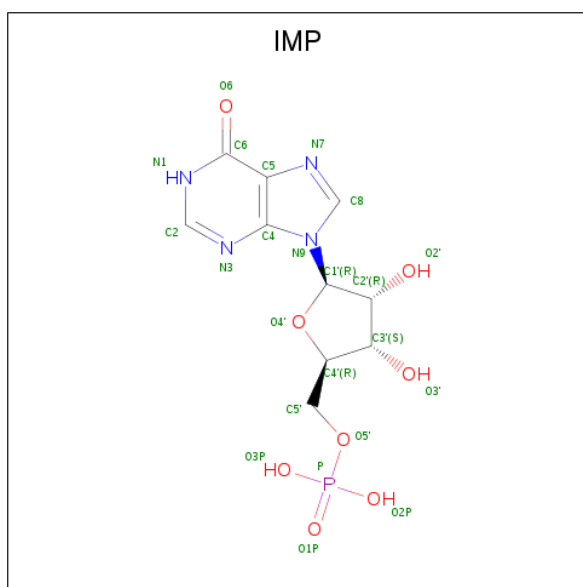
There are 4 unique types of molecules in this entry. The entry contains 13369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenylosuccinate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3165	2003	577	582	3			
1	B	407	Total	C	N	O	S	0	1	0
			3173	2008	580	582	3			
1	C	407	Total	C	N	O	S	0	0	0
			3165	2003	577	582	3			
1	D	407	Total	C	N	O	S	0	0	0
			3165	2003	577	582	3			

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		

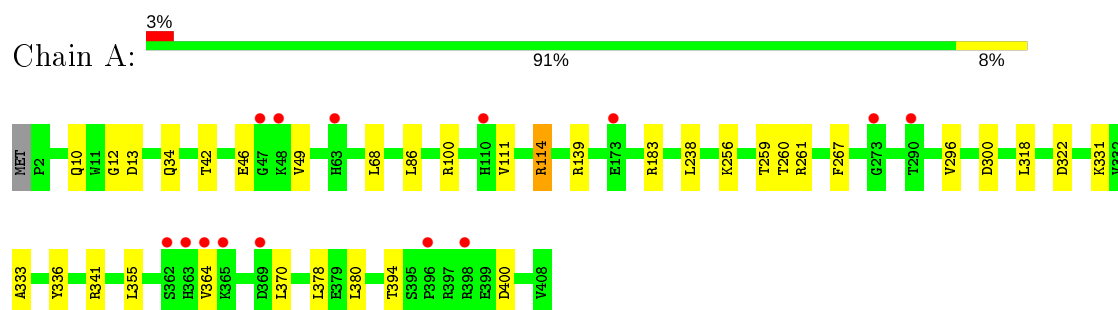
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	127	Total	O	0	0
			127	127		
4	C	158	Total	O	0	0
			158	158		
4	D	123	Total	O	0	0
			123	123		

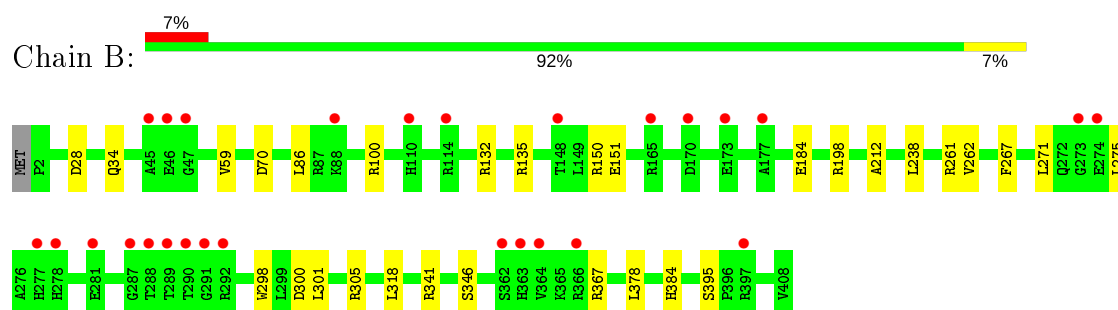
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

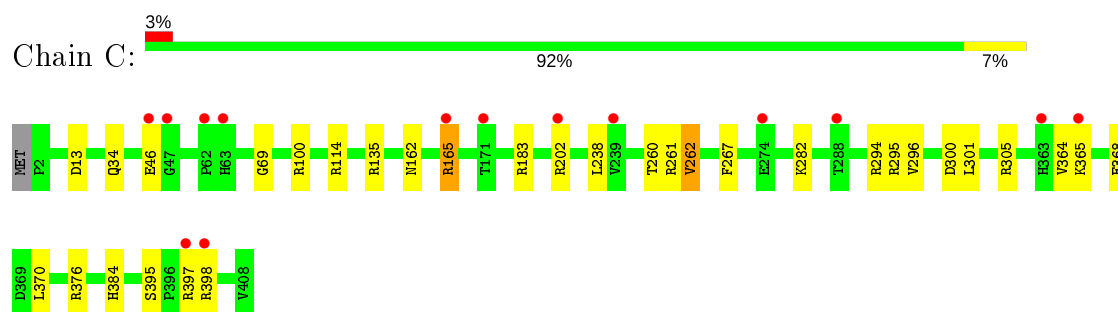
- Molecule 1: Adenylosuccinate synthetase



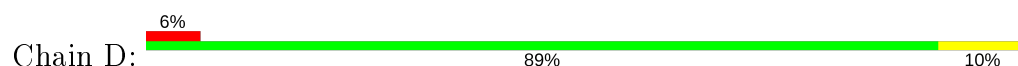
- Molecule 1: Adenylosuccinate synthetase

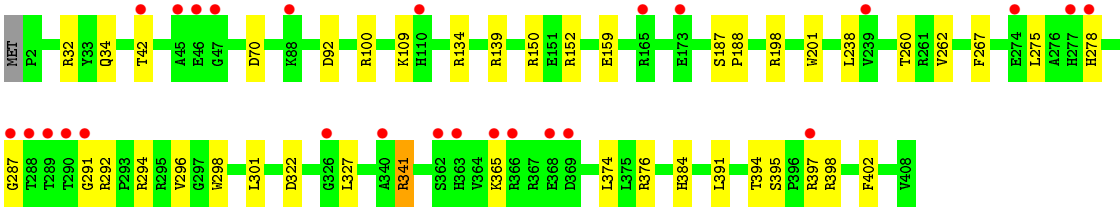


- Molecule 1: Adenylosuccinate synthetase



- Molecule 1: Adenylosuccinate synthetase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.85Å 106.39Å 114.53Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	34.47 – 2.10 34.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.47-2.10) 99.1 (34.47-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.183 , 0.226 0.193 , 0.235	Depositor DCC
$R_{free}$ test set	5094 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: IMP, EDO

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	0.91	0/3235	0.99	10/4384 (0.2%)
1	B	0.89	0/3246	0.97	13/4398 (0.3%)
1	C	0.93	1/3235 (0.0%)	1.01	15/4384 (0.3%)
1	D	0.88	1/3235 (0.0%)	0.98	13/4384 (0.3%)
All	All	0.90	2/12951 (0.0%)	0.99	51/17550 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	GLY	C-O	6.62	1.34	1.23
1	D	201	TRP	CG-CD1	5.18	1.44	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	D	341	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	C	183	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	139	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	70	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	C	135	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	262	VAL	CB-CA-C	-7.10	97.90	111.40
1	A	341	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	198	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	300	ASP	CB-CG-OD1	6.84	124.45	118.30
1	C	100	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	135	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	261	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	100	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	150	ARG	NE-CZ-NH1	6.39	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	28	ASP	CB-CG-OD1	-6.24	112.68	118.30
1	A	183	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	183	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	341	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	165	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	305	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	32	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	294	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	134	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	C	295	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	261	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	261	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	150	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	28	ASP	CB-CG-OD2	5.65	123.39	118.30
1	D	152	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	300	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	336	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	B	132	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	261	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	261	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	D	70	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	100	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	13	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	294	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	D	92	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	262	VAL	CB-CA-C	-5.26	101.41	111.40
1	C	305	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	139	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	13	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	32	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	198	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	100	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	398	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	397	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	341	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	3165	0	3172	17	0
1	B	3173	0	3185	8	0
1	C	3165	0	3172	7	0
1	D	3165	0	3172	11	0
2	A	23	0	10	0	0
2	B	23	0	10	0	0
2	C	23	0	10	1	0
2	D	23	0	10	0	0
3	A	16	0	24	5	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	D	8	0	12	0	0
4	A	161	0	0	1	0
4	B	127	0	0	0	0
4	C	158	0	0	0	0
4	D	123	0	0	0	0
All	All	13369	0	12801	40	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 2.

All (40) 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:A:12:GLY:O	3:A:504:EDO:H11	1.54	1.08
1:A:10:GLN:HB2	3:A:504:EDO:H12	1.67	0.76
1:A:331:LYS:NZ	4:A:601:HOH:O	2.34	0.59
1:A:259:THR:HA	3:A:504:EDO:O2	2.02	0.59
1:A:318:LEU:HD23	1:A:378:LEU:CD2	2.34	0.58
1:D:301:LEU:HD13	1:D:384:HIS:HB2	1.86	0.57
1:A:364:VAL:HG11	1:A:370:LEU:HD23	1.87	0.55
1:C:260:THR:HG22	1:C:296:VAL:HG12	1.89	0.54
1:A:111:VAL:O	1:A:114:ARG:HD3	2.08	0.53
1:A:238:LEU:HD22	1:B:238:LEU:HD22	1.91	0.53
1:C:162:ASN:OD1	1:C:165:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:VAL:HG11	1:C:370:LEU:HD23	1.91	0.52
1:D:322:ASP:HB3	1:D:394:THR:O	2.10	0.51
1:C:114:ARG:NH2	1:D:159:GLU:OE2	2.44	0.51
1:C:238:LEU:HD22	1:D:238:LEU:HD22	1.92	0.51
1:A:260:THR:HG22	1:A:296:VAL:HG12	1.94	0.50
1:A:42:THR:HG23	1:A:49:VAL:HG13	1.94	0.49
1:D:278:HIS:CD2	1:D:327:LEU:HD21	2.48	0.49
1:D:374:LEU:HD23	1:D:374:LEU:C	2.34	0.48
1:D:275:LEU:HD21	1:D:298:TRP:CZ2	2.48	0.47
1:A:256:LYS:HE2	3:A:504:EDO:H21	1.97	0.47
1:B:318:LEU:HD23	1:B:378:LEU:CD2	2.45	0.47
1:C:301:LEU:HD13	1:C:384:HIS:HB2	1.97	0.46
1:B:59:VAL:HG21	1:B:86:LEU:HD11	1.99	0.45
1:A:256:LYS:HE2	3:A:504:EDO:C2	2.46	0.45
1:B:34:GLN:NE2	1:B:212:ALA:H	2.15	0.44
1:A:355:LEU:HD21	1:A:380:LEU:HD22	2.00	0.44
1:B:301:LEU:HD13	1:B:384:HIS:HB2	2.00	0.44
1:D:287:GLY:O	1:D:291:GLY:HA2	2.18	0.44
1:A:300:ASP:HA	1:A:333:ALA:HB3	1.98	0.44
1:C:262:VAL:O	2:C:501:IMP:O2'	2.34	0.42
1:A:394:THR:OG1	1:A:400:ASP:HB3	2.18	0.42
1:B:271:LEU:HD22	1:B:275:LEU:HD23	2.01	0.42
1:A:68:LEU:N	1:A:68:LEU:HD12	2.35	0.41
1:B:151:GLU:OE1	1:B:151:GLU:HA	2.20	0.41
1:A:322:ASP:HB3	1:A:394:THR:O	2.21	0.41
1:D:187:SER:N	1:D:188:PRO:CD	2.83	0.41
1:D:391:LEU:HA	1:D:402:PHE:O	2.20	0.41
1:D:260:THR:HG22	1:D:296:VAL:HG12	2.03	0.40
1:B:275:LEU:HD21	1:B:298:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	405/408 (99%)	393 (97%)	12 (3%)	0	100	100
1	B	406/408 (100%)	391 (96%)	15 (4%)	0	100	100
1	C	405/408 (99%)	396 (98%)	9 (2%)	0	100	100
1	D	405/408 (99%)	390 (96%)	15 (4%)	0	100	100
All	All	1621/1632 (99%)	1570 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	327/328 (100%)	322 (98%)	5 (2%)	65	71
1	B	328/328 (100%)	323 (98%)	5 (2%)	65	71
1	C	327/328 (100%)	318 (97%)	9 (3%)	43	47
1	D	327/328 (100%)	316 (97%)	11 (3%)	37	39
All	All	1309/1312 (100%)	1279 (98%)	30 (2%)	50	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	46	GLU
1	A	86	LEU
1	A	114	ARG
1	A	267	PHE
1	B	184	GLU
1	B	267	PHE
1	B	346	SER
1	B	367	ARG
1	B	395	SER
1	C	34	GLN
1	C	46	GLU
1	C	202	ARG

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Mol	Chain	Res	Type
1	C	267	PHE
1	C	282	LYS
1	C	365	LYS
1	C	368	GLU
1	C	376	ARG
1	C	395	SER
1	D	34	GLN
1	D	42	THR
1	D	109	LYS
1	D	262	VAL
1	D	267	PHE
1	D	292	ARG
1	D	341	ARG
1	D	365	LYS
1	D	376	ARG
1	D	395	SER
1	D	398	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	61	HIS
1	B	278	HIS
1	D	61	HIS
1	D	278	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

14 ligands 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$
3	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.69	0
3	EDO	A	502	-	3,3,3	0.58	0	2,2,2	0.84	0
3	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.18	0
3	EDO	A	503	-	3,3,3	0.56	0	2,2,2	0.51	0
3	EDO	C	503	-	3,3,3	0.68	0	2,2,2	0.31	0
3	EDO	A	504	-	3,3,3	0.66	0	2,2,2	0.96	0
2	IMP	B	501	-	21,25,25	1.47	4 (19%)	23,38,38	2.15	7 (30%)
2	IMP	A	501	-	21,25,25	1.21	4 (19%)	23,38,38	1.91	7 (30%)
2	IMP	D	501	-	21,25,25	1.53	5 (23%)	23,38,38	2.09	10 (43%)
2	IMP	C	501	-	21,25,25	1.52	4 (19%)	23,38,38	1.97	9 (39%)
3	EDO	D	503	-	3,3,3	0.54	0	2,2,2	0.46	0
3	EDO	A	505	-	3,3,3	0.66	0	2,2,2	0.32	0
3	EDO	B	503	-	3,3,3	0.60	0	2,2,2	0.10	0
3	EDO	D	502	-	3,3,3	0.73	0	2,2,2	0.40	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	EDO	C	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
2	IMP	C	501	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	IMP	C2-N3	3.68	1.38	1.32
2	C	501	IMP	C6-C5	3.16	1.46	1.41
2	B	501	IMP	C6-C5	3.06	1.46	1.41
2	C	501	IMP	O4'-C4'	-3.04	1.38	1.45
2	B	501	IMP	C2'-C1'	-2.69	1.49	1.53
2	C	501	IMP	C5-C4	2.68	1.48	1.40
2	B	501	IMP	C2-N3	2.68	1.36	1.32
2	A	501	IMP	C6-C5	2.49	1.45	1.41
2	B	501	IMP	O4'-C4'	-2.41	1.39	1.45
2	C	501	IMP	C2-N1	2.38	1.38	1.33
2	A	501	IMP	C2-N3	2.31	1.35	1.32
2	D	501	IMP	C6-C5	2.26	1.45	1.41
2	A	501	IMP	O4'-C4'	-2.26	1.40	1.45
2	D	501	IMP	O3'-C3'	2.22	1.48	1.43
2	D	501	IMP	C5-C4	2.10	1.46	1.40
2	D	501	IMP	O4'-C1'	2.05	1.43	1.41
2	A	501	IMP	C5-C4	2.05	1.46	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IMP	C6-C5-C4	-4.65	116.36	120.80
2	B	501	IMP	C5'-C4'-C3'	4.40	131.68	115.18
2	B	501	IMP	C6-C5-C4	-4.25	116.74	120.80
2	C	501	IMP	C6-C5-C4	-4.12	116.87	120.80
2	B	501	IMP	C1'-N9-C4	-3.90	119.79	126.64
2	D	501	IMP	C5'-C4'-C3'	3.84	129.56	115.18
2	B	501	IMP	C2-N1-C6	3.81	122.26	115.88
2	C	501	IMP	C2-N1-C6	3.78	122.21	115.88
2	A	501	IMP	O4'-C4'-C5'	3.42	120.63	109.37
2	D	501	IMP	C2-N1-C6	3.41	121.59	115.88
2	C	501	IMP	C5'-C4'-C3'	3.28	127.46	115.18
2	B	501	IMP	N3-C2-N1	-3.24	123.61	128.68
2	D	501	IMP	C2'-C3'-C4'	-3.23	96.37	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IMP	N3-C2-N1	-3.18	123.72	128.68
2	A	501	IMP	C2-N1-C6	3.13	121.12	115.88
2	D	501	IMP	C1'-N9-C4	-3.00	121.37	126.64
2	D	501	IMP	N3-C2-N1	-2.97	124.04	128.68
2	D	501	IMP	C6-C5-C4	-2.79	118.13	120.80
2	C	501	IMP	N3-C2-N1	-2.77	124.35	128.68
2	B	501	IMP	C3'-C2'-C1'	-2.65	96.99	100.98
2	A	501	IMP	C2'-C3'-C4'	-2.60	97.59	102.64
2	D	501	IMP	C4-C5-N7	-2.49	106.80	109.40
2	C	501	IMP	O4'-C4'-C5'	2.46	117.47	109.37
2	C	501	IMP	C2'-C3'-C4'	-2.40	97.98	102.64
2	D	501	IMP	O5'-C5'-C4'	-2.33	100.97	108.99
2	C	501	IMP	P-O5'-C5'	2.33	124.71	118.30
2	D	501	IMP	O4'-C4'-C5'	2.28	116.86	109.37
2	C	501	IMP	O5'-C5'-C4'	-2.22	101.33	108.99
2	A	501	IMP	O5'-C5'-C4'	-2.20	101.41	108.99
2	A	501	IMP	C5'-C4'-C3'	2.12	123.13	115.18
2	B	501	IMP	C2'-C3'-C4'	-2.08	98.59	102.64
2	D	501	IMP	O3'-C3'-C4'	2.08	117.06	111.05
2	C	501	IMP	O4'-C4'-C3'	2.03	109.12	105.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2

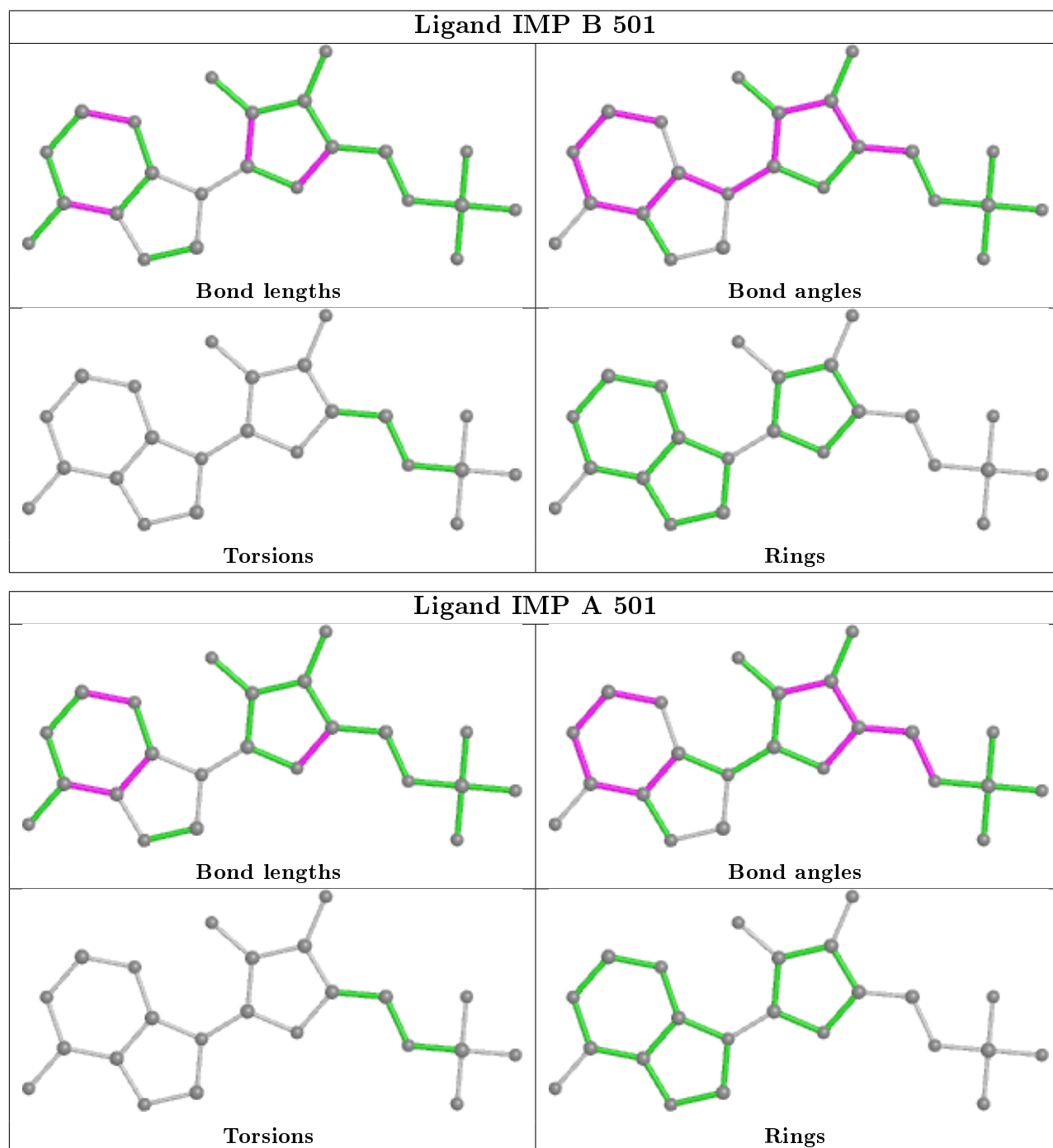
There are no ring outliers.

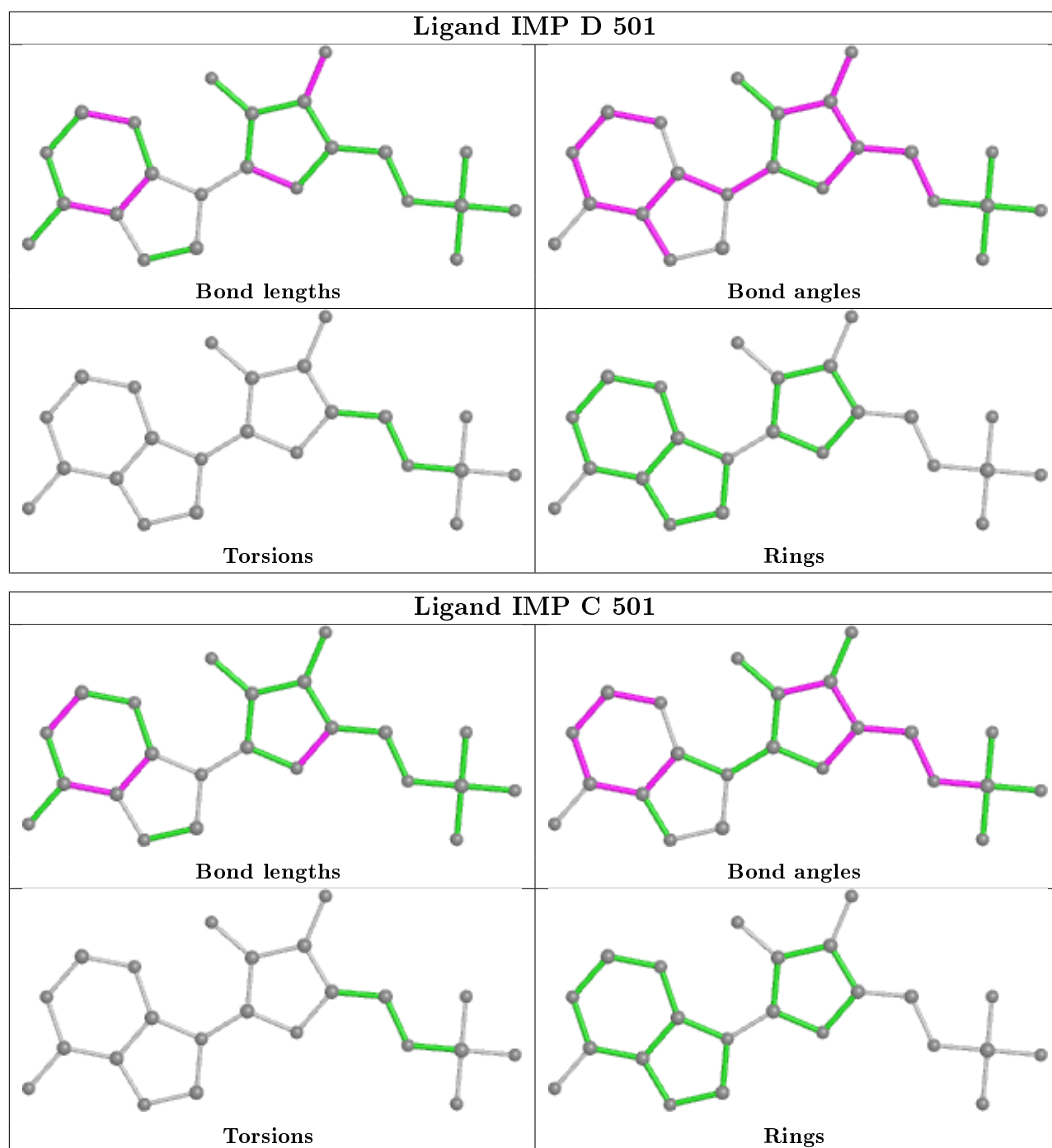
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	5	0
2	C	501	IMP	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 than 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.





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/408 (99%)	0.22	14 (3%) 45 51	9, 16, 36, 64	0
1	B	407/408 (99%)	0.36	27 (6%) 18 23	8, 16, 44, 80	0
1	C	407/408 (99%)	0.21	14 (3%) 45 51	9, 15, 36, 57	0
1	D	407/408 (99%)	0.48	26 (6%) 19 24	9, 19, 46, 106	0
All	All	1628/1632 (99%)	0.32	81 (4%) 28 34	8, 16, 41, 106	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	291	GLY	15.2
1	B	291	GLY	7.8
1	D	363	HIS	6.5
1	D	289	THR	5.3
1	D	47	GLY	5.2
1	B	47	GLY	5.1
1	B	397	ARG	4.3
1	C	363	HIS	4.2
1	B	363	HIS	4.2
1	D	278	HIS	3.9
1	D	397	ARG	3.8
1	D	362	SER	3.7
1	A	363	HIS	3.7
1	B	366	ARG	3.7
1	A	273	GLY	3.6
1	D	173	GLU	3.4
1	B	273	GLY	3.3
1	B	110	HIS	3.3
1	D	287	GLY	3.2
1	B	288	THR	3.2
1	C	62	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	288	THR	3.2
1	C	63	HIS	3.1
1	A	365	LYS	3.1
1	D	274	GLU	3.1
1	A	63	HIS	3.1
1	B	46	GLU	3.1
1	D	340	ALA	3.1
1	B	165	ARG	3.0
1	C	365	LYS	3.0
1	B	292	ARG	3.0
1	B	45	ALA	2.9
1	D	290	THR	2.9
1	A	362	SER	2.9
1	D	277	HIS	2.8
1	C	165	ARG	2.8
1	B	287	GLY	2.8
1	B	170	ASP	2.8
1	A	47	GLY	2.8
1	D	45	ALA	2.7
1	B	277	HIS	2.7
1	B	362	SER	2.7
1	B	289	THR	2.7
1	B	278	HIS	2.7
1	D	366	ARG	2.7
1	B	173	GLU	2.6
1	A	396	PRO	2.6
1	C	171	THR	2.5
1	D	110	HIS	2.5
1	B	177	ALA	2.4
1	A	110	HIS	2.4
1	D	88	LYS	2.4
1	C	46	GLU	2.4
1	C	398	ARG	2.3
1	D	46	GLU	2.3
1	C	47	GLY	2.2
1	B	274	GLU	2.2
1	A	364	VAL	2.2
1	D	368	GLU	2.2
1	A	369	ASP	2.2
1	C	274	GLU	2.2
1	B	364	VAL	2.2
1	B	114	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	290	THR	2.1
1	C	397	ARG	2.1
1	D	365	LYS	2.1
1	A	398	ARG	2.1
1	B	88	LYS	2.1
1	C	288	THR	2.1
1	B	148	THR	2.1
1	A	173	GLU	2.0
1	D	42	THR	2.0
1	B	290	THR	2.0
1	B	281	GLU	2.0
1	C	239	VAL	2.0
1	D	239	VAL	2.0
1	C	202	ARG	2.0
1	D	165	ARG	2.0
1	D	326	GLY	2.0
1	A	48	LYS	2.0
1	D	369	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	505	4/4	0.90	0.16	24,25,25,28	0
3	EDO	A	503	4/4	0.94	0.12	15,16,16,20	0
3	EDO	C	502	4/4	0.94	0.15	17,17,18,21	0
3	EDO	D	503	4/4	0.95	0.16	18,21,21,22	0
3	EDO	C	503	4/4	0.95	0.10	14,16,16,16	0

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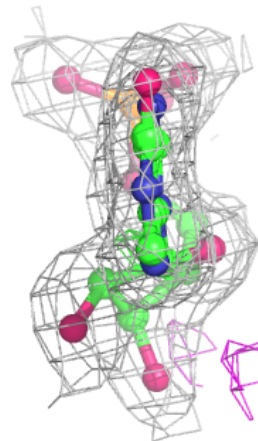
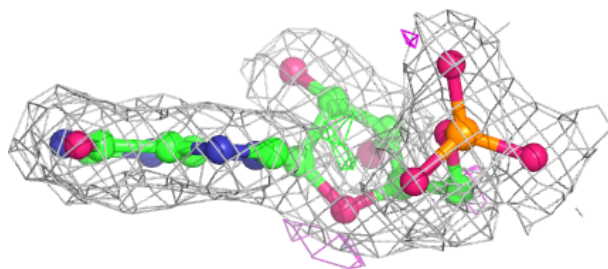
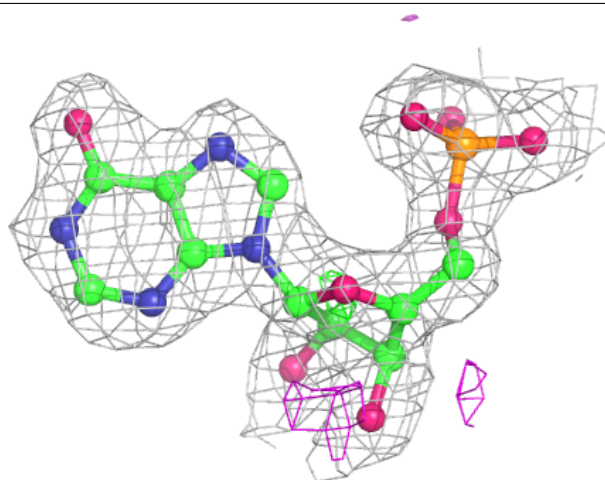
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	503	4/4	0.95	0.14	18,20,21,21	0
3	EDO	D	502	4/4	0.95	0.11	17,17,18,18	0
3	EDO	A	502	4/4	0.96	0.10	16,18,19,19	0
3	EDO	B	502	4/4	0.96	0.10	13,15,16,17	0
2	IMP	C	501	23/23	0.97	0.10	10,11,13,13	0
3	EDO	A	504	4/4	0.97	0.15	16,17,18,19	0
2	IMP	B	501	23/23	0.97	0.10	11,13,14,15	0
2	IMP	A	501	23/23	0.97	0.09	10,12,14,14	0
2	IMP	D	501	23/23	0.97	0.10	12,15,16,17	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 IMP C 501:**

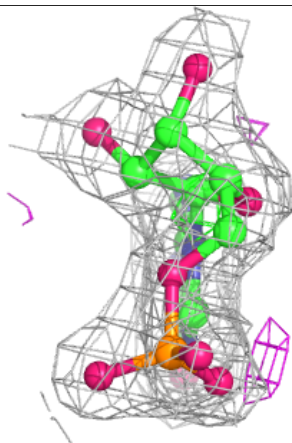
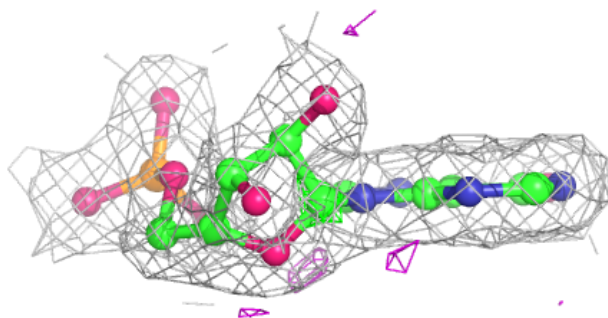
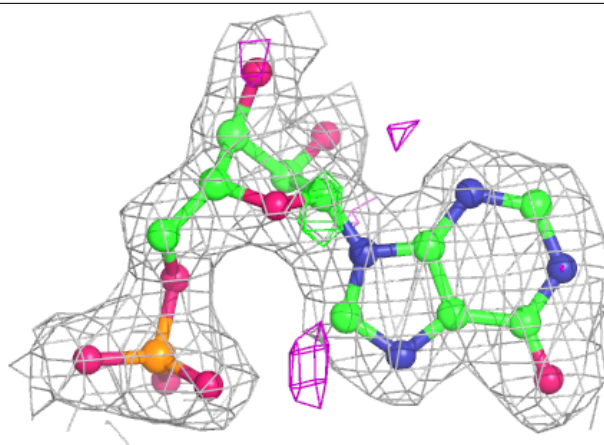
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





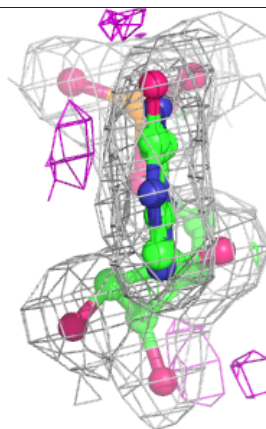
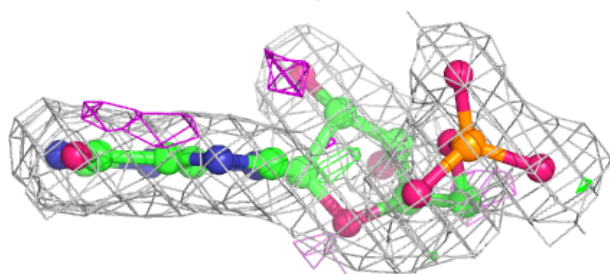
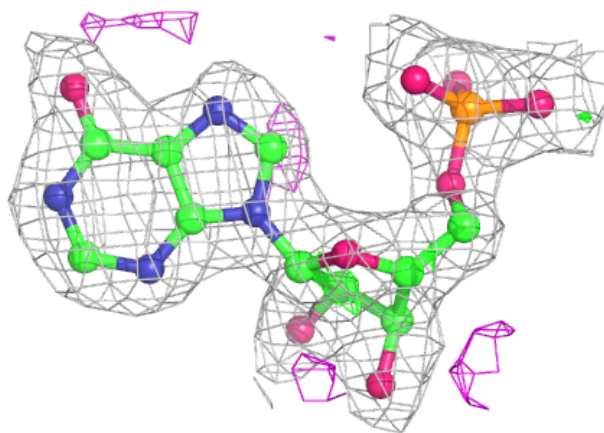
**Electron density around IMP B 501:**

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

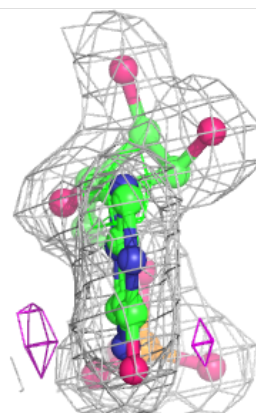
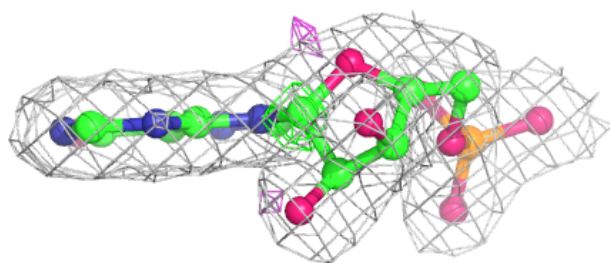
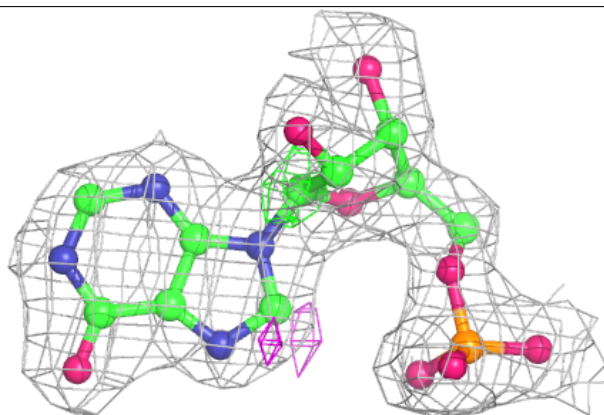


**Electron density around IMP A 501:**

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

**Electron density around IMP D 501:**

$2mF_o-DF_c$  (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.