



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:48 am BST

PDB ID : 1C0A  
Title : CRYSTAL STRUCTURE OF THE E. COLI ASPARTYL-TRNA SYN-  
THETASE : TRNAASP : ASPARTYL-ADENYLATE COMPLEX  
Authors : Eiler, S.; Dock-Bregeon, A.-C.; Moulinier, L.; Thierry, J.-C.; Moras, D.  
Deposited on : 1999-07-15  
Resolution : 2.40 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](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

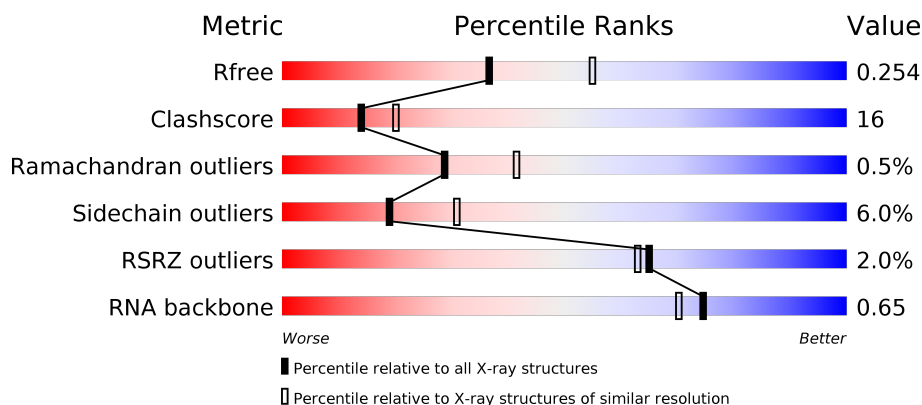
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	B	77	<div> <div>5%</div> <div> <div></div> <div>36%</div> <div>52%</div> <div>12%</div> </div> </div>
2	A	585	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>.</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	H2U	B	620	-	-	-	X
1	H2U	B	620(A)	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6820 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.

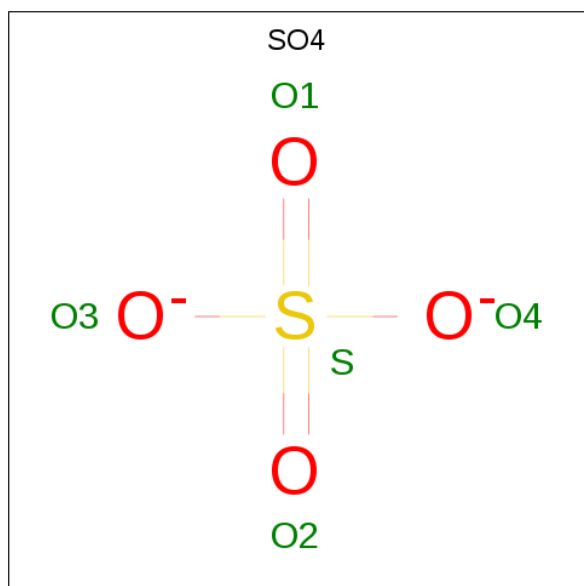
- Molecule 1 is a RNA chain called ASPARTYL TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	B	77	Total	C	N	O	P	S	0	0	0
			1655	740	290	547	77	1			

- Molecule 2 is a protein called ASPARTYL TRNA SYNTHETASE.

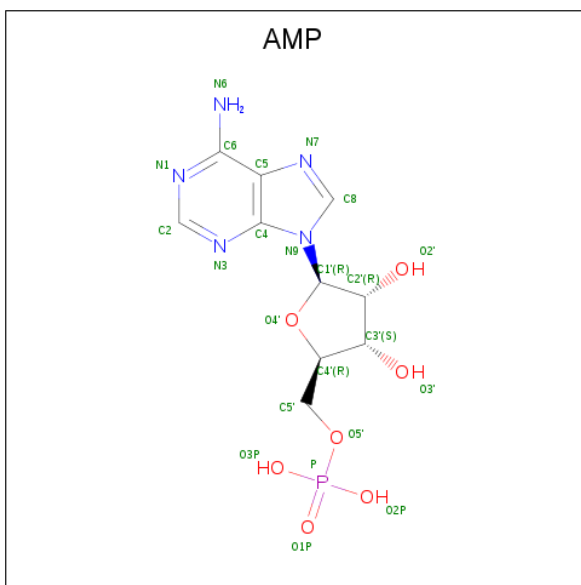
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	585	Total	C	N	O	S	0	0	0
			4592	2900	804	862	26			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



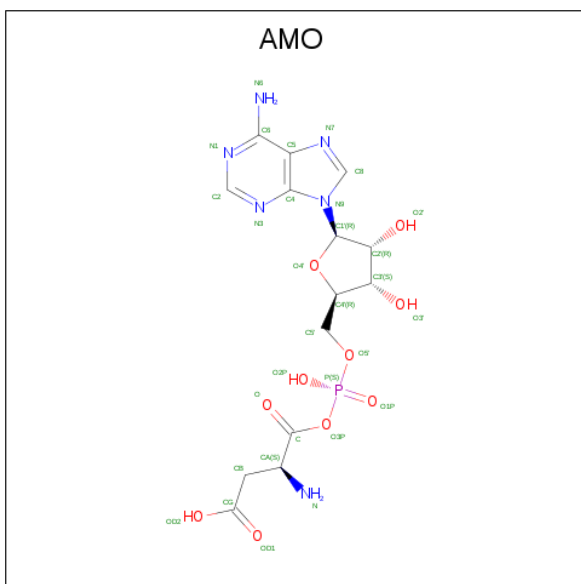
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

- Molecule 5 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (three-letter code: AMO) (formula:  $C_{14}H_{19}N_6O_{10}P$ ).

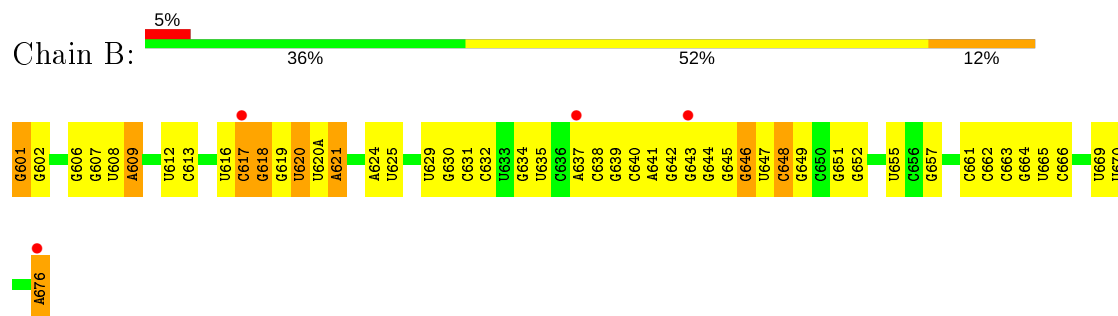


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	107	Total 107	O 107	0	0
6	A	407	Total 407	O 407	0	0

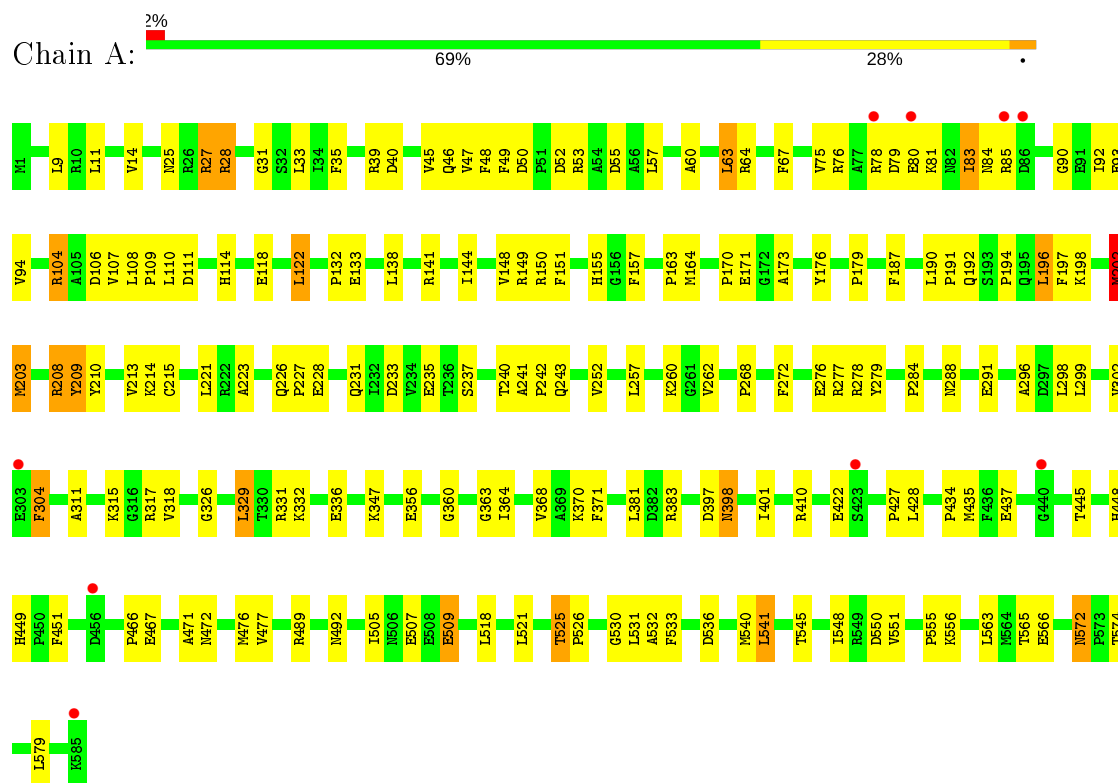
### 3 Residue-property plots

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: ASPARTYL TRNA



#### • Molecule 2: ASPARTYL TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.20Å 101.20Å 231.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40 14.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (12.00-2.40) 98.1 (14.89-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.78 (at 2.39Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.208 , 0.249 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	3555 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: 5MU, AMO, G7M, H2U, SO4, AMP, 4SU, QUO, PSU

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	B	0.73	3/1628 (0.2%)	0.99	6/2534 (0.2%)
2	A	0.52	1/4678 (0.0%)	0.79	7/6320 (0.1%)
All	All	0.58	4/6306 (0.1%)	0.85	13/8854 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	648	C	O3'-P	-18.15	1.39	1.61
1	B	646	G7M	O3'-P	-10.43	1.48	1.61
1	B	601	G	OP3-P	-7.26	1.52	1.61
2	A	398	ASN	C-N	-7.18	1.17	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	C	P-O3'-C3'	26.13	151.06	119.70
1	B	648	C	OP2-P-O3'	-13.40	75.72	105.20
2	A	398	ASN	O-C-N	-10.16	106.44	122.70
1	B	648	C	OP1-P-O3'	8.89	124.77	105.20
1	B	646	G7M	P-O3'-C3'	8.72	130.16	119.70
1	B	648	C	O5'-P-OP1	-7.32	99.11	105.70
2	A	398	ASN	CA-C-N	6.87	132.31	117.20
2	A	208	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	A	202	MET	CG-SD-CE	6.13	110.00	100.20
1	B	648	C	O3'-P-O5'	5.86	115.14	104.00
2	A	203	MET	CG-SD-CE	5.74	109.39	100.20
2	A	489	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	A	398	ASN	C-N-CA	5.17	134.61	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1655	0	850	43	0
2	A	4592	0	4589	144	0
3	B	5	0	0	0	0
4	A	23	0	12	2	0
5	A	31	0	17	0	0
6	A	407	0	0	12	0
6	B	107	0	0	1	0
All	All	6820	0	5468	185	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 16.

All (185) 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)
2:A:202:MET:HG3	2:A:237:SER:OG	1.65	0.96
2:A:78:ARG:HD2	2:A:83:ILE:HA	1.48	0.95
2:A:202:MET:HA	2:A:202:MET:HE2	1.50	0.94
2:A:505:ILE:HG23	2:A:509:GLU:HG2	1.51	0.92
1:B:647:U:H4'	1:B:648:C:H5'	1.56	0.86
2:A:226:GLN:HE22	2:A:556:LYS:H	1.21	0.84
2:A:202:MET:CE	2:A:202:MET:HA	2.12	0.80
2:A:521:LEU:HA	2:A:525:THR:HG21	1.61	0.80
1:B:620:H2U:H62	1:B:620:H2U:OP2	1.82	0.79
2:A:260:LYS:HB2	2:A:262:VAL:HG12	1.63	0.78
2:A:572:ASN:HD22	2:A:574:THR:H	1.32	0.77
2:A:214:LYS:HE3	2:A:228:GLU:OE2	1.86	0.76
2:A:428:LEU:CD2	2:A:477:VAL:HG22	2.17	0.75
2:A:25:ASN:HD22	2:A:39:ARG:HH11	1.36	0.73
1:B:642:G:O2'	1:B:643:G:H5'	1.90	0.72
1:B:617:C:H4'	1:B:618:G:OP2	1.90	0.71
2:A:332:LYS:O	2:A:336:GLU:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:LEU:O	2:A:14:VAL:HG23	1.91	0.70
2:A:428:LEU:HD21	2:A:477:VAL:HG22	1.75	0.67
2:A:315:LYS:HB3	6:A:1378:HOH:O	1.94	0.67
1:B:635:U:O3'	1:B:638:C:H1'	1.95	0.66
2:A:84:ASN:O	2:A:90:GLY:HA3	1.95	0.65
2:A:108:LEU:N	2:A:108:LEU:HD22	2.13	0.64
1:B:609:A:O4'	1:B:646:G7M:H1'	1.97	0.64
2:A:78:ARG:CD	2:A:83:ILE:HA	2.25	0.63
1:B:629:U:O2'	1:B:630:G:H5'	1.99	0.63
1:B:621:A:H4'	6:B:1234:HOH:O	1.99	0.62
2:A:210:TYR:HA	2:A:233:ASP:O	2.00	0.62
2:A:347:LYS:HB2	4:A:800:AMP:N6	2.15	0.62
2:A:196:LEU:HD11	2:A:451:PHE:CZ	2.35	0.61
1:B:644:G:O2'	1:B:645:G:H5'	2.01	0.61
2:A:304:PHE:HB2	2:A:371:PHE:HB3	1.82	0.60
2:A:572:ASN:ND2	2:A:574:THR:H	2.00	0.60
2:A:157:PHE:CD2	2:A:208:ARG:HB3	2.37	0.60
2:A:47:VAL:HG22	2:A:94:VAL:CG2	2.31	0.59
2:A:241:ALA:HB3	2:A:242:PRO:HD3	1.84	0.59
2:A:467:GLU:CD	2:A:467:GLU:H	2.06	0.58
2:A:144:ILE:O	2:A:148:VAL:HG23	2.04	0.57
1:B:640:C:H2'	1:B:641:A:H8	1.67	0.57
2:A:25:ASN:HD22	2:A:39:ARG:NH1	2.00	0.57
1:B:640:C:H2'	1:B:641:A:C8	2.38	0.57
2:A:55:ASP:HB2	6:A:1185:HOH:O	2.04	0.57
2:A:428:LEU:HD23	2:A:477:VAL:HG22	1.85	0.57
2:A:27:ARG:O	2:A:27:ARG:HD3	2.05	0.56
2:A:78:ARG:HG3	2:A:83:ILE:HG22	1.86	0.56
2:A:151:PHE:O	2:A:155:HIS:HD2	1.88	0.56
2:A:149:ARG:HG2	2:A:149:ARG:HH11	1.70	0.56
1:B:676:A:H1'	2:A:449:HIS:HB3	1.86	0.56
2:A:46:GLN:HB3	2:A:78:ARG:NH2	2.20	0.56
2:A:173:ALA:O	2:A:192:GLN:NE2	2.38	0.55
2:A:33:LEU:HD11	2:A:48:PHE:CZ	2.41	0.55
1:B:631:C:H2'	1:B:632:C:C6	2.42	0.55
2:A:33:LEU:HD11	2:A:48:PHE:HZ	1.70	0.55
2:A:111:ASP:HB3	2:A:114:HIS:CD2	2.41	0.55
2:A:545:THR:HG21	2:A:550:ASP:CB	2.36	0.55
2:A:40:ASP:OD1	2:A:40:ASP:C	2.46	0.54
2:A:435:MET:HA	2:A:471:ALA:HB2	1.90	0.54
2:A:226:GLN:NE2	2:A:556:LYS:H	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:448:HIS:HB2	6:A:1117:HOH:O	2.07	0.53
2:A:202:MET:CA	2:A:202:MET:CE	2.85	0.53
2:A:268:PRO:HD2	2:A:427:PRO:O	2.09	0.53
2:A:278:ARG:HD2	2:A:291:GLU:OE1	2.09	0.53
2:A:50:ASP:HB3	2:A:52:ASP:H	1.72	0.53
1:B:669:U:H2'	1:B:670:U:C6	2.43	0.53
2:A:260:LYS:HB2	2:A:262:VAL:CG1	2.36	0.53
2:A:198:LYS:HD2	2:A:235:GLU:HB2	1.91	0.52
2:A:46:GLN:CB	2:A:78:ARG:HH22	2.23	0.52
2:A:79:ASP:O	2:A:81:LYS:N	2.43	0.52
2:A:536:ASP:O	2:A:540:MET:HG3	2.10	0.51
2:A:78:ARG:HH21	2:A:93:GLU:HB3	1.75	0.51
2:A:50:ASP:HB3	2:A:52:ASP:HB2	1.91	0.51
2:A:60:ALA:HA	2:A:63:LEU:HD22	1.91	0.51
2:A:108:LEU:H	2:A:108:LEU:HD22	1.75	0.51
2:A:356:GLU:O	2:A:363:GLY:HA3	2.11	0.51
2:A:360:GLY:HA3	6:A:1181:HOH:O	2.11	0.51
2:A:277:ARG:O	2:A:317:ARG:NH2	2.43	0.51
2:A:108:LEU:H	2:A:108:LEU:CD2	2.24	0.51
2:A:203:MET:HG2	2:A:525:THR:HB	1.92	0.51
2:A:196:LEU:HD11	2:A:451:PHE:CE1	2.47	0.50
2:A:235:GLU:OE1	2:A:530:GLY:HA3	2.11	0.50
1:B:643:G:H2'	1:B:644:G:C8	2.46	0.50
1:B:631:C:H2'	1:B:632:C:H6	1.76	0.50
2:A:252:VAL:HG21	2:A:476:MET:SD	2.52	0.50
2:A:428:LEU:HD21	2:A:477:VAL:CG2	2.42	0.50
1:B:630:G:O2'	1:B:631:C:H5'	2.12	0.49
2:A:14:VAL:HA	2:A:75:VAL:HG12	1.94	0.49
1:B:638:C:H2'	1:B:639:G:O4'	2.12	0.49
2:A:118:GLU:O	2:A:122:LEU:HD22	2.11	0.49
1:B:634:QUO:H4'	1:B:635:U:H5'	1.94	0.49
2:A:46:GLN:HB3	2:A:78:ARG:HH22	1.75	0.49
2:A:565:THR:O	2:A:566:GLU:HB2	2.13	0.49
2:A:104:ARG:CG	2:A:104:ARG:HH11	2.25	0.48
2:A:57:LEU:HD12	6:A:1490:HOH:O	2.14	0.48
2:A:109:PRO:O	2:A:110:LEU:HD23	2.14	0.48
2:A:92:ILE:C	2:A:92:ILE:HD12	2.35	0.48
2:A:521:LEU:HA	2:A:525:THR:CG2	2.39	0.47
2:A:299:LEU:CD1	2:A:318:VAL:HG11	2.44	0.47
2:A:57:LEU:C	2:A:57:LEU:HD13	2.35	0.47
2:A:83:ILE:HD11	2:A:85:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:U:C4'	1:B:648:C:H5'	2.38	0.47
2:A:179:PRO:HB3	2:A:187:PHE:CE2	2.50	0.47
2:A:326:GLY:O	2:A:329:LEU:HD22	2.15	0.47
2:A:364:ILE:O	2:A:364:ILE:HD12	2.15	0.47
1:B:663:C:O2'	1:B:664:G:H5'	2.15	0.46
2:A:505:ILE:HG23	2:A:509:GLU:CG	2.34	0.46
2:A:50:ASP:HB3	2:A:52:ASP:CB	2.45	0.46
1:B:616:H2U:C2'	1:B:616:H2U:O2	2.63	0.46
1:B:663:C:H2'	1:B:664:G:H8	1.80	0.46
1:B:606:G:O2'	1:B:607:G:H5'	2.16	0.46
1:B:616:H2U:O2	1:B:616:H2U:H2'	2.16	0.46
2:A:79:ASP:C	2:A:81:LYS:N	2.69	0.46
2:A:108:LEU:N	2:A:108:LEU:CD2	2.76	0.46
2:A:209:TYR:C	2:A:209:TYR:CD1	2.89	0.46
2:A:231:GLN:HA	2:A:533:PHE:O	2.16	0.46
2:A:223:ALA:O	2:A:548:ILE:HG22	2.16	0.46
2:A:11:LEU:HA	2:A:14:VAL:HG23	1.98	0.45
1:B:651:G:O2'	1:B:652:G:H5'	2.15	0.45
2:A:9:LEU:HD12	2:A:45:VAL:HG21	1.97	0.45
2:A:132:PRO:HD2	2:A:133:GLU:OE1	2.16	0.45
2:A:221:LEU:N	2:A:221:LEU:HD12	2.32	0.45
1:B:644:G:C2'	1:B:645:G:H5'	2.46	0.45
2:A:83:ILE:O	2:A:83:ILE:HG13	2.17	0.45
1:B:612:U:H2'	1:B:613:C:C6	2.52	0.45
2:A:410:ARG:HD3	6:A:1018:HOH:O	2.15	0.45
2:A:284:PRO:HG2	2:A:428:LEU:HD11	1.99	0.44
2:A:279:TYR:HD2	2:A:410:ARG:CZ	2.30	0.44
2:A:437:GLU:O	2:A:445:THR:HG22	2.17	0.44
2:A:164:MET:O	2:A:191:PRO:HD3	2.18	0.44
2:A:531:LEU:HD23	2:A:532:ALA:N	2.32	0.44
2:A:260:LYS:CB	2:A:262:VAL:HG12	2.39	0.44
2:A:277:ARG:HA	6:A:1340:HOH:O	2.16	0.44
1:B:631:C:O2'	1:B:632:C:H5'	2.18	0.44
1:B:661:C:H2'	1:B:662:C:C6	2.53	0.44
2:A:104:ARG:CG	2:A:104:ARG:NH1	2.81	0.44
2:A:302:VAL:CG2	2:A:371:PHE:O	2.66	0.44
2:A:64:ARG:HB2	2:A:67:PHE:CE1	2.52	0.44
1:B:624:A:H2'	1:B:625:U:O4'	2.18	0.44
1:B:663:C:H2'	1:B:664:G:C8	2.53	0.43
2:A:302:VAL:HG23	2:A:371:PHE:O	2.18	0.43
2:A:240:THR:OG1	2:A:243:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:276:GLU:HB2	6:A:1104:HOH:O	2.19	0.43
1:B:630:G:C6	1:B:631:C:C4	3.07	0.43
2:A:14:VAL:HG13	2:A:76:ARG:HA	2.00	0.43
1:B:665:PSU:H2'	1:B:666:C:C6	2.53	0.43
2:A:111:ASP:HB3	2:A:114:HIS:HD2	1.83	0.43
2:A:49:PHE:O	2:A:57:LEU:HD23	2.19	0.43
2:A:57:LEU:O	2:A:57:LEU:HD13	2.18	0.43
2:A:108:LEU:HA	2:A:109:PRO:HD3	1.83	0.42
2:A:150:ARG:HD2	6:A:1444:HOH:O	2.18	0.42
2:A:83:ILE:HD12	2:A:83:ILE:C	2.40	0.42
2:A:398:ASN:HD21	2:A:401:ILE:HG13	1.84	0.42
2:A:298:LEU:HD21	2:A:383:ARG:NH2	2.35	0.42
2:A:370:LYS:HB3	6:A:1481:HOH:O	2.19	0.42
2:A:521:LEU:CA	2:A:525:THR:HG21	2.43	0.42
2:A:149:ARG:HG2	2:A:149:ARG:NH1	2.34	0.42
2:A:296:ALA:HB1	2:A:311:ALA:HA	2.02	0.42
2:A:466:PRO:HD2	2:A:467:GLU:OE2	2.20	0.42
1:B:638:C:O2'	1:B:639:G:H5'	2.20	0.42
1:B:655:PSU:H2'	1:B:657:G:OP2	2.19	0.42
2:A:257:LEU:HD12	2:A:257:LEU:HA	1.88	0.42
2:A:215:CYS:SG	2:A:231:GLN:HG3	2.59	0.41
2:A:28:ARG:HB2	2:A:35:PHE:HB2	2.02	0.41
1:B:632:C:C4	2:A:31:GLY:N	2.88	0.41
2:A:525:THR:HG23	6:A:1022:HOH:O	2.20	0.41
2:A:545:THR:HG21	2:A:550:ASP:HB2	2.02	0.41
2:A:209:TYR:CG	2:A:210:TYR:N	2.87	0.41
1:B:639:G:C6	1:B:640:C:C4	3.08	0.41
2:A:288:ASN:O	2:A:410:ARG:NH2	2.52	0.41
2:A:467:GLU:HG2	6:A:1383:HOH:O	2.20	0.41
1:B:620(A):H2U:H61	1:B:620(A):H2U:H2'	1.79	0.41
2:A:176:TYR:OH	2:A:227:PRO:HB2	2.20	0.41
2:A:170:PRO:C	2:A:171:GLU:HG2	2.40	0.41
2:A:163:PRO:HG2	2:A:197:PHE:CE2	2.55	0.41
2:A:299:LEU:HD12	2:A:318:VAL:HG11	2.03	0.41
2:A:541:LEU:HA	2:A:541:LEU:HD12	1.87	0.41
1:B:629:U:H2'	1:B:630:G:H8	1.85	0.41
2:A:347:LYS:HB2	4:A:800:AMP:HN61	1.85	0.41
1:B:608:4SU:H5''	1:B:649:G:OP2	2.20	0.41
1:B:601:G:O2'	1:B:602:G:H5'	2.21	0.40
2:A:179:PRO:HG2	2:A:579:LEU:HD13	2.03	0.40
2:A:194:PRO:HG2	2:A:213:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:141:ARG:NH1	2:A:551:VAL:O	2.55	0.40
1:B:643:G:H2'	1:B:644:G:H8	1.85	0.40
2:A:138:LEU:HA	2:A:138:LEU:HD23	1.91	0.40
2:A:272:PHE:CD2	2:A:434:PRO:HD3	2.56	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	
2	A	583/585 (100%)	551 (94%)	29 (5%)	3 (0%)	29	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	80	GLU
2	A	304	PHE
2	A	106	ASP

### 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	
2	A	486/486 (100%)	457 (94%)	29 (6%)	19	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	27	ARG
2	A	28	ARG
2	A	53	ARG
2	A	63	LEU
2	A	83	ILE
2	A	104	ARG
2	A	107	VAL
2	A	122	LEU
2	A	190	LEU
2	A	196	LEU
2	A	202	MET
2	A	209	TYR
2	A	329	LEU
2	A	331	ARG
2	A	368	VAL
2	A	381	LEU
2	A	397	ASP
2	A	422	GLU
2	A	472	ASN
2	A	492	ASN
2	A	507	GLU
2	A	509	GLU
2	A	518	LEU
2	A	525	THR
2	A	526	PRO
2	A	541	LEU
2	A	555	PRO
2	A	563	LEU
2	A	572	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	25	ASN
2	A	65	ASN
2	A	113	ASN
2	A	114	HIS
2	A	155	HIS
2	A	226	GLN
2	A	312	ASN
2	A	339	ASN

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Mol	Chain	Res	Type
2	A	355	ASN
2	A	365	ASN
2	A	387	GLN
2	A	472	ASN
2	A	572	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	75/77 (97%)	8 (10%)	2 (2%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	609	A
1	B	617	C
1	B	618	G
1	B	619	G
1	B	620	H2U
1	B	621	A
1	B	637	A
1	B	676	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	617	C
1	B	619	G

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

9 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	5MU	B	654	1	15,22,23	1.18	2 (13%)	16,32,35	3.61	2 (12%)
1	4SU	B	608	1	14,21,22	5.78	3 (21%)	15,30,33	2.94	2 (13%)
1	QUO	B	634	1	28,35,36	1.22	3 (10%)	32,52,55	3.83	10 (31%)
1	PSU	B	655	1	17,21,22	1.92	4 (23%)	20,30,33	5.74	5 (25%)
1	G7M	B	646	1	20,26,27	1.39	3 (15%)	20,39,42	2.66	4 (20%)
1	H2U	B	616	1	18,21,22	0.94	1 (5%)	21,30,33	0.82	1 (4%)
1	PSU	B	665	1	17,21,22	2.17	4 (23%)	20,30,33	5.67	5 (25%)
1	H2U	B	620(A)	1	18,21,22	0.57	0	21,30,33	0.75	1 (4%)
1	H2U	B	620	1	18,21,22	0.69	1 (5%)	21,30,33	0.83	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
1	5MU	B	654	1	-	0/5/25/26	0/2/2/2
1	4SU	B	608	1	-	0/5/25/26	0/2/2/2
1	QUO	B	634	1	-	0/6/43/44	0/4/4/4
1	PSU	B	655	1	-	0/7/25/26	0/2/2/2
1	G7M	B	646	1	-	0/3/25/26	0/3/3/3
1	H2U	B	616	1	-	2/7/38/39	0/2/2/2
1	PSU	B	665	1	-	0/7/25/26	0/2/2/2
1	H2U	B	620(A)	1	-	4/7/38/39	0/2/2/2
1	H2U	B	620	1	-	1/7/38/39	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	4SU	C4-S4	-20.77	1.29	1.67
1	B	665	PSU	C5-C1'	-6.18	1.47	1.52
1	B	608	4SU	C5-C4	5.16	1.44	1.38
1	B	655	PSU	C6-N1	-4.71	1.24	1.34
1	B	665	PSU	C6-N1	-4.69	1.24	1.34
1	B	655	PSU	C5-C1'	-4.57	1.48	1.52
1	B	646	G7M	C6-N1	4.26	1.40	1.33
1	B	634	QUO	C6-N1	3.91	1.39	1.33
1	B	654	5MU	C4-N3	3.50	1.39	1.33
1	B	616	H2U	C2-N1	3.45	1.40	1.35
1	B	634	QUO	C7-C5	-3.35	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	646	G7M	C8-N9	2.99	1.38	1.33
1	B	655	PSU	C4-N3	2.63	1.37	1.33
1	B	655	PSU	C6-C5	-2.59	1.34	1.38
1	B	665	PSU	C6-C5	-2.57	1.34	1.38
1	B	620	H2U	C2-N1	2.47	1.39	1.35
1	B	646	G7M	C2-N1	2.21	1.39	1.35
1	B	665	PSU	C4-N3	2.21	1.36	1.33
1	B	634	QUO	C5-C4	-2.16	1.37	1.43
1	B	654	5MU	C6-C5	-2.03	1.34	1.40
1	B	608	4SU	C6-N1	2.01	1.38	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	PSU	N1-C2-N3	-17.38	114.61	128.43
1	B	665	PSU	N1-C2-N3	-17.06	114.87	128.43
1	B	634	QUO	C5-C6-N1	-15.05	110.73	124.09
1	B	654	5MU	C4-N3-C2	14.08	127.03	115.14
1	B	665	PSU	C4-N3-C2	12.44	125.65	115.14
1	B	655	PSU	C4-N3-C2	12.24	125.48	115.14
1	B	655	PSU	O4'-C1'-C5	10.22	125.76	109.93
1	B	665	PSU	O4'-C1'-C5	9.69	124.94	109.93
1	B	634	QUO	C6-C5-C4	9.20	120.21	115.01
1	B	646	G7M	C5-C6-N1	-9.04	111.07	123.43
1	B	665	PSU	C5-C4-N3	-8.83	113.98	125.36
1	B	655	PSU	C5-C4-N3	-8.81	114.01	125.36
1	B	608	4SU	C2-N3-C4	8.48	127.44	115.15
1	B	634	QUO	C10-N11-C12	8.32	132.38	114.90
1	B	608	4SU	C5-C4-N3	-7.38	113.96	123.83
1	B	646	G7M	C6-N1-C2	5.71	125.00	115.93
1	B	634	QUO	C6-N1-C2	5.65	124.91	115.93
1	B	655	PSU	C6-N1-C2	4.43	122.67	115.36
1	B	665	PSU	C6-N1-C2	4.35	122.54	115.36
1	B	634	QUO	C7-C10-N11	3.57	123.13	112.75
1	B	634	QUO	C8-N9-C1'	3.24	128.35	125.48
1	B	634	QUO	C2-N3-C4	-3.11	111.81	115.36
1	B	646	G7M	C2-N3-C4	-3.03	111.89	115.36
1	B	646	G7M	N3-C2-N1	-2.50	123.88	127.22
1	B	634	QUO	N3-C2-N1	-2.34	124.11	127.22
1	B	616	H2U	N3-C2-N1	-2.20	114.33	116.65
1	B	634	QUO	O3'-C3'-C2'	-2.13	104.95	111.82
1	B	620(A)	H2U	N3-C2-N1	-2.08	114.45	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	5MU	C5M-C5-C6	2.07	123.05	118.68
1	B	634	QUO	O4'-C1'-C2'	-2.05	103.92	106.93

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	620(A)	H2U	O4'-C1'-N1-C6
1	B	616	H2U	C2'-C1'-N1-C2
1	B	616	H2U	C2'-C1'-N1-C6
1	B	620(A)	H2U	C2'-C1'-N1-C6
1	B	620(A)	H2U	C2'-C1'-N1-C2
1	B	620(A)	H2U	O4'-C1'-N1-C2
1	B	620	H2U	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	608	4SU	1	0
1	B	634	QUO	1	0
1	B	655	PSU	1	0
1	B	646	G7M	1	0
1	B	616	H2U	2	0
1	B	665	PSU	1	0
1	B	620(A)	H2U	1	0
1	B	620	H2U	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	SO4	B	701	-	4,4,4	0.46	0	6,6,6	0.28	0
5	AMO	A	831	-	26,33,33	1.03	1 (3%)	28,49,49	1.60	2 (7%)
4	AMP	A	800	-	22,25,25	0.67	0	25,38,38	0.95	3 (12%)

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
5	AMO	A	831	-	-	1/15/39/39	0/3/3/3
4	AMP	A	800	-	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	831	AMO	P-O3P	4.03	1.68	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	831	AMO	O3P-P-O5'	6.43	121.70	102.92
5	A	831	AMO	O2P-P-O3P	-4.19	90.44	104.14
4	A	800	AMP	O2P-P-O1P	2.31	119.74	110.68
4	A	800	AMP	C5-C6-N6	2.14	123.60	120.35
4	A	800	AMP	O3P-P-O5'	-2.03	101.34	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

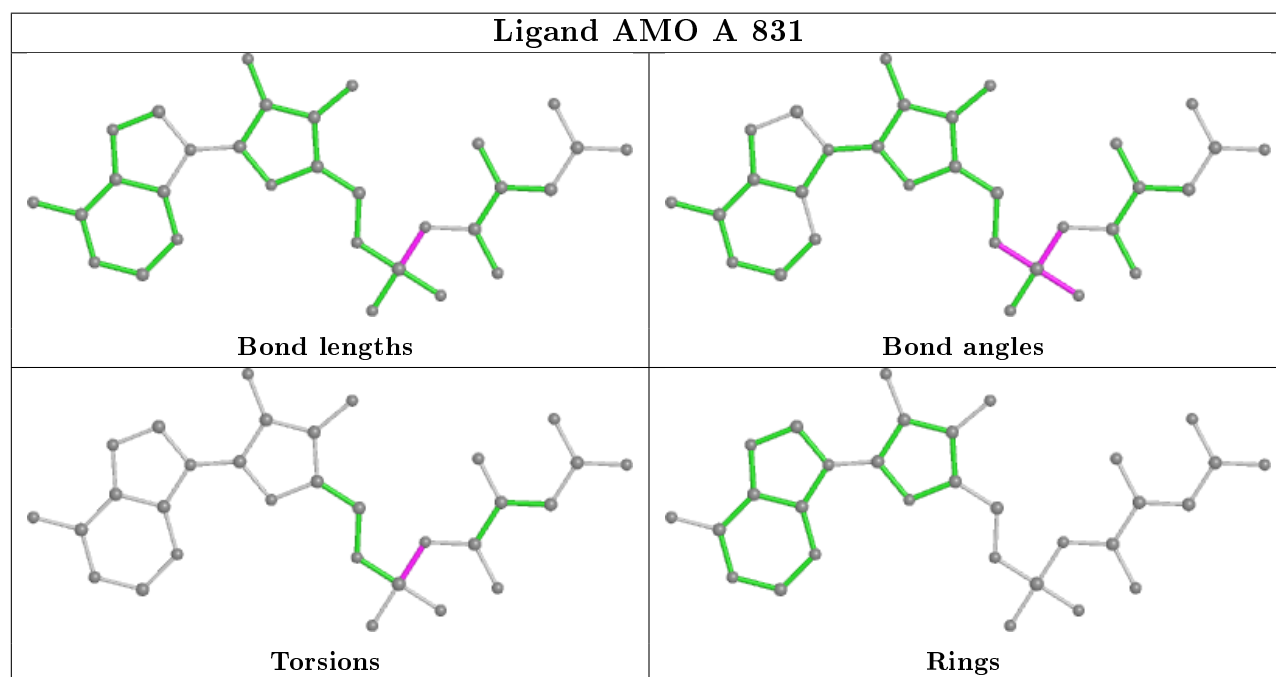
Mol	Chain	Res	Type	Atoms
5	A	831	AMO	C-O3P-P-O5'

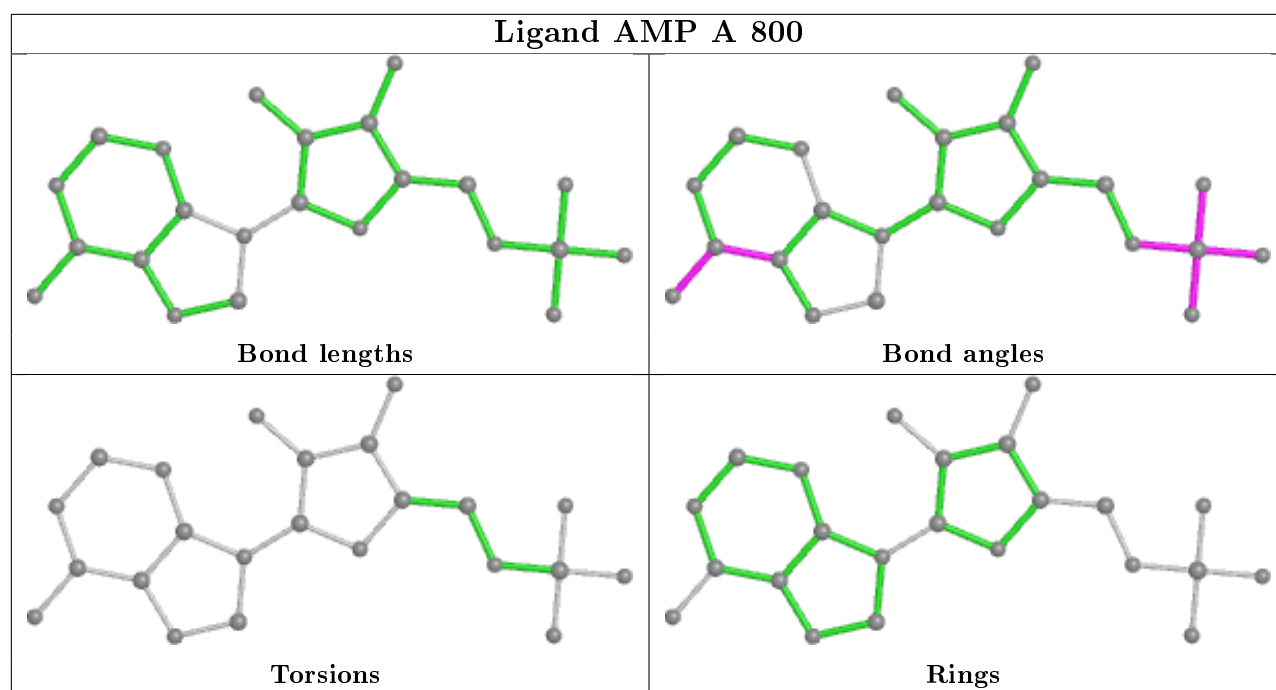
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	AMP	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	648:C	O3'	649:G	P	1.39
1	A	398:ASN	C	399:LYS	N	1.17

## 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	B	68/77 (88%)	0.08	4 (5%) 22 21	16, 38, 67, 89	0
2	A	585/585 (100%)	-0.40	9 (1%) 73 72	7, 22, 45, 65	0
All	All	653/662 (98%)	-0.35	13 (1%) 65 63	7, 24, 50, 89	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	617	C	7.4
2	A	585	LYS	4.0
1	B	643	G	3.6
2	A	440	GLY	3.1
2	A	85	ARG	2.6
2	A	423	SER	2.6
1	B	637	A	2.5
2	A	80	GLU	2.4
2	A	303	GLU	2.3
2	A	78	ARG	2.2
2	A	86	ASP	2.2
2	A	456	ASP	2.1
1	B	676	A	2.0

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

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(Å <sup>2</sup> )	Q<0.9
1	H2U	B	620	20/21	0.71	0.40	72,82,83,83	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	H2U	B	620(A)	20/21	0.76	0.41	72,80,83,83	0
1	H2U	B	616	20/21	0.79	0.37	51,79,83,83	0
1	QUO	B	634	32/33	0.80	0.25	59,65,76,76	0
1	PSU	B	655	20/21	0.81	0.23	35,46,51,52	0
1	5MU	B	654	21/22	0.84	0.24	37,44,47,50	0
1	PSU	B	665	20/21	0.91	0.15	27,33,36,38	0
1	G7M	B	646	24/25	0.92	0.16	42,45,47,48	0
1	4SU	B	608	20/21	0.98	0.09	23,26,29,31	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

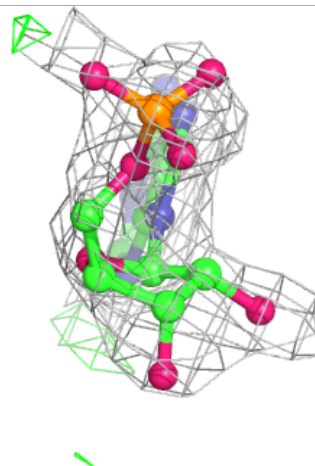
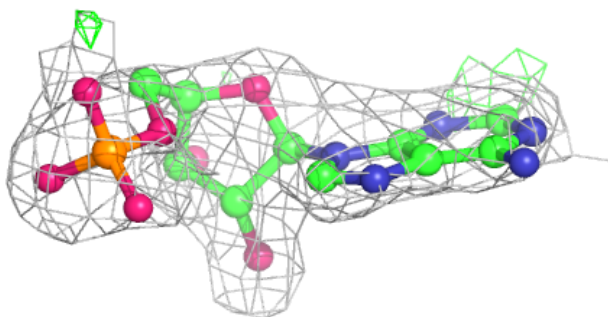
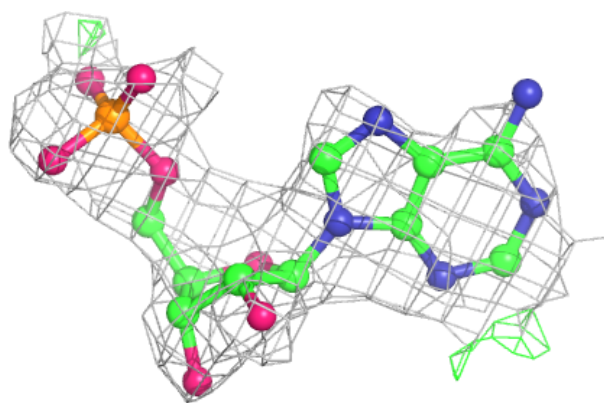
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

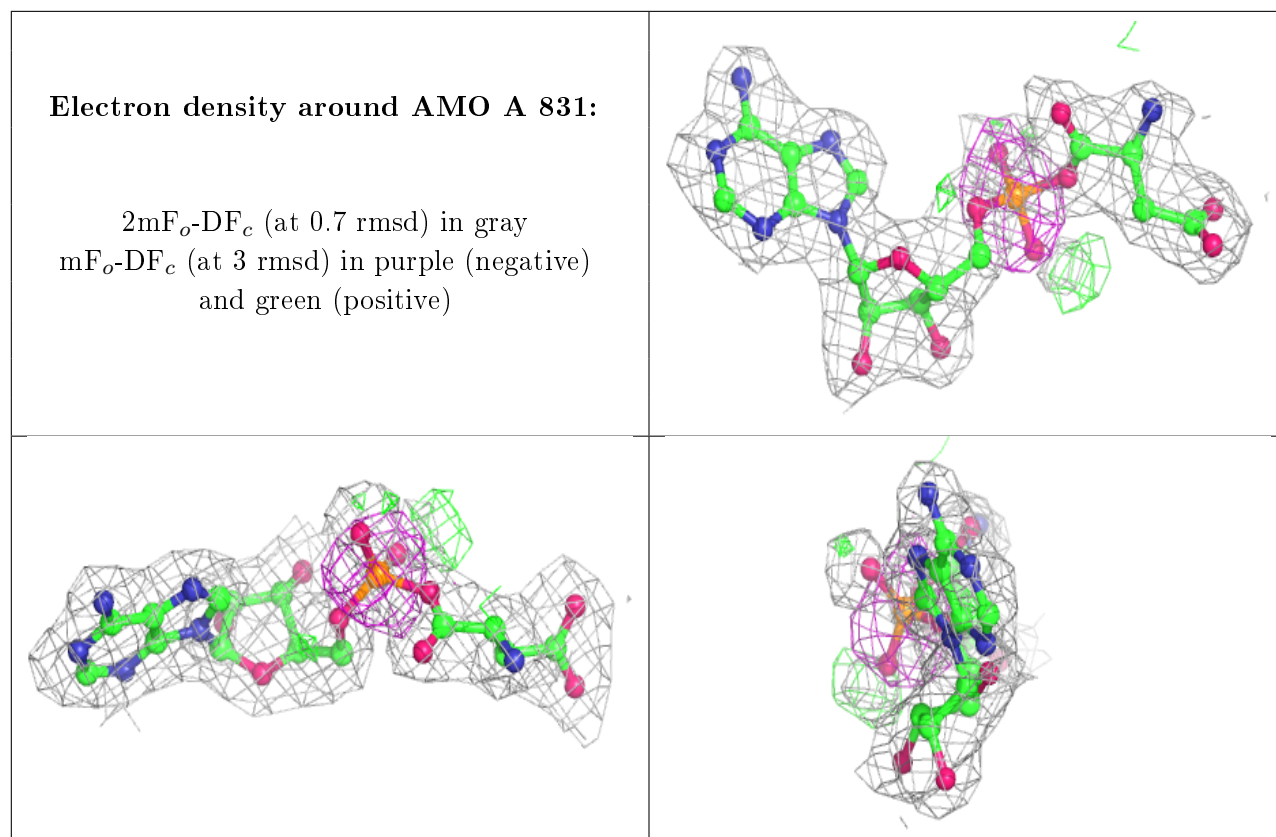
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	AMP	A	800	23/23	0.73	0.27	77,79,89,89	0
5	AMO	A	831	31/31	0.87	0.17	8,15,32,40	0
3	SO4	B	701	5/5	0.97	0.20	50,51,51,52	0

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 A 800:**

$2mF_o-DF_c$  (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.