



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:34 am BST

PDB ID : 6EZU  
Title : Schistosoma mansoni Phosphodiesterase 4A  
Authors : Brown, D.G.; Schroeder, S.; Gil, C.  
Deposited on : 2017-11-16  
Resolution : 2.04 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

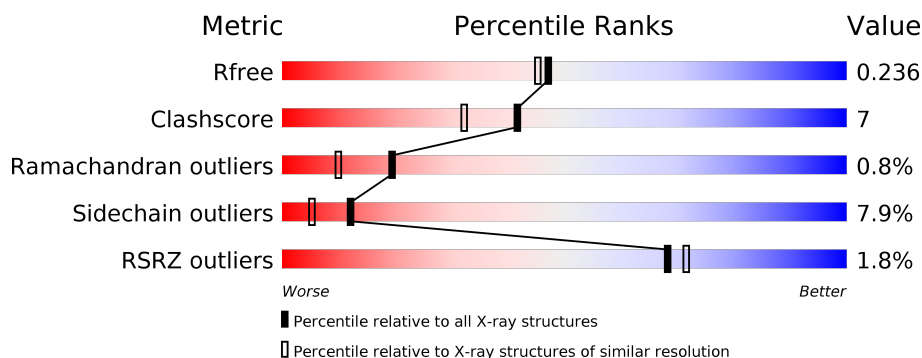
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	371	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 67%, yellow 16%, orange 5%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>67%</span> <span>16%</span> <span>5%</span> <span>10%</span> </div> </div>
1	B	371	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 64%, yellow 18%, orange 1%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>2%</span> <span>64%</span> <span>18%</span> <span>.</span> <span>13%</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5340 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 Phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2677	1701	459	500	17			
1	B	324	Total	C	N	O	S	0	0	0
			2558	1634	432	475	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	GLY	-	expression tag	UNP G4VPI6
A	302	PRO	-	expression tag	UNP G4VPI6
B	301	GLY	-	expression tag	UNP G4VPI6
B	302	PRO	-	expression tag	UNP G4VPI6

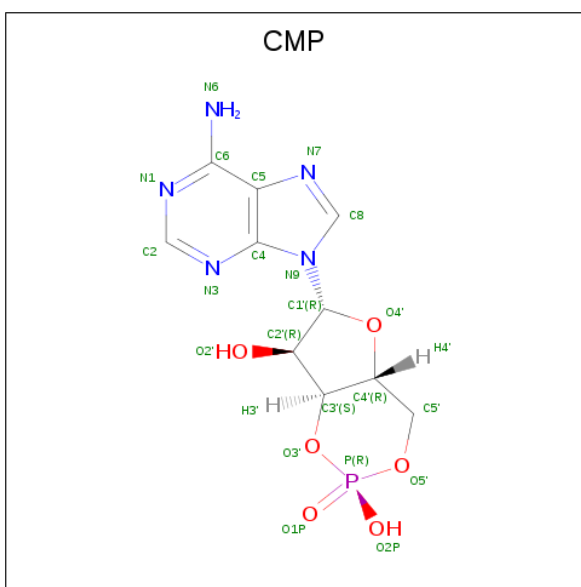
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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

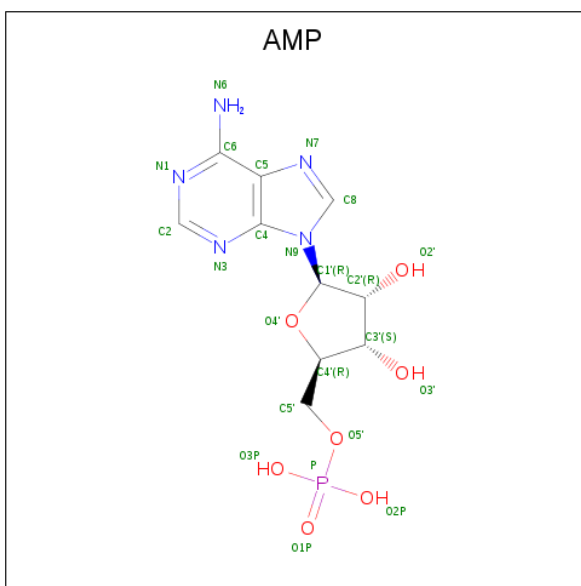
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



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

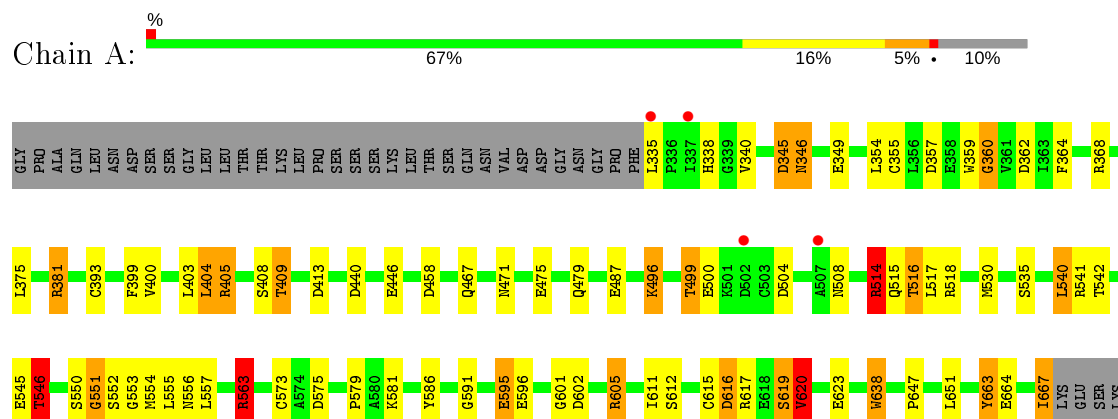
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total 34	O 34	0	0
6	B	22	Total 22	O 22	0	0

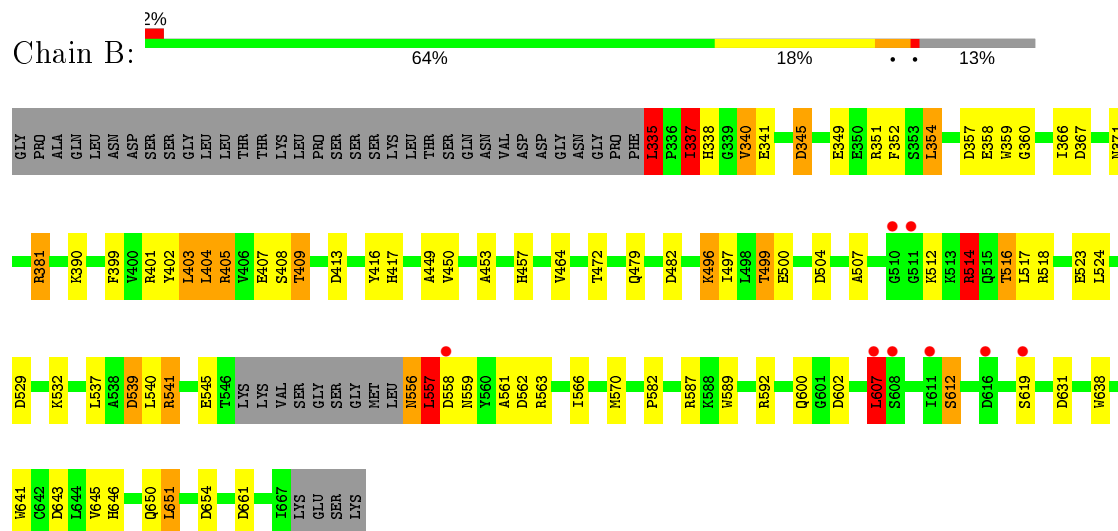
### 3 Residue-property plots [i](#)

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: Phosphodiesterase



#### • Molecule 1: Phosphodiesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.55Å 81.55Å 255.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.44 – 2.04 47.41 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.44-2.04) 100.0 (47.41-2.04)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.199 , 0.233 0.205 , 0.236	Depositor DCC
$R_{free}$ test set	3042 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, ZN, MG, CMP

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	1.59	22/2737 (0.8%)	1.46	35/3720 (0.9%)
1	B	1.57	22/2616 (0.8%)	1.59	56/3562 (1.6%)
All	All	1.58	44/5353 (0.8%)	1.52	91/7282 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	GLY	N-CA	13.00	1.65	1.46
1	A	360	GLY	N-CA	12.25	1.64	1.46
1	A	619	SER	CB-OG	-11.86	1.26	1.42
1	B	612	SER	CB-OG	10.06	1.55	1.42
1	A	546	THR	CB-CG2	-9.21	1.22	1.52
1	A	596	GLU	CD-OE2	-8.33	1.16	1.25
1	A	355	CYS	CB-SG	8.23	1.96	1.82
1	B	358	GLU	CD-OE2	7.44	1.33	1.25
1	A	535	SER	CB-OG	-7.04	1.33	1.42
1	B	523	GLU	CD-OE2	6.89	1.33	1.25
1	B	514	ARG	CZ-NH1	6.80	1.41	1.33
1	A	487	GLU	CD-OE1	-6.73	1.18	1.25
1	B	504	ASP	CB-CG	6.67	1.65	1.51
1	B	408	SER	CA-CB	6.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	TYR	CZ-OH	6.61	1.49	1.37
1	A	364	PHE	N-CA	6.58	1.59	1.46
1	B	407	GLU	CD-OE2	6.46	1.32	1.25
1	B	499	THR	CB-CG2	-6.41	1.31	1.52
1	A	638	TRP	CB-CG	6.39	1.61	1.50
1	A	545	GLU	CD-OE2	6.35	1.32	1.25
1	A	545	GLU	CD-OE1	-6.07	1.19	1.25
1	A	663	TYR	CG-CD2	-6.07	1.31	1.39
1	B	341	GLU	CG-CD	6.07	1.61	1.51
1	B	612	SER	CA-CB	5.91	1.61	1.52
1	A	651	LEU	CA-C	5.83	1.68	1.52
1	A	551	GLY	N-CA	5.81	1.54	1.46
1	A	612	SER	CB-OG	-5.71	1.34	1.42
1	A	360	GLY	C-O	-5.70	1.14	1.23
1	B	612	SER	CA-C	5.63	1.67	1.52
1	A	647	PRO	N-CA	5.62	1.56	1.47
1	A	595	GLU	CG-CD	5.57	1.60	1.51
1	A	602	ASP	CB-CG	5.43	1.63	1.51
1	A	591	GLY	N-CA	5.40	1.54	1.46
1	B	401	ARG	CG-CD	5.37	1.65	1.51
1	B	341	GLU	CD-OE2	5.32	1.31	1.25
1	A	362	ASP	CB-CG	5.27	1.62	1.51
1	B	449	ALA	C-O	5.24	1.33	1.23
1	B	612	SER	C-O	5.24	1.33	1.23
1	B	416	TYR	CG-CD1	5.16	1.45	1.39
1	B	638	TRP	CE3-CZ3	-5.11	1.29	1.38
1	B	589	TRP	CB-CG	-5.09	1.41	1.50
1	A	617	ARG	CZ-NH2	-5.06	1.26	1.33
1	B	638	TRP	CD2-CE2	-5.03	1.35	1.41
1	B	661	ASP	N-CA	5.03	1.56	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	B	592	ARG	NE-CZ-NH2	-14.19	113.20	120.30
1	B	401	ARG	NE-CZ-NH2	-13.63	113.48	120.30
1	B	404	LEU	CB-CG-CD1	12.36	132.01	111.00
1	B	381	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	B	381	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	B	592	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	B	651	LEU	CA-CB-CG	11.24	141.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	B	514	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	B	403	LEU	CB-CG-CD1	-10.65	92.89	111.00
1	B	612	SER	CB-CA-C	10.47	129.99	110.10
1	A	359	TRP	C-N-CA	-9.12	103.15	122.30
1	A	413	ASP	CB-CG-OD1	8.74	126.16	118.30
1	B	367	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	A	345	ASP	CB-CG-OD1	8.64	126.08	118.30
1	B	359	TRP	C-N-CA	-8.58	104.29	122.30
1	B	354	LEU	CB-CG-CD1	8.35	125.19	111.00
1	B	335	LEU	CB-CG-CD2	8.34	125.18	111.00
1	A	616	ASP	CB-CG-OD1	8.26	125.74	118.30
1	B	541	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	B	405	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	607	LEU	CA-CB-CG	7.97	133.62	115.30
1	B	340	VAL	CB-CA-C	-7.96	96.28	111.40
1	B	340	VAL	CG1-CB-CG2	7.88	123.51	110.90
1	A	514	ARG	CG-CD-NE	-7.76	95.50	111.80
1	B	558	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	631	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	540	LEU	CB-CG-CD2	7.54	123.81	111.00
1	A	602	ASP	CB-CG-OD1	7.42	124.97	118.30
1	A	620	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	A	619	SER	CB-CA-C	-7.37	96.11	110.10
1	B	504	ASP	CB-CG-OD2	7.36	124.92	118.30
1	B	345	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	401	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	605	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	539	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	605	ARG	CD-NE-CZ	7.00	133.41	123.60
1	A	357	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	458	ASP	CB-CG-OD1	6.95	124.56	118.30
1	B	408	SER	CA-CB-OG	-6.92	92.50	111.20
1	A	375	LEU	CB-CG-CD1	6.87	122.68	111.00
1	A	345	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	359	TRP	CA-C-N	6.70	129.59	116.20
1	A	617	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	499	THR	CA-CB-CG2	6.67	121.74	112.40
1	B	403	LEU	CB-CG-CD2	-6.53	99.90	111.00
1	B	518	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	587	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	351	ARG	NE-CZ-NH1	6.44	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	530	MET	CG-SD-CE	6.43	110.49	100.20
1	B	351	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	563	ARG	N-CA-CB	-6.30	99.25	110.60
1	B	529	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	408	SER	CB-CA-C	-6.07	98.57	110.10
1	B	401	ARG	CG-CD-NE	-5.95	99.31	111.80
1	B	337	ILE	CB-CA-C	-5.94	99.72	111.60
1	A	563	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	B	587	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	475	GLU	CG-CD-OE2	5.70	129.71	118.30
1	B	500	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	B	514	ARG	CD-NE-CZ	5.70	131.58	123.60
1	B	563	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	595	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	B	563	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	570	MET	CG-SD-CE	5.58	109.13	100.20
1	A	541	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	546	THR	CA-CB-CG2	5.57	120.20	112.40
1	B	607	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	518	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	482	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	B	482	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	541	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	401	ARG	CD-NE-CZ	5.39	131.15	123.60
1	B	359	TRP	O-C-N	-5.37	114.07	123.20
1	A	405	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	631	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	405	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	575	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	413	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	602	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	545	GLU	CG-CD-OE2	5.27	128.85	118.30
1	A	550	SER	C-N-CA	-5.26	111.25	122.30
1	A	616	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	345	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	516	THR	N-CA-CB	5.11	120.02	110.30
1	B	340	VAL	CA-CB-CG2	5.11	118.56	110.90
1	A	404	LEU	CB-CG-CD1	5.10	119.67	111.00
1	B	504	ASP	OD1-CG-OD2	-5.03	113.74	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	THR	Peptide
1	A	551	GLY	Peptide
1	A	605	ARG	Sidechain
1	B	619	SER	Peptide

## 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	2677	0	2578	35	0
1	B	2558	0	2426	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	22	0	11	2	0
5	B	23	0	12	2	0
6	A	34	0	0	1	1
6	B	22	0	0	1	0
All	All	5340	0	5027	72	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (72) 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)
4:A:703:CMP:H2	4:A:703:CMP:C2	0.97	1.48
1:B:405:ARG:O	1:B:409:THR:HG23	1.81	0.81
1:B:349:GLU:OE2	1:B:381:ARG:NH2	2.15	0.78
1:A:405:ARG:O	1:A:409:THR:HG23	1.83	0.78
1:A:611:ILE:HG21	1:A:616:ASP:HB2	1.71	0.73
1:A:542:THR:O	1:A:546:THR:HG23	1.91	0.70
1:A:446:GLU:OE1	1:A:563:ARG:NH1	2.25	0.69
1:B:559:ASN:ND2	1:B:562:ASP:H	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:ASN:HD21	1:B:562:ASP:CG	1.98	0.67
1:B:399:PHE:CE2	1:B:403:LEU:HD11	2.31	0.66
1:A:664:GLU:O	1:A:667:ILE:HG13	1.95	0.65
1:B:417:HIS:NE2	5:B:703:AMP:O1P	2.30	0.64
1:A:400:VAL:O	1:A:404:LEU:HD23	1.98	0.63
1:A:552:SER:O	1:A:552:SER:OG	2.18	0.61
1:A:499:THR:HG22	1:A:500:GLU:HA	1.83	0.60
1:B:556:ASN:C	1:B:556:ASN:ND2	2.55	0.59
1:B:496:LYS:O	1:B:499:THR:HB	2.01	0.59
1:A:399:PHE:CE2	1:A:403:LEU:HD11	2.39	0.58
1:A:496:LYS:O	1:A:499:THR:HB	2.04	0.57
5:B:703:AMP:P	6:B:801:HOH:O	2.62	0.57
1:B:556:ASN:HD22	1:B:557:LEU:N	2.02	0.56
1:B:335:LEU:HD13	1:B:335:LEU:C	2.28	0.54
1:B:607:LEU:HD23	1:B:607:LEU:O	2.09	0.52
1:A:616:ASP:O	1:A:620:VAL:HG13	2.09	0.52
1:A:479:GLN:NE2	1:B:479:GLN:CD	2.63	0.51
1:A:504:ASP:OD2	1:A:514:ARG:NH2	2.44	0.51
1:B:399:PHE:CE2	1:B:403:LEU:CD1	2.93	0.51
1:A:517:LEU:HD23	1:A:517:LEU:C	2.31	0.50
1:B:557:LEU:HD22	1:B:566:ILE:HD11	1.95	0.49
1:A:405:ARG:O	1:A:409:THR:CG2	2.55	0.49
1:B:399:PHE:CZ	1:B:403:LEU:HD11	2.48	0.49
1:B:337:ILE:HD11	1:B:345:ASP:HB3	1.95	0.49
1:A:346:ASN:HD22	1:A:346:ASN:H	1.61	0.47
1:A:611:ILE:CG2	1:A:616:ASP:HB2	2.43	0.47
1:B:559:ASN:HD21	1:B:562:ASP:CB	2.28	0.47
1:A:579:PRO:HA	1:A:586:TYR:CD1	2.50	0.46
1:B:559:ASN:ND2	1:B:562:ASP:N	2.60	0.46
1:A:346:ASN:ND2	1:A:346:ASN:H	2.13	0.46
1:B:641:TRP:O	1:B:645:VAL:HG22	2.15	0.46
1:B:409:THR:HG21	1:B:497:ILE:HD11	1.97	0.46
1:A:552:SER:O	1:A:554:MET:N	2.49	0.45
1:B:464:VAL:HG12	1:B:600:GLN:HG3	1.96	0.45
1:A:349:GLU:OE1	1:A:381:ARG:NH2	2.49	0.45
1:A:399:PHE:CE2	1:A:403:LEU:CD1	3.00	0.45
1:B:514:ARG:HG2	1:B:514:ARG:HH11	1.80	0.45
1:A:573:CYS:HB3	1:A:638:TRP:CH2	2.52	0.45
1:A:623:GLU:HG3	1:A:663:TYR:CD1	2.52	0.44
1:B:559:ASN:HD22	1:B:561:ALA:HB3	1.82	0.44
1:B:556:ASN:ND2	1:B:557:LEU:N	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LYS:O	1:B:516:THR:HG23	2.17	0.44
1:A:338:HIS:HE1	1:A:345:ASP:O	2.00	0.44
1:B:337:ILE:HD13	1:B:338:HIS:CE1	2.53	0.43
1:B:650:GLN:NE2	1:B:654:ASP:OD1	2.50	0.43
1:A:479:GLN:HE21	1:B:479:GLN:NE2	2.17	0.43
1:A:601:GLY:HA3	1:A:615:CYS:O	2.19	0.43
1:A:360:GLY:HA2	1:A:581:LYS:HD2	2.01	0.43
1:B:450:VAL:HA	1:B:524:LEU:HD13	2.00	0.42
1:B:338:HIS:HE1	1:B:345:ASP:O	2.03	0.42
1:B:650:GLN:HE21	1:B:654:ASP:CG	2.22	0.42
1:B:556:ASN:O	1:B:557:LEU:HD23	2.19	0.42
1:A:400:VAL:O	1:A:404:LEU:CD2	2.68	0.42
1:A:393:CYS:HB3	1:A:508:ASN:HD22	1.85	0.41
1:B:453:ALA:O	1:B:457:HIS:HB3	2.20	0.41
1:A:479:GLN:NE2	1:B:479:GLN:NE2	2.69	0.41
1:A:467:GLN:HG3	1:A:471:ASN:ND2	2.36	0.41
4:A:703:CMP:P	6:A:802:HOH:O	2.78	0.41
1:B:352:PHE:HE1	1:B:366:ILE:HD13	1.86	0.41
1:B:556:ASN:C	1:B:556:ASN:HD22	2.22	0.41
1:A:499:THR:HG22	1:A:500:GLU:CA	2.51	0.41
1:A:623:GLU:HG3	1:A:663:TYR:HD1	1.85	0.41
1:A:399:PHE:CZ	1:A:403:LEU:HD11	2.56	0.40
1:B:537:LEU:CD2	1:B:541:ARG:NH2	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:832:HOH:O	6:A:832:HOH:O[5_554]	1.46	0.74

## 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	331/371 (89%)	311 (94%)	19 (6%)	1 (0%)	41	31
1	B	320/371 (86%)	304 (95%)	12 (4%)	4 (1%)	12	4
All	All	651/742 (88%)	615 (94%)	31 (5%)	5 (1%)	19	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	GLU
1	B	507	ALA
1	A	553	GLY
1	B	557	LEU
1	B	646	HIS

### 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	290/333 (87%)	269 (93%)	21 (7%)	14	7
1	B	270/333 (81%)	247 (92%)	23 (8%)	10	4
All	All	560/666 (84%)	516 (92%)	44 (8%)	12	5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	340	VAL
1	A	346	ASN
1	A	354	LEU
1	A	381	ARG
1	A	409	THR
1	A	440	ASP
1	A	496	LYS
1	A	514	ARG
1	A	515	GLN
1	A	516	THR

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Mol	Chain	Res	Type
1	A	540	LEU
1	A	546	THR
1	A	555	LEU
1	A	556	ASN
1	A	557	LEU
1	A	563	ARG
1	A	595	GLU
1	A	619	SER
1	A	620	VAL
1	A	667	ILE
1	B	335	LEU
1	B	337	ILE
1	B	340	VAL
1	B	354	LEU
1	B	371	ASN
1	B	390	LYS
1	B	404	LEU
1	B	409	THR
1	B	472	THR
1	B	496	LYS
1	B	514	ARG
1	B	516	THR
1	B	517	LEU
1	B	532	LYS
1	B	539	ASP
1	B	540	LEU
1	B	556	ASN
1	B	557	LEU
1	B	582	PRO
1	B	607	LEU
1	B	612	SER
1	B	643	ASP
1	B	651	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	346	ASN
1	A	371	ASN
1	A	434	GLN
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	556	ASN
1	A	565	GLN
1	B	338	HIS
1	B	371	ASN
1	B	479	GLN
1	B	556	ASN
1	B	559	ASN
1	B	650	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
5	AMP	B	703	3,2	22,25,25	1.72	6 (27%)	25,38,38	2.13	10 (40%)
4	CMP	A	703	3,2	22,25,25	5.32	10 (45%)	24,39,39	8.09	17 (70%)

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	AMP	B	703	3,2	-	2/6/26/26	0/3/3/3
4	CMP	A	703	3,2	-	0/0/31/31	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CMP	P-O3'	16.43	1.84	1.57
4	A	703	CMP	O3'-C3'	11.69	1.62	1.44
4	A	703	CMP	P-O5'	7.54	1.66	1.57
4	A	703	CMP	C2'-C1'	7.36	1.64	1.53
4	A	703	CMP	C8-N7	4.92	1.43	1.34
4	A	703	CMP	C2'-C3'	4.13	1.62	1.52
4	A	703	CMP	P-O1P	4.05	1.65	1.50
4	A	703	CMP	O4'-C1'	3.60	1.46	1.41
5	B	703	AMP	P-O3P	3.46	1.68	1.54
4	A	703	CMP	O4'-C4'	3.11	1.51	1.45
4	A	703	CMP	O5'-C5'	-3.04	1.41	1.46
5	B	703	AMP	C5-C4	2.93	1.48	1.40
5	B	703	AMP	P-O1P	2.78	1.59	1.50
5	B	703	AMP	O4'-C4'	2.48	1.50	1.45
5	B	703	AMP	P-O5'	2.47	1.68	1.60
5	B	703	AMP	O4'-C1'	2.42	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CMP	O3'-C3'-C2'	30.93	145.94	115.61
4	A	703	CMP	O5'-P-O3'	-14.55	85.63	105.68
4	A	703	CMP	O3'-P-O1P	9.14	129.96	110.39
4	A	703	CMP	C2'-C3'-C4'	-7.29	90.30	103.22
4	A	703	CMP	O2'-C2'-C1'	-6.32	87.50	110.85
4	A	703	CMP	O3'-C3'-C4'	6.23	115.41	110.71
4	A	703	CMP	N6-C6-N1	5.29	129.56	118.57
4	A	703	CMP	O2'-C2'-C3'	5.09	125.63	111.17
4	A	703	CMP	N3-C2-N1	-4.67	121.39	128.68
4	A	703	CMP	C5-C6-N6	-4.25	113.89	120.35
5	B	703	AMP	C2-N1-C6	4.05	125.67	118.75
5	B	703	AMP	N3-C2-N1	-3.91	122.57	128.68
4	A	703	CMP	O2P-P-O1P	3.74	120.44	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CMP	C4-C5-N7	3.74	113.29	109.40
4	A	703	CMP	C2-N1-C6	3.69	125.07	118.75
5	B	703	AMP	C1'-N9-C4	-3.51	120.47	126.64
4	A	703	CMP	O2P-P-O5'	-3.48	98.67	107.16
4	A	703	CMP	C1'-N9-C4	-3.08	121.23	126.64
5	B	703	AMP	O3'-C3'-C4'	3.07	119.92	111.05
4	A	703	CMP	O4'-C4'-C3'	2.75	110.77	104.87
5	B	703	AMP	O5'-P-O1P	-2.72	98.86	106.47
4	A	703	CMP	O4'-C1'-C2'	-2.69	102.99	106.93
5	B	703	AMP	P-O5'-C5'	2.53	125.26	118.30
5	B	703	AMP	N6-C6-N1	2.42	123.60	118.57
5	B	703	AMP	O3P-P-O5'	2.34	112.96	106.73
5	B	703	AMP	C5-C6-N1	-2.32	115.10	120.35
5	B	703	AMP	O4'-C4'-C5'	-2.13	102.36	109.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

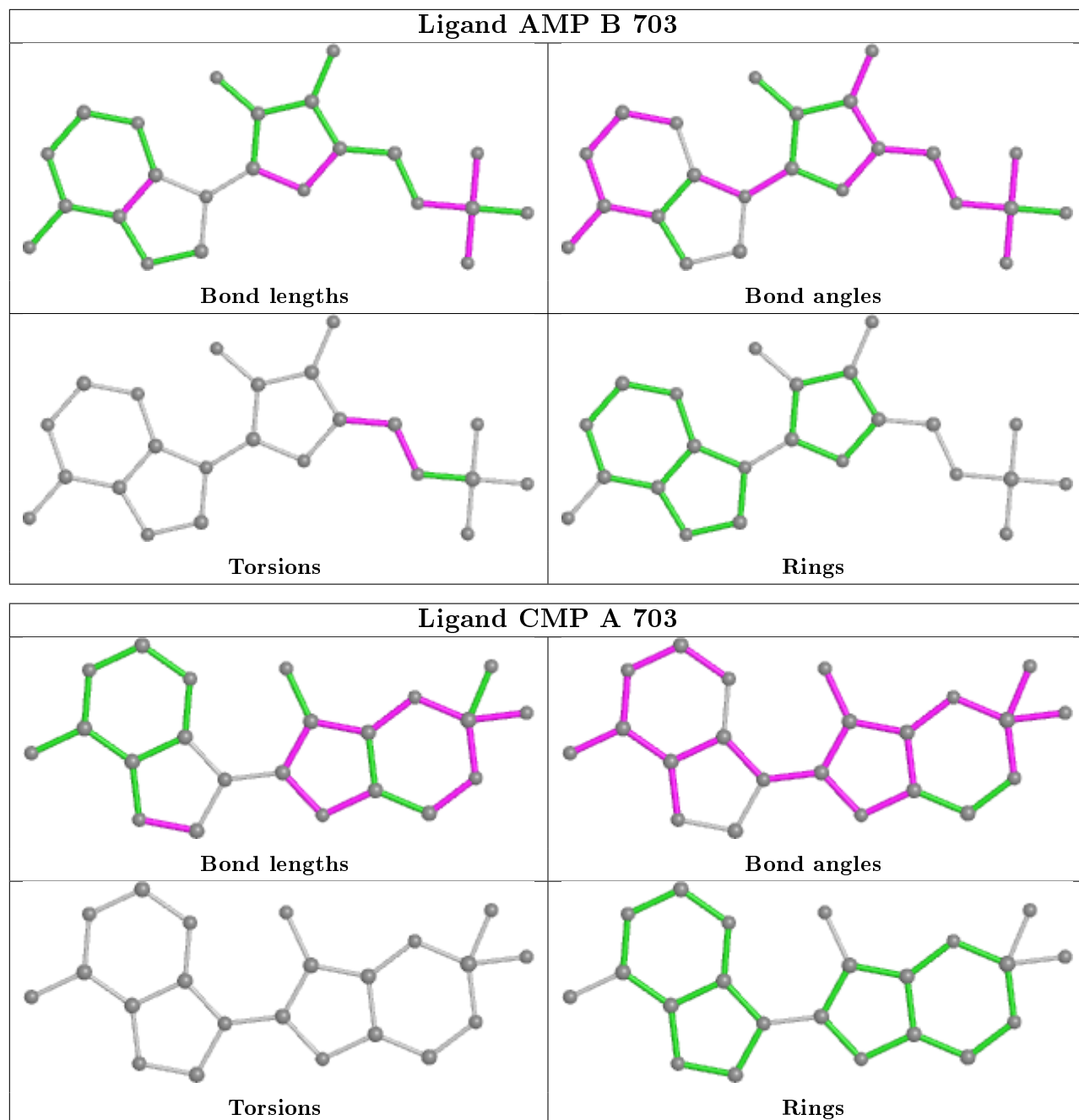
Mol	Chain	Res	Type	Atoms
5	B	703	AMP	C4'-C5'-O5'-P
5	B	703	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	703	AMP	2	0
4	A	703	CMP	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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	333/371 (89%)	-0.12	4 (1%) 79 81	37, 56, 82, 93	0
1	B	324/371 (87%)	0.03	8 (2%) 57 61	39, 61, 104, 132	0
All	All	657/742 (88%)	-0.05	12 (1%) 68 71	37, 58, 92, 132	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ILE	4.1
1	B	510	GLY	3.8
1	B	558	ASP	3.7
1	A	507	ALA	3.1
1	B	616	ASP	2.9
1	B	619	SER	2.9
1	A	502	ASP	2.9
1	B	611	ILE	2.9
1	B	607	LEU	2.6
1	A	335	LEU	2.5
1	B	608	SER	2.2
1	B	511	GLY	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](#)

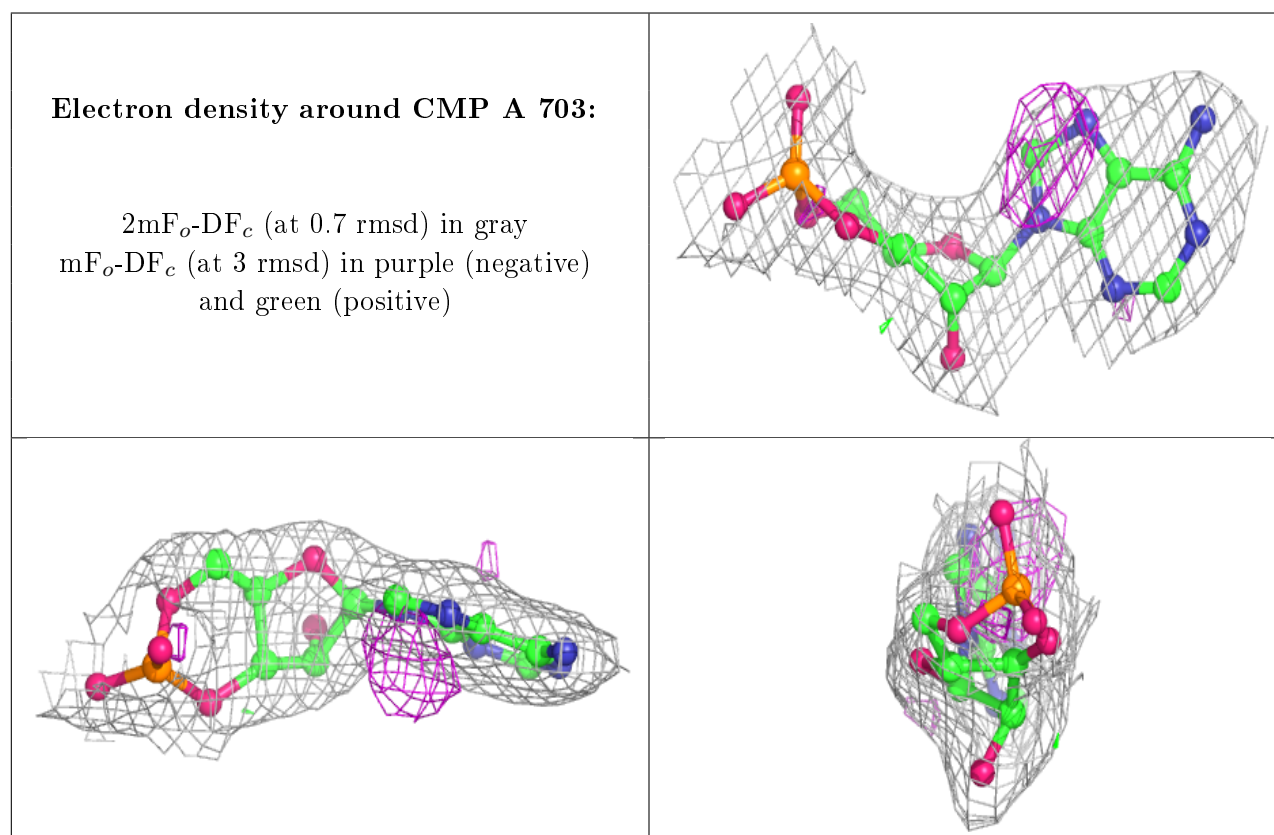
There are no carbohydrates in this entry.

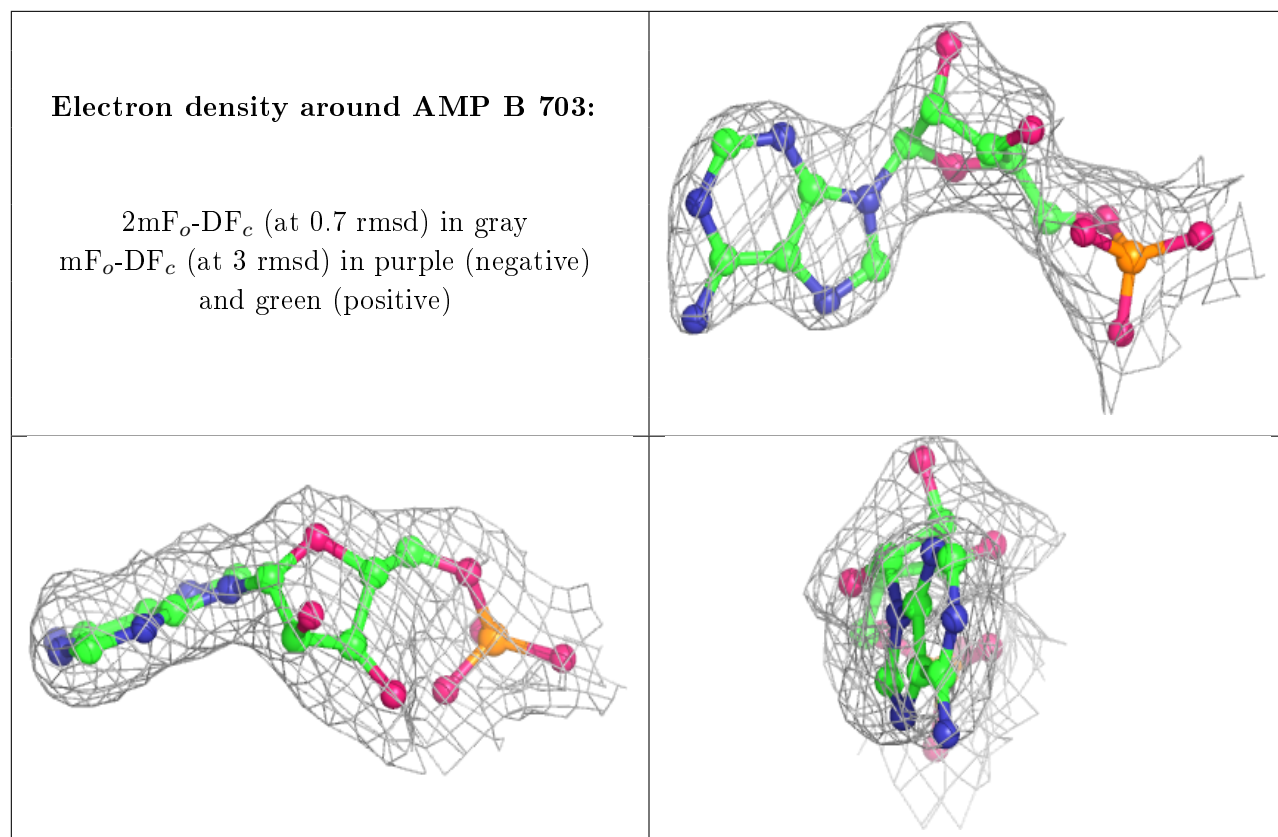
## 6.4 Ligands ⓘ

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
4	CMP	A	703	22/22	0.96	0.10	43,51,63,69	0
3	MG	B	702	1/1	0.96	0.07	44,44,44,44	0
5	AMP	B	703	23/23	0.97	0.10	49,64,70,71	0
3	MG	A	702	1/1	0.99	0.09	40,40,40,40	0
2	ZN	B	701	1/1	1.00	0.14	47,47,47,47	0
2	ZN	A	701	1/1	1.00	0.12	43,43,43,43	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.