



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 AM UTC

PDB ID : 4ZCF / pdb_00004zcf
Title : Structural basis of asymmetric DNA methylation and ATP-triggered long-range diffusion by EcoP15I
Authors : Gupta, Y.K.; Chan, S.H.; Xu, S.Y.; Aggarwal, A.K.
Deposited on : 2015-04-15
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

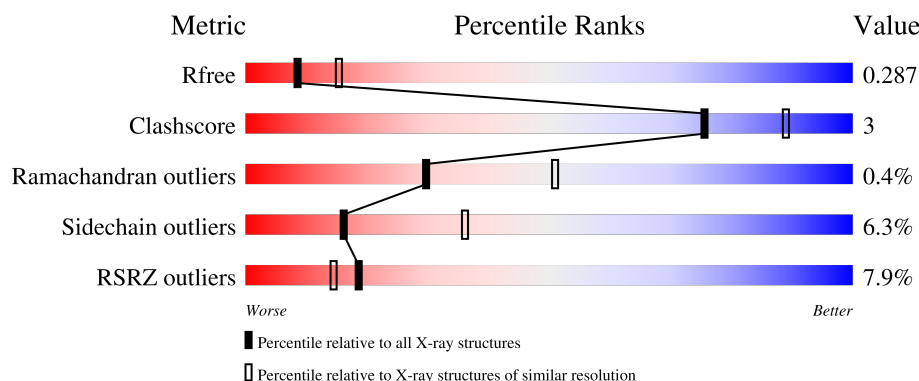
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	644	3% 82% 12% • •
1	B	644	6% 82% 11% • 5%
2	C	970	9% 57% 7% • 35%
3	D	20	5% 75% 25%
4	E	20	50% 45% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14929 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 Restriction endonuclease EcoP15I, modification subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4833	3096	803	920	14			
1	B	612	Total	C	N	O	S	0	0	0
			4705	3001	784	905	15			

- Molecule 2 is a protein called Restriction endonuclease EcoP15I, restriction subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	627	Total	C	N	O	S	0	0	0
			4452	2848	766	827	11			

- Molecule 3 is a DNA chain called DNA 20-mer ATACAGCAGTAGACTATGAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			413	197	79	117	20			

- Molecule 4 is a DNA chain called DNA 20-mer AATCATAGTCTACTGCTGTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	20	Total	C	N	O	P	0	0	0
			405	196	71	119	19			

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mn	0	0
			2	2		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Ca	0	0
			1	1		

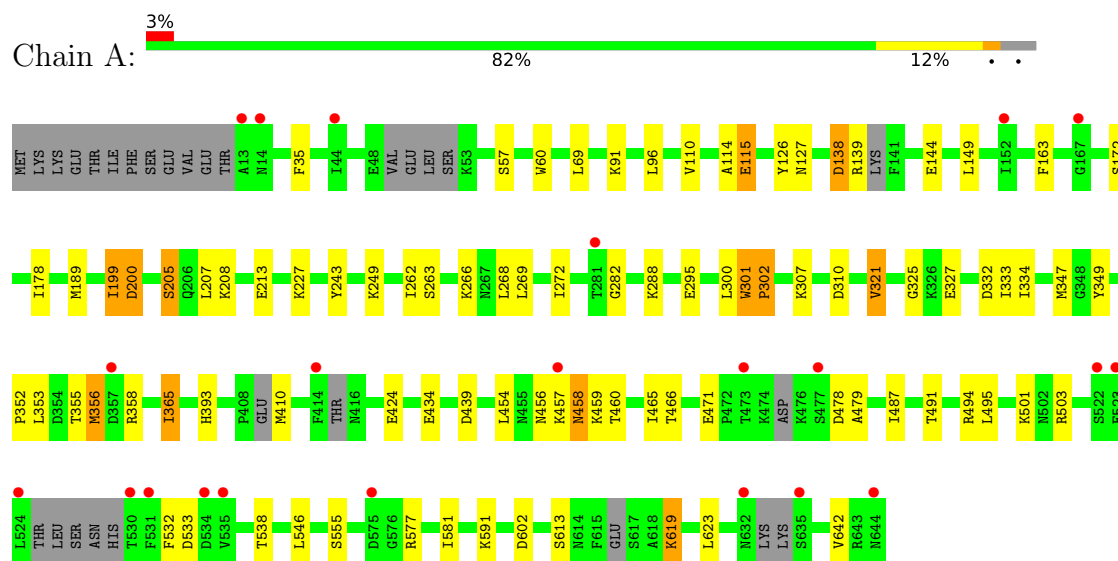
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	B	36	Total	O	0	0
			36	36		
8	C	4	Total	O	0	0
			4	4		
8	D	7	Total	O	0	0
			7	7		
8	E	5	Total	O	0	0
			5	5		

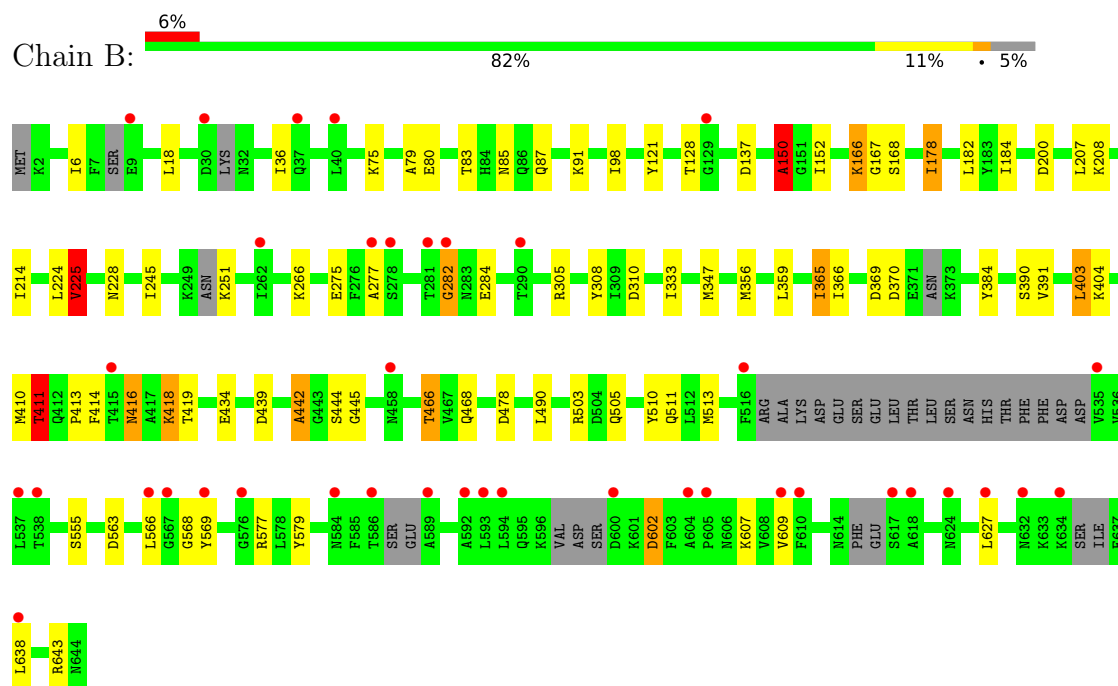
3 Residue-property plots

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

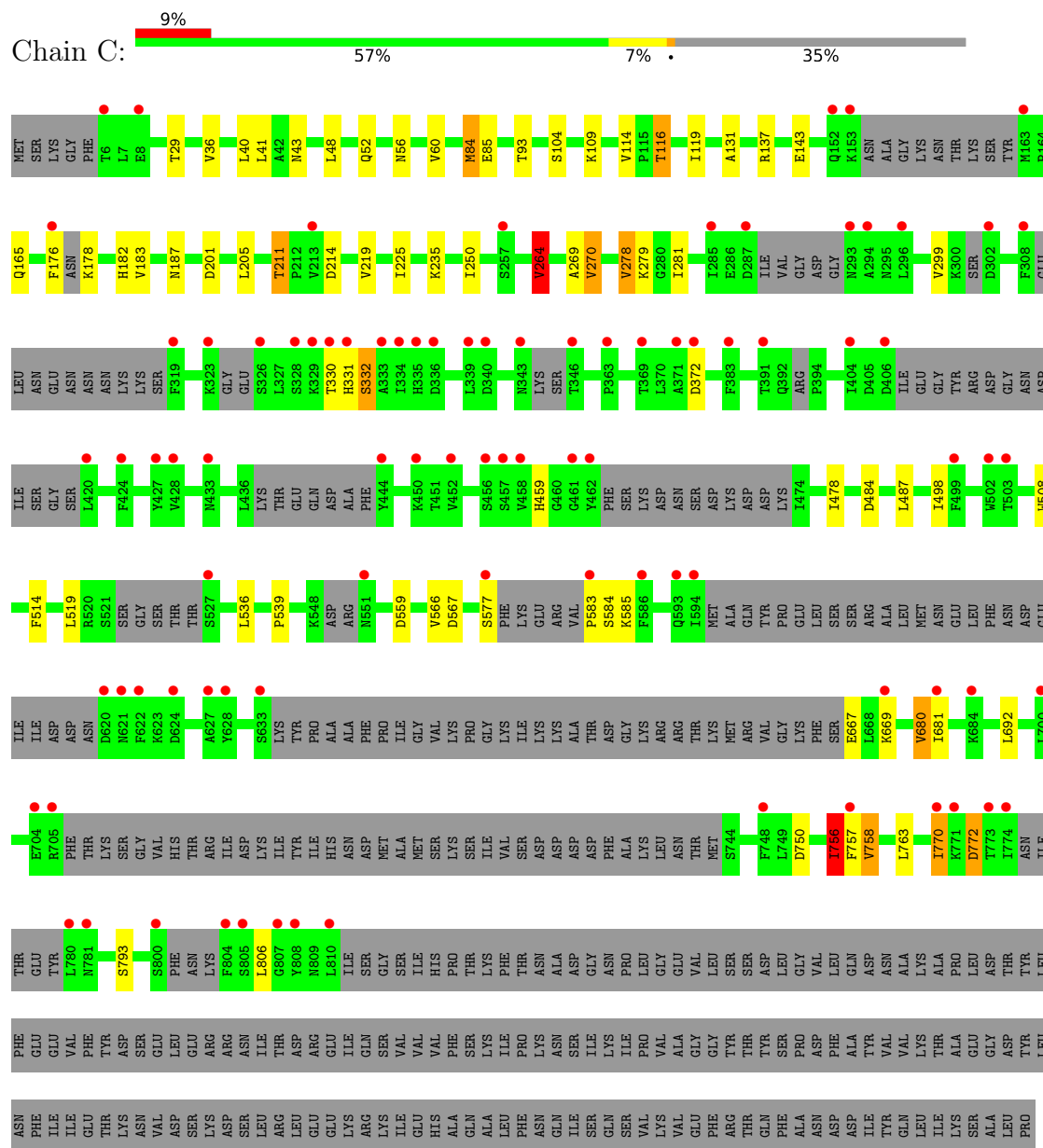
- Molecule 1: Restriction endonuclease EcoP15I, modification subunit



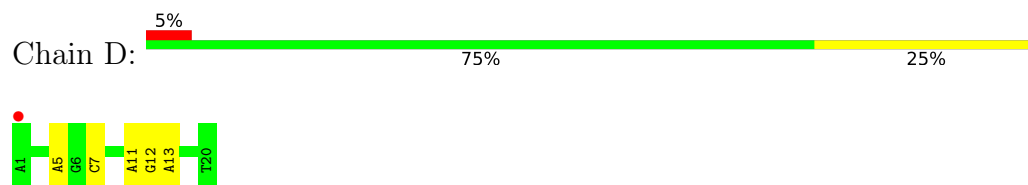
- Molecule 1: Restriction endonuclease EcoP15I, modification subunit



- Molecule 2: Restriction endonuclease EcoP15I, restriction subunit



- Molecule 3: DNA 20-mer ATACAGCAGTAGACTATGAT



- Molecule 4: DNA 20-mer AATCATAGTCTACTGCTGTA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.84Å 101.84Å 533.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-2.60) 97.4 (40.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.263 0.237 , 0.287	Depositor DCC
R_{free} test set	4329 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14929	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, MN, AMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	1/4932 (0.0%)	1.43	29/6678 (0.4%)
1	B	0.88	0/4798	1.45	34/6509 (0.5%)
2	C	0.89	1/4518 (0.0%)	1.46	24/6136 (0.4%)
3	D	0.45	0/464	1.40	5/714 (0.7%)
4	E	0.48	0/453	1.51	10/697 (1.4%)
All	All	0.87	2/15165 (0.0%)	1.45	102/20734 (0.5%)

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	3
2	C	0	5
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	MET	SD-CE	-8.49	1.58	1.79
2	C	84	MET	SD-CE	-5.43	1.66	1.79

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	LYS	N-CA-C	-10.19	96.80	110.55
3	D	7	DC	P-O5'-C5'	9.16	133.74	120.00
2	C	756	ILE	N-CA-C	8.80	121.55	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ALA	N-CA-C	8.76	121.78	111.71
4	E	1	DA	P-O3'-C3'	8.44	132.85	120.20
1	A	301	TRP	C-N-CD	8.37	139.02	120.60
1	B	128	THR	N-CA-C	-8.24	99.89	110.53
2	C	299	VAL	N-CA-C	8.23	118.27	110.53
1	A	127	ASN	CA-C-N	8.09	131.46	120.38
1	A	127	ASN	C-N-CA	8.09	131.46	120.38
1	A	200	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	225	VAL	N-CA-CB	7.80	121.28	111.46
1	B	310	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	503	ARG	N-CA-C	7.27	121.55	111.74
2	C	201	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	228	ASN	N-CA-C	7.15	122.89	113.30
1	B	167	GLY	N-CA-C	6.94	120.97	111.54
1	A	178	ILE	N-CA-C	6.75	117.54	110.72
2	C	459	HIS	CA-C-N	6.57	126.71	122.18
2	C	459	HIS	C-N-CA	6.57	126.71	122.18
2	C	183	VAL	N-CA-C	6.43	117.29	107.77
1	B	137	ASP	N-CA-C	6.39	121.43	112.93
2	C	583	PRO	N-CA-CB	6.38	110.02	103.00
1	B	419	THR	CA-C-N	6.29	129.07	120.46
1	B	419	THR	C-N-CA	6.29	129.07	120.46
3	D	13	DA	P-O3'-C3'	6.26	129.59	120.20
1	A	126	TYR	N-CA-C	-6.14	102.61	110.53
4	E	13	DC	O4'-C1'-N1	6.10	117.55	108.40
2	C	372	ASP	N-CA-C	-6.05	104.75	111.71
2	C	201	ASP	CA-C-N	6.04	131.04	122.09
2	C	201	ASP	C-N-CA	6.04	131.04	122.09
2	C	584	SER	N-CA-C	6.00	116.35	107.88
4	E	7	DA	P-O3'-C3'	6.00	129.19	120.20
1	A	546	LEU	CA-C-N	5.93	128.16	120.44
1	A	546	LEU	C-N-CA	5.93	128.16	120.44
2	C	264	VAL	CB-CA-C	5.92	116.27	111.06
4	E	13	DC	P-O5'-C5'	-5.89	111.17	120.00
3	D	12	DG	P-O5'-C5'	5.88	128.82	120.00
1	A	321	VAL	N-CA-CB	-5.86	104.20	112.12
1	B	602	ASP	CA-C-N	5.85	130.56	121.26
1	B	602	ASP	C-N-CA	5.85	130.56	121.26
2	C	519	LEU	N-CA-C	5.79	117.46	111.03
1	B	178	ILE	N-CA-C	5.79	116.57	110.72
1	B	166	LYS	CA-C-N	5.79	126.21	120.31
1	B	166	LYS	C-N-CA	5.79	126.21	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	11	DA	P-O3'-C3'	5.78	128.87	120.20
1	B	442	ALA	N-CA-C	5.73	117.98	111.11
1	A	138	ASP	CA-C-N	5.69	131.95	121.70
1	A	138	ASP	C-N-CA	5.69	131.95	121.70
2	C	806	LEU	N-CA-C	5.67	115.50	108.19
1	A	310	ASP	CA-CB-CG	5.67	118.27	112.60
4	E	8	DG	P-O3'-C3'	5.66	128.69	120.20
1	B	445	GLY	CA-C-N	5.63	128.14	120.54
1	B	445	GLY	C-N-CA	5.63	128.14	120.54
1	B	643	ARG	N-CA-C	5.60	117.86	108.96
2	C	43	ASN	CA-CB-CG	5.58	118.18	112.60
2	C	131	ALA	CA-C-N	5.57	128.01	120.44
2	C	131	ALA	C-N-CA	5.57	128.01	120.44
4	E	13	DC	C5'-C4'-O4'	5.54	117.72	109.40
1	B	91	LYS	N-CA-C	5.53	117.31	111.28
1	B	416	ASN	CA-CB-CG	5.53	118.13	112.60
2	C	104	SER	N-CA-C	5.52	117.30	111.28
1	A	332	ASP	CA-CB-CG	5.49	118.08	112.60
4	E	16	DC	P-O3'-C3'	5.46	128.39	120.20
1	A	144	GLU	CA-C-N	5.45	127.52	120.44
1	A	144	GLU	C-N-CA	5.45	127.52	120.44
1	A	126	TYR	CA-C-N	-5.42	111.19	121.54
1	A	126	TYR	C-N-CA	-5.42	111.19	121.54
4	E	17	DT	P-O5'-C5'	5.34	128.01	120.00
1	A	365	ILE	N-CA-C	5.34	116.27	108.58
1	B	184	ILE	N-CA-CB	5.32	116.66	110.65
1	B	200	ASP	CA-CB-CG	5.31	117.91	112.60
3	D	5	DA	P-O3'-C3'	5.28	128.12	120.20
1	A	127	ASN	CA-CB-CG	5.24	117.83	112.60
1	A	302	PRO	CA-N-CD	-5.21	104.20	111.50
2	C	165	GLN	N-CA-C	5.20	116.95	111.28
4	E	4	DC	P-O3'-C3'	5.20	128.01	120.20
1	A	35	PHE	N-CA-C	5.20	117.23	109.59
1	B	369	ASP	N-CA-C	-5.19	106.79	113.23
1	B	569	TYR	CA-C-N	5.19	131.04	121.70
1	B	569	TYR	C-N-CA	5.19	131.04	121.70
1	A	532	PHE	CA-C-N	5.18	128.98	121.26
1	A	532	PHE	C-N-CA	5.18	128.98	121.26
1	B	83	THR	CA-C-N	5.15	127.45	120.44
1	B	83	THR	C-N-CA	5.15	127.45	120.44
1	B	411	THR	CB-CA-C	5.13	118.93	110.88
2	C	52	GLN	CA-C-N	5.13	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	52	GLN	C-N-CA	5.13	127.15	120.28
4	E	3	DT	P-O5'-C5'	5.12	127.69	120.00
1	A	619	LYS	CA-C-N	5.11	127.13	120.28
1	A	619	LYS	C-N-CA	5.11	127.13	120.28
1	A	57	SER	N-CA-C	5.11	116.83	108.55
1	B	404	LYS	CA-C-N	5.11	127.38	120.44
1	B	404	LYS	C-N-CA	5.11	127.38	120.44
1	B	466	THR	CB-CA-C	5.11	119.46	109.35
1	A	110	VAL	N-CA-C	5.07	115.68	110.36
2	C	235	LYS	N-CA-C	5.04	117.03	110.53
1	B	277	ALA	CA-C-N	5.02	127.01	120.28
1	B	277	ALA	C-N-CA	5.02	127.01	120.28
1	B	168	SER	N-CA-C	5.01	117.89	110.48
2	C	680	VAL	CA-C-N	5.00	127.20	120.50
2	C	680	VAL	C-N-CA	5.00	127.20	120.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ALA	Peptide
1	A	456	ASN	Peptide
1	A	458	ASN	Peptide
1	B	150	ALA	Peptide
1	B	166	LYS	Peptide
1	B	282	GLY	Peptide
2	C	330	THR	Peptide
2	C	332	SER	Peptide
2	C	585	LYS	Peptide
2	C	667	GLU	Peptide
2	C	756	ILE	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	4833	0	4603	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4705	0	4394	30	0
2	C	4452	0	3830	28	0
3	D	413	0	226	0	0
4	E	405	0	229	3	0
5	A	2	0	0	0	0
6	C	23	0	12	0	0
7	D	1	0	0	0	0
8	A	43	0	0	0	0
8	B	36	0	0	1	0
8	C	4	0	0	0	0
8	D	7	0	0	0	0
8	E	5	0	0	0	0
All	All	14929	0	13294	85	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 3.

All (85) 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:458:ASN:CB	1:A:460:THR:H	1.82	0.93
1:A:457:LYS:O	1:A:457:LYS:HD2	1.85	0.76
1:B:503:ARG:HG3	1:B:503:ARG:NH1	2.02	0.73
1:B:503:ARG:HG3	1:B:503:ARG:HH11	1.54	0.73
1:B:333:ILE:HD13	1:B:356:MET:HE2	1.70	0.73
2:C:84:MET:HE1	2:C:93:THR:HG21	1.71	0.72
2:C:757:PHE:H	2:C:757:PHE:HD1	1.39	0.69
4:E:10:DC:H2"	4:E:11:DT:H71	1.80	0.63
1:B:150:ALA:HB3	1:B:152:ILE:HG12	1.79	0.63
1:A:458:ASN:CB	1:A:460:THR:N	2.60	0.62
2:C:56:ASN:O	2:C:60:VAL:HG23	2.01	0.61
2:C:116:THR:HG22	2:C:119:ILE:H	1.66	0.61
1:B:207:LEU:HD23	1:B:245:ILE:HD12	1.84	0.58
2:C:756:ILE:HD12	2:C:758:VAL:HG13	1.85	0.58
2:C:84:MET:CE	2:C:93:THR:HG21	2.33	0.58
1:B:511:GLN:HG3	1:B:513:MET:HE3	1.84	0.57
1:A:356:MET:HE1	1:A:365:ILE:HD11	1.87	0.57
2:C:270:VAL:HG13	2:C:577:SER:OG	2.04	0.57
2:C:757:PHE:CD1	2:C:757:PHE:N	2.73	0.57
1:A:356:MET:HE1	1:A:365:ILE:CD1	2.34	0.56
1:B:359:LEU:HB2	1:B:365:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:THR:HG23	1:A:358:ARG:HH21	1.73	0.54
1:B:182:LEU:HB2	1:B:214:ILE:HD13	1.90	0.54
2:C:85:GLU:HG2	2:C:269:ALA:HB2	1.90	0.53
1:B:442:ALA:HB3	1:B:468:GLN:HB2	1.91	0.52
2:C:498:ILE:HG21	2:C:508:TRP:CH2	2.45	0.52
1:A:115:GLU:HB3	1:A:189:MET:O	2.09	0.52
2:C:211:THR:HG22	2:C:214:ASP:H	1.74	0.52
1:A:410:MET:HE1	1:A:479:ALA:HA	1.92	0.52
1:B:577:ARG:HG2	1:B:607:LYS:HB3	1.91	0.51
1:B:579:TYR:HA	1:B:609:VAL:O	2.10	0.51
1:B:410:MET:HE2	1:B:413:PRO:HA	1.92	0.50
2:C:281:ILE:HD11	2:C:536:LEU:HD21	1.94	0.50
1:A:96:LEU:HD12	1:A:465:ILE:HG12	1.94	0.49
1:B:121:TYR:OH	1:B:418:LYS:HD2	2.13	0.49
2:C:770:ILE:HG23	2:C:772:ASP:HB2	1.93	0.49
2:C:137:ARG:HD3	2:C:143:GLU:OE2	2.12	0.49
2:C:278:VAL:HG13	2:C:536:LEU:HD22	1.94	0.48
1:A:333:ILE:HD12	1:A:349:TYR:CZ	2.48	0.48
2:C:279:LYS:HE3	2:C:539:PRO:HD3	1.95	0.48
2:C:514:PHE:CZ	2:C:539:PRO:HG3	2.48	0.48
2:C:756:ILE:HD11	2:C:763:LEU:HD21	1.96	0.47
1:A:268:LEU:HD22	1:B:347:MET:HE3	1.96	0.47
1:B:503:ARG:HH11	1:B:503:ARG:CG	2.21	0.47
1:A:227:LYS:HG2	1:A:393:HIS:ND1	2.30	0.46
1:A:471:GLU:O	1:A:487:ILE:HG12	2.15	0.46
2:C:484:ASP:HA	2:C:487:LEU:HD12	1.96	0.46
1:B:98:ILE:HG12	1:B:510:TYR:HB2	1.97	0.46
1:A:491:THR:O	1:A:495:LEU:HD13	2.16	0.46
1:A:138:ASP:CG	1:A:139:ARG:H	2.24	0.45
2:C:681:ILE:HD12	2:C:681:ILE:H	1.80	0.45
1:B:80:GLU:HG2	1:B:85:ASN:HD22	1.82	0.45
2:C:278:VAL:HG22	2:C:536:LEU:HB3	1.99	0.45
1:A:356:MET:HE1	1:A:365:ILE:HG13	1.99	0.45
1:B:439:ASP:O	1:B:466:THR:HA	2.17	0.44
1:B:79:ALA:HB2	1:B:513:MET:HG3	1.99	0.44
1:A:301:TRP:CG	1:A:302:PRO:HA	2.52	0.44
2:C:514:PHE:HZ	2:C:539:PRO:HG3	1.82	0.44
2:C:758:VAL:HG22	2:C:763:LEU:HG	2.00	0.44
1:A:439:ASP:HB3	1:A:466:THR:HG22	2.00	0.44
1:A:199:ILE:HG12	1:A:207:LEU:HD23	2.01	0.43
1:B:225:VAL:HG22	1:B:391:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LYS:HD2	1:B:384:TYR:HB3	1.99	0.43
2:C:114:VAL:O	2:C:187:ASN:HA	2.19	0.43
2:C:756:ILE:CD1	2:C:758:VAL:HG13	2.49	0.43
1:A:199:ILE:HD12	1:A:243:TYR:HB2	1.99	0.43
1:A:269:LEU:HD11	1:A:300:LEU:HD22	2.00	0.43
1:B:403:LEU:HD21	1:B:414:PHE:HD2	1.85	0.42
1:A:454:LEU:O	1:A:457:LYS:O	2.38	0.41
1:A:347:MET:HE1	1:B:411:THR:HG23	2.01	0.41
1:A:439:ASP:O	1:A:466:THR:HA	2.19	0.41
1:A:205:SER:OG	1:B:208:LYS:HG2	2.20	0.41
1:B:6:ILE:O	1:B:6:ILE:HG13	2.20	0.41
1:B:305:ARG:HB2	8:B:730:HOH:O	2.19	0.41
1:A:263:SER:HB2	1:A:266:LYS:HB3	2.03	0.41
1:B:414:PHE:CZ	1:B:444:SER:HA	2.55	0.41
1:A:149:LEU:HD22	2:C:176:PHE:HE1	1.85	0.41
1:A:352:PRO:HD3	4:E:13:DC:OP2	2.21	0.41
2:C:60:VAL:HG11	2:C:264:VAL:HG22	2.03	0.41
4:E:10:DC:H2"	4:E:11:DT:C7	2.49	0.41
2:C:109:LYS:HG2	2:C:182:HIS:HB2	2.02	0.40
1:A:60:TRP:HB2	1:A:172:SER:HB3	2.02	0.40
1:B:224:LEU:HD23	1:B:390:SER:HA	2.03	0.40
1:B:282:GLY:HA2	1:B:284:GLU:N	2.35	0.40
1:B:359:LEU:HB2	1:B:365:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	598/644 (93%)	569 (95%)	26 (4%)	3 (0%)	24 46
1	B	592/644 (92%)	558 (94%)	33 (6%)	1 (0%)	43 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	587/970 (60%)	558 (95%)	26 (4%)	3 (0%)	24	46
All	All	1777/2258 (79%)	1685 (95%)	85 (5%)	7 (0%)	30	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
2	C	332	SER
2	C	331	HIS
2	C	669	LYS
1	A	282	GLY
1	B	568	GLY
1	A	325	GLY

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	502/580 (87%)	468 (93%)	34 (7%)	14	32
1	B	478/580 (82%)	452 (95%)	26 (5%)	20	42
2	C	377/876 (43%)	351 (93%)	26 (7%)	14	32
All	All	1357/2036 (67%)	1271 (94%)	86 (6%)	16	36

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	115	GLU
1	A	163	PHE
1	A	199	ILE
1	A	200	ASP
1	A	205	SER
1	A	208	LYS
1	A	213	GLU

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Mol	Chain	Res	Type
1	A	249	LYS
1	A	262	ILE
1	A	272	ILE
1	A	288	LYS
1	A	295	GLU
1	A	307	LYS
1	A	321	VAL
1	A	327	GLU
1	A	334	ILE
1	A	353	LEU
1	A	424	GLU
1	A	434	GLU
1	A	459	LYS
1	A	478	ASP
1	A	494	ARG
1	A	533	ASP
1	A	538	THR
1	A	555	SER
1	A	577	ARG
1	A	581	ILE
1	A	591	LYS
1	A	602	ASP
1	A	613	SER
1	A	619	LYS
1	A	623	LEU
1	A	642	VAL
1	B	18	LEU
1	B	36	ILE
1	B	75	LYS
1	B	87	GLN
1	B	178	ILE
1	B	225	VAL
1	B	251	LYS
1	B	275	GLU
1	B	308	TYR
1	B	365	ILE
1	B	366	ILE
1	B	370	ASP
1	B	403	LEU
1	B	411	THR
1	B	416	ASN
1	B	418	LYS

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Mol	Chain	Res	Type
1	B	434	GLU
1	B	478	ASP
1	B	490	LEU
1	B	505	GLN
1	B	555	SER
1	B	563	ASP
1	B	566	LEU
1	B	602	ASP
1	B	627	LEU
1	B	638	LEU
2	C	29	THR
2	C	36	VAL
2	C	40	LEU
2	C	41	LEU
2	C	48	LEU
2	C	116	THR
2	C	178	LYS
2	C	205	LEU
2	C	211	THR
2	C	219	VAL
2	C	225	ILE
2	C	250	ILE
2	C	264	VAL
2	C	270	VAL
2	C	278	VAL
2	C	478	ILE
2	C	559	ASP
2	C	566	VAL
2	C	567	ASP
2	C	680	VAL
2	C	692	LEU
2	C	750	ASP
2	C	758	VAL
2	C	770	ILE
2	C	772	ASP
2	C	793	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	84	HIS

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Mol	Chain	Res	Type
1	A	323	ASN
1	A	386	GLN
1	A	624	ASN
1	B	59	ASN
1	B	71	ASN
1	B	87	GLN
1	B	218	GLN
1	B	219	ASN
1	B	453	ASN
1	B	482	HIS
1	B	541	GLN
2	C	31	HIS
2	C	35	ASN
2	C	51	GLN
2	C	72	ASN
2	C	168	HIS
2	C	208	GLN
2	C	373	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
6	AMP	C	1001	-	25,25,25	1.96	7 (28%)	37,38,38	2.78	15 (40%)

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
6	AMP	C	1001	-	-	4/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	AMP	C5-C4	4.72	1.47	1.39
6	C	1001	AMP	C5-N7	4.52	1.47	1.39
6	C	1001	AMP	C6-N6	3.17	1.42	1.34
6	C	1001	AMP	C8-N9	-3.09	1.32	1.37
6	C	1001	AMP	C8-N7	2.58	1.36	1.31
6	C	1001	AMP	C4-N9	-2.30	1.32	1.37
6	C	1001	AMP	C2'-C3'	-2.01	1.47	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1001	AMP	C4-N9-C8	8.64	114.81	105.74
6	C	1001	AMP	C5-C4-N3	-5.93	118.55	126.72
6	C	1001	AMP	N3-C4-N9	5.70	136.86	127.17
6	C	1001	AMP	C4-C5-N7	-4.82	105.08	110.58
6	C	1001	AMP	N3-C2-N1	-4.04	122.46	128.58
6	C	1001	AMP	C2-N3-C4	3.86	121.25	111.83
6	C	1001	AMP	O2P-P-O5'	3.70	116.31	106.67
6	C	1001	AMP	C6-C5-N7	3.12	138.11	132.09
6	C	1001	AMP	N9-C8-N7	-3.06	109.60	113.94
6	C	1001	AMP	O5'-P-O1P	2.92	114.34	106.44
6	C	1001	AMP	O3P-P-O5'	2.48	113.14	106.67
6	C	1001	AMP	C3'-C2'-C1'	2.26	105.73	101.46
6	C	1001	AMP	O4'-C1'-N9	2.06	112.06	108.09
6	C	1001	AMP	C2-N1-C6	2.05	122.11	118.73
6	C	1001	AMP	C4-N9-C1'	-2.05	121.83	126.63

There are no chirality outliers.

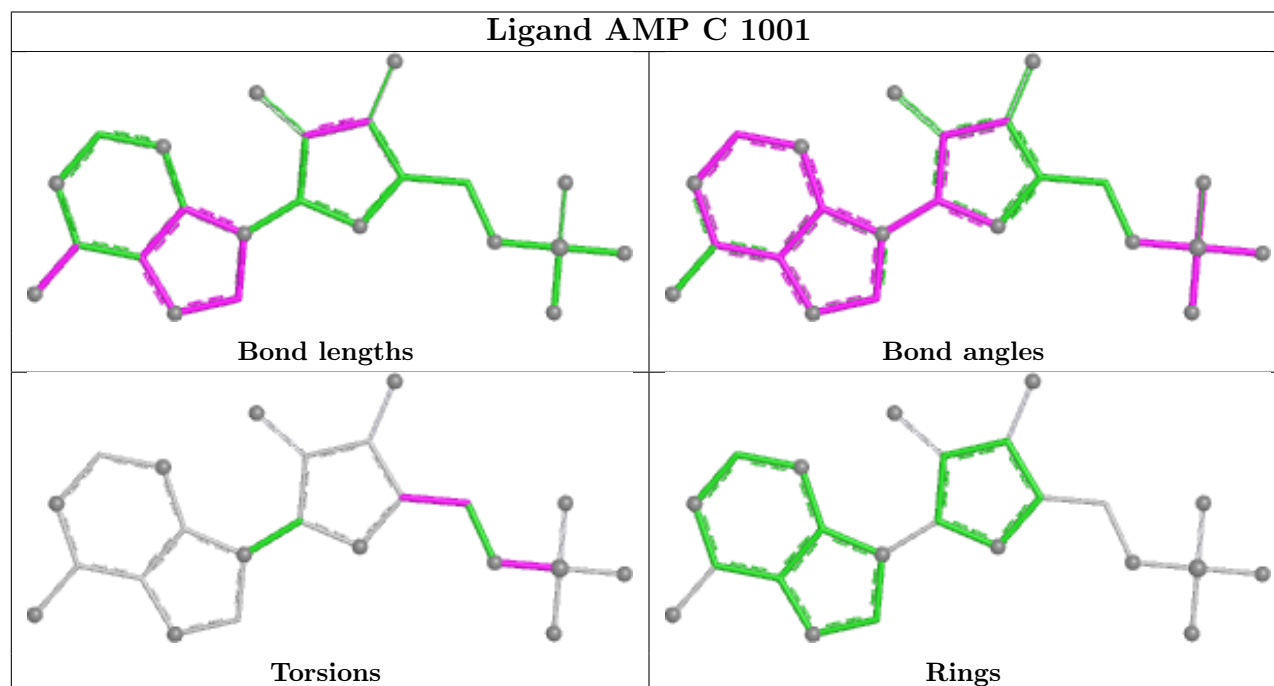
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1001	AMP	C5'-O5'-P-O1P
6	C	1001	AMP	C5'-O5'-P-O2P
6	C	1001	AMP	C5'-O5'-P-O3P
6	C	1001	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	616/644 (95%)	0.29	22 (3%) 46 40	27, 51, 80, 101	0
1	B	612/644 (95%)	0.34	39 (6%) 25 20	29, 55, 101, 124	0
2	C	627/970 (64%)	0.90	88 (14%) 6 5	40, 71, 99, 111	0
3	D	20/20 (100%)	-0.08	1 (5%) 34 28	34, 49, 73, 73	0
4	E	20/20 (100%)	-0.20	0 100 100	32, 48, 74, 87	0
All	All	1895/2298 (82%)	0.50	150 (7%) 18 14	27, 59, 97, 124	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	632	ASN	5.7
2	C	804	PHE	5.3
1	A	524	LEU	4.7
2	C	335	HIS	4.6
2	C	800	SER	4.6
2	C	774	ILE	4.3
1	A	635	SER	4.3
2	C	343	ASN	4.2
1	B	277	ALA	4.0
2	C	334	ILE	4.0
2	C	406	ASP	4.0
1	B	9	GLU	4.0
2	C	371	ALA	3.9
2	C	808	TYR	3.9
1	A	575	ASP	3.9
1	B	30	ASP	3.9
2	C	620	ASP	3.9
2	C	586	PHE	3.8
1	B	627	LEU	3.7
2	C	681	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	771	LYS	3.6
2	C	153	LYS	3.5
2	C	583	PRO	3.4
1	B	589	ALA	3.4
2	C	319	PHE	3.4
1	B	569	TYR	3.3
2	C	457	SER	3.3
2	C	577	SER	3.3
2	C	628	TYR	3.2
1	B	535	VAL	3.2
2	C	331	HIS	3.2
2	C	330	THR	3.1
2	C	427	TYR	3.1
2	C	163	MET	3.1
2	C	293	ASN	3.1
2	C	781	ASN	3.1
2	C	810	LEU	3.1
2	C	308	PHE	3.1
1	B	618	ALA	3.0
2	C	757	PHE	3.0
2	C	621	ASN	3.0
1	B	617	SER	3.0
2	C	456	SER	2.9
2	C	462	TYR	2.9
1	A	152	ILE	2.9
2	C	326	SER	2.9
2	C	458	VAL	2.9
2	C	372	ASP	2.9
2	C	420	LEU	2.9
1	A	473	THR	2.9
2	C	294	ALA	2.9
2	C	624	ASP	2.8
2	C	780	LEU	2.8
2	C	770	ILE	2.8
2	C	336	ASP	2.8
2	C	329	LYS	2.8
2	C	461	GLY	2.8
1	A	644	ASN	2.7
1	A	457	LYS	2.7
1	A	522	SER	2.7
1	B	129	GLY	2.7
1	B	634	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	444	TYR	2.7
2	C	383	PHE	2.7
2	C	323	LYS	2.7
1	B	576	GLY	2.7
1	B	600	ASP	2.7
1	B	458	ASN	2.6
2	C	287	ASP	2.6
1	B	638	LEU	2.6
2	C	622	PHE	2.6
2	C	257	SER	2.6
2	C	213	VAL	2.6
2	C	593	GLN	2.6
2	C	669	LYS	2.5
1	B	516	PHE	2.5
1	B	415	THR	2.5
1	B	632	ASN	2.5
2	C	369	THR	2.5
3	D	1	DA	2.5
2	C	503	THR	2.5
1	A	357	ASP	2.5
2	C	594	ILE	2.5
2	C	346	THR	2.5
2	C	296	LEU	2.5
1	B	592	ALA	2.5
2	C	748	PHE	2.5
1	B	624	ASN	2.4
2	C	433	ASN	2.4
2	C	340	ASP	2.4
2	C	704	GLU	2.4
1	B	282	GLY	2.4
1	B	567	GLY	2.4
1	B	281	THR	2.4
2	C	404	ILE	2.4
1	B	604	ALA	2.4
2	C	176	PHE	2.4
2	C	773	THR	2.4
1	B	40	LEU	2.3
2	C	551	ASN	2.3
1	A	13	ALA	2.3
1	B	594	LEU	2.3
2	C	627	ALA	2.3
1	B	262	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	586	THR	2.3
1	A	523	GLU	2.3
1	B	584	ASN	2.3
1	A	530	THR	2.3
2	C	684	LYS	2.3
2	C	363	PRO	2.3
2	C	700	LEU	2.3
2	C	502	TRP	2.2
1	B	610	PHE	2.2
2	C	8	GLU	2.2
1	B	37	GLN	2.2
1	A	167	GLY	2.2
2	C	633	SER	2.2
1	B	566	LEU	2.2
2	C	333	ALA	2.2
2	C	391	THR	2.2
2	C	807	GLY	2.2
1	A	414	PHE	2.2
1	A	281	THR	2.2
1	B	290	THR	2.2
1	B	537	LEU	2.2
1	A	477	SER	2.2
2	C	328	SER	2.2
2	C	285	ILE	2.2
2	C	450	LYS	2.1
1	B	593	LEU	2.1
2	C	302	ASP	2.1
1	A	531	PHE	2.1
1	A	44	ILE	2.1
2	C	452	VAL	2.1
2	C	424	PHE	2.1
1	B	538	THR	2.1
2	C	152	GLN	2.1
2	C	428	VAL	2.1
1	A	534	ASP	2.1
1	B	278	SER	2.1
2	C	705	ARG	2.1
1	A	14	ASN	2.1
1	A	535	VAL	2.1
1	B	609	VAL	2.1
2	C	805	SER	2.0
2	C	6	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	605	PRO	2.0
2	C	499	PHE	2.0
2	C	527	SER	2.0
2	C	339	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

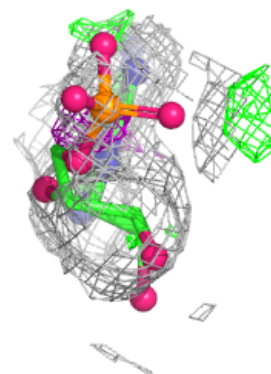
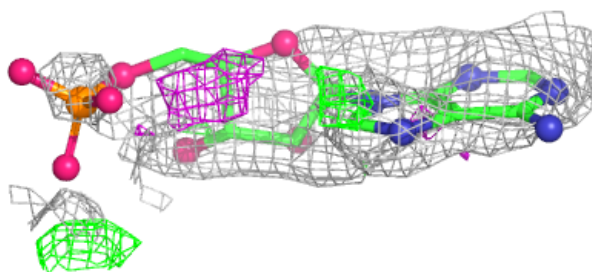
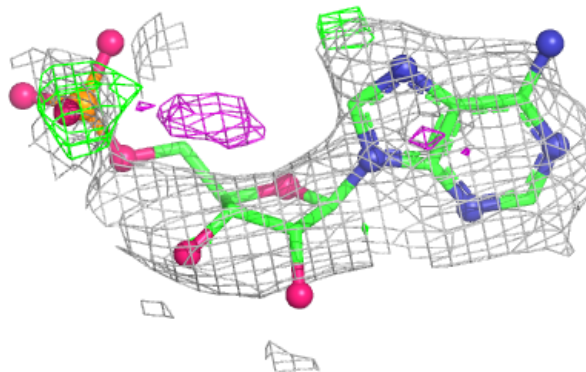
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	AMP	C	1001	23/23	0.65	0.28	128,133,149,150	0
5	MN	A	701	1/1	0.91	0.18	113,113,113,113	0
5	MN	A	702	1/1	0.96	0.18	75,75,75,75	0
7	CA	D	101	1/1	0.96	0.08	31,31,31,31	0

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

Electron density around AMP C 1001:

$2mF_o-DF_c$ (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.