



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 PM UTC

PDB ID : 1NKS / pdb_00001nks
Title : ADENYLATE KINASE FROM SULFOLOBUS ACIDOCALDARIUS
Authors : Vonnrhein, C.; Schulz, G.E.
Deposited on : 1998-07-16
Resolution : 2.57 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

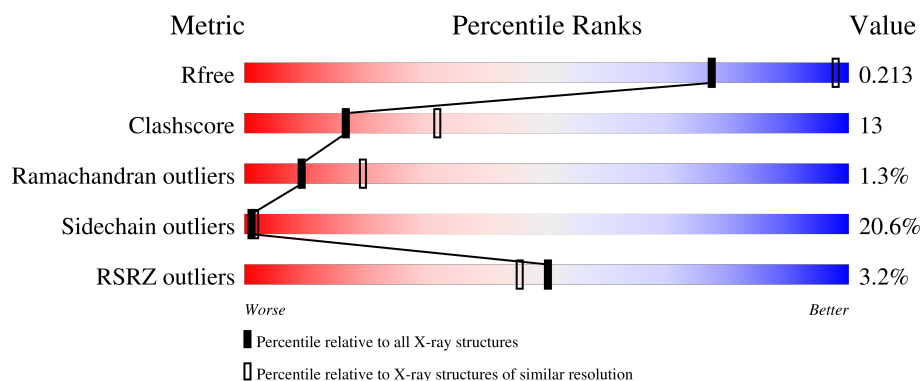
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	194	4% 63% 24% 11% .
1	B	194	4% 56% 29% 14% .
1	C	194	3% 61% 30% 6% .
1	D	194	4% 62% 31% 6% .
1	E	194	4% 51% 31% 14% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	194	% 68% 24% 7%

2 Entry composition [i](#)

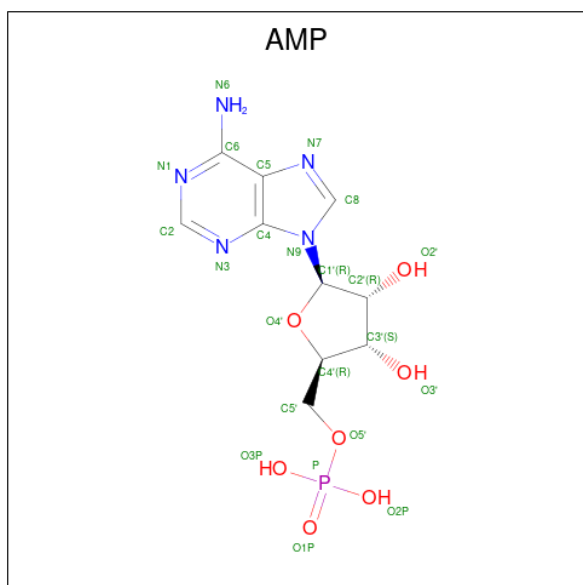
There are 4 unique types of molecules in this entry. The entry contains 9332 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENYLATE KINASE.

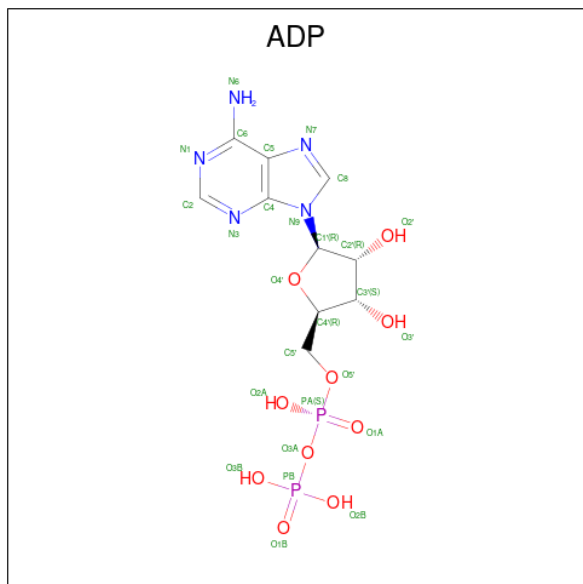
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	B	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	C	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	D	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	E	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	F	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

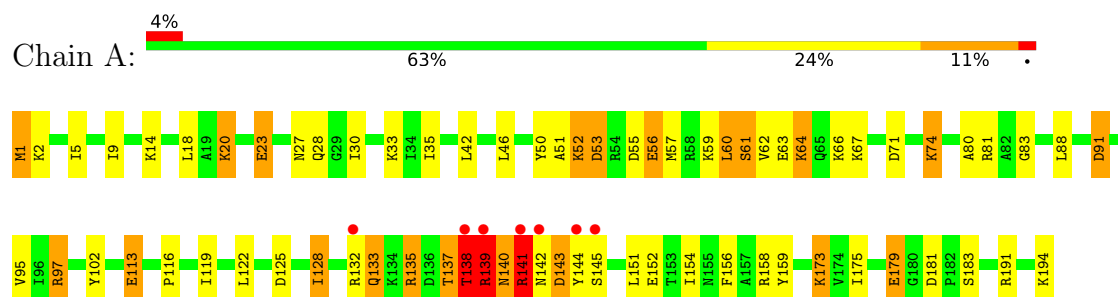
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	67	Total	O	0	0
			67	67		
4	C	41	Total	O	0	0
			41	41		
4	D	61	Total	O	0	0
			61	61		
4	E	67	Total	O	0	0
			67	67		
4	F	52	Total	O	0	0
			52	52		

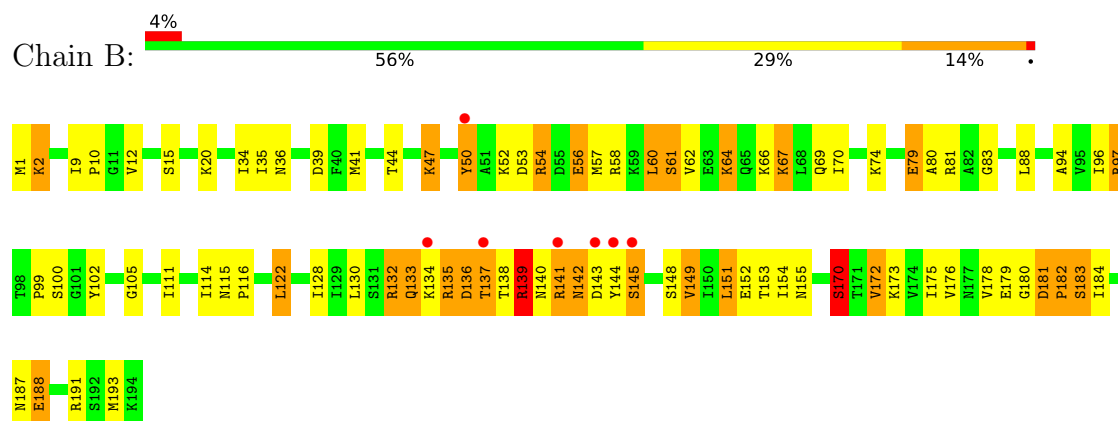
3 Residue-property plots

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.

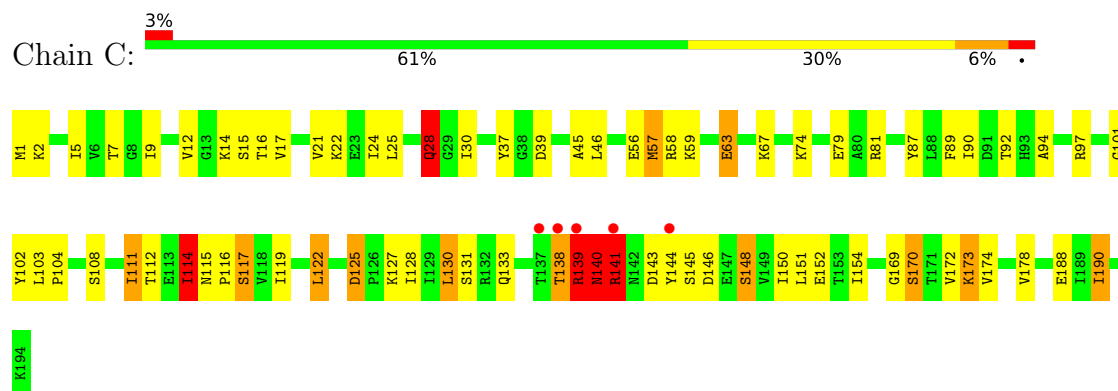
• Molecule 1: ADENYLATE KINASE



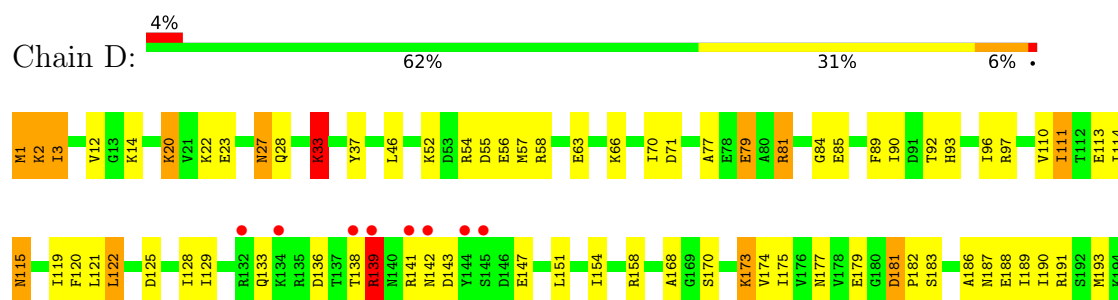
• Molecule 1: ADENYLATE KINASE



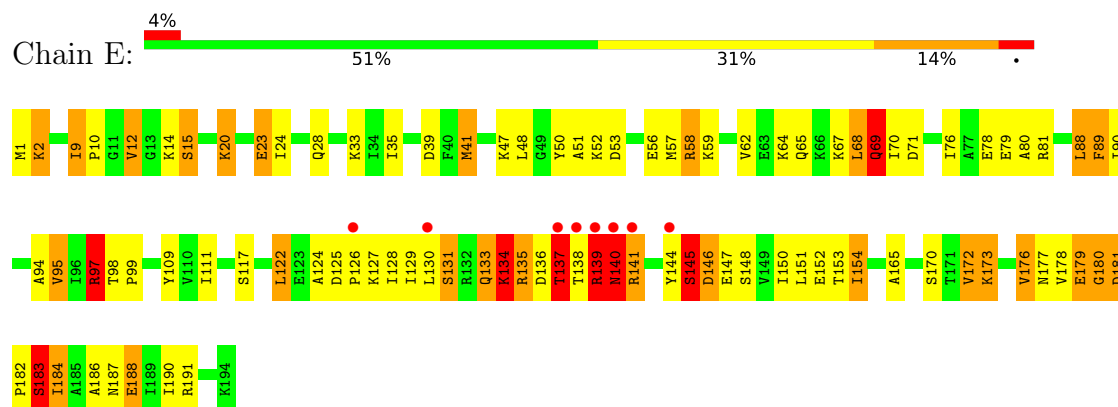
• Molecule 1: ADENYLATE KINASE



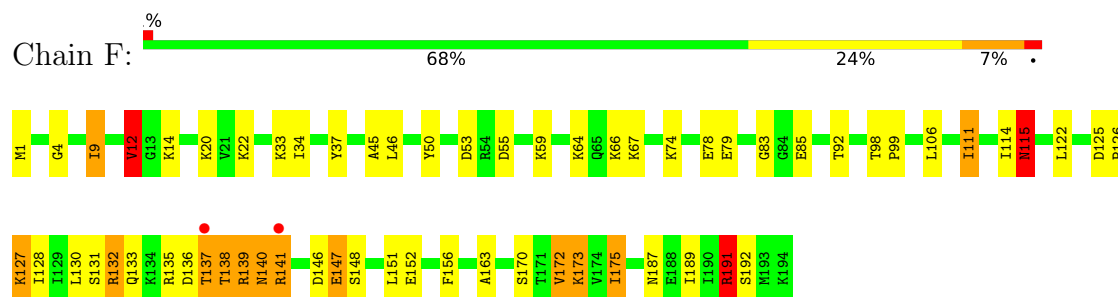
• Molecule 1: ADENYLATE KINASE



• Molecule 1: ADENYLATE KINASE



• Molecule 1: ADENYLATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.51Å 145.69Å 172.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.57 40.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-2.57) 92.0 (40.00-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.218 (Not available) , 0.213	Depositor DCC
R_{free} test set	1148 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9332	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: AMP, ADP

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	1.15	3/1502 (0.2%)	2.20	37/2026 (1.8%)
1	B	0.91	0/1502	1.81	38/2026 (1.9%)
1	C	0.83	0/1502	1.72	28/2026 (1.4%)
1	D	0.89	0/1502	1.72	26/2026 (1.3%)
1	E	1.09	1/1502 (0.1%)	1.98	37/2026 (1.8%)
1	F	0.84	1/1502 (0.1%)	1.73	14/2026 (0.7%)
All	All	0.96	5/9012 (0.1%)	1.87	180/12156 (1.5%)

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	2
1	E	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	THR	C-N	-23.68	1.00	1.33
1	E	137	THR	C-N	-21.17	1.07	1.33
1	A	137	THR	C-N	-7.82	1.23	1.33
1	A	141	ARG	CD-NE	-5.55	1.38	1.46
1	F	4	GLY	CA-C	5.09	1.56	1.51

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	CD-NE-CZ	31.06	167.88	124.40
1	A	138	THR	CA-C-N	22.10	163.75	121.54
1	A	138	THR	C-N-CA	22.10	163.75	121.54
1	E	137	THR	CA-C-N	20.97	153.25	122.21
1	E	137	THR	C-N-CA	20.97	153.25	122.21
1	A	138	THR	O-C-N	-19.14	96.98	122.43
1	E	137	THR	O-C-N	-14.98	102.85	122.33
1	D	27	ASN	CA-CB-CG	13.78	126.38	112.60
1	A	139	ARG	CD-NE-CZ	13.30	143.02	124.40
1	A	140	ASN	N-CA-CB	12.84	132.19	110.49
1	A	138	THR	CB-CA-C	11.99	136.46	110.21
1	E	58	ARG	CD-NE-CZ	9.93	138.30	124.40
1	D	114	ILE	N-CA-C	9.21	120.01	111.45
1	A	53	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	191	ARG	CD-NE-CZ	9.13	137.18	124.40
1	E	81	ARG	CD-NE-CZ	9.05	137.07	124.40
1	A	138	THR	N-CA-C	-9.05	102.01	112.87
1	E	53	ASP	CA-CB-CG	8.96	121.56	112.60
1	E	137	THR	CB-CA-C	8.75	129.78	110.18
1	F	191	ARG	CD-NE-CZ	8.69	136.57	124.40
1	F	45	ALA	CA-C-N	8.50	131.49	120.44
1	F	45	ALA	C-N-CA	8.50	131.49	120.44
1	D	143	ASP	CA-CB-CG	8.27	120.87	112.60
1	B	69	GLN	OE1-CD-NE2	8.21	130.81	122.60
1	C	139	ARG	CD-NE-CZ	8.18	135.84	124.40
1	F	115	ASN	CA-CB-CG	-8.14	104.45	112.60
1	B	97	ARG	N-CA-CB	8.08	122.16	109.71
1	D	28	GLN	N-CA-C	-7.91	101.83	114.09
1	F	132	ARG	CD-NE-CZ	7.89	135.45	124.40
1	F	12	VAL	CB-CA-C	-7.80	99.62	112.26
1	B	176	VAL	CB-CA-C	-7.75	101.07	111.15
1	A	139	ARG	CA-C-N	7.58	136.01	121.54
1	A	139	ARG	C-N-CA	7.58	136.01	121.54
1	E	140	ASN	CA-CB-CG	7.47	120.07	112.60
1	E	188	GLU	CB-CG-CD	7.20	124.83	112.60
1	D	89	PHE	CA-CB-CG	-7.08	106.72	113.80
1	A	141	ARG	CA-C-O	7.00	128.07	120.58
1	B	94	ALA	N-CA-C	-6.88	103.23	111.69
1	E	50	TYR	CA-CB-CG	6.85	126.23	113.90
1	E	69	GLN	OE1-CD-NE2	6.84	129.44	122.60
1	C	115	ASN	CA-CB-CG	-6.66	105.94	112.60
1	A	159	TYR	O-C-N	6.66	128.93	122.07
1	C	172	VAL	CA-C-O	-6.56	113.41	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	97	ARG	CD-NE-CZ	6.55	133.58	124.40
1	D	3	ILE	CA-C-O	6.53	127.56	120.57
1	C	37	TYR	CA-C-N	6.49	127.18	119.98
1	C	37	TYR	C-N-CA	6.49	127.18	119.98
1	E	23	GLU	CA-CB-CG	6.49	127.07	114.10
1	B	114	ILE	CA-C-O	-6.48	113.78	120.71
1	C	45	ALA	CA-C-N	6.39	129.16	120.54
1	C	45	ALA	C-N-CA	6.39	129.16	120.54
1	D	14	LYS	CA-CB-CG	6.38	126.87	114.10
1	A	191	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	B	188	GLU	CA-CB-CG	6.33	126.75	114.10
1	E	94	ALA	N-CA-C	-6.32	103.92	111.69
1	C	169	GLY	N-CA-C	-6.29	106.56	115.43
1	F	12	VAL	N-CA-CB	6.26	122.11	110.77
1	D	110	VAL	CA-C-N	6.25	129.02	120.46
1	D	110	VAL	C-N-CA	6.25	129.02	120.46
1	A	97	ARG	CD-NE-CZ	6.25	133.15	124.40
1	C	39	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	142	ASN	CA-CB-CG	6.24	118.84	112.60
1	A	139	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	B	172	VAL	CB-CA-C	-6.14	101.55	110.63
1	D	115	ASN	CA-CB-CG	-6.13	106.47	112.60
1	E	176	VAL	N-CA-CB	6.12	117.98	111.00
1	E	180	GLY	CA-C-N	6.11	132.55	120.94
1	E	180	GLY	C-N-CA	6.11	132.55	120.94
1	B	188	GLU	CB-CG-CD	6.11	122.98	112.60
1	B	181	ASP	CA-C-N	6.09	126.98	120.47
1	B	181	ASP	C-N-CA	6.09	126.98	120.47
1	A	179	GLU	N-CA-CB	-6.08	101.25	110.07
1	D	119	ILE	CA-C-O	-6.03	114.12	120.39
1	A	139	ARG	O-C-N	-6.02	114.58	122.59
1	B	105	GLY	O-C-N	-6.02	115.13	122.71
1	B	184	ILE	CB-CA-C	6.01	119.90	112.02
1	E	39	ASP	CA-CB-CG	-6.00	106.59	112.60
1	C	188	GLU	CA-CB-CG	5.99	126.07	114.10
1	D	77	ALA	CA-C-N	5.96	128.26	120.28
1	D	77	ALA	C-N-CA	5.96	128.26	120.28
1	B	181	ASP	N-CA-C	5.92	117.11	109.72
1	E	89	PHE	CA-CB-CG	-5.90	107.90	113.80
1	C	117	SER	N-CA-C	-5.89	105.75	113.12
1	E	183	SER	CA-C-N	5.89	127.91	120.72
1	E	183	SER	C-N-CA	5.89	127.91	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	LYS	N-CA-CB	5.89	118.78	110.12
1	A	95	VAL	CA-C-O	-5.88	115.04	121.28
1	B	36	ASN	CA-CB-CG	-5.88	106.72	112.60
1	C	119	ILE	CA-C-O	-5.85	114.31	120.39
1	D	71	ASP	CA-CB-CG	-5.83	106.77	112.60
1	B	81	ARG	CD-NE-CZ	5.80	132.52	124.40
1	D	90	ILE	N-CA-CB	5.79	117.98	111.21
1	C	89	PHE	CA-CB-CG	-5.76	108.04	113.80
1	C	56	GLU	CA-C-O	5.75	125.23	118.90
1	B	172	VAL	N-CA-CB	5.75	119.35	111.41
1	B	181	ASP	N-CA-CB	-5.75	101.81	110.32
1	C	28	GLN	N-CA-CB	5.74	120.10	110.92
1	A	156	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	141	ARG	CB-CA-C	5.72	120.25	110.81
1	B	97	ARG	CB-CA-C	-5.71	101.69	110.26
1	C	170	SER	CA-C-O	-5.71	115.21	121.89
1	B	182	PRO	CA-C-O	5.68	126.73	118.78
1	D	187	ASN	O-C-N	5.67	128.62	122.15
1	C	178	VAL	N-CA-CB	5.66	117.10	110.82
1	A	181	ASP	N-CA-C	5.65	119.47	108.85
1	B	111	ILE	N-CA-C	5.65	116.38	110.62
1	B	81	ARG	CA-C-N	5.62	130.23	120.68
1	B	81	ARG	C-N-CA	5.62	130.23	120.68
1	C	94	ALA	N-CA-C	-5.62	104.64	112.45
1	E	172	VAL	CA-C-O	-5.61	114.41	120.36
1	C	87	TYR	N-CA-C	5.60	117.87	108.96
1	B	67	LYS	CA-C-O	5.58	126.45	120.70
1	E	152	GLU	CB-CG-CD	5.58	122.09	112.60
1	B	176	VAL	CA-C-O	-5.57	114.50	120.85
1	E	69	GLN	CA-C-O	-5.53	113.86	120.10
1	C	56	GLU	N-CA-CB	-5.52	103.26	110.88
1	C	57	MET	CA-C-O	5.50	126.30	119.97
1	E	184	ILE	O-C-N	5.50	127.82	121.94
1	E	176	VAL	CA-C-N	-5.48	115.72	122.84
1	E	176	VAL	C-N-CA	-5.48	115.72	122.84
1	C	63	GLU	CB-CG-CD	5.47	121.89	112.60
1	D	56	GLU	CA-CB-CG	5.47	125.03	114.10
1	C	114	ILE	N-CA-C	5.46	116.86	111.67
1	B	151	LEU	CA-C-O	5.44	126.54	120.82
1	E	181	ASP	N-CA-C	5.44	116.51	109.65
1	B	170	SER	N-CA-CB	-5.44	102.47	110.85
1	D	115	ASN	OD1-CG-ND2	5.43	128.03	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	SER	CA-C-N	-5.42	113.73	120.56
1	A	183	SER	C-N-CA	-5.42	113.73	120.56
1	A	27	ASN	CB-CA-C	-5.41	104.52	111.22
1	C	138	THR	CA-C-N	5.39	128.69	121.90
1	C	138	THR	C-N-CA	5.39	128.69	121.90
1	C	174	VAL	CB-CA-C	-5.39	104.44	110.96
1	D	174	VAL	CB-CA-C	-5.39	104.78	111.08
1	A	81	ARG	CA-CB-CG	5.38	124.87	114.10
1	E	2	LYS	N-CA-C	-5.37	101.71	110.20
1	E	71	ASP	CA-CB-CG	-5.37	107.23	112.60
1	F	156	PHE	CA-CB-CG	-5.36	108.44	113.80
1	B	96	ILE	CA-C-O	-5.35	114.80	120.53
1	D	121	LEU	CA-C-O	-5.34	114.61	120.70
1	D	147	GLU	CA-C-N	5.33	127.36	120.44
1	D	147	GLU	C-N-CA	5.33	127.36	120.44
1	A	27	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	141	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	175	ILE	CB-CA-C	-5.31	103.23	110.77
1	E	139	ARG	N-CA-C	-5.31	99.49	110.80
1	F	138	THR	N-CA-C	-5.31	106.97	113.50
1	E	15	SER	N-CA-CB	5.29	117.90	110.12
1	C	125	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	170	SER	CA-C-O	-5.27	115.18	121.56
1	B	79	GLU	CA-CB-CG	5.27	124.64	114.10
1	D	12	VAL	N-CA-CB	5.25	122.90	111.76
1	B	41	MET	N-CA-C	-5.25	104.99	111.40
1	E	95	VAL	CB-CA-C	-5.23	101.35	110.71
1	A	141	ARG	CG-CD-NE	5.22	123.49	112.00
1	B	2	LYS	CB-CA-C	5.22	118.35	109.84
1	A	119	ILE	CA-C-O	-5.21	114.74	120.48
1	E	111	ILE	N-CA-C	5.19	115.91	110.62
1	D	181	ASP	N-CA-C	5.18	119.93	108.27
1	D	33	LYS	O-C-N	-5.18	116.64	123.21
1	B	35	ILE	N-CA-C	5.16	115.52	107.99
1	B	115	ASN	CA-C-O	5.15	124.45	120.48
1	A	71	ASP	CA-C-N	-5.13	113.77	120.44
1	A	71	ASP	C-N-CA	-5.13	113.77	120.44
1	F	172	VAL	CB-CA-C	-5.12	103.51	110.42
1	F	137	THR	N-CA-CB	5.11	117.42	110.42
1	C	9	ILE	CB-CA-C	5.10	120.65	111.36
1	B	15	SER	N-CA-CB	5.10	117.70	110.16
1	B	155	ASN	CA-CB-CG	5.08	117.68	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	THR	CA-C-N	5.08	127.08	120.28
1	B	44	THR	C-N-CA	5.08	127.08	120.28
1	F	163	ALA	N-CA-C	-5.07	105.66	111.14
1	A	159	TYR	CA-C-O	-5.07	115.50	120.82
1	A	158	ARG	O-C-N	5.06	127.92	122.15
1	E	172	VAL	N-CA-CB	5.06	118.90	111.52
1	D	97	ARG	CD-NE-CZ	5.04	131.46	124.40
1	B	50	TYR	CA-CB-CG	5.04	122.97	113.90
1	F	55	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	134	LYS	CA-CB-CG	5.03	124.16	114.10
1	E	181	ASP	CA-C-O	5.00	124.21	119.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	THR	Mainchain,Peptide
1	E	137	THR	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	1484	0	1548	48	0
1	B	1484	0	1549	41	0
1	C	1484	0	1549	28	0
1	D	1484	0	1549	33	0
1	E	1484	0	1548	62	0
1	F	1484	0	1549	25	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
2	F	23	0	12	0	0
3	F	27	0	12	0	0
4	A	44	0	0	8	0
4	B	67	0	0	8	0
4	C	41	0	0	1	0
4	D	61	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	67	0	0	10	0
4	F	52	0	0	4	0
All	All	9332	0	9340	234	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 13.

All (234) 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:E:137:THR:O	1:E:140:ASN:HB3	1.30	1.30
1:E:188:GLU:HG2	4:E:222:HOH:O	1.56	1.02
1:C:140:ASN:O	1:C:141:ARG:HB2	1.69	0.92
1:D:20:LYS:HD3	1:D:183:SER:HB3	1.57	0.87
1:E:137:THR:C	1:E:140:ASN:HB3	2.04	0.82
1:A:1:MET:SD	4:A:225:HOH:O	2.37	0.82
1:A:139:ARG:HH11	1:A:141:ARG:NH2	1.78	0.81
1:C:125:ASP:HB3	1:C:128:ILE:HD13	1.63	0.81
1:A:1:MET:HE2	1:A:83:GLY:HA3	1.63	0.79
1:B:133:GLN:HG2	4:B:260:HOH:O	1.81	0.79
1:A:143:ASP:HB2	4:A:233:HOH:O	1.81	0.79
1:E:9:ILE:O	1:E:12:VAL:HG23	1.82	0.78
1:A:125:ASP:HB3	1:A:128:ILE:HG12	1.65	0.78
1:A:137:THR:HG23	1:A:140:ASN:HB2	1.66	0.77
1:A:80:ALA:HB2	1:A:88:LEU:HD23	1.66	0.77
1:B:80:ALA:HB2	1:B:88:LEU:HD23	1.67	0.76
1:A:139:ARG:HH11	1:A:141:ARG:HH22	1.35	0.74
1:E:138:THR:O	1:E:139:ARG:HB2	1.87	0.74
1:D:179:GLU:HA	4:D:254:HOH:O	1.88	0.73
1:A:139:ARG:HB3	1:A:141:ARG:HE	1.54	0.72
1:C:139:ARG:HH11	1:C:139:ARG:HG3	1.55	0.72
1:B:128:ILE:HD13	1:B:179:GLU:HB2	1.72	0.71
1:A:61:SER:HB3	1:A:64:LYS:HD3	1.72	0.71
1:B:1:MET:HE2	1:B:83:GLY:HA3	1.72	0.71
1:A:1:MET:HE3	1:A:80:ALA:HA	1.74	0.69
1:E:144:TYR:HB2	4:E:243:HOH:O	1.93	0.69
1:F:139:ARG:HG2	1:F:141:ARG:HH21	1.57	0.69
1:B:99:PRO:O	1:C:173:LYS:NZ	2.26	0.68
1:A:135:ARG:HH11	1:A:135:ARG:HB3	1.58	0.67
1:A:51:ALA:HB1	1:A:56:GLU:HG3	1.76	0.67
1:B:10:PRO:HD2	1:B:144:TYR:OH	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:HD1	1:B:149:VAL:HG12	1.61	0.65
1:E:1:MET:N	4:E:245:HOH:O	2.20	0.65
1:F:125:ASP:HB3	1:F:128:ILE:HD12	1.79	0.65
1:E:41:MET:HE2	1:E:68:LEU:HD13	1.80	0.64
1:E:98:THR:HB	1:E:99:PRO:CD	2.27	0.64
1:A:137:THR:HG23	1:A:140:ASN:CB	2.28	0.64
1:E:139:ARG:NH1	1:E:141:ARG:HD2	2.12	0.64
1:A:97:ARG:HD3	4:A:227:HOH:O	1.97	0.63
1:B:47:LYS:HD2	4:B:231:HOH:O	1.97	0.62
1:D:27:ASN:HB2	4:D:226:HOH:O	1.99	0.62
1:A:135:ARG:HB3	1:A:135:ARG:NH1	2.15	0.61
1:E:178:VAL:HG21	1:E:184:ILE:HD13	1.80	0.61
1:B:138:THR:O	1:B:139:ARG:HB2	2.01	0.61
1:B:39:ASP:OD1	1:B:54:ARG:NH2	2.31	0.61
1:E:139:ARG:HH11	1:E:141:ARG:HD2	1.66	0.61
1:E:178:VAL:HG21	1:E:184:ILE:HG21	1.81	0.61
1:F:191:ARG:HH11	1:F:191:ARG:HG2	1.66	0.60
1:E:9:ILE:HD13	1:E:154:ILE:HG12	1.82	0.60
1:F:50:TYR:CE1	1:F:64:LYS:HD3	2.36	0.60
1:D:138:THR:O	1:D:139:ARG:HB2	2.02	0.59
1:A:5:ILE:HD12	1:A:116:PRO:HG3	1.83	0.59
1:E:137:THR:O	1:E:140:ASN:CB	2.26	0.59
1:B:54:ARG:HD2	4:B:261:HOH:O	2.02	0.58
1:D:66:LYS:O	1:D:70:ILE:HG13	2.04	0.58
1:C:12:VAL:HG21	1:C:122:LEU:HB3	1.84	0.58
1:B:137:THR:HG23	1:B:140:ASN:HB2	1.84	0.58
1:C:114:ILE:HG22	1:C:116:PRO:HD3	1.85	0.58
1:A:139:ARG:HB3	1:A:141:ARG:CD	2.34	0.58
1:D:141:ARG:O	1:D:142:ASN:HB2	2.03	0.57
1:A:57:MET:HA	1:A:60:LEU:CD1	2.35	0.57
1:E:9:ILE:CG2	1:E:153:THR:HG22	2.35	0.57
1:B:135:ARG:HB3	4:B:237:HOH:O	2.04	0.57
1:B:137:THR:HG23	1:B:140:ASN:CB	2.34	0.57
1:E:181:ASP:OD1	1:E:183:SER:HB2	2.05	0.56
1:C:144:TYR:HD2	1:C:150:ILE:HG13	1.70	0.56
1:D:125:ASP:HB3	1:D:128:ILE:HD12	1.87	0.56
1:C:139:ARG:O	1:C:140:ASN:HB2	2.05	0.55
1:E:187:ASN:HB3	1:E:191:ARG:NH2	2.21	0.55
1:C:141:ARG:HG3	1:C:143:ASP:OD1	2.06	0.55
1:B:141:ARG:NH2	4:B:248:HOH:O	2.40	0.55
1:A:173:LYS:HG2	1:C:101:GLY:CA	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE3	1:B:80:ALA:HA	1.88	0.55
1:D:58:ARG:NH1	4:D:207:HOH:O	2.40	0.55
1:E:12:VAL:O	1:E:177:ASN:ND2	2.37	0.55
1:E:134:LYS:HG2	4:E:261:HOH:O	2.05	0.55
1:A:139:ARG:HD2	1:A:141:ARG:NH2	2.22	0.55
1:C:108:SER:O	1:C:112:THR:HG23	2.06	0.54
1:A:137:THR:CG2	1:A:140:ASN:HB2	2.36	0.54
1:E:33:LYS:HD3	4:E:211:HOH:O	2.07	0.54
1:A:139:ARG:HB3	1:A:141:ARG:NE	2.22	0.54
1:B:178:VAL:HG13	1:E:178:VAL:HG13	1.90	0.54
1:C:102:TYR:OH	1:C:152:GLU:HG2	2.08	0.54
1:F:128:ILE:O	1:F:132:ARG:HG3	2.08	0.54
1:D:141:ARG:HD3	4:D:247:HOH:O	2.08	0.54
1:E:9:ILE:HG21	1:E:153:THR:HG22	1.89	0.54
1:D:125:ASP:HB3	1:D:128:ILE:CD1	2.37	0.53
1:C:128:ILE:HD12	1:C:128:ILE:H	1.74	0.53
1:E:186:ALA:O	1:E:190:ILE:HG13	2.09	0.53
1:F:140:ASN:ND2	4:F:212:HOH:O	2.41	0.53
1:E:124:ALA:HB3	1:E:129:ILE:HD11	1.91	0.53
1:E:125:ASP:HB2	4:E:206:HOH:O	2.07	0.53
1:E:128:ILE:HD13	1:E:179:GLU:HG2	1.91	0.52
1:C:17:VAL:O	1:C:21:VAL:HG23	2.09	0.52
1:B:9:ILE:HD13	1:B:154:ILE:HG13	1.92	0.52
1:C:146:ASP:OD2	1:C:148:SER:HB2	2.09	0.52
1:E:147:GLU:HA	1:E:150:ILE:HD12	1.91	0.52
1:B:136:ASP:HB2	4:B:237:HOH:O	2.09	0.52
1:A:102:TYR:OH	1:A:152:GLU:HG2	2.10	0.52
1:C:128:ILE:HD12	1:C:128:ILE:N	2.25	0.52
1:C:24:ILE:O	1:C:28:GLN:HG3	2.09	0.52
1:F:50:TYR:CZ	1:F:64:LYS:HD3	2.45	0.52
1:A:137:THR:HG22	1:A:137:THR:O	2.10	0.51
1:B:181:ASP:OD1	1:B:183:SER:HB2	2.09	0.51
1:D:2:LYS:HE3	1:D:193:MET:O	2.09	0.51
1:F:152:GLU:HG3	4:F:230:HOH:O	2.09	0.51
1:B:66:LYS:O	1:B:70:ILE:HG13	2.10	0.51
1:E:35:ILE:HD12	1:E:88:LEU:HD11	1.92	0.51
1:B:132:ARG:NH1	4:B:197:HOH:O	2.43	0.51
1:E:173:LYS:HE3	4:E:250:HOH:O	2.09	0.51
1:E:20:LYS:HD2	1:E:24:ILE:HD11	1.93	0.51
1:F:1:MET:HB2	4:F:239:HOH:O	2.11	0.51
1:A:57:MET:HA	1:A:60:LEU:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:HD1	1:B:149:VAL:CG1	2.23	0.50
1:E:14:LYS:HG3	1:E:122:LEU:HD23	1.93	0.50
1:F:175:ILE:HD12	1:F:189:ILE:HG12	1.92	0.50
1:F:125:ASP:OD1	1:F:127:LYS:HB2	2.11	0.50
1:A:51:ALA:HB2	1:A:60:LEU:HD11	1.93	0.50
1:A:1:MET:HG3	1:A:80:ALA:O	2.10	0.50
1:E:65:GLN:O	1:E:69:GLN:HG2	2.12	0.50
1:A:139:ARG:HH11	1:A:141:ARG:CZ	2.25	0.49
1:D:188:GLU:OE2	1:D:191:ARG:NH1	2.45	0.49
1:F:139:ARG:HG2	1:F:141:ARG:NH2	2.26	0.49
1:D:63:GLU:HG2	4:D:216:HOH:O	2.11	0.49
1:B:53:ASP:OD1	1:B:56:GLU:HB2	2.13	0.49
1:D:154:ILE:O	1:D:158:ARG:HG3	2.13	0.49
1:E:51:ALA:HB1	1:E:56:GLU:HB3	1.93	0.49
1:B:2:LYS:HE2	1:B:193:MET:O	2.14	0.48
1:D:33:LYS:NZ	1:D:79:GLU:HG3	2.29	0.48
1:D:129:ILE:O	1:D:133:GLN:HG3	2.14	0.48
1:E:76:ILE:HG21	1:E:90:ILE:HD11	1.94	0.48
1:E:97:ARG:HD2	1:E:144:TYR:HE1	1.78	0.48
1:E:178:VAL:CG2	1:E:184:ILE:HG21	2.42	0.48
1:E:141:ARG:NH1	1:E:141:ARG:HB2	2.29	0.48
1:E:141:ARG:HB2	1:E:141:ARG:HH11	1.78	0.47
1:B:58:ARG:HD3	4:B:246:HOH:O	2.14	0.47
1:C:7:THR:HA	1:C:92:THR:O	2.14	0.47
1:E:98:THR:CB	1:E:99:PRO:CD	2.91	0.47
1:F:127:LYS:HG3	1:F:147:GLU:OE2	2.14	0.47
1:A:61:SER:HB3	1:A:64:LYS:CD	2.42	0.47
1:B:12:VAL:HG21	1:B:122:LEU:HB3	1.97	0.47
1:E:88:LEU:HD12	1:E:89:PHE:N	2.29	0.47
1:A:20:LYS:HE2	1:A:23:GLU:OE2	2.15	0.47
1:B:187:ASN:HB3	1:B:191:ARG:NH2	2.30	0.47
1:F:98:THR:HB	1:F:99:PRO:CD	2.45	0.46
1:D:133:GLN:HE22	1:D:141:ARG:CG	2.29	0.46
1:E:133:GLN:NE2	4:E:243:HOH:O	2.40	0.46
1:F:187:ASN:HB3	1:F:191:ARG:NH2	2.31	0.46
1:A:9:ILE:HD13	1:A:154:ILE:HG13	1.98	0.46
1:A:139:ARG:HD2	1:A:141:ARG:HH21	1.81	0.46
1:F:173:LYS:NZ	1:F:192:SER:OG	2.41	0.46
1:D:84:GLY:N	4:D:253:HOH:O	2.45	0.46
1:D:173:LYS:HE2	1:D:188:GLU:OE1	2.15	0.46
1:A:66:LYS:NZ	4:A:229:HOH:O	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:O	1:E:12:VAL:HG12	2.16	0.46
1:F:74:LYS:HE2	4:F:242:HOH:O	2.15	0.46
1:D:186:ALA:O	1:D:190:ILE:HD12	2.16	0.46
1:A:125:ASP:HB3	1:A:128:ILE:CG1	2.40	0.45
1:A:97:ARG:NH1	4:A:227:HOH:O	2.40	0.45
1:D:37:TYR:HB2	1:D:92:THR:HB	1.97	0.45
1:E:126:PRO:HG2	1:E:151:LEU:HD21	1.99	0.45
1:E:145:SER:HB2	1:E:146:ASP:H	1.64	0.45
1:D:111:ILE:HG23	1:D:168:ALA:HB2	1.99	0.45
1:D:175:ILE:HD13	1:D:189:ILE:HG13	1.99	0.45
1:D:81:ARG:NH1	4:D:242:HOH:O	2.50	0.45
1:E:165:ALA:HB1	1:E:170:SER:O	2.17	0.45
1:B:61:SER:OG	1:B:64:LYS:HG3	2.17	0.45
1:D:2:LYS:HE2	4:D:223:HOH:O	2.17	0.45
1:D:181:ASP:HA	1:D:182:PRO:HD2	1.85	0.45
1:E:10:PRO:HD3	4:E:226:HOH:O	2.15	0.45
1:A:42:LEU:HD12	1:A:42:LEU:O	2.17	0.44
1:A:141:ARG:HB3	4:A:237:HOH:O	2.17	0.44
1:A:141:ARG:HG3	4:A:233:HOH:O	2.15	0.44
1:D:115:ASN:HA	4:D:255:HOH:O	2.17	0.44
1:C:111:ILE:HD13	1:C:111:ILE:HA	1.85	0.44
1:F:114:ILE:O	1:F:115:ASN:C	2.58	0.44
1:B:34:ILE:HD13	1:B:34:ILE:HG21	1.79	0.44
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.82	0.44
1:D:54:ARG:HD2	4:D:240:HOH:O	2.18	0.44
1:F:146:ASP:OD2	1:F:148:SER:HB2	2.18	0.44
1:B:57:MET:O	1:B:60:LEU:HB2	2.18	0.43
1:C:140:ASN:O	1:C:141:ARG:CB	2.52	0.43
1:B:122:LEU:HD12	1:B:175:ILE:HB	2.00	0.43
4:E:257:HOH:O	1:F:191:ARG:HB3	2.18	0.43
1:A:18:LEU:HD11	1:A:91:ASP:HB2	2.00	0.43
1:B:116:PRO:O	1:B:170:SER:HB2	2.18	0.43
1:A:46:LEU:HD23	1:A:52:LYS:HA	1.99	0.43
1:B:137:THR:O	1:B:137:THR:HG22	2.18	0.43
1:E:24:ILE:O	1:E:28:GLN:HG3	2.19	0.43
1:C:103:LEU:HA	1:C:104:PRO:HD3	1.92	0.43
1:F:126:PRO:HB2	1:F:147:GLU:HG2	2.01	0.43
1:C:5:ILE:HD13	1:C:90:ILE:HD12	2.01	0.42
1:E:130:LEU:HG	1:E:150:ILE:CD1	2.50	0.42
1:F:9:ILE:O	1:F:12:VAL:HG22	2.20	0.42
1:E:20:LYS:O	1:E:24:ILE:HD12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LEU:HD12	1:D:177:ASN:HB2	2.01	0.42
1:E:98:THR:HB	1:E:99:PRO:HD3	2.02	0.42
1:A:139:ARG:HD2	1:A:139:ARG:HA	1.80	0.42
1:C:130:LEU:HD23	1:C:130:LEU:HA	1.91	0.42
1:E:12:VAL:HG13	1:E:124:ALA:HB2	2.01	0.42
1:A:74:LYS:HG3	1:A:113:GLU:HG3	2.01	0.42
1:D:120:PHE:CD2	1:D:175:ILE:HD12	2.55	0.42
1:E:9:ILE:HG13	1:E:12:VAL:CG2	2.50	0.42
1:E:144:TYR:CD2	1:E:150:ILE:HG12	2.54	0.42
1:F:136:ASP:OD1	1:F:138:THR:HG22	2.19	0.42
1:A:145:SER:HB2	4:A:223:HOH:O	2.19	0.42
1:B:130:LEU:O	1:B:133:GLN:HB2	2.20	0.42
1:A:133:GLN:OE1	1:A:144:TYR:HB2	2.20	0.41
1:C:25:LEU:HG	1:C:190:ILE:HD13	2.01	0.41
1:E:131:SER:O	1:E:135:ARG:HB2	2.20	0.41
1:E:80:ALA:HB2	1:E:88:LEU:HD23	2.01	0.41
1:B:144:TYR:CD1	1:B:149:VAL:HG12	2.47	0.41
1:B:102:TYR:OH	1:B:152:GLU:HG2	2.21	0.41
1:D:96:ILE:N	1:D:96:ILE:HD12	2.35	0.41
1:B:181:ASP:HA	1:B:182:PRO:HD3	1.75	0.41
1:E:70:ILE:HD11	1:E:109:TYR:HB2	2.02	0.41
1:E:138:THR:O	1:E:139:ARG:CB	2.63	0.41
1:F:37:TYR:HB2	1:F:92:THR:HB	2.02	0.41
1:D:1:MET:HA	4:D:218:HOH:O	2.20	0.41
1:A:35:ILE:HD12	1:A:88:LEU:HD11	2.02	0.41
1:B:9:ILE:HG21	1:B:153:THR:HG22	2.03	0.41
1:B:9:ILE:O	1:B:12:VAL:HG13	2.20	0.41
1:C:97:ARG:HD3	1:C:143:ASP:OD2	2.21	0.41
1:D:92:THR:OG1	1:D:93:HIS:N	2.53	0.41
1:E:47:LYS:O	1:E:48:LEU:HD23	2.21	0.41
1:E:181:ASP:HA	1:E:182:PRO:HD3	1.87	0.41
1:C:22:LYS:NZ	4:C:223:HOH:O	2.53	0.41
1:A:1:MET:N	1:A:80:ALA:O	2.48	0.40
1:C:128:ILE:H	1:C:128:ILE:CD1	2.33	0.40
1:E:9:ILE:HG22	1:E:153:THR:HG22	2.02	0.40
1:E:88:LEU:HD12	1:E:88:LEU:C	2.46	0.40
1:A:46:LEU:CD2	1:A:52:LYS:HA	2.51	0.40
1:C:15:SER:O	1:C:16:THR:C	2.65	0.40
1:F:106:LEU:HB3	1:F:111:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/194 (99%)	178 (93%)	12 (6%)	2 (1%)	12	26
1	B	192/194 (99%)	181 (94%)	6 (3%)	5 (3%)	4	7
1	C	192/194 (99%)	181 (94%)	9 (5%)	2 (1%)	12	26
1	D	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	24	44
1	E	192/194 (99%)	181 (94%)	7 (4%)	4 (2%)	5	10
1	F	192/194 (99%)	186 (97%)	5 (3%)	1 (0%)	24	44
All	All	1152/1164 (99%)	1088 (94%)	49 (4%)	15 (1%)	9	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ARG
1	B	145	SER
1	C	140	ASN
1	C	141	ARG
1	E	139	ARG
1	B	139	ARG
1	B	142	ASN
1	D	139	ARG
1	E	140	ASN
1	E	145	SER
1	B	50	TYR
1	E	180	GLY
1	F	83	GLY
1	A	28	GLN
1	B	180	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	160/160 (100%)	125 (78%)	35 (22%)	1	1
1	B	160/160 (100%)	126 (79%)	34 (21%)	1	1
1	C	160/160 (100%)	127 (79%)	33 (21%)	1	2
1	D	160/160 (100%)	138 (86%)	22 (14%)	3	6
1	E	160/160 (100%)	119 (74%)	41 (26%)	0	1
1	F	160/160 (100%)	127 (79%)	33 (21%)	1	2
All	All	960/960 (100%)	762 (79%)	198 (21%)	1	2

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	14	LYS
1	A	20	LYS
1	A	23	GLU
1	A	30	ILE
1	A	33	LYS
1	A	50	TYR
1	A	52	LYS
1	A	53	ASP
1	A	55	ASP
1	A	56	GLU
1	A	59	LYS
1	A	60	LEU
1	A	61	SER
1	A	62	VAL
1	A	63	GLU
1	A	64	LYS
1	A	67	LYS
1	A	74	LYS
1	A	91	ASP
1	A	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	LEU
1	A	128	ILE
1	A	132	ARG
1	A	133	GLN
1	A	135	ARG
1	A	138	THR
1	A	139	ARG
1	A	141	ARG
1	A	143	ASP
1	A	151	LEU
1	A	173	LYS
1	A	179	GLU
1	A	194	LYS
1	B	20	LYS
1	B	47	LYS
1	B	52	LYS
1	B	54	ARG
1	B	56	GLU
1	B	60	LEU
1	B	61	SER
1	B	62	VAL
1	B	64	LYS
1	B	67	LYS
1	B	74	LYS
1	B	79	GLU
1	B	97	ARG
1	B	100	SER
1	B	122	LEU
1	B	132	ARG
1	B	133	GLN
1	B	134	LYS
1	B	135	ARG
1	B	136	ASP
1	B	137	THR
1	B	139	ARG
1	B	141	ARG
1	B	142	ASN
1	B	143	ASP
1	B	145	SER
1	B	148	SER
1	B	149	VAL
1	B	151	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	SER
1	B	172	VAL
1	B	173	LYS
1	B	183	SER
1	B	188	GLU
1	C	1	MET
1	C	2	LYS
1	C	14	LYS
1	C	28	GLN
1	C	30	ILE
1	C	46	LEU
1	C	57	MET
1	C	58	ARG
1	C	59	LYS
1	C	63	GLU
1	C	67	LYS
1	C	74	LYS
1	C	79	GLU
1	C	81	ARG
1	C	111	ILE
1	C	114	ILE
1	C	117	SER
1	C	122	LEU
1	C	127	LYS
1	C	130	LEU
1	C	131	SER
1	C	133	GLN
1	C	138	THR
1	C	139	ARG
1	C	140	ASN
1	C	141	ARG
1	C	145	SER
1	C	148	SER
1	C	151	LEU
1	C	154	ILE
1	C	170	SER
1	C	173	LYS
1	C	190	ILE
1	D	1	MET
1	D	2	LYS
1	D	3	ILE
1	D	20	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	22	LYS
1	D	23	GLU
1	D	33	LYS
1	D	46	LEU
1	D	52	LYS
1	D	55	ASP
1	D	57	MET
1	D	79	GLU
1	D	81	ARG
1	D	85	GLU
1	D	111	ILE
1	D	113	GLU
1	D	122	LEU
1	D	136	ASP
1	D	139	ARG
1	D	151	LEU
1	D	170	SER
1	D	173	LYS
1	E	2	LYS
1	E	9	ILE
1	E	12	VAL
1	E	15	SER
1	E	20	LYS
1	E	23	GLU
1	E	41	MET
1	E	52	LYS
1	E	57	MET
1	E	58	ARG
1	E	59	LYS
1	E	62	VAL
1	E	64	LYS
1	E	67	LYS
1	E	68	LEU
1	E	69	GLN
1	E	78	GLU
1	E	79	GLU
1	E	88	LEU
1	E	95	VAL
1	E	97	ARG
1	E	117	SER
1	E	122	LEU
1	E	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	131	SER
1	E	133	GLN
1	E	134	LYS
1	E	135	ARG
1	E	136	ASP
1	E	139	ARG
1	E	140	ASN
1	E	141	ARG
1	E	145	SER
1	E	146	ASP
1	E	148	SER
1	E	154	ILE
1	E	172	VAL
1	E	173	LYS
1	E	176	VAL
1	E	179	GLU
1	E	183	SER
1	F	9	ILE
1	F	12	VAL
1	F	14	LYS
1	F	20	LYS
1	F	22	LYS
1	F	33	LYS
1	F	34	ILE
1	F	46	LEU
1	F	53	ASP
1	F	59	LYS
1	F	67	LYS
1	F	78	GLU
1	F	79	GLU
1	F	85	GLU
1	F	111	ILE
1	F	115	ASN
1	F	122	LEU
1	F	127	LYS
1	F	130	LEU
1	F	131	SER
1	F	133	GLN
1	F	135	ARG
1	F	137	THR
1	F	139	ARG
1	F	140	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	141	ARG
1	F	147	GLU
1	F	151	LEU
1	F	170	SER
1	F	172	VAL
1	F	173	LYS
1	F	175	ILE
1	F	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	140	ASN
1	B	28	GLN
1	B	69	GLN
1	B	115	ASN
1	B	133	GLN
1	B	140	ASN
1	B	142	ASN
1	C	28	GLN
1	C	133	GLN
1	D	133	GLN
1	D	142	ASN
1	E	28	GLN
1	E	65	GLN
1	F	28	GLN
1	F	115	ASN
1	F	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	AMP	D	195	-	25,25,25	1.33	3 (12%)	37,38,38	1.78	9 (24%)
2	AMP	C	195	-	25,25,25	1.33	5 (20%)	37,38,38	1.65	10 (27%)
3	ADP	F	196	-	28,29,29	1.39	5 (17%)	43,45,45	2.09	10 (23%)
2	AMP	F	195	-	25,25,25	1.34	2 (8%)	37,38,38	1.72	9 (24%)

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
2	AMP	D	195	-	-	0/10/26/26	0/3/3/3
2	AMP	C	195	-	-	0/10/26/26	0/3/3/3
3	ADP	F	196	-	-	4/16/32/32	0/3/3/3
2	AMP	F	195	-	-	0/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	196	ADP	C5-N7	-4.11	1.31	1.39
2	F	195	AMP	P-O5'	-3.34	1.49	1.60
3	F	196	ADP	PA-O3A	-3.07	1.56	1.59
2	D	195	AMP	P-O5'	-3.02	1.50	1.60
2	C	195	AMP	P-O5'	-2.59	1.52	1.60
2	C	195	AMP	C2'-C3'	-2.46	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	195	AMP	C5-C4	2.41	1.43	1.39
2	D	195	AMP	C5-C4	2.40	1.43	1.39
2	D	195	AMP	C2'-C3'	-2.36	1.47	1.53
3	F	196	ADP	C4-N9	-2.34	1.32	1.37
2	C	195	AMP	P-O2P	-2.34	1.46	1.54
3	F	196	ADP	C8-N9	-2.28	1.33	1.37
3	F	196	ADP	PB-O2B	2.20	1.63	1.54
2	C	195	AMP	P-O3P	2.09	1.62	1.54
2	C	195	AMP	C5-C4	2.08	1.42	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	196	ADP	N3-C2-N1	-5.89	119.66	128.58
3	F	196	ADP	C5-C4-N3	-5.59	119.02	126.72
2	D	195	AMP	O4'-C1'-N9	5.27	118.21	108.09
3	F	196	ADP	C2-N3-C4	4.22	122.12	111.83
3	F	196	ADP	N3-C4-N9	4.03	134.01	127.17
3	F	196	ADP	C5-N7-C8	3.97	109.68	103.45
3	F	196	ADP	N9-C8-N7	-3.93	108.36	113.94
2	C	195	AMP	O2P-P-O1P	3.89	125.99	110.83
2	F	195	AMP	O4'-C1'-N9	3.60	115.00	108.09
3	F	196	ADP	C4-C5-N7	-3.57	106.50	110.58
2	F	195	AMP	C4-C5-N7	-3.54	106.53	110.58
2	F	195	AMP	C2-N1-C6	3.28	124.11	118.73
2	D	195	AMP	C3'-C2'-C1'	-3.06	95.67	101.46
2	D	195	AMP	O3P-P-O5'	-3.03	98.77	106.67
2	C	195	AMP	O3'-C3'-C4'	2.98	119.64	111.08
2	F	195	AMP	C3'-C2'-C1'	-2.97	95.85	101.46
2	D	195	AMP	C4-C5-N7	-2.88	107.29	110.58
2	F	195	AMP	C2'-C1'-N9	2.82	120.32	113.30
2	C	195	AMP	C4-C5-N7	-2.82	107.36	110.58
2	C	195	AMP	O3P-P-O2P	-2.80	97.31	107.80
2	C	195	AMP	O5'-C5'-C4'	2.76	118.40	108.99
2	C	195	AMP	O4'-C1'-N9	2.70	113.28	108.09
3	F	196	ADP	O3B-PB-O3A	2.65	113.53	104.64
3	F	196	ADP	C4-N9-C8	2.62	108.48	105.74
2	F	195	AMP	O4'-C1'-C2'	2.61	112.21	106.62
2	F	195	AMP	O3P-P-O5'	-2.59	99.92	106.67
2	D	195	AMP	C2'-C1'-N9	2.41	119.30	113.30
2	D	195	AMP	C5-N7-C8	2.40	107.23	103.45
2	F	195	AMP	C4'-O4'-C1'	-2.35	104.28	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	195	AMP	O4'-C1'-C2'	2.32	111.58	106.62
2	C	195	AMP	C3'-C2'-C1'	-2.30	97.10	101.46
2	D	195	AMP	C2-N1-C6	2.30	122.51	118.73
2	D	195	AMP	O3P-P-O1P	2.27	119.68	110.83
2	F	195	AMP	C5-N7-C8	2.27	107.01	103.45
2	C	195	AMP	C4'-O4'-C1'	-2.16	104.70	109.47
3	F	196	ADP	O4'-C1'-N9	2.13	112.19	108.09
2	C	195	AMP	C5-N7-C8	2.10	106.76	103.45
2	D	195	AMP	O3P-P-O2P	-2.06	100.09	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

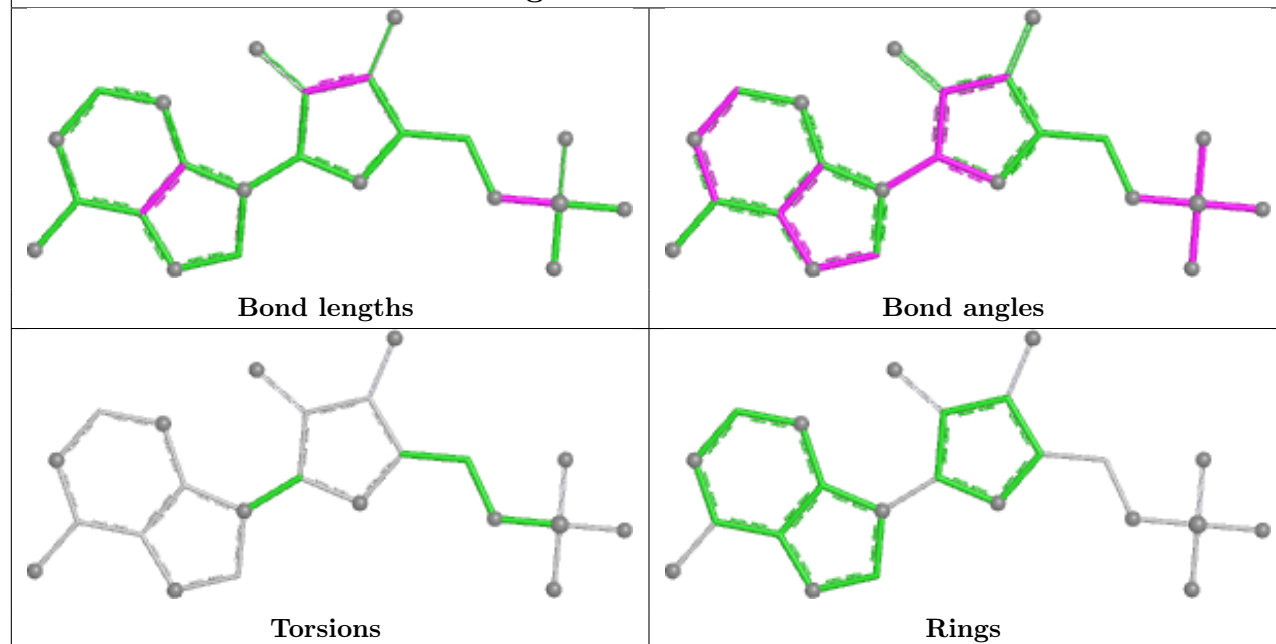
Mol	Chain	Res	Type	Atoms
3	F	196	ADP	C5'-O5'-PA-O1A
3	F	196	ADP	C5'-O5'-PA-O2A
3	F	196	ADP	C5'-O5'-PA-O3A
3	F	196	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

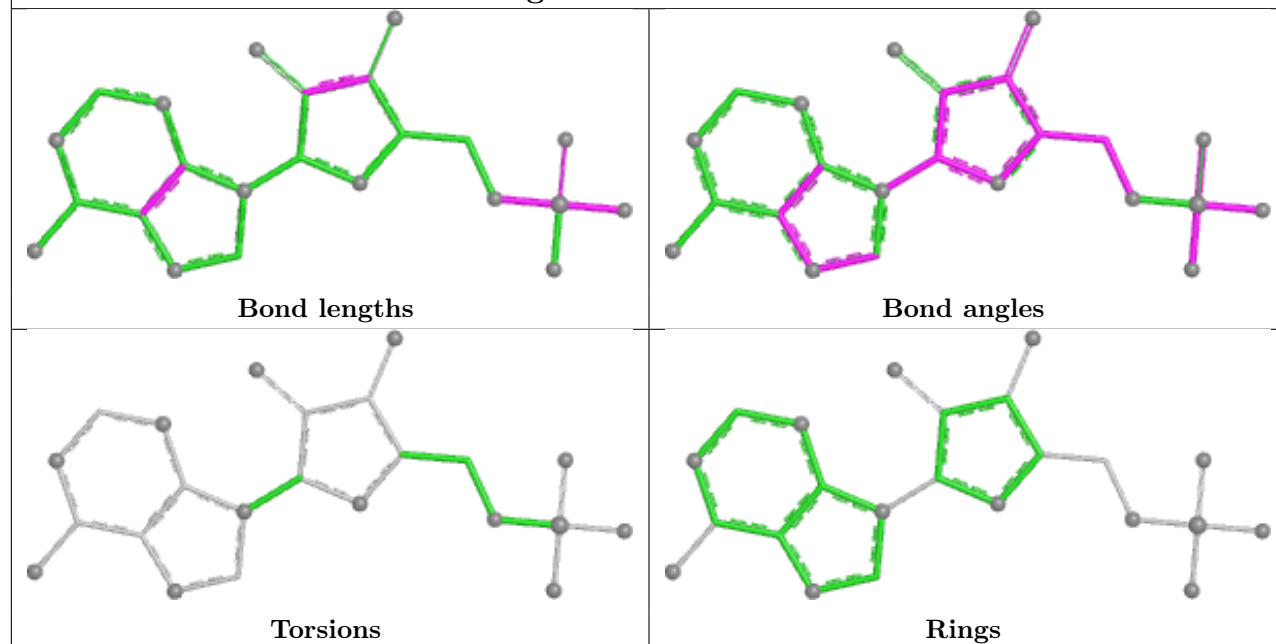
No monomer is involved in short contacts.

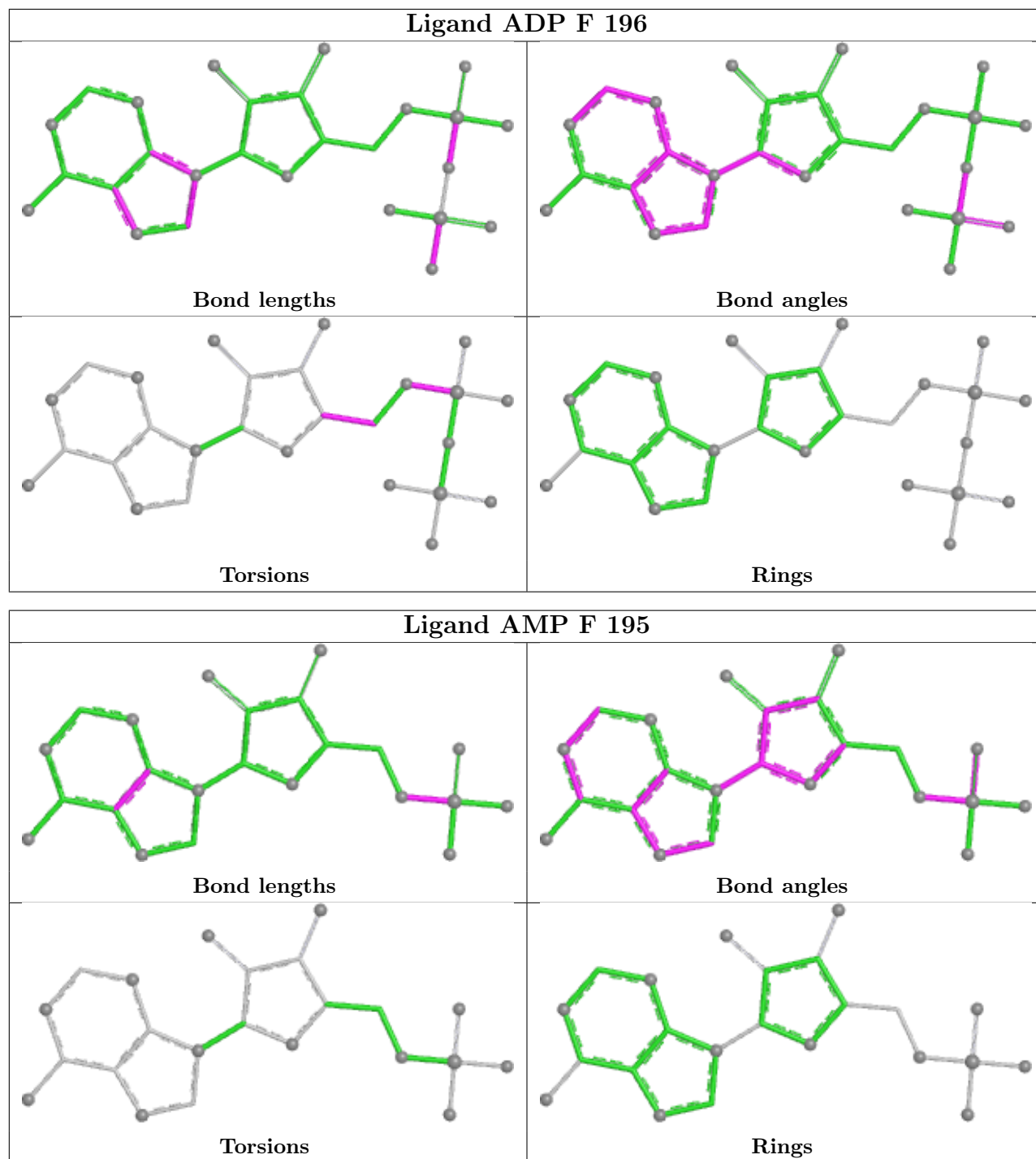
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand AMP D 195



Ligand AMP C 195





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	E	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	137:THR	C	138:THR	N	1.07
1	A	138:THR	C	139:ARG	N	1.00

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	194/194 (100%)	-0.23	7 (3%) 46 41	26, 53, 134, 188	0
1	B	194/194 (100%)	-0.21	7 (3%) 46 41	26, 50, 134, 188	0
1	C	194/194 (100%)	-0.24	5 (2%) 57 52	28, 59, 134, 182	0
1	D	194/194 (100%)	-0.18	8 (4%) 41 37	27, 57, 133, 182	0
1	E	194/194 (100%)	-0.12	8 (4%) 41 37	26, 50, 135, 189	0
1	F	194/194 (100%)	-0.32	2 (1%) 79 77	27, 56, 112, 132	0
All	All	1164/1164 (100%)	-0.22	37 (3%) 50 45	26, 54, 130, 189	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	138	THR	4.4
1	D	144	TYR	4.0
1	E	137	THR	3.9
1	B	144	TYR	3.7
1	C	138	THR	3.5
1	D	134	LYS	3.5
1	A	145	SER	3.2
1	A	144	TYR	3.2
1	C	144	TYR	3.2
1	E	144	TYR	3.1
1	D	141	ARG	3.1
1	D	138	THR	3.0
1	A	138	THR	3.0
1	D	142	ASN	2.9
1	B	137	THR	2.9
1	B	145	SER	2.8
1	D	132	ARG	2.7
1	E	140	ASN	2.7
1	B	141	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	141	ARG	2.6
1	D	145	SER	2.6
1	E	130	LEU	2.6
1	E	141	ARG	2.4
1	B	143	ASP	2.4
1	A	139	ARG	2.3
1	B	50	TYR	2.3
1	C	137	THR	2.3
1	F	137	THR	2.3
1	A	132	ARG	2.3
1	D	139	ARG	2.3
1	E	139	ARG	2.3
1	B	134	LYS	2.3
1	A	141	ARG	2.2
1	E	126	PRO	2.1
1	A	142	ASN	2.1
1	C	139	ARG	2.1
1	C	141	ARG	2.1

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](#)

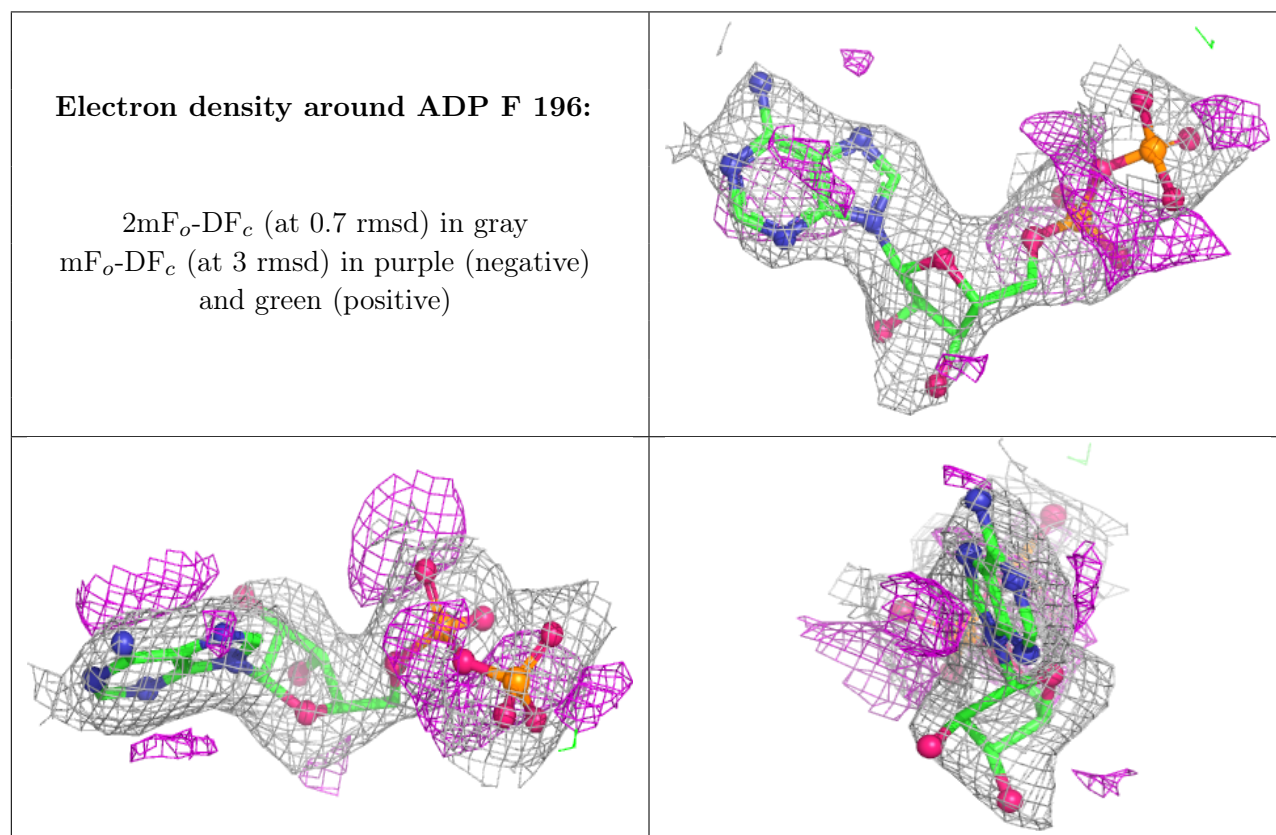
There are no oligosaccharides in this entry.

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.

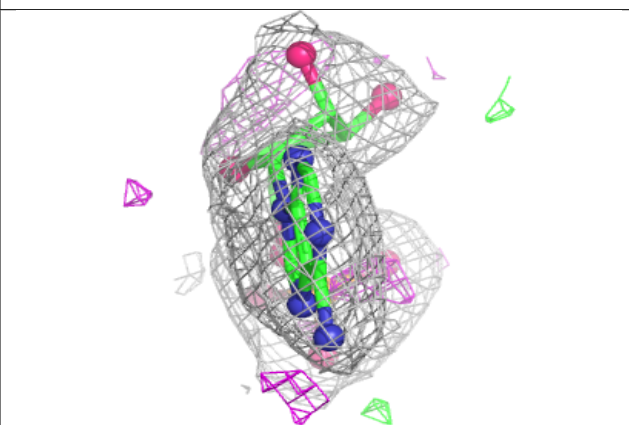
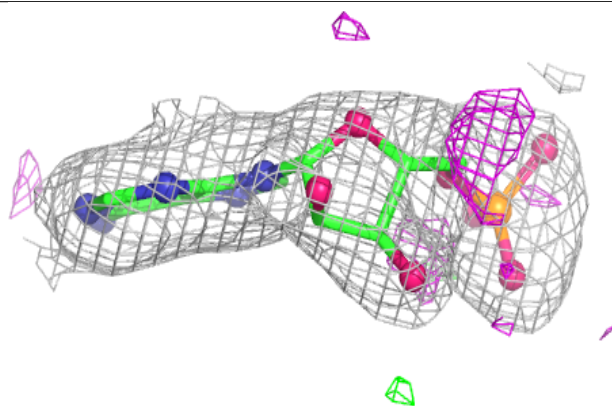
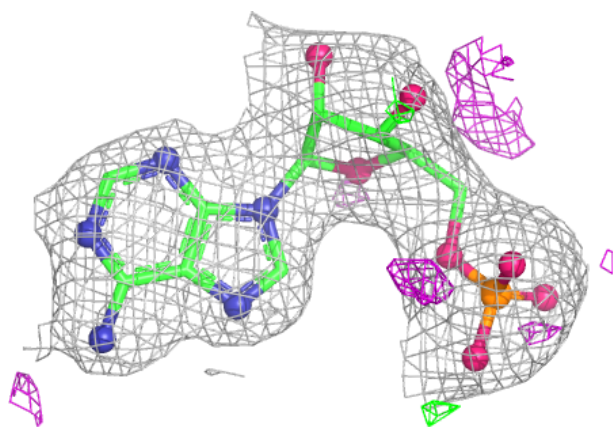
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	F	196	27/27	0.91	0.13	84,114,119,119	0
2	AMP	D	195	23/23	0.97	0.05	29,44,52,64	0
2	AMP	C	195	23/23	0.97	0.06	44,50,56,70	0
2	AMP	F	195	23/23	0.98	0.05	30,43,50,57	0

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.



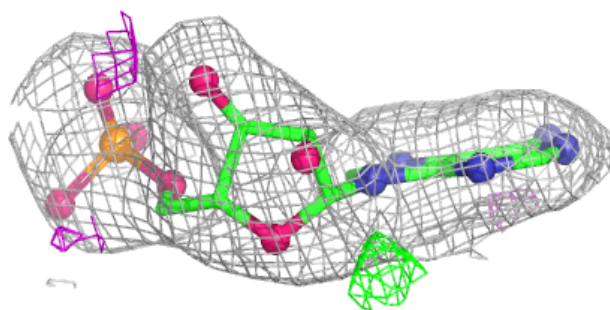
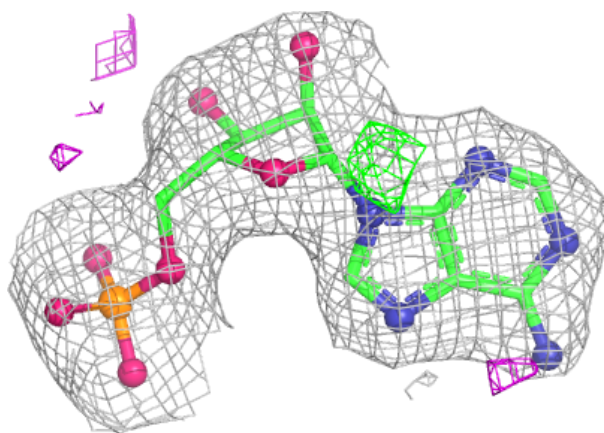
Electron density around AMP D 195:

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

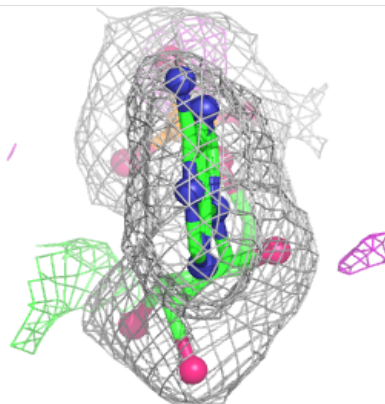
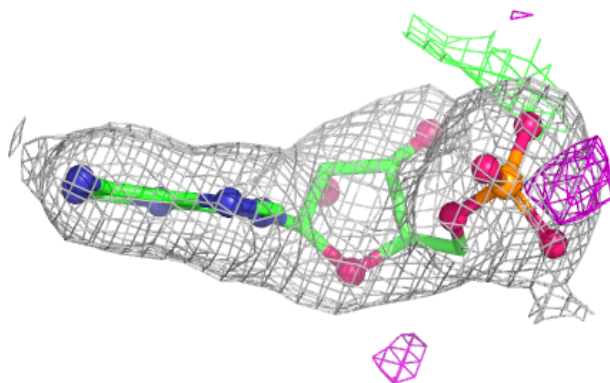
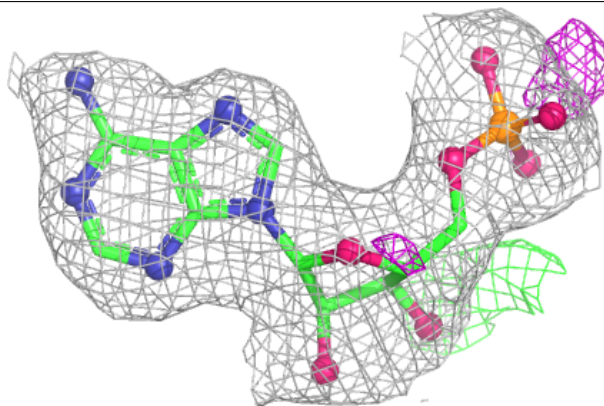


Electron density around AMP C 195:

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

**Electron density around AMP F 195:**

$2mF_o-DF_c$ (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.