



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:49 PM GMT

PDB ID : 1F9A  
Title : CRYSTAL STRUCTURE ANALYSIS OF NMN ADENYLYLTRANSFERASE FROM METHANOCOCCUS JANNASCHII  
Authors : D'Angelo, I.; Raffaelli, N.; Dabusti, V.; Lorenzi, T.; Magni, G.; Rizzi, M.  
Deposited on : 2000-07-09  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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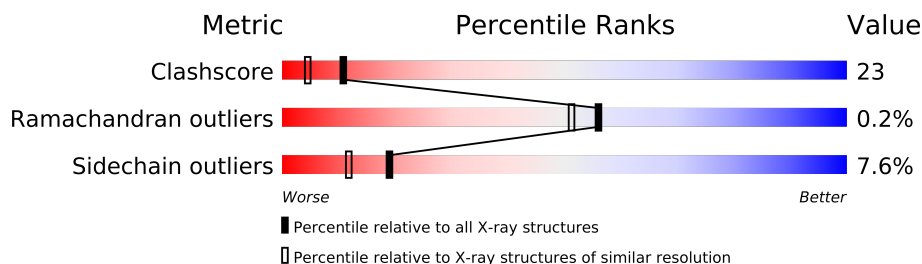
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	
1	B	168	
1	C	168	
1	D	168	
1	E	168	
1	F	168	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8923 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HYPOTHETICAL PROTEIN MJ0541.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	C	164	Total	C	N	O	S	0	0	0
			1338	866	231	238	3			
1	D	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	E	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	F	164	Total	C	N	O	S	0	0	0
			1351	876	231	241	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	CONFLICT	UNP Q57961
B	1	LEU	MET	CONFLICT	UNP Q57961
C	1	LEU	MET	CONFLICT	UNP Q57961
D	1	LEU	MET	CONFLICT	UNP Q57961
E	1	LEU	MET	CONFLICT	UNP Q57961
F	1	LEU	MET	CONFLICT	UNP Q57961

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

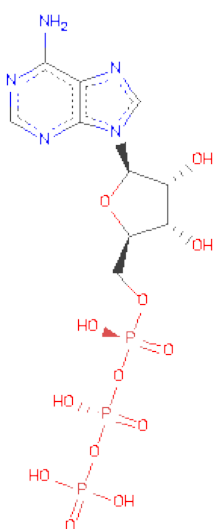
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	100	Total 100	O 100	0	0
4	C	103	Total 103	O 103	0	0
4	D	93	Total 93	O 93	0	0
4	E	122	Total 122	O 122	0	0
4	F	141	Total 141	O 141	0	0

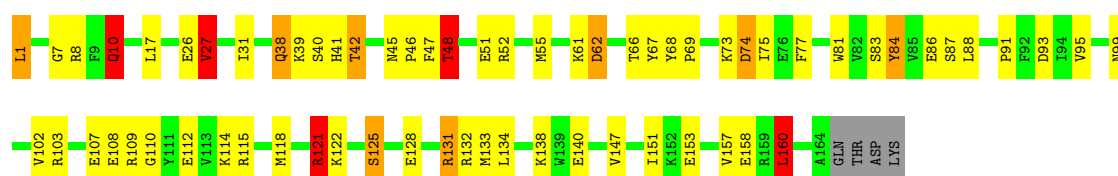
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

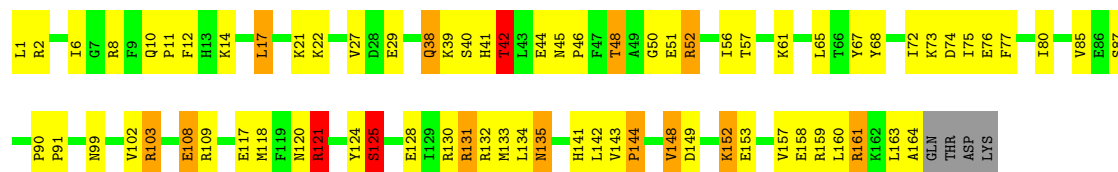
#### • Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain A: 



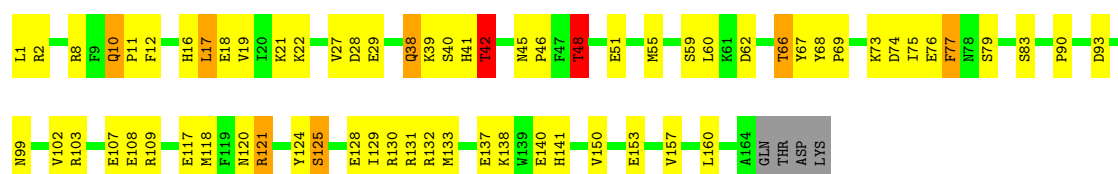
#### • Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain B: 



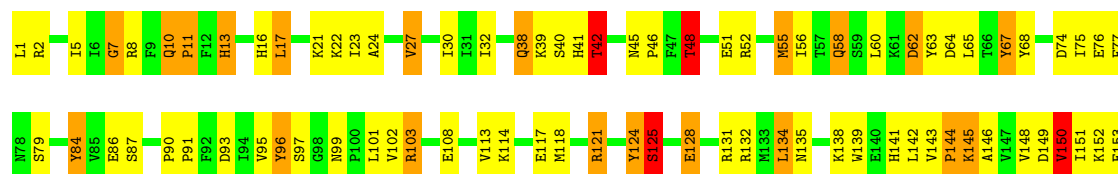
#### • Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain C: 



#### • Molecule 1: HYPOTHETICAL PROTEIN MJ0541

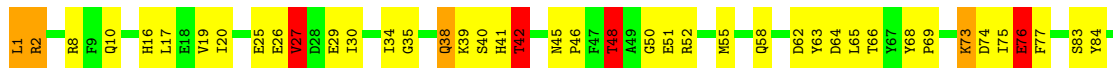
Chain D: 





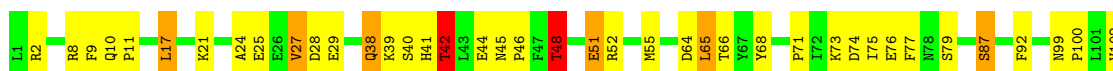
• Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain E:



• Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain F:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.77Å 112.64Å 79.87Å 90.00° 116.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.0 (20.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

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

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	0.76	1/1371 (0.1%)	1.86	34/1849 (1.8%)
1	B	0.72	0/1371	1.89	34/1849 (1.8%)
1	C	0.78	1/1368 (0.1%)	1.61	24/1845 (1.3%)
1	D	0.77	1/1379 (0.1%)	1.76	33/1860 (1.8%)
1	E	0.77	1/1379 (0.1%)	1.76	32/1860 (1.7%)
1	F	0.82	1/1382 (0.1%)	1.59	29/1864 (1.6%)
All	All	0.77	5/8250 (0.1%)	1.75	186/11127 (1.7%)

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	5
1	B	1	4
1	C	1	3
1	D	0	14
1	E	1	9
1	F	1	2
All	All	4	37

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	87	SER	CA-CB	6.45	1.62	1.52
1	A	87	SER	CA-CB	5.96	1.61	1.52
1	F	79	SER	CA-CB	5.74	1.61	1.52
1	C	137	GLU	CD-OE1	5.69	1.31	1.25
1	D	79	SER	CA-CB	5.46	1.61	1.52

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH2	32.76	136.68	120.30
1	B	8	ARG	NE-CZ-NH1	-20.83	109.88	120.30
1	B	2	ARG	NE-CZ-NH1	19.05	129.82	120.30
1	E	8	ARG	NE-CZ-NH1	-16.98	111.81	120.30
1	B	109	ARG	NE-CZ-NH2	-16.02	112.29	120.30
1	D	93	ASP	CB-CG-OD2	14.83	131.65	118.30
1	E	109	ARG	NE-CZ-NH2	14.41	127.51	120.30
1	A	52	ARG	NE-CZ-NH2	-13.78	113.41	120.30
1	D	161	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	A	109	ARG	NH1-CZ-NH2	-12.74	105.39	119.40
1	E	161	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	E	52	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	E	130	ARG	NE-CZ-NH1	11.75	126.18	120.30
1	B	161	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	B	52	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	F	121	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	E	140	GLU	OE1-CD-OE2	-10.63	110.54	123.30
1	C	8	ARG	NE-CZ-NH1	-10.56	115.02	120.30
1	B	109	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	E	52	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	C	130	ARG	CD-NE-CZ	10.05	137.67	123.60
1	F	130	ARG	CD-NE-CZ	9.90	137.46	123.60
1	A	131	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	F	121	ARG	CD-NE-CZ	9.60	137.04	123.60
1	A	132	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	D	52	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	C	140	GLU	OE1-CD-OE2	-9.22	112.23	123.30
1	A	93	ASP	CB-CG-OD1	-8.98	110.22	118.30
1	E	161	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	103	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	2	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	C	68	TYR	CB-CG-CD1	-8.92	115.65	121.00
1	F	132	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	B	8	ARG	NH1-CZ-NH2	8.88	129.16	119.40
1	A	48	THR	N-CA-CB	-8.83	93.52	110.30
1	C	48	THR	N-CA-CB	-8.82	93.55	110.30
1	F	68	TYR	CB-CG-CD1	-8.45	115.93	121.00
1	B	108	GLU	OE1-CD-OE2	-8.37	113.25	123.30
1	D	8	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	C	153	GLU	OE1-CD-OE2	-8.29	113.35	123.30
1	F	75	ILE	O-C-N	-8.09	109.75	122.70
1	E	75	ILE	O-C-N	-7.95	109.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	48	THR	N-CA-CB	-7.55	95.95	110.30
1	D	68	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	A	86	GLU	OE1-CD-OE2	-7.46	114.35	123.30
1	E	48	THR	N-CA-CB	-7.35	96.34	110.30
1	B	132	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	61	LYS	O-C-N	7.30	134.37	122.70
1	A	8	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	C	109	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	E	8	ARG	CD-NE-CZ	-7.19	113.54	123.60
1	A	74	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	F	107	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	F	48	THR	N-CA-CB	-7.05	96.90	110.30
1	C	48	THR	CA-CB-CG2	7.03	122.25	112.40
1	D	2	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	C	109	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	A	103	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	146	ALA	CB-CA-C	7.00	120.60	110.10
1	D	161	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	160	LEU	CB-CG-CD1	6.95	122.81	111.00
1	D	96	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	D	48	THR	OG1-CB-CG2	6.91	125.89	110.00
1	C	42	THR	N-CA-CB	-6.88	97.23	110.30
1	D	42	THR	N-CA-CB	-6.85	97.29	110.30
1	B	42	THR	N-CA-CB	-6.83	97.31	110.30
1	E	8	ARG	NH1-CZ-NH2	6.76	126.84	119.40
1	F	48	THR	CA-CB-OG1	6.76	123.19	109.00
1	D	2	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	48	THR	N-CA-CB	-6.69	97.58	110.30
1	B	159	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	E	73	LYS	N-CA-CB	-6.68	98.57	110.60
1	E	48	THR	OG1-CB-CG2	6.67	125.35	110.00
1	D	150	VAL	O-C-N	-6.66	112.05	122.70
1	F	68	TYR	CB-CG-CD2	6.65	124.99	121.00
1	A	48	THR	OG1-CB-CG2	6.59	125.17	110.00
1	A	107	GLU	OE1-CD-OE2	-6.58	115.40	123.30
1	A	121	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	121	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	F	132	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	121	ARG	CD-NE-CZ	6.48	132.68	123.60
1	F	75	ILE	N-CA-C	-6.47	93.54	111.00
1	D	160	LEU	CA-CB-CG	6.46	130.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	THR	N-CA-CB	-6.46	98.02	110.30
1	A	84	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	B	48	THR	OG1-CB-CG2	6.38	124.68	110.00
1	C	153	GLU	CG-CD-OE1	6.38	131.06	118.30
1	D	93	ASP	OD1-CG-OD2	-6.36	111.22	123.30
1	C	66	THR	CA-CB-CG2	-6.35	103.52	112.40
1	E	140	GLU	CG-CD-OE2	6.34	130.99	118.30
1	F	52	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	24	ALA	N-CA-CB	-6.28	101.31	110.10
1	C	68	TYR	CB-CG-CD2	6.23	124.74	121.00
1	A	8	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	10	GLN	N-CA-CB	6.15	121.68	110.60
1	F	27	VAL	CA-CB-CG1	6.15	120.12	110.90
1	B	42	THR	OG1-CB-CG2	6.14	124.13	110.00
1	D	103	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	F	28	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	75	ILE	O-C-N	-6.07	112.99	122.70
1	B	153	GLU	CA-CB-CG	6.02	126.64	113.40
1	F	64	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	161	ARG	NH1-CZ-NH2	6.01	126.01	119.40
1	D	58	GLN	CG-CD-OE1	-6.00	109.60	121.60
1	D	68	TYR	CB-CG-CD2	6.00	124.60	121.00
1	E	27	VAL	CG1-CB-CG2	6.00	120.49	110.90
1	A	75	ILE	O-C-N	-6.00	113.11	122.70
1	F	51	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	D	87	SER	CA-CB-OG	-5.99	95.03	111.20
1	C	8	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	F	87	SER	CB-CA-C	-5.89	98.91	110.10
1	D	84	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	F	42	THR	N-CA-CB	-5.87	99.14	110.30
1	B	130	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	86	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	E	127	THR	CA-CB-CG2	5.81	120.53	112.40
1	A	121	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	E	76	GLU	CA-C-O	-5.78	107.97	120.10
1	F	149	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	48	THR	CA-CB-OG1	5.72	121.02	109.00
1	A	75	ILE	N-CA-C	-5.72	95.56	111.00
1	C	132	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	2	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	121	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	148	VAL	CA-CB-CG1	5.68	119.42	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	GLU	CA-CB-CG	5.67	125.88	113.40
1	B	68	TYR	CB-CG-CD2	5.64	124.38	121.00
1	A	61	LYS	CA-C-N	-5.64	104.80	117.20
1	C	132	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	A	27	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	F	164	ALA	CA-C-O	-5.57	108.41	120.10
1	E	87	SER	CB-CA-C	-5.56	99.53	110.10
1	D	75	ILE	O-C-N	-5.55	113.82	122.70
1	A	115	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	153	GLU	CA-CB-CG	5.51	125.53	113.40
1	A	27	VAL	CA-CB-CG1	5.50	119.16	110.90
1	F	92	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	E	76	GLU	CB-CA-C	5.46	121.32	110.40
1	E	75	ILE	N-CA-C	-5.46	96.27	111.00
1	F	2	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	28	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	27	VAL	CA-CB-CG2	5.44	119.06	110.90
1	B	12	PHE	CB-CG-CD1	5.43	124.60	120.80
1	B	2	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	C	48	THR	CA-CB-OG1	5.42	120.38	109.00
1	E	75	ILE	CA-C-N	5.41	129.10	117.20
1	D	161	ARG	CD-NE-CZ	5.41	131.17	123.60
1	B	121	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	152	LYS	CA-C-O	-5.39	108.79	120.10
1	C	93	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	103	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	F	2	ARG	CD-NE-CZ	5.34	131.07	123.60
1	A	69	PRO	N-CD-CG	-5.33	95.20	103.20
1	E	109	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	A	68	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	B	149	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	31	ILE	CG1-CB-CG2	-5.31	99.73	111.40
1	C	132	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	D	124	TYR	N-CA-CB	-5.30	101.07	110.60
1	D	16	HIS	N-CA-CB	5.28	120.11	110.60
1	D	128	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	A	91	PRO	O-C-N	-5.28	114.25	122.70
1	C	130	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	F	42	THR	OG1-CB-CG2	5.26	122.09	110.00
1	D	42	THR	CA-CB-CG2	5.26	119.76	112.40
1	F	75	ILE	CA-C-N	5.25	128.75	117.20
1	D	146	ALA	O-C-N	-5.25	114.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	153	GLU	CA-CB-CG	5.22	124.88	113.40
1	E	119	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	E	25	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	153	GLU	CG-CD-OE1	5.14	128.58	118.30
1	A	62	ASP	N-CA-CB	-5.14	101.35	110.60
1	E	87	SER	CA-CB-OG	-5.12	97.36	111.20
1	E	121	ARG	CA-C-O	-5.11	109.37	120.10
1	F	153	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	B	159	ARG	NH1-CZ-NH2	-5.09	113.81	119.40
1	B	29	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	A	66	THR	CA-CB-CG2	-5.08	105.29	112.40
1	E	131	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	92	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	C	75	ILE	O-C-N	-5.04	114.63	122.70
1	D	67	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	B	131	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	125	SER	N-CA-CB	-5.00	103.00	110.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	48	THR	CB
1	C	48	THR	CB
1	E	48	THR	CB
1	F	48	THR	CB

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLY	Mainchain
1	A	125	SER	Mainchain
1	A	7	GLY	Mainchain
1	A	81	TRP	Mainchain
1	A	95	VAL	Mainchain
1	B	103	ARG	Mainchain
1	B	135	ASN	Mainchain
1	B	80	ILE	Mainchain
1	B	87	SER	Mainchain
1	C	107	GLU	Mainchain
1	C	77	PHE	Mainchain
1	C	83	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	D	11	PRO	Mainchain
1	D	125	SER	Mainchain
1	D	13	HIS	Mainchain
1	D	134	LEU	Mainchain
1	D	144	PRO	Mainchain
1	D	145	LYS	Mainchain
1	D	150	VAL	Mainchain
1	D	151	ILE	Mainchain
1	D	155	LYS	Mainchain
1	D	32	ILE	Mainchain
1	D	55	MET	Mainchain
1	D	56	ILE	Mainchain
1	D	7	GLY	Mainchain
1	D	84	TYR	Mainchain
1	E	111	TYR	Mainchain
1	E	163	LEU	Mainchain
1	E	2	ARG	Mainchain
1	E	26	GLU	Mainchain
1	E	34	ILE	Mainchain
1	E	50	GLY	Mainchain
1	E	69	PRO	Mainchain
1	E	76	GLU	Mainchain
1	E	90	PRO	Mainchain
1	F	153	GLU	Mainchain
1	F	71	PRO	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1341	0	1375	55	0
1	B	1341	0	1375	67	0
1	C	1338	0	1366	62	0
1	D	1348	0	1382	75	0
1	E	1348	0	1382	61	0
1	F	1351	0	1384	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	11	1	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	6	0
3	E	31	0	11	0	0
3	F	31	0	12	0	0
4	A	105	0	0	16	0
4	B	100	0	0	16	0
4	C	103	0	0	9	0
4	D	93	0	0	13	0
4	E	122	0	0	18	0
4	F	141	0	0	19	0
All	All	8923	0	8334	378	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:MET:SD	4:A:791:HOH:O	2.07	1.13
1:B:134:LEU:HD21	1:B:161:ARG:HA	1.18	1.10
1:D:42:THR:HG21	4:D:728:HOH:O	1.52	1.10
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.12	1.07
1:D:42:THR:HG22	1:D:45:ASN:H	1.13	1.07
1:E:121:ARG:HH21	1:E:125:SER:HB2	1.19	1.04
1:D:121:ARG:HH21	1:D:125:SER:HB2	1.21	1.04
1:B:118:MET:CE	1:B:121:ARG:HD2	1.87	1.03
1:A:48:THR:HG21	4:F:814:HOH:O	1.59	1.02
1:B:134:LEU:HD22	4:B:785:HOH:O	1.58	1.01
1:E:118:MET:CE	1:E:121:ARG:HD2	1.91	1.01
1:A:42:THR:HG22	1:A:45:ASN:H	1.24	1.00
1:A:42:THR:HG21	4:A:733:HOH:O	1.62	0.99
1:C:42:THR:HG21	4:C:714:HOH:O	1.60	0.99
1:C:42:THR:HG22	1:C:45:ASN:H	1.23	0.99
1:C:38:GLN:HE21	1:C:38:GLN:H	1.06	0.97
1:B:61:LYS:HE3	4:B:783:HOH:O	1.63	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:158:GLU:HG3	4:D:743:HOH:O	1.62	0.96
1:B:133:MET:HE2	1:B:160:LEU:HD23	1.47	0.96
1:B:163:LEU:HD11	4:B:767:HOH:O	1.66	0.95
1:B:118:MET:HE2	1:B:121:ARG:HD2	1.46	0.95
1:B:42:THR:HG22	1:B:45:ASN:H	1.29	0.94
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.31	0.94
1:E:118:MET:HE1	1:E:121:ARG:HD2	1.46	0.93
1:F:42:THR:HG22	1:F:45:ASN:H	1.33	0.93
1:D:38:GLN:HE21	1:D:38:GLN:H	1.01	0.92
1:A:121:ARG:HH21	1:A:125:SER:HB2	1.33	0.91
1:F:131:ARG:HH11	1:F:131:ARG:HG2	1.34	0.91
1:C:118:MET:CE	1:C:121:ARG:HD2	2.01	0.90
1:F:42:THR:HG21	4:F:817:HOH:O	1.69	0.90
1:B:38:GLN:H	1:B:38:GLN:HE21	1.20	0.90
1:E:152:LYS:HD2	4:E:842:HOH:O	1.69	0.90
1:F:38:GLN:H	1:F:38:GLN:HE21	1.20	0.90
1:B:133:MET:HE3	1:B:157:VAL:HG22	1.52	0.90
1:E:131:ARG:HH11	1:E:131:ARG:HG2	1.38	0.89
1:E:42:THR:HG22	1:E:45:ASN:H	1.37	0.89
1:A:73:LYS:HE3	4:A:780:HOH:O	1.73	0.87
1:C:73:LYS:HE3	4:C:778:HOH:O	1.73	0.87
1:C:118:MET:HE1	1:C:121:ARG:HD2	1.56	0.87
1:A:131:ARG:NH1	1:A:131:ARG:HG2	1.89	0.87
1:C:38:GLN:HE22	1:C:74:ASP:H	1.19	0.86
1:A:131:ARG:HH11	1:A:131:ARG:CG	1.88	0.85
1:E:38:GLN:HE21	1:E:38:GLN:H	1.19	0.85
3:D:703:ATP:H5'1	4:D:786:HOH:O	1.76	0.84
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.43	0.83
1:E:39:LYS:HE3	1:E:74:ASP:OD2	1.78	0.83
1:A:38:GLN:HE22	1:A:74:ASP:H	1.26	0.83
1:D:48:THR:HG22	1:D:51:GLU:H	1.40	0.83
1:B:134:LEU:HD23	1:B:161:ARG:HG2	1.61	0.83
1:C:48:THR:HG21	4:E:811:HOH:O	1.79	0.82
1:E:38:GLN:HE22	1:E:74:ASP:H	1.25	0.82
4:C:723:HOH:O	1:E:48:THR:HG21	1.79	0.82
1:C:39:LYS:NZ	1:C:74:ASP:OD2	2.12	0.81
1:B:42:THR:HG21	4:B:711:HOH:O	1.80	0.81
1:E:63:TYR:O	1:E:64:ASP:CB	2.26	0.81
1:B:118:MET:HE3	1:B:121:ARG:HD2	1.61	0.81
1:D:42:THR:HG22	1:D:45:ASN:N	1.95	0.81
1:B:134:LEU:CD2	1:B:161:ARG:HA	2.08	0.81
1:B:48:THR:HG21	4:D:726:HOH:O	1.79	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:103:ARG:HG3	1:D:113:VAL:HG11	1.63	0.81
1:D:38:GLN:HE22	1:D:74:ASP:H	1.26	0.81
1:D:7:GLY:HA2	4:D:786:HOH:O	1.81	0.80
1:B:121:ARG:HH21	1:B:125:SER:HB2	1.46	0.80
1:A:118:MET:CE	1:A:121:ARG:HD2	2.12	0.80
1:E:128:GLU:OE1	1:E:131:ARG:NH2	2.15	0.80
1:C:42:THR:HG22	1:C:45:ASN:N	1.97	0.79
1:B:48:THR:HG22	1:B:51:GLU:H	1.48	0.79
1:F:135:ASN:ND2	1:F:137:GLU:OE2	2.16	0.79
1:E:42:THR:HG21	4:E:826:HOH:O	1.83	0.79
4:A:710:HOH:O	1:F:48:THR:HG21	1.81	0.79
1:F:42:THR:CG2	1:F:45:ASN:H	1.96	0.78
1:A:38:GLN:HE21	1:A:38:GLN:H	1.27	0.78
1:B:158:GLU:HG3	4:B:725:HOH:O	1.84	0.78
1:C:40:SER:OG	1:C:41:HIS:HD2	1.67	0.78
3:D:703:ATP:C5'	4:D:786:HOH:O	2.30	0.78
1:A:147:VAL:HG12	1:A:151:ILE:HD12	1.65	0.78
1:F:158:GLU:HG3	4:F:895:HOH:O	1.84	0.77
1:F:131:ARG:NH1	4:F:939:HOH:O	2.18	0.77
1:D:17:LEU:HD22	1:D:21:LYS:HE3	1.67	0.77
1:A:41:HIS:HE1	1:C:108:GLU:OE1	1.68	0.77
1:F:131:ARG:HG2	1:F:131:ARG:NH1	1.99	0.76
1:C:76:GLU:HB2	4:C:750:HOH:O	1.85	0.76
1:B:133:MET:CE	1:B:160:LEU:HD23	2.15	0.76
1:B:38:GLN:HE22	1:B:74:ASP:H	1.33	0.75
4:B:733:HOH:O	1:D:48:THR:HG21	1.87	0.75
1:F:42:THR:HG22	1:F:45:ASN:N	2.02	0.75
1:D:38:GLN:N	1:D:38:GLN:HE21	1.82	0.75
1:E:118:MET:HE3	1:E:121:ARG:HD2	1.67	0.75
1:D:128:GLU:OE1	1:D:131:ARG:NH2	2.20	0.74
1:D:22:LYS:HE2	1:D:117:GLU:OE2	1.87	0.74
1:C:42:THR:CG2	1:C:45:ASN:H	1.99	0.74
1:C:131:ARG:NH1	1:C:131:ARG:HG2	2.03	0.74
1:F:40:SER:OG	1:F:41:HIS:HD2	1.70	0.74
1:D:121:ARG:HG2	3:D:703:ATP:N6	2.03	0.73
1:C:128:GLU:OE1	1:C:131:ARG:NH2	2.22	0.73
1:F:25:GLU:CD	4:F:937:HOH:O	2.28	0.72
1:A:128:GLU:OE1	1:A:131:ARG:NH2	2.24	0.71
1:E:99:ASN:HD22	1:E:102:VAL:H	1.36	0.71
1:B:128:GLU:OE1	1:B:131:ARG:NH2	2.24	0.71
1:A:118:MET:HE3	1:A:121:ARG:HD2	1.72	0.70
1:B:48:THR:CG2	1:B:51:GLU:H	2.04	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:720:HOH:O	1:C:79:SER:HB2	1.91	0.69
1:A:48:THR:HG22	1:A:51:GLU:H	1.57	0.69
1:A:138:LYS:HE3	4:A:782:HOH:O	1.93	0.69
1:B:76:GLU:HB2	4:B:788:HOH:O	1.92	0.68
1:E:41:HIS:HE1	1:F:108:GLU:OE1	1.75	0.68
1:C:118:MET:HE3	1:C:121:ARG:HD2	1.75	0.68
1:A:133:MET:HE3	1:A:157:VAL:HG22	1.75	0.68
1:F:145:LYS:HG2	4:F:858:HOH:O	1.93	0.68
1:F:158:GLU:CD	4:F:926:HOH:O	2.32	0.68
1:E:42:THR:HG22	1:E:45:ASN:N	2.09	0.67
1:D:40:SER:OG	1:D:41:HIS:HD2	1.75	0.67
1:F:38:GLN:HE22	1:F:74:ASP:H	1.40	0.67
1:E:48:THR:HG22	1:E:51:GLU:H	1.59	0.67
1:A:26:GLU:HG2	4:A:774:HOH:O	1.94	0.66
1:A:99:ASN:HD22	1:A:102:VAL:H	1.44	0.66
1:E:76:GLU:HB2	4:E:848:HOH:O	1.94	0.66
1:A:48:THR:CG2	1:A:51:GLU:H	2.07	0.66
1:E:30:ILE:HG13	1:E:65:LEU:HD11	1.77	0.66
1:F:132:ARG:HD3	4:F:876:HOH:O	1.95	0.66
1:A:1:LEU:HB2	4:A:755:HOH:O	1.96	0.65
1:E:42:THR:CG2	1:E:45:ASN:H	2.08	0.65
1:A:1:LEU:HB3	1:A:27:VAL:HG22	1.79	0.65
1:C:99:ASN:HD22	1:C:102:VAL:H	1.42	0.65
1:A:39:LYS:HE3	1:A:74:ASP:OD2	1.97	0.65
1:C:51:GLU:O	1:C:55:MET:HG3	1.97	0.65
1:D:21:LYS:HE2	1:D:63:TYR:CE2	2.32	0.65
1:B:131:ARG:NH1	1:B:131:ARG:HG2	2.12	0.65
1:D:76:GLU:HB2	4:D:771:HOH:O	1.97	0.64
1:D:121:ARG:NH2	1:D:125:SER:HB2	2.04	0.64
1:A:42:THR:HG22	1:A:45:ASN:N	2.06	0.63
1:B:42:THR:HG22	1:B:45:ASN:N	2.09	0.63
1:C:59:SER:O	1:C:62:ASP:OD2	2.17	0.63
1:E:131:ARG:NH1	1:E:131:ARG:HG2	2.01	0.63
1:B:108:GLU:OE1	1:C:41:HIS:HE1	1.81	0.63
1:F:139:TRP:HA	4:F:876:HOH:O	1.97	0.63
1:D:162:LYS:HE2	4:E:876:HOH:O	1.97	0.63
1:E:38:GLN:HE21	1:E:38:GLN:N	1.96	0.62
1:E:20:ILE:HG23	1:E:30:ILE:HD12	1.81	0.62
1:A:131:ARG:NH2	4:A:740:HOH:O	2.33	0.61
1:D:42:THR:CG2	1:D:45:ASN:H	2.01	0.61
1:E:91:PRO:HD3	4:E:855:HOH:O	2.00	0.61
1:A:62:ASP:HA	4:A:750:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:46:PRO:HB3	1:F:160:LEU:HD13	1.81	0.61
1:F:128:GLU:OE1	1:F:131:ARG:NH2	2.34	0.61
1:C:29:GLU:HG2	1:C:66:THR:HB	1.82	0.61
1:F:138:LYS:HG2	4:F:897:HOH:O	2.00	0.61
1:A:140:GLU:HG3	4:A:731:HOH:O	2.00	0.60
1:A:121:ARG:NH2	3:A:700:ATP:O2B	2.34	0.60
1:B:133:MET:CE	1:B:160:LEU:CD2	2.80	0.60
1:F:76:GLU:HB2	4:F:836:HOH:O	2.01	0.60
1:C:48:THR:HG22	1:C:51:GLU:CG	2.32	0.60
1:F:118:MET:CE	1:F:121:ARG:HD2	2.32	0.59
1:F:99:ASN:HD22	1:F:102:VAL:H	1.50	0.59
1:C:40:SER:OG	1:C:41:HIS:CD2	2.53	0.58
1:B:57:THR:HG23	1:B:67:TYR:OH	2.03	0.58
1:A:38:GLN:HE22	1:A:74:ASP:N	1.99	0.58
1:D:108:GLU:OE1	1:F:41:HIS:HE1	1.85	0.58
1:D:51:GLU:O	1:D:55:MET:HG3	2.03	0.58
1:D:124:TYR:O	3:D:703:ATP:N6	2.37	0.58
1:D:7:GLY:CA	4:D:786:HOH:O	2.47	0.58
1:B:133:MET:HE2	1:B:160:LEU:CD2	2.29	0.58
1:D:99:ASN:HD22	1:D:102:VAL:H	1.50	0.58
1:D:118:MET:CE	1:D:121:ARG:HD2	2.33	0.57
1:C:48:THR:HG22	1:C:51:GLU:H	1.68	0.57
1:D:103:ARG:HD2	4:D:753:HOH:O	2.04	0.57
1:C:48:THR:HG22	1:C:51:GLU:HG3	1.86	0.57
1:D:150:VAL:O	1:D:152:LYS:N	2.37	0.57
1:E:48:THR:CG2	1:E:51:GLU:H	2.17	0.57
1:D:99:ASN:ND2	1:D:101:LEU:H	2.03	0.57
1:B:39:LYS:HE3	1:B:74:ASP:OD2	2.05	0.57
1:F:51:GLU:O	1:F:55:MET:HG3	2.04	0.56
1:B:120:ASN:HB3	1:B:124:TYR:CD1	2.40	0.56
1:C:73:LYS:HD2	1:E:73:LYS:HZ3	1.71	0.56
1:B:17:LEU:HD22	1:B:21:LYS:HE3	1.88	0.56
1:C:90:PRO:HA	4:E:871:HOH:O	2.04	0.56
1:E:121:ARG:NH2	1:E:125:SER:HB2	2.04	0.56
1:F:29:GLU:HG2	1:F:66:THR:HB	1.87	0.56
1:E:38:GLN:NE2	1:E:38:GLN:H	1.97	0.56
1:D:62:ASP:CG	1:D:62:ASP:O	2.45	0.55
1:A:131:ARG:NH1	1:A:131:ARG:CG	2.54	0.55
1:B:134:LEU:CD2	4:B:785:HOH:O	2.35	0.55
1:C:38:GLN:NE2	1:C:38:GLN:H	1.90	0.55
1:E:133:MET:HE3	1:E:157:VAL:HG22	1.87	0.55
1:C:121:ARG:HG2	3:C:702:ATP:N6	2.22	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:HIS:HB3	4:B:767:HOH:O	2.06	0.55
1:E:131:ARG:HG3	1:E:135:ASN:HD22	1.71	0.55
1:A:122:LYS:HD3	4:A:748:HOH:O	2.06	0.54
1:D:118:MET:HA	3:D:703:ATP:C2	2.42	0.54
1:D:39:LYS:HE3	1:D:74:ASP:OD2	2.07	0.54
1:B:44:GLU:HG3	4:B:787:HOH:O	2.08	0.54
1:C:131:ARG:NH1	4:C:779:HOH:O	2.38	0.54
1:D:41:HIS:HE1	1:E:108:GLU:OE1	1.91	0.54
1:A:131:ARG:NE	4:A:811:HOH:O	2.22	0.53
1:A:42:THR:CG2	1:A:45:ASN:H	2.09	0.53
1:F:25:GLU:OE1	4:F:937:HOH:O	2.18	0.53
1:E:29:GLU:HG2	1:E:66:THR:HB	1.90	0.53
1:A:133:MET:CE	1:A:157:VAL:HG22	2.39	0.53
1:B:40:SER:OG	1:B:41:HIS:HD2	1.91	0.53
1:F:17:LEU:HD22	1:F:21:LYS:HE3	1.90	0.53
1:D:48:THR:CG2	1:D:51:GLU:H	2.15	0.53
1:B:73:LYS:HE3	4:B:793:HOH:O	2.08	0.53
1:D:64:ASP:C	4:D:762:HOH:O	2.47	0.53
1:B:42:THR:HG23	1:B:44:GLU:H	1.73	0.53
1:F:132:ARG:CD	4:F:876:HOH:O	2.53	0.52
1:B:134:LEU:CD2	1:B:161:ARG:HG2	2.37	0.52
1:A:48:THR:HG22	1:A:51:GLU:CB	2.39	0.52
1:C:69:PRO:HG2	4:C:804:HOH:O	2.10	0.52
1:E:120:ASN:HB3	1:E:124:TYR:CD1	2.45	0.52
1:B:152:LYS:HD3	4:B:776:HOH:O	2.09	0.52
1:E:46:PRO:HB3	1:E:160:LEU:HD13	1.91	0.52
1:D:63:TYR:HB3	1:D:65:LEU:HG	1.91	0.51
1:F:38:GLN:H	1:F:38:GLN:NE2	1.99	0.51
1:B:38:GLN:HE22	1:B:74:ASP:N	2.04	0.51
1:F:103:ARG:HD3	4:F:846:HOH:O	2.10	0.51
1:B:152:LYS:HB3	4:B:776:HOH:O	2.10	0.51
1:C:17:LEU:HD22	1:C:21:LYS:HE3	1.92	0.51
1:C:18:GLU:HG2	4:C:781:HOH:O	2.10	0.51
1:B:42:THR:CG2	1:B:45:ASN:H	2.13	0.51
1:A:118:MET:HE2	1:A:121:ARG:HD2	1.88	0.51
1:F:103:ARG:NH1	4:F:846:HOH:O	2.43	0.51
1:A:48:THR:HG22	1:A:51:GLU:HB2	1.93	0.50
1:D:148:VAL:O	1:D:149:ASP:C	2.49	0.50
1:E:114:LYS:NZ	4:E:892:HOH:O	2.39	0.50
1:D:17:LEU:CD2	1:D:21:LYS:HE3	2.39	0.50
1:E:133:MET:CE	1:E:157:VAL:HG22	2.41	0.50
1:B:39:LYS:CE	1:B:74:ASP:OD2	2.59	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:21:LYS:HE2	1:D:63:TYR:CZ	2.46	0.50
1:D:128:GLU:O	1:D:132:ARG:HG3	2.12	0.50
1:D:144:PRO:O	1:D:145:LYS:C	2.50	0.50
1:F:39:LYS:HE3	1:F:74:ASP:OD2	2.11	0.50
1:E:141:HIS:HE1	4:E:803:HOH:O	1.95	0.50
4:B:746:HOH:O	1:D:58:GLN:NE2	2.45	0.50
1:C:133:MET:HE1	1:C:160:LEU:CD2	2.42	0.49
1:F:42:THR:HG22	1:F:45:ASN:HB2	1.95	0.49
1:C:17:LEU:CD2	1:C:21:LYS:HE3	2.43	0.49
1:D:157:VAL:O	1:D:161:ARG:HG3	2.12	0.49
1:B:46:PRO:HB3	1:B:160:LEU:HD13	1.93	0.49
1:F:48:THR:CG2	1:F:51:GLU:H	2.26	0.49
1:D:60:LEU:HB3	1:D:65:LEU:HD12	1.95	0.49
1:B:17:LEU:CD2	1:B:21:LYS:HE3	2.42	0.49
1:C:22:LYS:NZ	4:C:767:HOH:O	2.45	0.49
1:C:48:THR:CG2	1:C:51:GLU:H	2.26	0.49
1:E:38:GLN:HE22	1:E:74:ASP:N	2.01	0.48
1:B:65:LEU:HD23	1:B:65:LEU:N	2.27	0.48
1:D:97:SER:HB2	4:D:768:HOH:O	2.12	0.48
1:D:118:MET:HE3	1:D:121:ARG:HD2	1.95	0.48
1:F:133:MET:HE3	1:F:157:VAL:HG22	1.94	0.48
1:B:22:LYS:HE2	1:B:117:GLU:OE2	2.13	0.48
1:D:38:GLN:NE2	1:D:38:GLN:H	1.86	0.48
1:E:133:MET:HE1	1:E:160:LEU:HD22	1.94	0.48
1:D:135:ASN:OD1	1:D:135:ASN:O	2.31	0.48
1:A:46:PRO:HB3	1:A:160:LEU:HD13	1.95	0.48
1:B:14:LYS:NZ	1:B:141:HIS:O	2.35	0.48
1:B:143:VAL:HG23	1:B:144:PRO:O	2.13	0.48
1:F:24:ALA:CB	1:F:65:LEU:HD21	2.44	0.48
1:F:48:THR:HG22	1:F:51:GLU:H	1.78	0.47
1:B:41:HIS:CB	4:B:767:HOH:O	2.62	0.47
1:D:138:LYS:HG3	1:D:139:TRP:N	2.28	0.47
1:D:13:HIS:HA	1:D:143:VAL:HG12	1.95	0.47
1:A:48:THR:HG22	1:A:51:GLU:CG	2.44	0.47
1:A:138:LYS:CE	4:A:782:HOH:O	2.56	0.47
1:E:1:LEU:N	4:E:880:HOH:O	2.24	0.47
1:C:133:MET:HE2	1:C:133:MET:HB3	1.71	0.47
1:C:138:LYS:NZ	1:C:141:HIS:CG	2.83	0.47
1:F:135:ASN:ND2	4:F:939:HOH:O	2.47	0.47
1:E:131:ARG:HD2	4:E:885:HOH:O	2.14	0.47
1:E:62:ASP:HB2	4:E:883:HOH:O	2.14	0.47
1:B:133:MET:HE3	1:B:157:VAL:CG2	2.35	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:ARG:HH21	1:C:125:SER:HB2	1.80	0.46
1:F:48:THR:HG22	1:F:51:GLU:CG	2.45	0.46
1:A:40:SER:OG	1:A:41:HIS:HD2	1.98	0.46
1:D:23:ILE:HG22	1:D:30:ILE:HD11	1.96	0.46
1:A:84:TYR:CZ	1:A:88:LEU:HD11	2.50	0.46
1:B:141:HIS:CE1	1:B:142:LEU:HD21	2.51	0.46
1:F:118:MET:HE3	1:F:121:ARG:HD2	1.97	0.45
1:B:72:ILE:HD13	1:B:85:VAL:HG22	1.99	0.45
1:F:131:ARG:HH11	1:F:131:ARG:CG	2.14	0.45
1:C:46:PRO:HB3	1:C:160:LEU:HD13	1.98	0.45
1:F:38:GLN:HE21	1:F:38:GLN:N	2.01	0.45
1:E:51:GLU:O	1:E:55:MET:HG3	2.16	0.45
1:E:122:LYS:NZ	4:E:850:HOH:O	2.17	0.45
1:C:120:ASN:HB3	1:C:124:TYR:CD1	2.51	0.45
1:E:40:SER:OG	1:E:41:HIS:HD2	1.99	0.45
1:D:10:GLN:HG2	1:D:46:PRO:CD	2.46	0.45
1:B:99:ASN:HD22	1:B:102:VAL:H	1.64	0.45
1:D:158:GLU:N	4:D:743:HOH:O	2.39	0.45
1:D:40:SER:OG	1:D:41:HIS:CD2	2.64	0.45
1:F:118:MET:HE2	1:F:121:ARG:HD2	1.98	0.45
1:A:108:GLU:OE1	1:B:41:HIS:HE1	2.00	0.44
1:E:131:ARG:NH1	4:E:828:HOH:O	2.25	0.44
1:A:38:GLN:H	1:A:38:GLN:NE2	2.07	0.44
1:F:133:MET:HE1	1:F:160:LEU:HD22	1.98	0.44
1:D:10:GLN:HG2	1:D:46:PRO:HG2	2.00	0.44
1:A:147:VAL:CG1	1:A:151:ILE:HD12	2.42	0.44
1:D:96:TYR:HA	1:D:114:LYS:O	2.18	0.44
1:E:131:ARG:CG	1:E:131:ARG:NH1	2.73	0.44
1:C:133:MET:HE1	1:C:160:LEU:HD22	2.00	0.44
1:A:41:HIS:CE1	1:C:108:GLU:OE1	2.59	0.44
1:D:95:VAL:HB	1:D:113:VAL:HG22	2.00	0.44
1:C:10:GLN:HA	1:C:11:PRO:HA	1.77	0.44
1:F:141:HIS:CD2	1:F:141:HIS:H	2.36	0.44
1:F:158:GLU:CG	4:F:895:HOH:O	2.54	0.43
1:C:60:LEU:C	1:C:62:ASP:N	2.71	0.43
1:E:58:GLN:HB3	1:E:146:ALA:HB1	2.00	0.43
1:B:1:LEU:HD12	1:B:1:LEU:HA	1.80	0.43
1:F:99:ASN:HA	1:F:100:PRO:HD3	1.87	0.43
1:C:12:PHE:H	1:C:55:MET:HE3	1.83	0.43
1:A:147:VAL:HG12	1:A:151:ILE:CD1	2.42	0.43
1:D:138:LYS:HG3	1:D:139:TRP:H	1.83	0.43
1:D:30:ILE:O	1:D:67:TYR:HA	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:90:PRO:HA	1:D:91:PRO:HD3	1.83	0.43
1:D:118:MET:HE1	1:D:121:ARG:HD2	1.99	0.43
1:C:133:MET:CE	1:C:160:LEU:HD23	2.48	0.43
1:D:23:ILE:HG22	1:D:30:ILE:CD1	2.48	0.43
1:B:118:MET:HE3	1:B:121:ARG:CD	2.38	0.43
1:E:122:LYS:CE	4:E:850:HOH:O	2.65	0.43
1:E:68:TYR:CD1	1:E:68:TYR:N	2.87	0.43
1:F:55:MET:HG2	1:F:150:VAL:HG11	2.00	0.43
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.84	0.43
1:D:125:SER:O	1:D:125:SER:OG	2.36	0.43
1:C:138:LYS:HZ1	1:C:141:HIS:HB3	1.82	0.42
1:C:129:ILE:HG21	1:C:129:ILE:HD13	1.81	0.42
1:F:48:THR:HG22	1:F:51:GLU:HG3	2.01	0.42
1:E:84:TYR:CZ	1:E:88:LEU:HD11	2.54	0.42
1:C:118:MET:HE3	1:C:121:ARG:CD	2.46	0.42
1:E:16:HIS:O	1:E:19:VAL:HG12	2.19	0.42
1:E:42:THR:HG22	1:E:45:ASN:HB2	2.01	0.42
1:F:145:LYS:HE2	4:F:858:HOH:O	2.20	0.42
1:E:1:LEU:HB3	1:E:27:VAL:HG22	2.01	0.42
3:D:703:ATP:O2G	4:D:745:HOH:O	2.21	0.42
1:B:134:LEU:HD13	1:B:164:ALA:HB2	2.00	0.42
1:A:133:MET:HE3	1:A:157:VAL:CG2	2.46	0.42
1:F:103:ARG:HG3	1:F:113:VAL:HG11	2.01	0.42
1:B:135:ASN:OD1	1:B:135:ASN:C	2.58	0.42
1:F:42:THR:HG22	1:F:45:ASN:CA	2.51	0.41
1:D:103:ARG:HG3	1:D:113:VAL:CG1	2.44	0.41
1:E:118:MET:HE3	1:E:121:ARG:CD	2.46	0.41
1:E:1:LEU:N	4:E:909:HOH:O	2.41	0.41
1:A:67:TYR:HE2	4:A:714:HOH:O	2.03	0.41
1:F:42:THR:CG2	1:F:45:ASN:N	2.73	0.41
1:D:132:ARG:HD3	1:D:138:LYS:O	2.20	0.41
1:C:22:LYS:HE2	1:C:117:GLU:OE2	2.20	0.41
1:E:131:ARG:NH2	4:E:849:HOH:O	2.51	0.41
1:B:52:ARG:O	1:B:56:ILE:HG13	2.21	0.41
1:D:134:LEU:HD11	1:D:164:ALA:HB2	2.02	0.41
1:F:42:THR:CG2	1:F:45:ASN:HB2	2.51	0.41
1:B:90:PRO:HA	1:B:91:PRO:HD3	1.94	0.41
1:A:133:MET:HB3	1:A:133:MET:HE2	1.81	0.41
1:F:133:MET:CE	1:F:157:VAL:HA	2.51	0.41
1:E:141:HIS:H	1:E:141:HIS:CD2	2.39	0.41
1:E:38:GLN:NE2	1:E:74:ASP:H	2.04	0.41
1:D:60:LEU:HD22	1:D:65:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:40:SER:OG	1:F:41:HIS:CD2	2.61	0.41
1:E:136:GLY:HA2	4:E:831:HOH:O	2.20	0.41
1:F:73:LYS:HE3	4:F:863:HOH:O	2.20	0.41
1:B:41:HIS:HA	4:B:767:HOH:O	2.21	0.41
1:F:42:THR:HG23	1:F:44:GLU:H	1.86	0.41
1:D:99:ASN:HD21	1:D:101:LEU:HB3	1.86	0.41
1:C:16:HIS:HA	1:C:19:VAL:HG12	2.02	0.41
1:F:9:PHE:O	1:F:11:PRO:HA	2.21	0.41
1:C:131:ARG:NH1	1:C:131:ARG:CG	2.71	0.40
1:C:131:ARG:NH1	4:C:790:HOH:O	2.53	0.40
1:F:10:GLN:OE1	1:F:45:ASN:OD1	2.39	0.40
1:C:55:MET:HG2	1:C:150:VAL:HG11	2.03	0.40
1:C:133:MET:CE	1:C:157:VAL:HA	2.51	0.40
1:D:23:ILE:CG2	1:D:30:ILE:CD1	2.99	0.40
1:D:5:ILE:HG21	1:D:5:ILE:HD13	1.74	0.40
1:C:67:TYR:CD2	1:C:67:TYR:N	2.87	0.40
1:A:158:GLU:HG3	4:A:743:HOH:O	2.21	0.40
1:D:38:GLN:HE22	1:D:74:ASP:N	2.05	0.40
1:B:48:THR:HG23	1:B:50:GLY:N	2.36	0.40
1:C:138:LYS:HZ1	1:C:141:HIS:CG	2.39	0.40
1:A:112:GLU:OE2	1:A:114:LYS:HE3	2.21	0.40
1:A:10:GLN:HG2	1:A:47:PHE:H	1.86	0.40
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.89	0.40
1:B:40:SER:OG	1:B:41:HIS:CD2	2.72	0.40
1:D:141:HIS:CE1	1:D:142:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/168 (96%)	157 (97%)	5 (3%)	0	100	100
1	B	162/168 (96%)	154 (95%)	7 (4%)	1 (1%)	33	24
1	C	162/168 (96%)	155 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	162/168 (96%)	152 (94%)	10 (6%)	0	100	100
1	E	162/168 (96%)	153 (94%)	8 (5%)	1 (1%)	33	24
1	F	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
All	All	972/1008 (96%)	926 (95%)	44 (4%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	35	GLY
1	B	148	VAL

### 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	146/152 (96%)	134 (92%)	12 (8%)	17	10
1	B	146/152 (96%)	135 (92%)	11 (8%)	19	12
1	C	145/152 (95%)	135 (93%)	10 (7%)	22	15
1	D	147/152 (97%)	135 (92%)	12 (8%)	17	10
1	E	147/152 (97%)	134 (91%)	13 (9%)	14	8
1	F	148/152 (97%)	139 (94%)	9 (6%)	26	19
All	All	879/912 (96%)	812 (92%)	67 (8%)	19	12

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	10	GLN
1	A	17	LEU
1	A	27	VAL
1	A	38	GLN
1	A	42	THR
1	A	48	THR
1	A	77	PHE

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Mol	Chain	Res	Type
1	A	83	SER
1	A	121	ARG
1	A	134	LEU
1	A	160	LEU
1	B	6	ILE
1	B	10	GLN
1	B	11	PRO
1	B	17	LEU
1	B	27	VAL
1	B	38	GLN
1	B	42	THR
1	B	77	PHE
1	B	121	ARG
1	B	125	SER
1	B	144	PRO
1	C	1	LEU
1	C	10	GLN
1	C	17	LEU
1	C	27	VAL
1	C	38	GLN
1	C	42	THR
1	C	48	THR
1	C	77	PHE
1	C	121	ARG
1	C	125	SER
1	D	1	LEU
1	D	10	GLN
1	D	11	PRO
1	D	17	LEU
1	D	27	VAL
1	D	38	GLN
1	D	42	THR
1	D	48	THR
1	D	62	ASP
1	D	77	PHE
1	D	121	ARG
1	D	125	SER
1	E	1	LEU
1	E	10	GLN
1	E	17	LEU
1	E	27	VAL
1	E	38	GLN

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Mol	Chain	Res	Type
1	E	42	THR
1	E	48	THR
1	E	77	PHE
1	E	83	SER
1	E	100	PRO
1	E	121	ARG
1	E	125	SER
1	E	152	LYS
1	F	17	LEU
1	F	27	VAL
1	F	38	GLN
1	F	42	THR
1	F	48	THR
1	F	65	LEU
1	F	77	PHE
1	F	87	SER
1	F	121	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	41	HIS
1	A	99	ASN
1	B	38	GLN
1	B	41	HIS
1	B	99	ASN
1	B	141	HIS
1	C	38	GLN
1	C	41	HIS
1	C	99	ASN
1	C	141	HIS
1	D	38	GLN
1	D	41	HIS
1	D	99	ASN
1	D	141	HIS
1	E	38	GLN
1	E	41	HIS
1	E	99	ASN
1	E	135	ASN
1	E	141	HIS
1	F	38	GLN

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Mol	Chain	Res	Type
1	F	41	HIS
1	F	99	ASN
1	F	141	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z  > 2$
3	ATP	A	700	2	33,33,33	1.43	8 (24%)	52,52,52	2.13	10 (19%)
3	ATP	B	701	-	33,33,33	1.25	5 (15%)	52,52,52	1.95	8 (15%)
3	ATP	C	702	2	33,33,33	1.32	6 (18%)	52,52,52	1.95	11 (21%)
3	ATP	D	703	2	33,33,33	1.27	2 (6%)	52,52,52	2.61	9 (17%)
3	ATP	E	704	2	33,33,33	1.42	6 (18%)	52,52,52	2.99	17 (32%)
3	ATP	F	705	2	33,33,33	1.42	5 (15%)	52,52,52	1.82	13 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	700	2	-	0/22/38/38	0/1/3/3
3	ATP	B	701	-	-	0/22/38/38	0/1/3/3
3	ATP	C	702	2	-	0/22/38/38	0/1/3/3
3	ATP	D	703	2	-	0/22/38/38	0/1/3/3
3	ATP	E	704	2	1/1/7/7	0/22/38/38	0/1/3/3
3	ATP	F	705	2	-	0/22/38/38	0/1/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	705	ATP	PG-O2G	-3.41	1.42	1.54
3	E	704	ATP	C2-N1	3.06	1.39	1.33
3	D	703	ATP	C8-N7	-2.91	1.28	1.34
3	F	705	ATP	C2-N1	2.85	1.39	1.33
3	C	702	ATP	C8-N7	-2.76	1.29	1.34
3	A	700	ATP	C2'-C3'	2.74	1.61	1.53
3	C	702	ATP	C2-N1	2.67	1.39	1.33
3	F	705	ATP	C8-N7	-2.66	1.29	1.34
3	B	701	ATP	PG-O2G	-2.64	1.45	1.54
3	A	700	ATP	O4'-C1'	-2.63	1.37	1.41
3	A	700	ATP	C8-N7	-2.53	1.29	1.34
3	B	701	ATP	C8-N7	-2.51	1.29	1.34
3	E	704	ATP	C8-N7	-2.49	1.29	1.34
3	E	704	ATP	C5-N7	-2.47	1.31	1.40
3	E	704	ATP	O2'-C2'	2.44	1.48	1.43
3	E	704	ATP	PG-O2G	-2.40	1.45	1.54
3	C	702	ATP	C5-N7	-2.35	1.31	1.40
3	A	700	ATP	PG-O2G	-2.32	1.46	1.54
3	D	703	ATP	C5-N7	-2.31	1.31	1.40
3	C	702	ATP	PG-O2G	-2.30	1.46	1.54
3	A	700	ATP	C1'-N9	-2.20	1.41	1.48
3	F	705	ATP	PB-O1B	-2.20	1.43	1.51
3	A	700	ATP	C4-N9	2.19	1.40	1.37
3	A	700	ATP	PA-O2A	-2.18	1.45	1.55
3	B	701	ATP	PB-O3A	-2.17	1.55	1.59
3	A	700	ATP	C5-N7	-2.16	1.32	1.40
3	F	705	ATP	C5-N7	-2.14	1.32	1.40
3	E	704	ATP	C1'-N9	-2.11	1.42	1.48
3	B	701	ATP	C5-N7	-2.09	1.32	1.40
3	B	701	ATP	PB-O2B	-2.07	1.45	1.55
3	C	702	ATP	C4-N9	2.07	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	ATP	PG-O3B	-2.05	1.56	1.60

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	ATP	O4'-C1'-N9	11.36	119.00	108.44
3	E	704	ATP	C8-N9-C4	-10.20	99.12	106.90
3	E	704	ATP	O4'-C1'-N9	10.18	117.91	108.44
3	D	703	ATP	C8-N9-C4	-9.76	99.45	106.90
3	B	701	ATP	C8-N9-C4	-8.54	100.38	106.90
3	C	702	ATP	O4'-C1'-N9	7.64	115.55	108.44
3	E	704	ATP	C2'-C1'-N9	7.56	132.67	113.27
3	A	700	ATP	O4'-C1'-N9	7.26	115.19	108.44
3	C	702	ATP	C8-N9-C4	-7.18	101.42	106.90
3	D	703	ATP	PA-O3A-PB	6.84	151.75	131.68
3	F	705	ATP	C8-N9-C4	-6.75	101.75	106.90
3	A	700	ATP	C8-N9-C4	-6.09	102.25	106.90
3	E	704	ATP	C4-C5-N7	6.02	114.68	109.52
3	B	701	ATP	O4'-C1'-N9	5.70	113.74	108.44
3	A	700	ATP	C2'-C1'-N9	5.69	127.87	113.27
3	E	704	ATP	PA-O3A-PB	5.55	147.95	131.68
3	F	705	ATP	O4'-C1'-N9	5.23	113.31	108.44
3	A	700	ATP	C4'-O4'-C1'	-5.17	104.14	109.75
3	E	704	ATP	C1'-N9-C4	5.03	135.33	126.64
3	B	701	ATP	PA-O3A-PB	4.24	144.12	131.68
3	B	701	ATP	C5-C6-N6	3.77	129.24	120.72
3	E	704	ATP	N3-C4-N9	3.53	131.81	125.43
3	A	700	ATP	C2'-C3'-C4'	-3.47	95.73	102.65
3	E	704	ATP	O2'-C2'-C3'	-3.41	100.74	111.83
3	C	702	ATP	C8-N9-C1'	3.35	132.98	126.38
3	A	700	ATP	O2'-C2'-C3'	-3.20	101.42	111.83
3	C	702	ATP	O3G-PG-O1G	-3.16	100.13	110.44
3	D	703	ATP	PB-O3B-PG	3.15	140.93	131.68
3	A	700	ATP	C4-C5-N7	3.14	112.22	109.52
3	D	703	ATP	C4-C5-N7	3.10	112.18	109.52
3	C	702	ATP	PA-O3A-PB	3.03	140.56	131.68
3	F	705	ATP	O2'-C2'-C3'	-3.00	102.08	111.83
3	C	702	ATP	PB-O3B-PG	2.88	140.13	131.68
3	E	704	ATP	PB-O3B-PG	2.88	140.12	131.68
3	A	700	ATP	C8-N9-C1'	2.87	132.04	126.38
3	F	705	ATP	C5-C6-N6	2.87	127.20	120.72
3	B	701	ATP	C8-N9-C1'	2.82	131.94	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	ATP	O4'-C1'-C2'	2.73	110.95	106.77
3	F	705	ATP	C5'-C4'-C3'	-2.68	104.48	115.21
3	E	704	ATP	C6-C5-C4	2.58	121.99	117.25
3	B	701	ATP	C2'-C1'-N9	2.58	119.89	113.27
3	C	702	ATP	O3A-PB-O3B	2.54	106.83	101.66
3	A	700	ATP	O2B-PB-O3B	2.51	117.05	105.14
3	F	705	ATP	C4'-O4'-C1'	2.50	112.47	109.75
3	E	704	ATP	O3A-PA-O5'	-2.50	92.23	103.41
3	F	705	ATP	O3G-PG-O2G	2.46	117.17	107.61
3	F	705	ATP	N6-C6-N1	-2.43	114.59	119.36
3	C	702	ATP	C4-C5-N7	2.33	111.52	109.52
3	D	703	ATP	O2G-PG-O3B	2.30	116.05	105.14
3	F	705	ATP	C8-N9-C1'	2.29	130.90	126.38
3	F	705	ATP	PA-O3A-PB	2.29	138.40	131.68
3	E	704	ATP	O2G-PG-O3B	2.29	115.98	105.14
3	B	701	ATP	N6-C6-N1	-2.28	114.90	119.36
3	D	703	ATP	C2'-C1'-N9	2.27	119.10	113.27
3	E	704	ATP	C4'-O4'-C1'	-2.20	107.36	109.75
3	C	702	ATP	O2'-C2'-C1'	-2.18	104.63	111.23
3	C	702	ATP	O2G-PG-O3B	2.18	115.48	105.14
3	E	704	ATP	C6-C5-N7	-2.16	123.10	131.34
3	D	703	ATP	C6-C5-C4	2.14	121.18	117.25
3	B	701	ATP	N3-C2-N1	2.13	130.49	128.71
3	F	705	ATP	O3'-C3'-C4'	-2.11	104.85	111.08
3	F	705	ATP	C4-C5-N7	2.11	111.33	109.52
3	E	704	ATP	N6-C6-N1	2.10	123.48	119.36
3	C	702	ATP	C2'-C3'-C4'	-2.08	98.50	102.65
3	E	704	ATP	N7-C8-N9	2.08	120.24	114.36
3	F	705	ATP	O2G-PG-O3B	2.04	114.81	105.14
3	D	703	ATP	C8-N9-C1'	2.01	130.34	126.38
3	E	704	ATP	O5'-PA-O1A	2.01	117.24	109.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	704	ATP	C1'

There are no torsion outliers.

There are no ring outliers.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.