Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:07 PM GMT

PDB ID	:	1NKS
Title	:	ADENYLATE KINASE FROM SULFOLOBUS ACIDOCALDARIUS
Authors	:	Vonrhein, 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

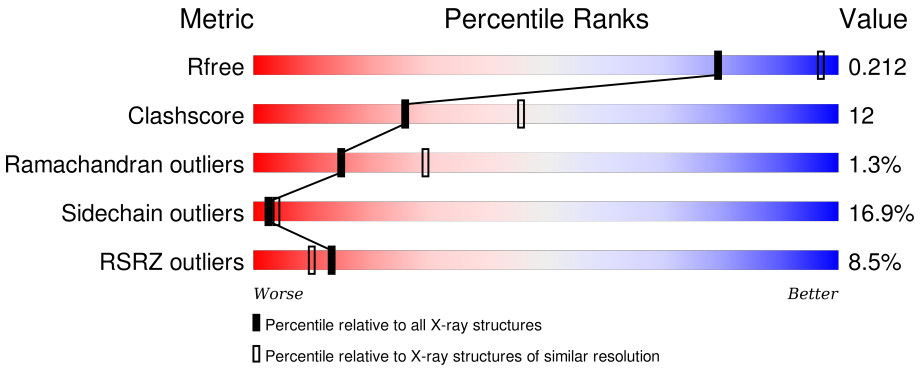
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	11% 67% 23% 9%
1	B	194	7% 64% 26% 8%
1	C	194	11% 71% 25%
1	D	194	6% 70% 24% 6%
1	E	194	9% 56% 34% 7%

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Mol	Chain	Length	Quality of chain
1	F	194	

2 Entry composition

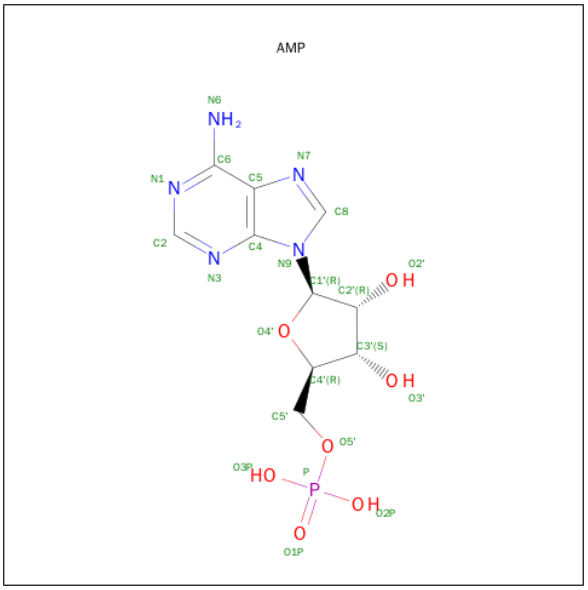
There are 4 unique types of molecules in this entry. The entry contains 9332 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

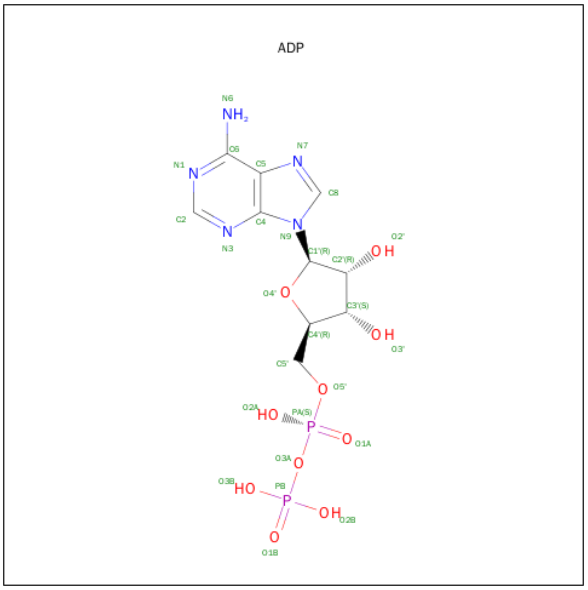
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	B	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	C	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	D	194	Total	C	N	O	S	0	0	0
			1484	939	256	285	4			
1	E	194	Total	C	N	O	S	0	0	0
			1484	939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

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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 (three-letter code: 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		

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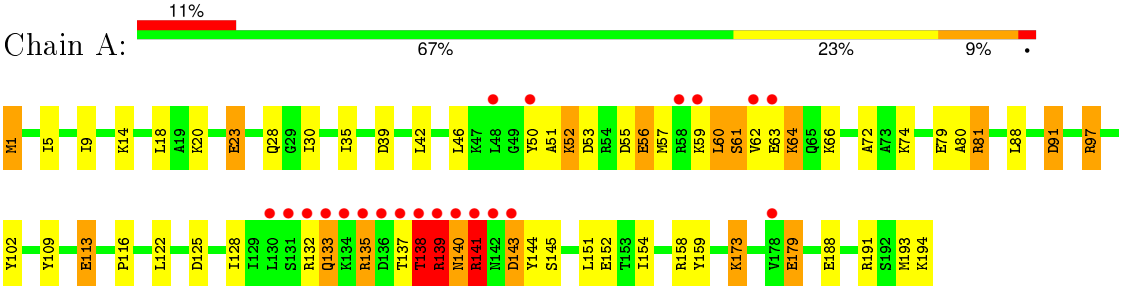
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	52	Total O 52 52	0	0

3 Residue-property plots (i)

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

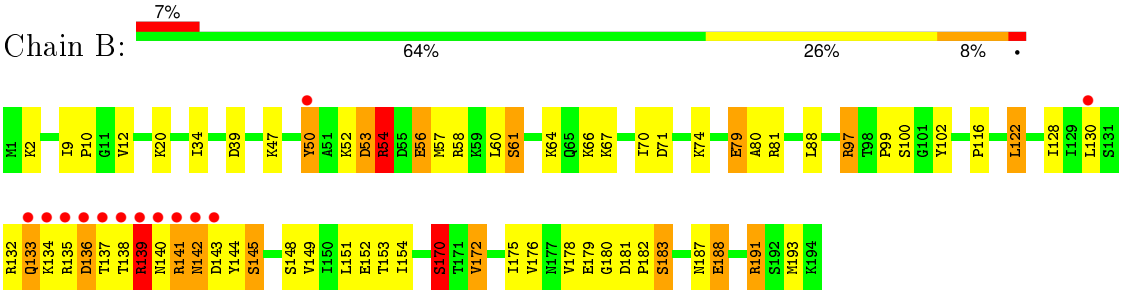
- Molecule 1: ADENYLATE KINASE

Chain A:



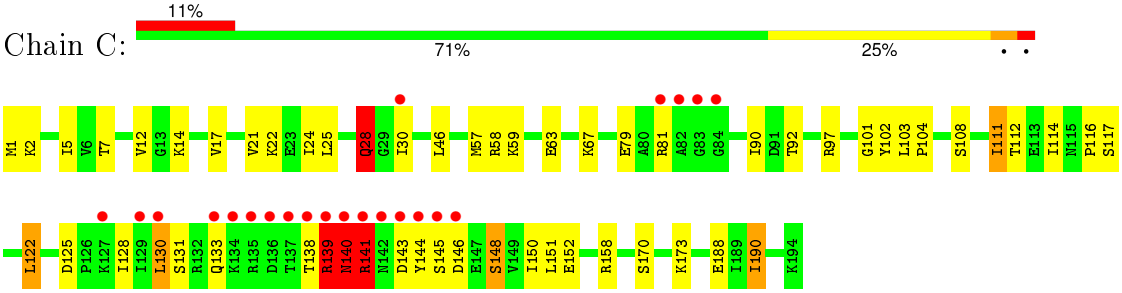
- Molecule 1: ADENYLATE KINASE

Chain B:



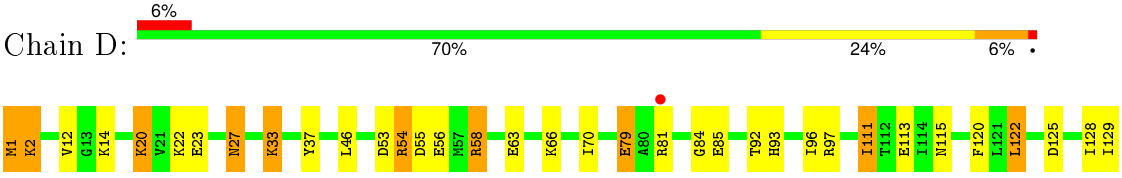
- Molecule 1: ADENYLATE KINASE

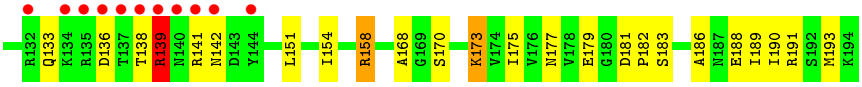
Chain C:



- Molecule 1: ADENYLATE KINASE

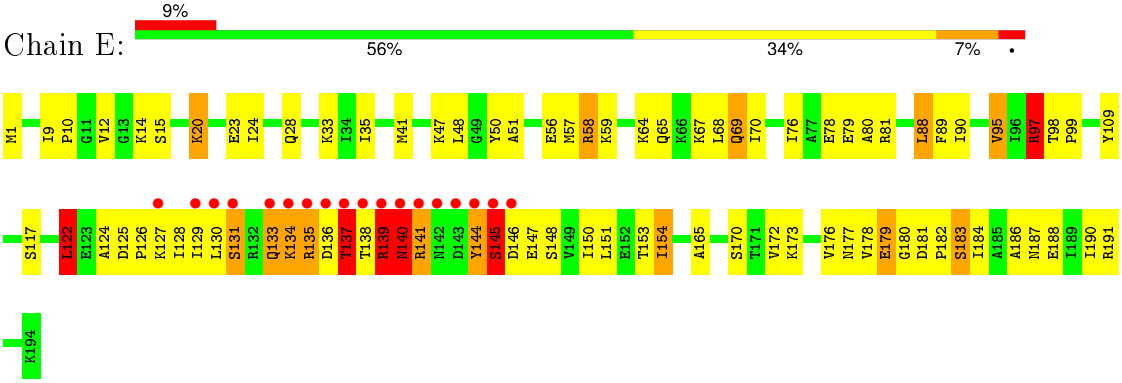
Chain D:





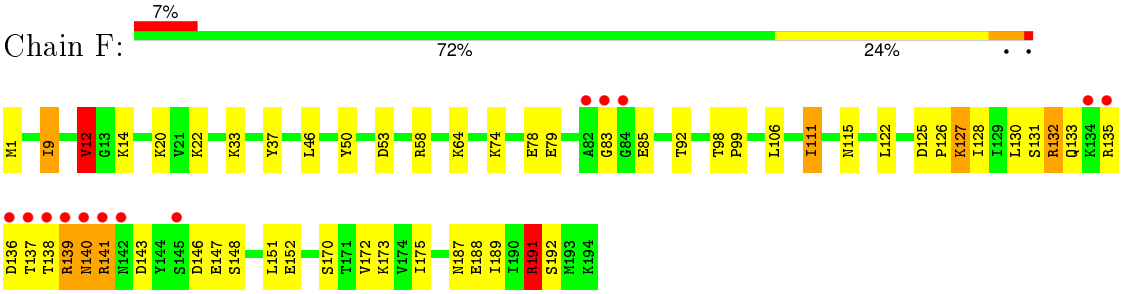
• Molecule 1: ADENYLATE KINASE

Chain E:



• Molecule 1: ADENYLATE KINASE

Chain F:



4 Data and refinement statistics (i)

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 39.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-2.57) 86.5 (39.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.218 0.162 , 0.212	Depositor DCC
R_{free} test set	1129 reflections (2.10%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 56027 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.84	1/1502 (0.1%)	1.86	31/2026 (1.5%)
1	B	0.68	0/1502	1.41	15/2026 (0.7%)
1	C	0.65	0/1502	1.30	6/2026 (0.3%)
1	D	0.66	0/1502	1.28	10/2026 (0.5%)
1	E	0.78	1/1502 (0.1%)	1.51	15/2026 (0.7%)
1	F	0.64	0/1502	1.32	9/2026 (0.4%)
All	All	0.71	2/9012 (0.0%)	1.46	86/12156 (0.7%)

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	2
1	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	THR	C-N	-14.57	1.00	1.34
1	E	137	THR	C-N	-11.62	1.07	1.34

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	ARG	CD-NE-CZ	31.63	167.88	123.60
1	A	138	THR	C-N-CA	16.82	163.75	121.70
1	A	138	THR	O-C-N	-16.07	96.98	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ARG	NE-CZ-NH1	15.07	127.83	120.30
1	A	139	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	A	139	ARG	CD-NE-CZ	13.87	143.02	123.60
1	E	137	THR	C-N-CA	12.62	153.25	121.70
1	E	137	THR	O-C-N	-12.40	102.85	122.70
1	A	140	ASN	N-CA-CB	12.00	132.19	110.60
1	B	191	ARG	NE-CZ-NH1	10.89	125.74	120.30
1	A	138	THR	CA-C-N	10.77	140.90	117.20
1	A	158	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	E	81	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	E	58	ARG	CD-NE-CZ	10.50	138.30	123.60
1	E	137	THR	CA-C-N	10.24	139.73	117.20
1	A	191	ARG	CD-NE-CZ	9.70	137.18	123.60
1	E	81	ARG	CD-NE-CZ	9.62	137.07	123.60
1	B	81	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	F	191	ARG	CD-NE-CZ	9.26	136.57	123.60
1	A	138	THR	CB-CA-C	9.21	136.46	111.60
1	D	158	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	D	58	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	139	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	C	139	ARG	CD-NE-CZ	8.75	135.84	123.60
1	F	191	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	F	132	ARG	CD-NE-CZ	8.46	135.45	123.60
1	A	39	ASP	CB-CG-OD1	-8.08	111.02	118.30
1	A	191	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	159	TYR	CB-CG-CD2	-7.92	116.25	121.00
1	D	54	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	97	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	141	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	139	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	F	58	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	F	58	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	E	97	ARG	CD-NE-CZ	7.13	133.58	123.60
1	A	97	ARG	CD-NE-CZ	6.82	133.15	123.60
1	E	50	TYR	CA-CB-CG	6.75	126.23	113.40
1	E	137	THR	CB-CA-C	6.73	129.78	111.60
1	E	81	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	97	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	97	ARG	N-CA-CB	6.42	122.16	110.60
1	B	81	ARG	CD-NE-CZ	6.37	132.52	123.60
1	E	23	GLU	CA-CB-CG	6.21	127.07	113.40
1	F	12	VAL	CB-CA-C	-6.20	99.62	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	132	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	14	LYS	CA-CB-CG	6.12	126.87	113.40
1	B	188	GLU	CA-CB-CG	6.07	126.75	113.40
1	F	191	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	57	MET	CA-CB-CG	5.97	123.44	113.30
1	D	27	ASN	CA-CB-CG	5.90	126.38	113.40
1	E	122	LEU	CA-CB-CG	5.87	128.79	115.30
1	E	57	MET	CA-CB-CG	5.85	123.25	113.30
1	A	79	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	139	ARG	CA-C-N	5.84	130.05	117.20
1	C	188	GLU	CA-CB-CG	5.76	126.07	113.40
1	C	158	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	139	ARG	C-N-CA	5.72	136.01	121.70
1	E	144	TYR	CB-CG-CD1	5.71	124.42	121.00
1	A	109	TYR	CB-CG-CD2	5.63	124.38	121.00
1	D	97	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	141	ARG	CG-CD-NE	5.57	123.49	111.80
1	D	97	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	188	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	B	191	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	140	ASN	CA-C-N	-5.47	105.18	117.20
1	B	176	VAL	CB-CA-C	-5.44	101.07	111.40
1	A	39	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	170	SER	N-CA-CB	-5.35	102.47	110.50
1	A	72	ALA	CB-CA-C	5.35	118.12	110.10
1	D	58	ARG	CD-NE-CZ	5.35	131.09	123.60
1	E	95	VAL	CB-CA-C	-5.29	101.35	111.40
1	D	56	GLU	CA-CB-CG	5.29	125.03	113.40
1	C	28	GLN	N-CA-CB	5.28	120.10	110.60
1	F	143	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	54	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	81	ARG	CA-CB-CG	5.21	124.87	113.40
1	A	179	GLU	N-CA-CB	-5.19	101.25	110.60
1	B	172	VAL	CB-CA-C	-5.19	101.55	111.40
1	D	12	VAL	N-CA-CB	5.18	122.90	111.50
1	A	81	ARG	CD-NE-CZ	5.15	130.81	123.60
1	B	79	GLU	CA-CB-CG	5.11	124.64	113.40
1	A	139	ARG	O-C-N	-5.07	114.58	122.70
1	A	193	MET	CG-SD-CE	5.07	108.31	100.20
1	B	71	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	50	TYR	CA-CB-CG	5.04	122.97	113.40

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	46	0
1	B	1484	0	1549	39	0
1	C	1484	0	1549	27	0
1	D	1484	0	1549	34	0
1	E	1484	0	1548	60	0
1	F	1484	0	1549	24	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
4	E	67	0	0	10	0
4	F	52	0	0	4	0
All	All	9332	0	9340	227	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 12.

All (227) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:137:THR:C	1:E:140:ASN:HB3	2.04	0.77
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:HG3	1:C:139:ARG:HH11	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: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:HB3	1:A:135:ARG:HH11	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
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: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:NH1	1:A:135:ARG:HB3	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:HG2	1:F:191:ARG:HH11	1.66	0.60
1:E:9:ILE:HD13	1:E:154:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:137:THR:O	1:E:140:ASN:CB	2.26	0.59
1:A:5:ILE:HD12	1:A:116:PRO:HG3	1.83	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:137:THR:HG23	1:B:140:ASN:CB	2.34	0.57
1:B:135:ARG:HB3	4:B:237:HOH:O	2.04	0.57
1:E:181:ASP:OD1	1:E:183:SER:HB2	2.05	0.56
1:C:139:ARG:O	1:C:140:ASN:HB2	2.05	0.56
1:D:125:ASP:HB3	1:D:128:ILE:HD12	1.87	0.56
1:C:144:TYR:HD2	1:C:150:ILE:HG13	1.70	0.56
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
1:E:12:VAL:O	1:E:177:ASN:ND2	2.37	0.55
1:D:58:ARG:NH1	4:D:207:HOH:O	2.40	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:F:128:ILE:O	1:F:132:ARG:HG3	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:147:GLU:HA	1:E:150:ILE:HD12	1.91	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: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:F:50:TYR:CZ	1:F:64:LYS:HD3	2.45	0.52
1:C:24:ILE:O	1:C:28:GLN:HG3	2.09	0.52
1:A:137:THR:HG22	1:A:137:THR:O	2.10	0.51
1:F:152:GLU:HG3	4:F:230:HOH:O	2.09	0.51
1:D:2:LYS:HE3	1:D:193:MET:O	2.09	0.51
1:B:181:ASP:OD1	1:B:183:SER:HB2	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
1:B:144:TYR:HD1	1:B:149:VAL:CG1	2.23	0.50
1:F:175:ILE:HD12	1:F:189:ILE:HG12	1.92	0.50
1:E:14:LYS:HG3	1:E:122:LEU:HD23	1.93	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:F:139:ARG:HG2	1:F:141:ARG:NH2	2.26	0.49
1:D:188:GLU:OE2	1:D:191:ARG:NH1	2.45	0.49
1:D:63:GLU:HG2	4:D:216:HOH:O	2.11	0.49
1:D:154:ILE:O	1:D:158:ARG:HG3	2.13	0.49
1:B:53:ASP:OD1	1:B:56:GLU:HB2	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:E:97:ARG:HD2	1:E:144:TYR:HE1	1.78	0.48
1:D:129:ILE:O	1:D:133:GLN:HG3	2.14	0.48
1:D:33:LYS:NZ	1:D:79:GLU:HG3	2.29	0.48
1:E:76:ILE:HG21	1:E:90:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:VAL:CG2	1:E:184:ILE:HG21	2.42	0.48
1:E:141:ARG:HB2	1:E:141:ARG:NH1	2.29	0.48
1:E:141:ARG:HH11	1:E:141:ARG:HB2	1.78	0.47
1:F:127:LYS:HG3	1:F:147:GLU:OE2	2.14	0.47
1:E:98:THR:CB	1:E:99:PRO:CD	2.91	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: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:B:187:ASN:HB3	1:B:191:ARG:NH2	2.30	0.47
1:A:20:LYS:HE2	1:A:23:GLU:OE2	2.15	0.47
1:F:98:THR:HB	1:F:99:PRO:CD	2.45	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:D:133:GLN:HE22	1:D:141:ARG:CG	2.29	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:33:LYS:HZ1	1:D:79:GLU:HG3	1.81	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: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:145:SER:HB2	1:E:146:ASP:H	1.64	0.45
1:E:126:PRO:HG2	1:E:151:LEU:HD21	1.99	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:E:165:ALA:HB1	1:E:170:SER:O	2.17	0.45
1:D:81:ARG:NH1	4:D:242:HOH:O	2.50	0.45
1:D:2:LYS:HE2	4:D:223:HOH:O	2.17	0.45
1:B:61:SER:OG	1:B:64:LYS:HG3	2.17	0.45
1:E:10:PRO:HD3	4:E:226:HOH:O	2.15	0.45
1:D:181:ASP:HA	1:D:182:PRO:HD2	1.85	0.45
1:A:141:ARG:HB3	4:A:237:HOH:O	2.17	0.44
1:A:42:LEU:O	1:A:42:LEU:HD12	2.17	0.44
1:A:141:ARG:HG3	4:A:233:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:122:LEU:HD12	1:B:122:LEU:HA	1.82	0.44
1:B:34:ILE:HD13	1:B:34:ILE:HG21	1.79	0.44
1:F:146:ASP:OD2	1:F:148:SER:HB2	2.18	0.44
1:D:54:ARG:HD2	4:D:240:HOH:O	2.18	0.44
1:C:140:ASN:O	1:C:141:ARG:CB	2.52	0.43
1:B:57:MET:O	1:B:60:LEU:HB2	2.18	0.43
4:E:257:HOH:O	1:F:191:ARG:HB3	2.18	0.43
1:B:122:LEU:HD12	1:B:175:ILE:HB	2.00	0.43
1:A:1:MET:HE2	1:A:80:ALA:HA	2.01	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:B:137:THR:O	1:B:137:THR:HG22	2.18	0.43
1:A:46:LEU:HD23	1:A:52:LYS:HA	1.99	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
1:E:98:THR:HB	1:E:99:PRO:HD3	2.02	0.42
1:D:122:LEU:HD12	1:D:177:ASN:HB2	2.01	0.42
1:A:139:ARG:HD2	1:A:139:ARG:HA	1.80	0.42
1:E:12:VAL:HG13	1:E:124:ALA:HB2	2.01	0.42
1:C:130:LEU:HA	1:C:130:LEU:HD23	1.91	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:D:120:PHE:CD2	1:D:175:ILE:HD12	2.55	0.42
1:F:136:ASP:OD1	1:F:138:THR:HG22	2.19	0.42
1:A:74:LYS:HG3	1:A:113:GLU:HG3	2.01	0.42
1:B:130:LEU:O	1:B:133:GLN:HB2	2.20	0.42
1:A:145:SER:HB2	4:A:223:HOH:O	2.19	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:D:96:ILE:N	1:D:96:ILE:HD12	2.35	0.41
1:B:102:TYR:OH	1:B:152:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:THR:O	1:E:139:ARG:CB	2.63	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: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:E:181:ASP:HA	1:E:182:PRO:HD3	1.87	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:C:22:LYS:NZ	4:C:223:HOH:O	2.53	0.41
1:A:66:LYS:NZ	4:A:229:HOH:O	2.36	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:A:46:LEU:CD2	1:A:52:LYS:HA	2.51	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 (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	192/194 (99%)	178 (93%)	12 (6%)	2 (1%)	19 38
1	B	192/194 (99%)	181 (94%)	6 (3%)	5 (3%)	7 11
1	C	192/194 (99%)	181 (94%)	9 (5%)	2 (1%)	19 38
1	D	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	34 58
1	E	192/194 (99%)	181 (94%)	7 (4%)	4 (2%)	9 16
1	F	192/194 (99%)	186 (97%)	5 (3%)	1 (0%)	34 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1152/1164 (99%)	1088 (94%)	49 (4%)	15 (1%)	15 29

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/160 (100%)	130 (81%)	30 (19%)	2 3
1	B	160/160 (100%)	134 (84%)	26 (16%)	3 4
1	C	160/160 (100%)	133 (83%)	27 (17%)	2 4
1	D	160/160 (100%)	141 (88%)	19 (12%)	6 11
1	E	160/160 (100%)	128 (80%)	32 (20%)	1 2
1	F	160/160 (100%)	132 (82%)	28 (18%)	2 3
All	All	960/960 (100%)	798 (83%)	162 (17%)	2 4

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	LYS
1	A	23	GLU
1	A	30	ILE
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	81	ARG
1	A	91	ASP
1	A	113	GLU
1	A	122	LEU
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	52	LYS
1	B	53	ASP
1	B	54	ARG
1	B	56	GLU
1	B	61	SER
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	133	GLN

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Mol	Chain	Res	Type
1	B	134	LYS
1	B	136	ASP
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	151	LEU
1	B	170	SER
1	B	172	VAL
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	58	ARG
1	C	59	LYS
1	C	63	GLU
1	C	67	LYS
1	C	79	GLU
1	C	81	ARG
1	C	111	ILE
1	C	117	SER
1	C	122	LEU
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	170	SER
1	C	190	ILE
1	D	1	MET
1	D	2	LYS

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Mol	Chain	Res	Type
1	D	20	LYS
1	D	22	LYS
1	D	23	GLU
1	D	33	LYS
1	D	46	LEU
1	D	53	ASP
1	D	55	ASP
1	D	79	GLU
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	15	SER
1	E	20	LYS
1	E	41	MET
1	E	58	ARG
1	E	59	LYS
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
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

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Mol	Chain	Res	Type
1	E	145	SER
1	E	148	SER
1	E	154	ILE
1	E	172	VAL
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	46	LEU
1	F	53	ASP
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
1	F	141	ARG
1	F	151	LEU
1	F	170	SER
1	F	172	VAL
1	F	188	GLU
1	F	191	ARG

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

Mol	Chain	Res	Type
1	A	28	GLN
1	A	140	ASN
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	133	GLN
1	B	140	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	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	C	195	-	20,25,25	1.47	5 (25%)	22,38,38	2.08	9 (40%)
2	AMP	D	195	-	20,25,25	1.53	3 (15%)	22,38,38	2.07	8 (36%)
2	AMP	F	195	-	20,25,25	1.37	3 (15%)	22,38,38	2.12	8 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ADP	F	196	-	22,29,29	1.09	3 (13%)	27,45,45	2.59	2 (7%)

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	C	195	-	-	0/6/26/26	0/3/3/3
2	AMP	D	195	-	-	0/6/26/26	0/3/3/3
2	AMP	F	195	-	-	0/6/26/26	0/3/3/3
3	ADP	F	196	-	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	195	AMP	P-O5'	-3.13	1.49	1.60
2	D	195	AMP	C8-N7	-3.03	1.28	1.34
2	D	195	AMP	P-O5'	-2.83	1.50	1.60
2	C	195	AMP	C8-N7	-2.58	1.29	1.34
2	C	195	AMP	C2'-C3'	-2.46	1.46	1.53
2	C	195	AMP	P-O5'	-2.42	1.52	1.60
2	C	195	AMP	P-O2P	-2.40	1.46	1.54
2	D	195	AMP	C2'-C3'	-2.36	1.47	1.53
3	F	196	ADP	C5-N7	-2.31	1.31	1.39
2	F	195	AMP	P-O1P	-2.08	1.44	1.51
2	F	195	AMP	C8-N7	-2.04	1.30	1.34
3	F	196	ADP	O4'-C1'	2.15	1.43	1.41
2	C	195	AMP	P-O3P	2.19	1.62	1.54
3	F	196	ADP	PB-O2B	2.30	1.63	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	196	ADP	N3-C2-N1	-12.06	119.66	128.89
2	F	195	AMP	C4'-O4'-C1'	-4.95	104.28	109.72
2	C	195	AMP	C4'-O4'-C1'	-4.57	104.70	109.72
2	D	195	AMP	C4'-O4'-C1'	-3.78	105.57	109.72
3	F	196	ADP	C4-C5-N7	-3.24	106.50	109.48
2	F	195	AMP	C4-C5-N7	-3.20	106.53	109.48
2	D	195	AMP	O3P-P-O5'	-2.71	98.77	106.56
2	C	195	AMP	O3P-P-O2P	-2.64	97.31	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	195	AMP	C4-C5-N7	-2.38	107.29	109.48
2	F	195	AMP	O3P-P-O5'	-2.31	99.92	106.56
2	C	195	AMP	C4-C5-N7	-2.31	107.36	109.48
2	F	195	AMP	O2P-P-O1P	2.09	117.31	110.58
2	D	195	AMP	C2-N1-C6	2.10	122.51	118.77
2	C	195	AMP	C2'-C1'-N9	2.11	117.51	114.29
2	D	195	AMP	O2P-P-O1P	2.16	117.55	110.58
2	C	195	AMP	O4'-C1'-N9	2.47	113.28	108.10
2	F	195	AMP	O3P-P-O1P	2.48	118.56	110.58
2	C	195	AMP	O5'-C5'-C4'	2.52	118.40	109.12
2	C	195	AMP	N3-C2-N1	2.55	130.85	128.89
2	D	195	AMP	O3P-P-O1P	2.83	119.68	110.58
2	C	195	AMP	O3'-C3'-C4'	2.86	119.64	111.05
2	F	195	AMP	C2-N1-C6	2.99	124.11	118.77
2	D	195	AMP	C2'-C1'-N9	3.28	119.30	114.29
2	F	195	AMP	O4'-C1'-N9	3.30	115.00	108.10
2	F	195	AMP	C2'-C1'-N9	3.94	120.32	114.29
2	C	195	AMP	O2P-P-O1P	4.79	125.99	110.58
2	D	195	AMP	O4'-C1'-N9	4.83	118.21	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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%)	0.33	21 (10%) 8 5	26, 53, 134, 188	0
1	B	194/194 (100%)	0.11	13 (6%) 21 17	26, 50, 134, 188	0
1	C	194/194 (100%)	0.37	22 (11%) 7 5	28, 59, 134, 182	0
1	D	194/194 (100%)	0.19	12 (6%) 24 20	27, 57, 133, 182	0
1	E	194/194 (100%)	0.56	18 (9%) 11 8	26, 50, 135, 189	0
1	F	194/194 (100%)	0.02	13 (6%) 21 17	27, 56, 112, 132	0
All	All	1164/1164 (100%)	0.26	99 (8%) 13 10	26, 54, 130, 189	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	139	ARG	12.9
1	E	138	THR	11.7
1	A	138	THR	11.7
1	E	137	THR	10.3
1	E	142	ASN	10.2
1	E	140	ASN	9.7
1	C	138	THR	9.4
1	A	139	ARG	8.9
1	A	137	THR	8.6
1	A	141	ARG	8.4
1	A	142	ASN	8.1
1	D	139	ARG	8.0
1	C	137	THR	7.9
1	B	137	THR	7.6
1	A	140	ASN	7.5
1	E	134	LYS	7.4
1	B	136	ASP	7.2
1	B	138	THR	7.1
1	D	138	THR	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	140	ASN	6.8
1	E	141	ARG	6.5
1	A	135	ARG	6.3
1	E	144	TYR	6.2
1	F	137	THR	6.2
1	C	142	ASN	6.2
1	B	139	ARG	6.1
1	E	136	ASP	6.1
1	E	143	ASP	6.0
1	C	135	ARG	5.6
1	C	133	GLN	5.5
1	E	133	GLN	5.4
1	D	137	THR	5.4
1	A	136	ASP	5.2
1	B	140	ASN	5.0
1	C	145	SER	5.0
1	D	135	ARG	5.0
1	C	136	ASP	4.9
1	B	135	ARG	4.8
1	C	134	LYS	4.8
1	E	130	LEU	4.7
1	E	135	ARG	4.6
1	C	141	ARG	4.6
1	E	145	SER	4.6
1	F	82	ALA	4.5
1	E	131	SER	4.4
1	D	140	ASN	4.4
1	B	134	LYS	4.3
1	C	130	LEU	4.1
1	D	136	ASP	4.1
1	F	142	ASN	4.1
1	C	139	ARG	4.0
1	F	134	LYS	4.0
1	C	144	TYR	3.9
1	C	143	ASP	3.9
1	B	141	ARG	3.9
1	A	132	ARG	3.8
1	C	84	GLY	3.7
1	C	83	GLY	3.6
1	B	142	ASN	3.5
1	F	138	THR	3.5
1	F	139	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	142	ASN	3.4
1	D	141	ARG	3.3
1	C	30	ILE	3.2
1	F	141	ARG	3.2
1	E	146	ASP	3.0
1	F	135	ARG	3.0
1	D	132	ARG	3.0
1	D	81	ARG	3.0
1	A	134	LYS	3.0
1	F	136	ASP	2.9
1	F	83	GLY	2.9
1	F	140	ASN	2.8
1	D	134	LYS	2.8
1	A	143	ASP	2.8
1	C	82	ALA	2.8
1	B	130	LEU	2.7
1	A	59	LYS	2.7
1	B	133	GLN	2.6
1	C	81	ARG	2.6
1	C	129	ILE	2.6
1	A	130	LEU	2.5
1	B	50	TYR	2.5
1	B	143	ASP	2.5
1	A	58	ARG	2.5
1	F	84	GLY	2.5
1	C	127	LYS	2.4
1	A	131	SER	2.4
1	F	145	SER	2.4
1	A	178	VAL	2.4
1	D	144	TYR	2.3
1	E	127	LYS	2.3
1	A	50	TYR	2.2
1	E	129	ILE	2.2
1	A	133	GLN	2.1
1	A	48	LEU	2.1
1	A	63	GLU	2.0
1	A	62	VAL	2.0
1	C	146	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	F	196	27/27	0.95	0.16	0.10	84,114,119,119	0
2	AMP	C	195	23/23	0.98	0.12	-0.50	44,50,56,70	0
2	AMP	D	195	23/23	0.99	0.11	-0.61	29,44,52,64	0
2	AMP	F	195	23/23	0.99	0.11	-0.70	30,43,50,57	0

6.5 Other polymers (i)

There are no such residues in this entry.