



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1ATP  
Title : 2.2 angstrom refined crystal structure of the catalytic subunit of cAMP-dependent protein kinase complexed with MNATP and a peptide inhibitor  
Authors : Zheng, J.; Trafny, E.A.; Knighton, D.R.; Xuong, N.-H.; Taylor, S.S.; Teneyck, L.F.; Sowadski, J.M.  
Deposited on : 1993-01-08  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

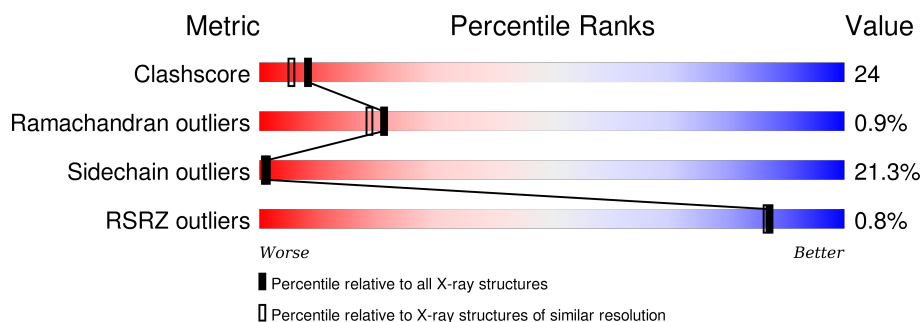
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	E	350	<div> <div></div> <div>44%</div> <div>33%</div> <div>16%</div> <div>• •</div> </div>
2	I	20	<div> <div>55%</div> <div>30%</div> <div>15%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3070 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 cAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	336	Total	C	N	O	P	S	0	0	0
			2777	1800	465	502	2	8			

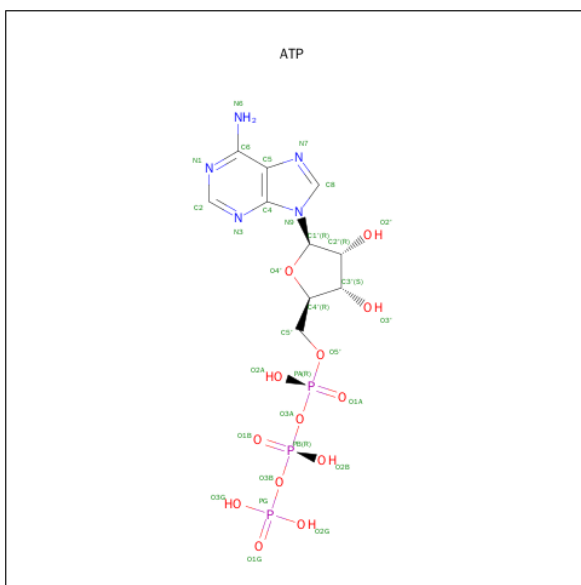
- Molecule 2 is a protein called PEPTIDE INHIBITOR PKI(5-24).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Mn	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

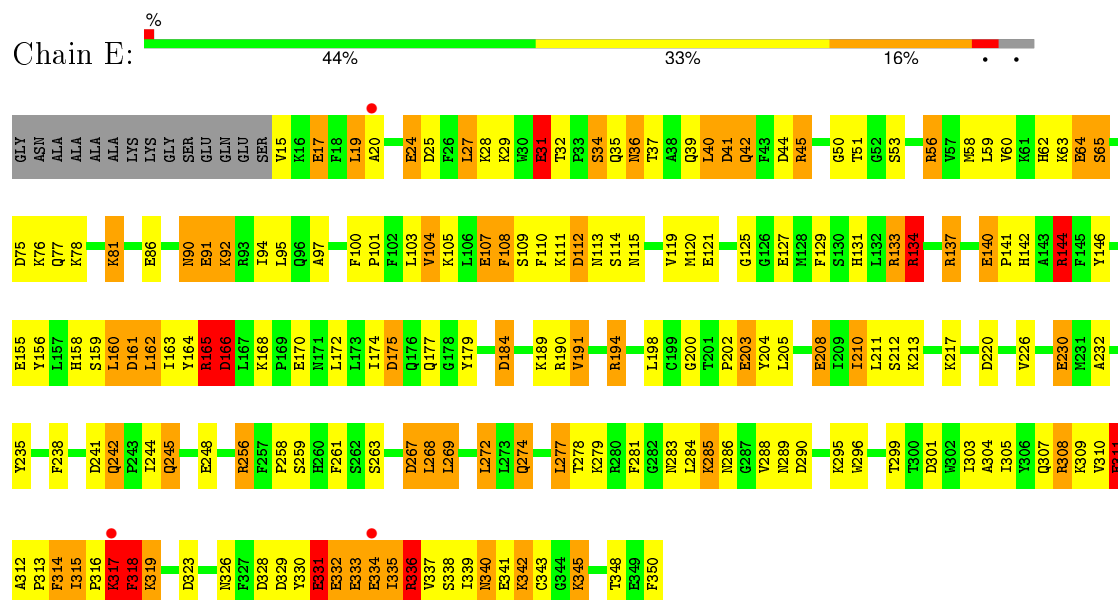
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	89	Total O 89 89	0	0
5	I	14	Total O 14 14	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.

#### • Molecule 1: cAMP-DEPENDENT PROTEIN KINASE



#### • Molecule 2: PEPTIDE INHIBITOR PKI(5-24)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.58Å 76.28Å 80.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 27.17 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 73.5 (27.17-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.15Å)	Xtriage
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.177 , (Not available) 0.195 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 109.6	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24564 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: TPO, MN, ATP, SEP

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	E	1.02	24/2825 (0.8%)	1.39	46/3804 (1.2%)
2	I	0.84	0/159	1.53	4/212 (1.9%)
All	All	1.01	24/2984 (0.8%)	1.40	50/4016 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	165	ARG	C-N	-8.64	1.14	1.34
1	E	170	GLU	CD-OE2	7.73	1.34	1.25
1	E	203	GLU	CD-OE2	7.44	1.33	1.25
1	E	333	GLU	CD-OE2	6.81	1.33	1.25
1	E	17	GLU	CD-OE2	6.65	1.32	1.25
1	E	331	GLU	CD-OE2	6.59	1.32	1.25
1	E	248	GLU	CD-OE1	6.50	1.32	1.25
1	E	64	GLU	CD-OE2	6.26	1.32	1.25
1	E	91	GLU	CD-OE2	-6.18	1.18	1.25
1	E	24	GLU	CD-OE2	6.17	1.32	1.25
1	E	31	GLU	CD-OE1	6.12	1.32	1.25
1	E	140	GLU	CD-OE2	6.05	1.32	1.25
1	E	311	GLU	CD-OE1	5.91	1.32	1.25
1	E	230	GLU	CD-OE1	5.84	1.32	1.25
1	E	332	GLU	CD-OE1	5.83	1.32	1.25
1	E	334	GLU	CD-OE1	5.83	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	121	GLU	CD-OE2	5.81	1.32	1.25
1	E	127	GLU	CD-OE2	5.72	1.31	1.25
1	E	230	GLU	CD-OE2	-5.64	1.19	1.25
1	E	86	GLU	CD-OE1	5.22	1.31	1.25
1	E	25	ASP	CG-OD2	5.22	1.37	1.25
1	E	341	GLU	CD-OE2	5.21	1.31	1.25
1	E	56	ARG	NE-CZ	-5.12	1.26	1.33
1	E	107	GLU	CD-OE2	5.10	1.31	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	165	ARG	O-C-N	-16.12	96.90	122.70
1	E	165	ARG	CA-C-N	10.80	140.95	117.20
1	E	56	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	E	267	ASP	CB-CG-OD1	-8.25	110.87	118.30
2	I	18	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	E	165	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	E	44	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	E	44	ASP	CB-CG-OD1	7.28	124.85	118.30
1	E	161	ASP	CB-CG-OD1	-7.06	111.94	118.30
1	E	112	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	E	194	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	E	241	ASP	CB-CG-OD2	-6.53	112.43	118.30
2	I	24	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	E	166	ASP	CA-C-N	-6.32	103.30	117.20
1	E	317	LYS	N-CA-CB	6.26	121.88	110.60
1	E	161	ASP	CB-CG-OD2	6.20	123.88	118.30
1	E	75	ASP	CB-CG-OD2	6.16	123.84	118.30
1	E	290	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	E	137	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	301	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	E	301	ASP	CB-CG-OD2	5.84	123.55	118.30
1	E	184	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	E	191	VAL	CB-CA-C	-5.77	100.44	111.40
1	E	318	PHE	CB-CG-CD1	5.69	124.78	120.80
1	E	144	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	E	329	ASP	CB-CG-OD2	5.59	123.33	118.30
2	I	24	ASP	CB-CG-OD2	5.59	123.33	118.30
1	E	112	ASP	CB-CG-OD1	5.48	123.23	118.30
1	E	133	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	I	15	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	328	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	E	90	ASN	CB-CA-C	-5.36	99.69	110.40
1	E	274	GLN	CB-CA-C	5.34	121.08	110.40
1	E	134	ARG	CB-CA-C	5.33	121.06	110.40
1	E	134	ARG	N-CA-CB	5.30	120.14	110.60
1	E	318	PHE	CG-CD2-CE2	5.26	126.59	120.80
1	E	175	ASP	CB-CG-OD1	-5.23	113.60	118.30
1	E	165	ARG	C-N-CA	5.21	134.73	121.70
1	E	41	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	E	329	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	E	137	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	104	VAL	CB-CA-C	-5.16	101.61	111.40
1	E	323	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	241	ASP	CB-CG-OD1	5.13	122.91	118.30
1	E	210	ILE	CA-CB-CG2	5.11	121.12	110.90
1	E	210	ILE	N-CA-CB	5.09	122.51	110.80
1	E	290	ASP	CB-CG-OD2	5.08	122.88	118.30
1	E	267	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	336	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	56	ARG	NH1-CZ-NH2	5.02	124.92	119.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	134	ARG	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	165	ARG	Mainchain
1	E	166	ASP	Mainchain

## 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	E	2777	0	2761	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	157	0	146	9	0
3	E	2	0	0	0	0
4	E	31	0	12	1	0
5	E	89	0	0	9	0
5	I	14	0	0	0	0
All	All	3070	0	2919	143	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 24.

All (143) 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:305:ILE:HG13	1:E:310:VAL:HG21	1.23	1.11
1:E:310:VAL:HG12	1:E:311:GLU:HG3	1.50	0.90
1:E:285:LYS:H	1:E:285:LYS:HD2	1.40	0.86
1:E:284:LEU:HB3	1:E:285:LYS:HD2	1.60	0.82
1:E:345:LYS:H	1:E:345:LYS:HD2	1.47	0.79
1:E:303:ILE:O	1:E:307:GLN:HG3	1.85	0.76
1:E:303:ILE:HD12	1:E:303:ILE:H	1.50	0.75
1:E:305:ILE:HG13	1:E:310:VAL:CG2	2.10	0.74
1:E:319:LYS:HD2	1:E:319:LYS:H	1.52	0.73
1:E:163:ILE:HG12	1:E:217:LYS:HD3	1.71	0.72
1:E:335:ILE:HD12	5:E:596:HOH:O	1.89	0.72
1:E:285:LYS:N	1:E:285:LYS:HD2	2.04	0.71
1:E:62:HIS:HD2	1:E:65:SER:HB3	1.54	0.71
1:E:285:LYS:HG2	1:E:286:ASN:N	2.07	0.70
1:E:203:GLU:OE2	2:I:15:ARG:HD3	1.91	0.70
1:E:334:GLU:HB2	1:E:336:ARG:HH12	1.58	0.68
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.26	0.68
1:E:277:LEU:O	1:E:283:ASN:ND2	2.27	0.68
1:E:36:ASN:ND2	1:E:110:PHE:HB2	2.10	0.67
1:E:64:GLU:CD	1:E:64:GLU:H	1.98	0.67
1:E:200:GLY:HA3	1:E:205:LEU:HD21	1.76	0.66
1:E:303:ILE:HD12	1:E:303:ILE:N	2.10	0.65
1:E:242:GLN:HG3	1:E:245:GLN:OE1	1.96	0.65
1:E:285:LYS:HG2	1:E:286:ASN:H	1.60	0.65
1:E:15:VAL:N	1:E:17:GLU:OE1	2.30	0.65
1:E:274:GLN:HG2	1:E:279:LYS:HB3	1.78	0.64
1:E:53:SER:OG	2:I:20:ASN:HB3	1.98	0.64
1:E:58:MET:CE	1:E:335:ILE:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ILE:HD13	1:E:335:ILE:N	2.12	0.64
1:E:90:ASN:O	1:E:94:ILE:HG13	1.99	0.63
1:E:45:ARG:NH2	1:E:333:GLU:O	2.31	0.63
1:E:77:GLN:NE2	1:E:342:LYS:HG3	2.13	0.63
1:E:56:ARG:HH12	1:E:333:GLU:CD	2.03	0.62
1:E:164:TYR:CE2	1:E:166:ASP:C	2.73	0.62
1:E:39:GLN:O	1:E:42:GLN:HG3	2.00	0.61
1:E:338:SEP:HB2	5:E:586:HOH:O	2.00	0.61
1:E:338:SEP:O2P	1:E:340:ASN:ND2	2.33	0.61
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.35	0.60
1:E:189:LYS:HD3	1:E:191:VAL:CG2	2.31	0.60
1:E:62:HIS:CD2	1:E:65:SER:HB3	2.37	0.59
1:E:163:ILE:HG22	1:E:165:ARG:HG3	1.83	0.59
1:E:125:GLY:HA3	1:E:174:ILE:O	2.02	0.59
1:E:204:TYR:CE2	1:E:226:VAL:HG12	2.37	0.59
1:E:56:ARG:NH2	1:E:333:GLU:OE1	2.25	0.59
1:E:285:LYS:H	1:E:285:LYS:CD	2.15	0.59
1:E:155:GLU:HG3	1:E:288:VAL:HG11	1.84	0.59
1:E:304:ALA:HA	1:E:309:LYS:HD3	1.83	0.59
1:E:304:ALA:HB1	1:E:309:LYS:HG2	1.86	0.58
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.86	0.58
1:E:286:ASN:O	1:E:289:ASN:HB2	2.04	0.57
1:E:189:LYS:HD3	1:E:191:VAL:HG21	1.86	0.57
1:E:144:ARG:HB2	1:E:296:TRP:CH2	2.40	0.56
1:E:160:LEU:O	1:E:162:LEU:HD13	2.04	0.56
1:E:331:GLU:O	1:E:331:GLU:HG3	2.04	0.56
1:E:175:ASP:OD2	1:E:308:ARG:NH1	2.29	0.55
1:E:310:VAL:HG12	1:E:311:GLU:CG	2.33	0.55
1:E:29:LYS:HD3	1:E:97:ALA:HA	1.88	0.54
1:E:45:ARG:O	1:E:45:ARG:HG2	1.98	0.54
1:E:310:VAL:HG12	1:E:311:GLU:N	2.23	0.54
1:E:303:ILE:H	1:E:303:ILE:CD1	2.20	0.54
1:E:162:LEU:HD12	1:E:190:ARG:HA	1.91	0.53
1:E:284:LEU:CB	1:E:285:LYS:HD2	2.36	0.53
1:E:56:ARG:NH1	1:E:333:GLU:HB2	2.23	0.52
2:I:23:HIS:CD2	2:I:24:ASP:N	2.77	0.52
1:E:131:HIS:HA	1:E:134:ARG:NH1	2.23	0.52
1:E:345:LYS:N	1:E:345:LYS:HD2	2.20	0.52
1:E:168:LYS:O	1:E:172:LEU:HG	2.11	0.51
1:E:76:LYS:HG3	1:E:114:SER:O	2.10	0.51
1:E:345:LYS:CD	1:E:345:LYS:H	2.06	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ASN:HD21	1:E:110:PHE:HB2	1.75	0.51
1:E:56:ARG:HH12	1:E:333:GLU:HB2	1.76	0.51
1:E:163:ILE:HG22	1:E:165:ARG:CG	2.41	0.51
1:E:58:MET:HE1	1:E:335:ILE:HD11	1.91	0.51
1:E:140:GLU:HB2	1:E:141:PRO:HD3	1.93	0.50
1:E:81:LYS:NZ	5:E:464:HOH:O	2.36	0.50
1:E:41:ASP:OD1	1:E:42:GLN:HG2	2.11	0.50
1:E:129:PHE:CE1	1:E:133:ARG:NH1	2.80	0.50
1:E:168:LYS:NZ	4:E:355:ATP:O2G	2.44	0.50
1:E:133:ARG:NH1	5:E:480:HOH:O	2.43	0.49
1:E:35:GLN:HE21	1:E:350:PHE:C	2.14	0.49
1:E:334:GLU:HB2	1:E:336:ARG:NH1	2.24	0.49
1:E:108:PHE:HD1	1:E:119:VAL:HB	1.78	0.49
1:E:34:SER:O	1:E:92:LYS:NZ	2.43	0.49
1:E:35:GLN:HG2	1:E:350:PHE:OXT	2.13	0.48
2:I:23:HIS:CD2	2:I:24:ASP:H	2.31	0.48
1:E:100:PHE:HB2	1:E:156:TYR:CE2	2.48	0.48
1:E:258:PRO:HG2	1:E:261:PHE:CE1	2.49	0.48
2:I:11:ILE:CD1	2:I:16:THR:HG21	2.44	0.48
1:E:334:GLU:C	1:E:335:ILE:HD13	2.33	0.48
1:E:256:ARG:HB3	1:E:256:ARG:CZ	2.40	0.47
1:E:76:LYS:HE2	1:E:112:ASP:O	2.13	0.47
2:I:23:HIS:CG	2:I:24:ASP:N	2.82	0.47
1:E:155:GLU:O	1:E:159:SER:HB3	2.14	0.47
1:E:17:GLU:O	1:E:20:ALA:HB3	2.14	0.47
2:I:23:HIS:O	2:I:24:ASP:O	2.33	0.47
1:E:29:LYS:HB2	1:E:97:ALA:CB	2.46	0.46
1:E:332:GLU:O	1:E:334:GLU:OE2	2.33	0.46
1:E:316:PRO:HA	5:E:535:HOH:O	2.16	0.46
1:E:268:LEU:HD22	1:E:272:LEU:HD22	1.99	0.45
1:E:312:ALA:HA	1:E:313:PRO:HD2	1.84	0.45
1:E:317:LYS:HA	1:E:317:LYS:HD2	1.44	0.45
1:E:319:LYS:CD	1:E:319:LYS:H	2.26	0.45
1:E:285:LYS:CG	1:E:286:ASN:N	2.79	0.45
1:E:208:GLU:HB3	1:E:213:LYS:HG2	1.99	0.45
1:E:338:SEP:OG	1:E:339:ILE:N	2.51	0.44
1:E:50:GLY:HA2	1:E:330:TYR:CE1	2.52	0.44
1:E:244:ILE:HG13	1:E:245:GLN:N	2.33	0.44
1:E:100:PHE:CD2	1:E:101:PRO:HD2	2.52	0.44
1:E:345:LYS:CD	1:E:345:LYS:N	2.78	0.44
1:E:211:LEU:HD23	1:E:211:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:HIS:CD2	1:E:146:TYR:CE2	3.06	0.43
1:E:230:GLU:HA	1:E:235:TYR:O	2.18	0.43
1:E:177:GLN:HG2	1:E:179:TYR:CD1	2.53	0.43
1:E:204:TYR:CE2	1:E:226:VAL:CG1	3.01	0.43
1:E:142:HIS:NE2	1:E:146:TYR:CE2	2.87	0.43
1:E:189:LYS:NZ	5:E:428:HOH:O	2.49	0.43
1:E:310:VAL:HG12	1:E:311:GLU:H	1.84	0.42
1:E:334:GLU:CB	1:E:336:ARG:HH12	2.30	0.42
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.89	0.42
1:E:105:LYS:O	1:E:120:MET:HB3	2.20	0.42
1:E:35:GLN:NE2	1:E:350:PHE:O	2.46	0.42
1:E:40:LEU:HA	1:E:40:LEU:HD23	1.80	0.42
1:E:77:GLN:CD	1:E:342:LYS:HG3	2.40	0.41
1:E:36:ASN:HA	1:E:109:SER:O	2.20	0.41
1:E:107:GLU:N	1:E:119:VAL:O	2.51	0.41
1:E:310:VAL:CG1	1:E:311:GLU:HG3	2.35	0.41
1:E:76:LYS:HG3	1:E:115:ASN:HA	2.02	0.41
1:E:269:LEU:HA	1:E:269:LEU:HD12	1.85	0.41
1:E:36:ASN:ND2	1:E:110:PHE:CB	2.81	0.41
1:E:212:SER:HA	5:E:415:HOH:O	2.20	0.41
1:E:137:ARG:NH1	1:E:232:ALA:O	2.53	0.41
1:E:319:LYS:HD2	1:E:319:LYS:N	2.28	0.41
1:E:41:ASP:OD1	1:E:42:GLN:N	2.54	0.41
1:E:100:PHE:HB3	1:E:103:LEU:HG	2.02	0.41
2:I:11:ILE:HD12	2:I:16:THR:HG21	2.03	0.41
1:E:343:CYS:N	5:E:659:HOH:O	2.24	0.41
1:E:318:PHE:HB3	5:E:684:HOH:O	2.19	0.41
1:E:194:ARG:HE	1:E:194:ARG:HB2	1.80	0.41
1:E:56:ARG:HD2	1:E:56:ARG:HH11	1.41	0.41
1:E:272:LEU:HA	1:E:272:LEU:HD12	1.87	0.40
1:E:314:PHE:C	1:E:315:ILE:HD13	2.42	0.40
1:E:27:LEU:O	1:E:31:GLU:HG2	2.21	0.40
2:I:10:PHE:O	2:I:13:SER:OG	2.28	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	E	332/350 (95%)	309 (93%)	20 (6%)	3 (1%)	21	19
2	I	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
All	All	350/370 (95%)	325 (93%)	22 (6%)	3 (1%)	21	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	184	ASP
1	E	36	ASN
1	E	202	PRO

### 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	E	295/303 (97%)	230 (78%)	65 (22%)	1	1
2	I	15/15 (100%)	14 (93%)	1 (7%)	20	21
All	All	310/318 (98%)	244 (79%)	66 (21%)	1	1

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	19	LEU
1	E	24	GLU
1	E	27	LEU

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Mol	Chain	Res	Type
1	E	28	LYS
1	E	31	GLU
1	E	32	THR
1	E	34	SER
1	E	37	THR
1	E	40	LEU
1	E	42	GLN
1	E	45	ARG
1	E	51	THR
1	E	59	LEU
1	E	60	VAL
1	E	63	LYS
1	E	65	SER
1	E	78	LYS
1	E	81	LYS
1	E	91	GLU
1	E	92	LYS
1	E	95	LEU
1	E	104	VAL
1	E	108	PHE
1	E	111	LYS
1	E	113	ASN
1	E	134	ARG
1	E	144	ARG
1	E	160	LEU
1	E	161	ASP
1	E	162	LEU
1	E	198	LEU
1	E	208	GLU
1	E	210	ILE
1	E	238	PHE
1	E	242	GLN
1	E	245	GLN
1	E	256	ARG
1	E	259	SER
1	E	263	SER
1	E	267	ASP
1	E	268	LEU
1	E	269	LEU
1	E	272	LEU
1	E	277	LEU
1	E	278	THR

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Mol	Chain	Res	Type
1	E	281	PHE
1	E	285	LYS
1	E	295	LYS
1	E	299	THR
1	E	308	ARG
1	E	311	GLU
1	E	314	PHE
1	E	315	ILE
1	E	317	LYS
1	E	318	PHE
1	E	319	LYS
1	E	326	ASN
1	E	331	GLU
1	E	335	ILE
1	E	336	ARG
1	E	337	VAL
1	E	340	ASN
1	E	342	LYS
1	E	345	LYS
1	E	348	THR
2	I	11	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	GLN
1	E	39	GLN
1	E	62	HIS
1	E	77	GLN
1	E	99	ASN
1	E	113	ASN
1	E	158	HIS
1	E	271	ASN
1	E	307	GLN
1	E	326	ASN
2	I	20	ASN
2	I	23	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	E	197	1	8,10,11	0.91	0	7,14,16	1.81	1 (14%)
1	SEP	E	338	1	8,9,10	1.05	0	8,12,14	5.53	2 (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
1	TPO	E	197	1	-	0/8/11/13	0/0/0/0
1	SEP	E	338	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	O3P-P-O1P	-11.55	73.39	110.58
1	E	197	TPO	C-CA-N	3.74	117.64	109.83
1	E	338	SEP	O2P-P-O1P	10.38	144.00	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	3	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ATP	E	355	3	24,33,33	1.09	1 (4%)	31,52,52	1.21	1 (3%)

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
4	ATP	E	355	3	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	355	ATP	PG-O3G	-3.14	1.43	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	355	ATP	C1'-N9-C4	4.73	134.08	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	355	ATP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	334/350 (95%)	-0.38	3 (0%) 85 85	15, 32, 67, 88	0
2	I	20/20 (100%)	-0.77	0 100 100	14, 26, 43, 86	0
All	All	354/370 (95%)	-0.40	3 (0%) 87 87	14, 32, 67, 88	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	GLU	2.4
1	E	20	ALA	2.3
1	E	317	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	E	338	10/11	0.96	0.10	-	35,45,61,100	0
1	TPO	E	197	11/12	0.99	0.07	-	13,18,45,78	0

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ATP	E	355	31/31	0.98	0.12	-0.25	1,19,45,58	0
3	MN	E	351	1/1	0.99	0.06	-2.39	23,23,23,23	0
3	MN	E	352	1/1	0.99	0.06	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.