



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:09 am GMT

PDB ID : 1VRP  
Title : The 2.1 Structure of T. californica Creatine Kinase Complexed with the Transition-State Analogue Complex, ADP-Mg <sup>2+</sup> /NO<sub>3</sub><sup>-</sup>/Creatine  
Authors : Lahiri, S.D.; Wang, P.F.; Babbitt, P.C.; McLeish, M.J.; Kenyon, G.L.; Allen, K.N.  
Deposited on : 2005-04-25  
Resolution : 2.10 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

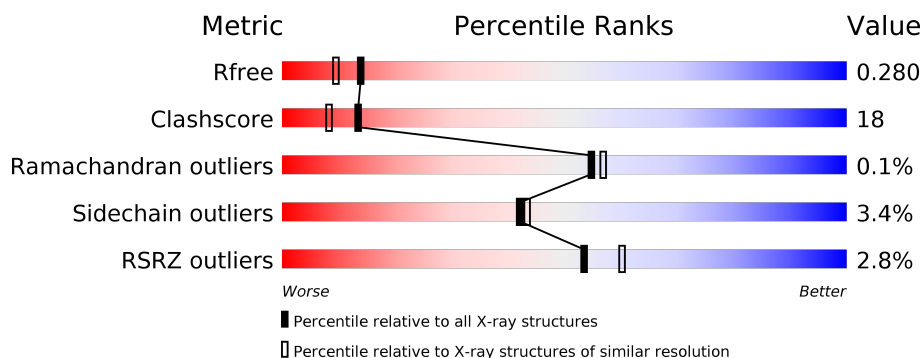
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	A	381	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
1	B	381	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	B	405	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6102 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.

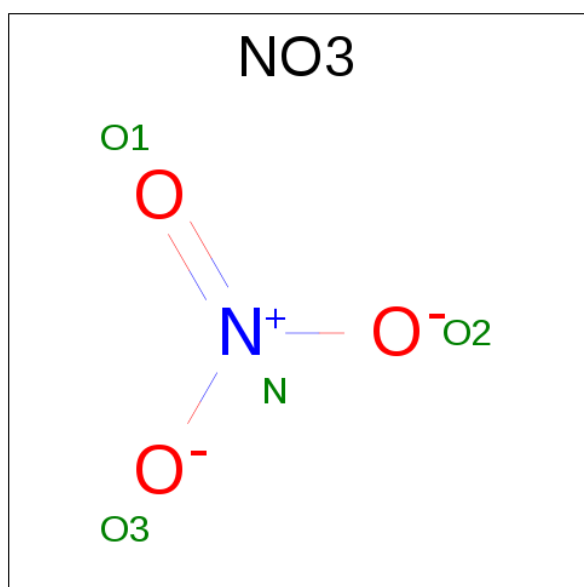
- Molecule 1 is a protein called Creatine Kinase, M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2921	1837	515	551	18			
1	B	374	Total	C	N	O	S	0	0	0
			2961	1864	523	556	18			

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

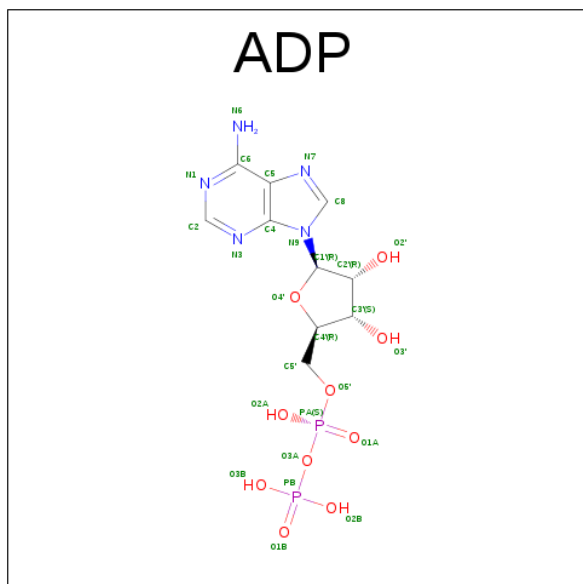
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



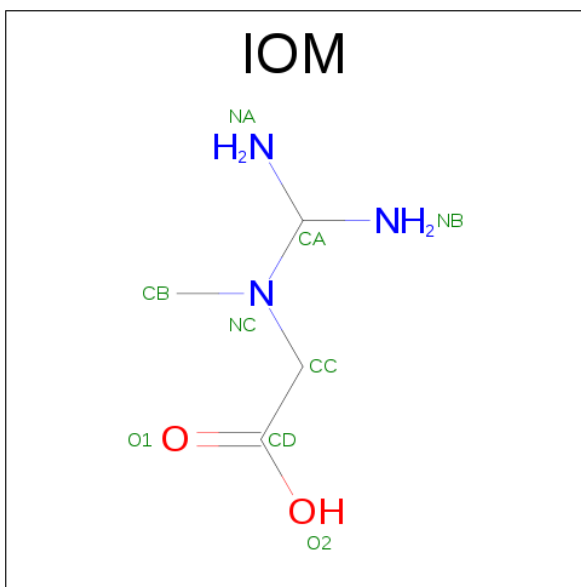
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is (DIAMINOMETHYL-METHYL-AMINO)-ACETIC ACID (three-letter code: IOM) (formula:  $C_4H_{11}N_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			9	4	3	2		

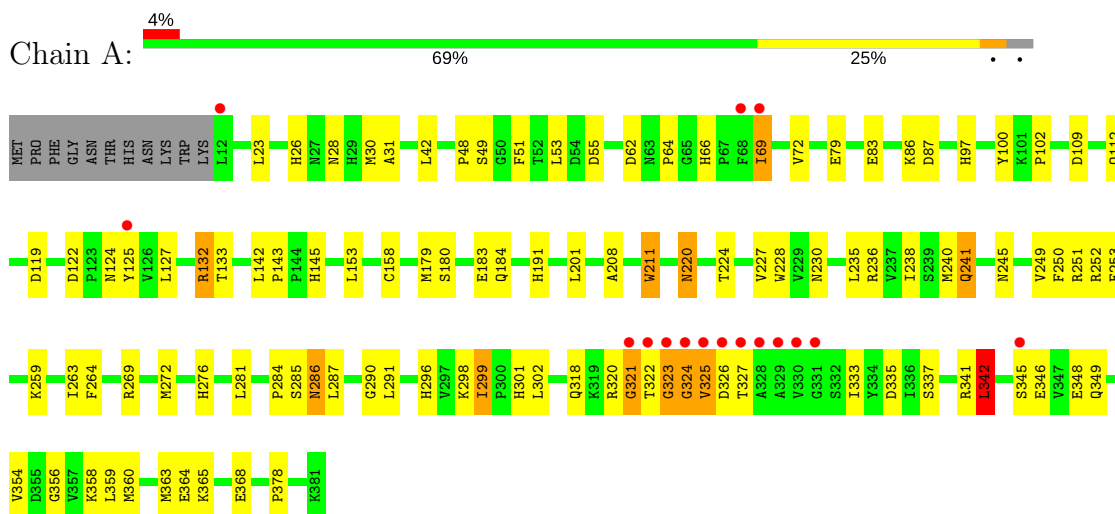
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	68	Total	O	0	0
			68	68		
6	B	83	Total	O	0	0
			83	83		

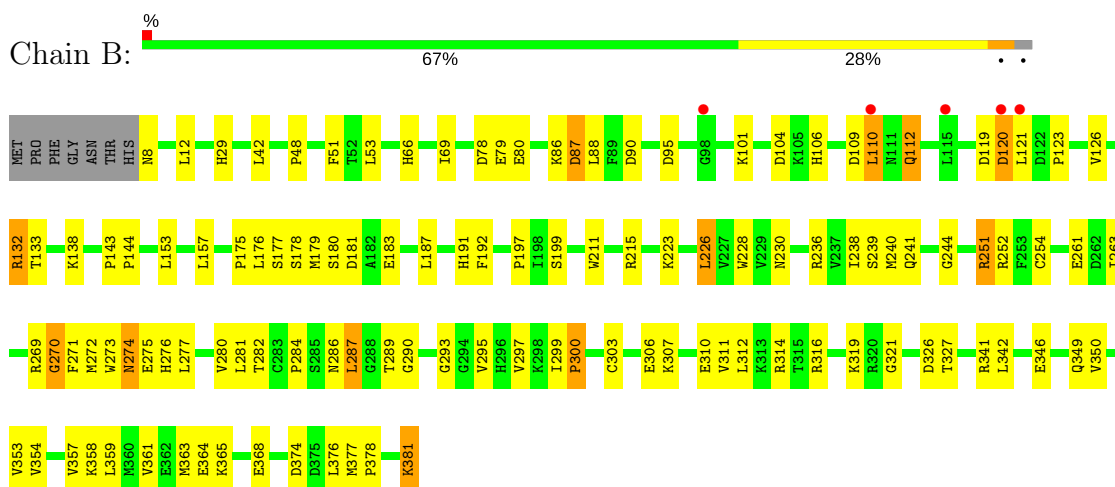
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Creatine Kinase, M chain



#### • Molecule 1: Creatine Kinase, M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.63Å 87.19Å 127.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.42 – 2.10 71.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (50.42-2.10) 91.2 (71.99-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.83 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.242 , 0.278 0.242 , 0.280	Depositor DCC
$R_{free}$ test set	4303 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IOM, ADP, NO3

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	0.60	1/2981 (0.0%)	0.84	7/4015 (0.2%)
1	B	0.48	0/3023	0.75	4/4071 (0.1%)
All	All	0.55	1/6004 (0.0%)	0.80	11/8086 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	C-O	-5.79	1.12	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	CB-CG-CD2	-10.34	93.42	111.00
1	B	287	LEU	CA-CB-CG	8.09	133.91	115.30
1	A	342	LEU	CB-CG-CD1	-7.24	98.70	111.00
1	A	324	GLY	N-CA-C	-6.60	96.60	113.10
1	B	109	ASP	N-CA-C	-6.51	93.42	111.00
1	A	211	TRP	C-N-CD	-6.50	106.31	120.60
1	A	342	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	321	GLY	N-CA-C	5.52	126.90	113.10
1	A	323	GLY	N-CA-C	5.47	126.77	113.10
1	A	324	GLY	C-N-CA	-5.45	108.07	121.70
1	B	110	LEU	CA-CB-CG	-5.10	103.56	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2921	0	2890	102	0
1	B	2961	0	2932	110	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	4	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	0	0
5	B	9	0	9	1	0
6	A	68	0	0	8	0
6	B	83	0	0	10	0
All	All	6102	0	5855	212	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 18.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD11	1:A:298:LYS:CE	1.77	1.12
1:A:127:LEU:HD11	1:A:298:LYS:HE3	1.05	1.01
1:B:191:HIS:HE1	6:B:472:HOH:O	1.45	0.99
1:B:119:ASP:OD1	1:B:120:ASP:OD1	1.81	0.99
1:B:300:PRO:HD2	1:B:364:GLU:OE2	1.65	0.97
1:B:48:PRO:HD2	1:B:80:GLU:HG3	1.48	0.96
1:A:127:LEU:CD1	1:A:298:LYS:HE3	1.96	0.94
1:A:322:THR:HG21	6:A:428:HOH:O	1.67	0.93
1:A:228:TRP:HB2	1:A:236:ARG:HB2	1.53	0.90
1:A:322:THR:CG2	6:A:428:HOH:O	2.19	0.90
1:A:298:LYS:HG2	1:A:333:ILE:HG12	1.55	0.89
1:A:158:CYS:SG	1:A:235:LEU:HD21	2.12	0.89
1:A:69:ILE:H	1:A:69:ILE:HD13	1.35	0.88
1:A:321:GLY:O	1:A:322:THR:HG23	1.75	0.86
1:A:298:LYS:HE2	1:A:333:ILE:HD11	1.59	0.85
1:B:199:SER:HA	1:B:326:ASP:OD1	1.78	0.82
1:A:179:MET:HE3	1:A:184:GLN:HG2	1.62	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:O	1:B:314:ARG:HG3	1.79	0.81
1:A:323:GLY:O	1:A:333:ILE:HB	1.81	0.80
1:B:269:ARG:O	1:B:270:GLY:O	2.00	0.80
1:B:287:LEU:O	1:B:342:LEU:HG	1.81	0.80
1:A:220:ASN:HD21	1:A:224:THR:H	1.31	0.78
1:A:320:ARG:HG2	1:A:335:ASP:HB3	1.64	0.78
1:B:121:LEU:HB2	1:B:244:GLY:HA3	1.67	0.77
1:B:110:LEU:O	1:B:254:CYS:SG	2.43	0.76
1:A:97:HIS:HE1	1:A:284:PRO:O	1.69	0.76
1:B:357:VAL:O	1:B:361:VAL:HG23	1.88	0.74
1:A:241:GLN:NE2	1:A:252:ARG:HH22	1.87	0.73
1:B:238:ILE:HG21	1:B:240:MET:HE1	1.70	0.72
1:A:133:THR:HA	1:A:290:GLY:O	1.88	0.72
1:A:49:SER:HB2	6:A:408:HOH:O	1.89	0.72
1:B:112:GLN:HG2	1:B:251:ARG:HA	1.69	0.72
1:A:321:GLY:O	1:A:322:THR:CG2	2.38	0.71
1:A:324:GLY:C	1:A:326:ASP:N	2.39	0.71
1:A:66:HIS:HB2	1:A:69:ILE:CD1	2.20	0.71
1:B:132:ARG:HG2	1:B:133:THR:N	2.04	0.71
1:A:66:HIS:HB2	1:A:69:ILE:HD11	1.72	0.70
1:B:215:ARG:HG3	1:B:230:ASN:O	1.90	0.70
1:A:201:LEU:HD22	6:A:435:HOH:O	1.92	0.70
1:B:176:LEU:HD12	1:B:179:MET:HE3	1.75	0.69
1:A:264:PHE:HB3	1:A:269:ARG:O	1.94	0.68
1:A:125:TYR:CE1	1:A:365:LYS:HE2	2.29	0.68
1:B:238:ILE:HG21	1:B:240:MET:CE	2.26	0.65
1:A:241:GLN:NE2	1:A:252:ARG:NH2	2.44	0.65
1:B:359:LEU:HD21	1:B:378:PRO:HD3	1.78	0.65
1:A:324:GLY:O	1:A:326:ASP:N	2.30	0.65
1:A:125:TYR:CE1	1:A:365:LYS:CE	2.79	0.65
1:A:324:GLY:C	1:A:326:ASP:H	2.00	0.64
1:B:364:GLU:O	1:B:368:GLU:HG3	1.97	0.64
1:A:109:ASP:O	1:A:346:GLU:HB2	1.98	0.64
1:B:300:PRO:CD	1:B:364:GLU:OE2	2.44	0.64
1:A:259:LYS:O	1:A:263:ILE:HG13	1.97	0.64
1:B:228:TRP:HB2	1:B:236:ARG:HB2	1.79	0.64
1:B:341:ARG:HA	1:B:349:GLN:NE2	2.12	0.63
1:A:69:ILE:H	1:A:69:ILE:CD1	2.11	0.63
1:B:80:GLU:H	1:B:80:GLU:CD	2.00	0.63
1:B:274:ASN:HD21	1:B:277:LEU:N	1.97	0.63
1:B:307:LYS:HE3	1:B:374:ASP:OD1	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:HIS:CE1	6:B:472:HOH:O	2.32	0.62
1:B:274:ASN:HD21	1:B:277:LEU:CA	2.12	0.62
1:A:354:VAL:HG12	1:A:358:LYS:HE2	1.82	0.62
1:A:320:ARG:CG	1:A:335:ASP:HB3	2.30	0.61
1:A:324:GLY:O	1:A:325:VAL:C	2.31	0.61
1:B:314:ARG:O	1:B:381:LYS:HG2	2.00	0.61
1:B:176:LEU:HA	1:B:179:MET:HE3	1.82	0.61
1:A:97:HIS:CE1	1:A:284:PRO:O	2.54	0.60
1:A:66:HIS:O	1:A:69:ILE:O	2.18	0.60
1:A:284:PRO:HA	1:A:287:LEU:HD11	1.84	0.60
1:A:345:SER:O	1:A:348:GLU:N	2.35	0.60
1:B:359:LEU:O	1:B:363:MET:HG3	2.02	0.60
1:A:359:LEU:O	1:A:363:MET:HG3	2.01	0.59
1:B:274:ASN:HD21	1:B:277:LEU:HB2	1.67	0.59
1:B:316:ARG:HD2	1:B:381:LYS:O	2.03	0.59
1:B:307:LYS:O	1:B:311:VAL:HG23	2.01	0.59
1:B:112:GLN:NE2	1:B:112:GLN:H	2.00	0.59
1:A:356:GLY:O	1:A:360:MET:HG3	2.02	0.58
1:B:226:LEU:HD13	1:B:240:MET:HE2	1.85	0.58
1:A:142:LEU:HB3	1:A:143:PRO:HD2	1.85	0.57
1:A:220:ASN:HD21	1:A:224:THR:N	2.02	0.57
1:A:28:ASN:OD1	1:A:31:ALA:CB	2.51	0.57
1:B:121:LEU:O	1:B:123:PRO:HD3	2.05	0.57
1:A:132:ARG:O	1:A:291:LEU:HA	2.05	0.57
1:B:126:VAL:HG22	1:B:297:VAL:CG1	2.34	0.57
1:A:245:ASN:O	1:A:249:VAL:HG23	2.05	0.56
1:B:101:LYS:HB2	1:B:104:ASP:OD2	2.05	0.56
1:B:286:ASN:O	1:B:290:GLY:HA2	2.06	0.56
1:B:78:ASP:OD1	1:B:80:GLU:HG2	2.06	0.56
1:B:274:ASN:HD21	1:B:277:LEU:H	1.55	0.55
1:A:42:LEU:HD11	1:A:87:ASP:HB2	1.87	0.55
1:B:261:GLU:HG2	1:B:271:PHE:HE2	1.72	0.55
1:A:180:SER:OG	1:A:183:GLU:HG3	2.06	0.55
1:A:100:TYR:CD2	1:A:342:LEU:HD21	2.42	0.54
1:B:354:VAL:O	1:B:358:LYS:HG3	2.07	0.54
1:A:238:ILE:HG21	1:A:240:MET:HE2	1.89	0.54
1:B:274:ASN:HD21	1:B:277:LEU:CB	2.21	0.54
1:B:69:ILE:HB	6:B:413:HOH:O	2.07	0.54
1:A:119:ASP:HB2	1:A:245:ASN:ND2	2.23	0.53
1:A:132:ARG:HG2	1:A:133:THR:N	2.24	0.53
1:A:28:ASN:OD1	1:A:31:ALA:N	2.36	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HB3	6:B:461:HOH:O	2.08	0.53
1:B:251:ARG:HD3	1:B:252:ARG:N	2.24	0.53
1:B:226:LEU:HD12	1:B:226:LEU:N	2.24	0.53
1:A:125:TYR:CE1	1:A:365:LYS:HE3	2.44	0.53
1:B:251:ARG:C	1:B:251:ARG:HD3	2.28	0.53
1:B:274:ASN:ND2	1:B:277:LEU:HB2	2.24	0.52
1:B:126:VAL:HG22	1:B:297:VAL:HG12	1.91	0.52
1:B:8:ASN:N	6:B:448:HOH:O	2.41	0.52
1:A:320:ARG:HG2	1:A:335:ASP:CB	2.38	0.52
1:B:121:LEU:HB2	1:B:244:GLY:CA	2.38	0.52
1:A:322:THR:HG23	6:A:428:HOH:O	1.96	0.52
1:B:197:PRO:HG3	1:B:211:TRP:CD2	2.45	0.51
1:B:120:ASP:OD1	1:B:120:ASP:N	2.43	0.51
1:A:125:TYR:OH	1:A:365:LYS:HG2	2.12	0.51
1:B:153:LEU:O	1:B:157:LEU:HG	2.11	0.51
1:B:180:SER:OG	1:B:183:GLU:HG3	2.10	0.51
1:B:361:VAL:HG12	1:B:365:LYS:HE2	1.93	0.50
1:A:79:GLU:HB2	1:A:272:MET:SD	2.52	0.50
1:B:177:SER:HB2	6:B:470:HOH:O	2.11	0.50
1:B:175:PRO:HG2	1:B:178:SER:HB3	1.94	0.50
1:B:353:VAL:O	1:B:357:VAL:HG23	2.12	0.49
1:B:86:LYS:HE2	1:B:90:ASP:OD2	2.12	0.49
1:B:312:LEU:HD11	1:B:319:LYS:HD3	1.93	0.49
1:B:181:ASP:HB2	6:B:445:HOH:O	2.12	0.49
1:B:66:HIS:HB3	1:B:69:ILE:O	2.13	0.49
1:B:86:LYS:HG2	6:B:464:HOH:O	2.12	0.49
1:B:192:PHE:CD2	1:B:223:LYS:HE3	2.48	0.49
1:B:311:VAL:HG22	1:B:377:MET:SD	2.52	0.48
1:B:289:THR:HB	1:B:346:GLU:HG3	1.94	0.48
1:A:250:PHE:O	1:A:253:PHE:HB3	2.12	0.48
1:A:341:ARG:O	1:A:349:GLN:NE2	2.46	0.48
1:B:112:GLN:H	1:B:112:GLN:HE21	1.60	0.48
1:A:301:HIS:CE1	1:A:368:GLU:HG2	2.49	0.48
1:B:42:LEU:HB2	1:B:53:LEU:HD22	1.96	0.47
1:B:284:PRO:HA	1:B:287:LEU:HG	1.96	0.47
1:A:28:ASN:OD1	1:A:31:ALA:HB2	2.13	0.47
1:B:69:ILE:HD11	5:B:402:IOM:HCB1	1.96	0.47
1:B:192:PHE:CE2	1:B:223:LYS:HE3	2.50	0.47
1:B:226:LEU:HD13	1:B:240:MET:CE	2.44	0.47
1:B:79:GLU:OE1	1:B:272:MET:HG2	2.15	0.47
1:A:227:VAL:CG1	1:A:235:LEU:HD22	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PRO:HG3	1:B:282:THR:HG23	1.97	0.47
1:B:273:TRP:CH2	1:B:275:GLU:OE2	2.68	0.47
1:A:23:LEU:HA	1:A:26:HIS:ND1	2.29	0.46
1:A:345:SER:OG	1:A:345:SER:O	2.31	0.46
1:A:83:GLU:O	1:A:86:LYS:HE3	2.15	0.46
1:A:364:GLU:O	1:A:368:GLU:HG3	2.15	0.46
1:B:274:ASN:ND2	1:B:277:LEU:H	2.12	0.46
1:B:42:LEU:HD11	1:B:87:ASP:HB2	1.96	0.46
1:B:261:GLU:HG2	1:B:271:PHE:CE2	2.49	0.46
1:B:126:VAL:HG13	1:B:295:VAL:HB	1.98	0.46
1:A:359:LEU:CD2	1:A:378:PRO:HG3	2.46	0.46
1:B:199:SER:CA	1:B:326:ASP:OD1	2.60	0.46
1:B:119:ASP:C	1:B:120:ASP:OD1	2.53	0.46
1:A:125:TYR:HE1	1:A:365:LYS:HE2	1.79	0.45
1:B:312:LEU:CD1	1:B:319:LYS:HD3	2.45	0.45
1:A:284:PRO:HA	1:A:287:LEU:CD1	2.44	0.45
1:A:179:MET:HE3	1:A:184:GLN:CG	2.39	0.45
1:B:176:LEU:HA	1:B:179:MET:CE	2.45	0.45
1:B:341:ARG:HA	1:B:349:GLN:HE22	1.77	0.45
1:B:29:HIS:HD2	1:B:95:ASP:OD1	1.98	0.45
1:A:211:TRP:C	1:A:211:TRP:CD1	2.91	0.45
1:B:350:VAL:O	1:B:354:VAL:HG23	2.16	0.45
1:A:354:VAL:O	1:A:358:LYS:HE2	2.17	0.45
1:B:138:LYS:HE3	1:B:271:PHE:O	2.17	0.45
1:B:321:GLY:HA3	1:B:327:THR:O	2.18	0.44
1:A:125:TYR:CZ	1:A:365:LYS:HE2	2.52	0.44
1:A:321:GLY:C	1:A:322:THR:HG23	2.38	0.44
1:A:191:HIS:HB3	4:A:400:ADP:HI'	1.98	0.44
1:B:299:ILE:O	1:B:299:ILE:HG13	2.18	0.44
1:A:276:HIS:HE1	6:A:466:HOH:O	2.00	0.44
1:A:230:ASN:ND2	6:A:419:HOH:O	2.50	0.44
1:A:318:GLN:HG2	1:A:337:SER:O	2.18	0.44
1:B:381:LYS:NZ	1:B:381:LYS:HB2	2.32	0.44
1:A:251:ARG:C	1:A:251:ARG:HD3	2.38	0.44
1:A:66:HIS:HB2	1:A:69:ILE:HD13	1.98	0.44
1:A:153:LEU:HD21	1:A:269:ARG:CZ	2.48	0.44
1:B:121:LEU:HB3	1:B:126:VAL:HG21	2.00	0.44
1:B:241:GLN:OE1	1:B:252:ARG:NH2	2.39	0.44
1:A:145:HIS:HE1	6:A:405:HOH:O	2.00	0.43
1:B:132:ARG:HG3	6:B:460:HOH:O	2.18	0.43
1:B:299:ILE:HG13	1:B:303:CYS:HB3	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:O	1:B:123:PRO:CD	2.67	0.43
1:A:69:ILE:N	1:A:69:ILE:HD13	2.12	0.43
1:A:30:MET:C	1:A:30:MET:SD	2.97	0.43
1:A:72:VAL:HG11	1:A:284:PRO:HG2	1.99	0.43
1:B:376:LEU:O	1:B:378:PRO:HD3	2.18	0.43
1:A:122:ASP:OD1	1:A:124:ASN:HB2	2.19	0.42
1:A:298:LYS:HG2	1:A:333:ILE:CG1	2.39	0.42
1:B:175:PRO:HG2	1:B:178:SER:CB	2.50	0.42
1:B:281:LEU:HD12	1:B:286:ASN:O	2.19	0.42
1:A:324:GLY:N	1:A:327:THR:O	2.52	0.42
1:A:102:PRO:HA	1:A:276:HIS:CE1	2.55	0.42
1:B:238:ILE:HG22	1:B:239:SER:N	2.34	0.42
1:B:106:HIS:HE1	1:B:289:THR:HG23	1.85	0.42
1:B:272:MET:HB3	1:B:280:VAL:HB	2.01	0.42
1:A:296:HIS:ND1	1:A:325:VAL:HG13	2.35	0.41
1:B:53:LEU:HD11	1:B:88:LEU:HD22	2.02	0.41
1:A:286:ASN:HD22	1:A:341:ARG:HE	1.69	0.41
1:A:69:ILE:N	1:A:69:ILE:CD1	2.76	0.41
1:A:299:ILE:HB	1:A:302:LEU:HB3	2.03	0.41
1:A:42:LEU:HB2	1:A:53:LEU:HD22	2.03	0.41
1:A:285:SER:O	1:A:341:ARG:HG3	2.21	0.41
1:A:51:PHE:CZ	1:A:55:ASP:HB3	2.56	0.41
1:A:62:ASP:O	1:A:64:PRO:HD3	2.20	0.41
1:A:208:ALA:O	1:A:211:TRP:HB2	2.21	0.40
1:A:281:LEU:HD12	1:A:286:ASN:O	2.21	0.40
1:A:291:LEU:HD23	1:A:291:LEU:C	2.41	0.40
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.83	0.40
1:B:263:ILE:HG21	1:B:263:ILE:HD13	1.89	0.40
1:B:276:HIS:NE2	6:B:446:HOH:O	2.37	0.40
1:B:293:GLY:O	1:B:353:VAL:HG21	2.22	0.40
1:B:132:ARG:HB2	1:B:238:ILE:HG12	2.04	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	368/381 (97%)	356 (97%)	12 (3%)	0	100	100
1	B	372/381 (98%)	357 (96%)	14 (4%)	1 (0%)	44	44
All	All	740/762 (97%)	713 (96%)	26 (4%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/330 (97%)	311 (97%)	9 (3%)	49	52
1	B	324/330 (98%)	311 (96%)	13 (4%)	36	36
All	All	644/660 (98%)	622 (97%)	22 (3%)	42	43

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
1	A	69	ILE
1	A	112	GLN
1	A	132	ARG
1	A	220	ASN
1	A	241	GLN
1	A	286	ASN
1	A	299	ILE
1	A	342	LEU
1	B	51	PHE
1	B	87	ASP
1	B	112	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	120	ASP
1	B	132	ARG
1	B	143	PRO
1	B	187	LEU
1	B	226	LEU
1	B	251	ARG
1	B	274	ASN
1	B	300	PRO
1	B	306	GLU
1	B	381	LYS

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

Mol	Chain	Res	Type
1	A	97	HIS
1	A	112	GLN
1	A	114	ASN
1	A	145	HIS
1	A	191	HIS
1	A	220	ASN
1	A	230	ASN
1	A	241	GLN
1	A	276	HIS
1	A	286	ASN
1	A	318	GLN
1	B	8	ASN
1	B	29	HIS
1	B	112	GLN
1	B	114	ASN
1	B	145	HIS
1	B	184	GLN
1	B	191	HIS
1	B	274	ASN
1	B	349	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ADP	A	400	2	25,29,29	1.63	3 (12%)	24,45,45	1.85	4 (16%)
4	ADP	B	401	2	25,29,29	2.40	3 (12%)	24,45,45	1.98	5 (20%)
5	IOM	B	402	-	2,8,8	6.97	1 (50%)	4,10,10	4.52	3 (75%)
3	NO3	B	405	2	1,3,3	3.86	1 (100%)	0,3,3	0.00	-

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	ADP	A	400	2	-	0/12/32/32	0/3/3/3
4	ADP	B	401	2	-	0/12/32/32	0/3/3/3
5	IOM	B	402	-	-	0/2/8/8	0/0/0/0
3	NO3	B	405	2	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	ADP	PB-O3A	-10.22	1.43	1.60
4	A	400	ADP	PA-O5'	-2.26	1.49	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	ADP	O4'-C1'	2.41	1.44	1.41
4	A	400	ADP	O4'-C1'	2.97	1.45	1.41
4	B	401	ADP	PA-O5'	3.79	1.75	1.59
3	B	405	NO3	O1-N	3.86	1.38	1.23
4	A	400	ADP	PB-O3A	5.98	1.69	1.60
5	B	402	IOM	CC-NC	9.83	1.57	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	N3-C2-N1	-6.99	122.77	128.86
4	A	400	ADP	N3-C2-N1	-6.92	122.83	128.86
4	B	401	ADP	C1'-N9-C4	-2.57	122.19	126.64
4	A	400	ADP	C1'-N9-C4	-2.30	122.67	126.64
4	B	401	ADP	C4'-O4'-C1'	-2.10	107.54	109.77
4	A	400	ADP	C4-C5-N7	2.04	111.38	109.41
4	B	401	ADP	C4-C5-N7	2.31	111.64	109.41
4	A	400	ADP	O5'-PA-O1A	2.41	118.98	109.25
5	B	402	IOM	CC-NC-CA	2.86	120.76	115.33
4	B	401	ADP	O2A-PA-O5'	3.40	124.18	108.14
5	B	402	IOM	CB-NC-CC	5.41	117.32	109.97
5	B	402	IOM	CD-CC-NC	6.38	121.09	111.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	ADP	1	0
5	B	402	IOM	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

### 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<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	A	370/381 (97%)	0.46	16 (4%) 36 43	12, 26, 43, 55	0
1	B	374/381 (98%)	0.28	5 (1%) 77 81	11, 27, 48, 81	0
All	All	744/762 (97%)	0.37	21 (2%) 53 60	11, 26, 45, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	GLY	8.7
1	A	329	ALA	8.1
1	A	330	VAL	6.8
1	A	327	THR	6.3
1	A	331	GLY	5.8
1	A	69	ILE	5.8
1	A	324	GLY	5.5
1	A	328	ALA	5.2
1	B	110	LEU	4.6
1	A	68	PHE	4.0
1	A	326	ASP	3.8
1	B	120	ASP	3.6
1	A	321	GLY	3.3
1	A	322	THR	3.1
1	A	125	TYR	2.9
1	A	345	SER	2.7
1	A	325	VAL	2.6
1	B	115	LEU	2.4
1	B	98	GLY	2.2
1	A	12	LEU	2.1
1	B	121	LEU	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
3	NO3	B	405	4/4	0.77	0.34	5.46	31,33,36,37	0
4	ADP	B	401	27/27	0.95	0.15	0.34	22,27,34,35	0
5	IOM	B	402	9/9	0.96	0.13	-0.33	17,20,23,25	0
4	ADP	A	400	27/27	0.96	0.13	-0.73	22,25,27,28	0
2	MG	B	403	1/1	0.96	0.12	-	26,26,26,26	0
2	MG	A	404	1/1	0.87	0.15	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.