



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:35 AM GMT

PDB ID : 2CCI  
Title : CRYSTAL STRUCTURE OF PHOSPHO-CDK2 CYCLIN A IN COMPLEX  
WITH A PEPTIDE CONTAINING BOTH THE SUBSTRATE AND RE-  
CRUITMENT SITES OF CDC6  
Authors : Cheng, K.Y.; Noble, M.E.M.; Skamnaki, V.; Brown, N.R.; Lowe, E.D.; Kon-  
togiannis, L.; Shen, K.; Cole, P.A.; Siligardi, G.; Johnson, L.N.  
Deposited on : 2006-01-16  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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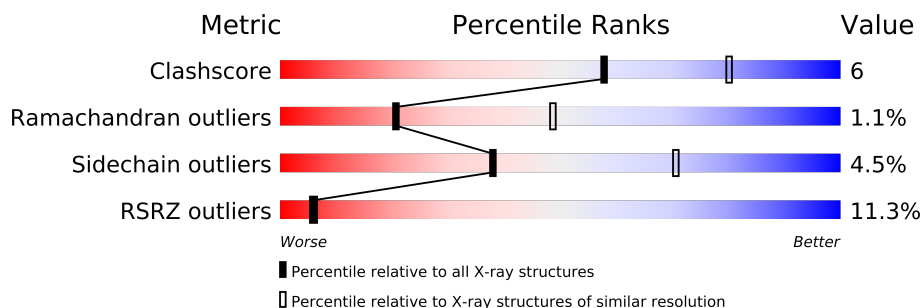
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	299	
1	C	299	
2	B	258	
2	D	258	
3	F	30	
3	I	30	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9391 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				
2	D	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				

- Molecule 3 is a protein called CELL DIVISION CONTROL PROTEIN 6 HOMOLOG.

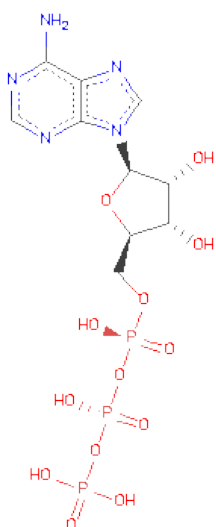
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	19	Total	C	N	O	0	0	0
			160	99	37	24			
3	I	14	Total	C	N	O	0	0	0
			114	73	25	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	67	HIS	PRO	ENGINEERED MUTATION	UNP Q99741
F	68	HIS	PRO	ENGINEERED MUTATION	UNP Q99741
F	69	ALA	CYS	ENGINEERED MUTATION	UNP Q99741
F	72	ARG	PRO	ENGINEERED MUTATION	UNP Q99741
I	69	ALA	CYS	ENGINEERED MUTATION	UNP Q99741
I	72	ARG	PRO	ENGINEERED MUTATION	UNP Q99741

- 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	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	23	Total	O	0	0
			23	23		
6	C	22	Total	O	0	0
			22	22		
6	D	12	Total	O	0	0
			12	12		
6	F	7	Total	O	0	0
			7	7		

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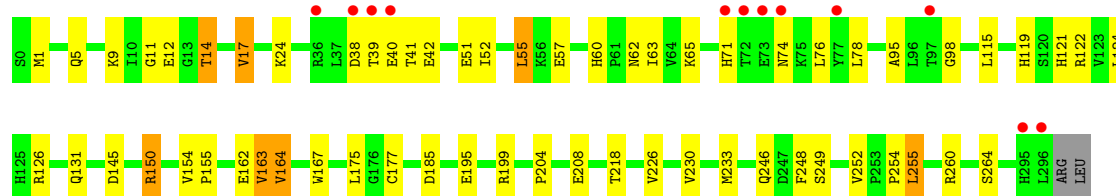
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	3	Total	O	0	0
			3	3		

### 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.

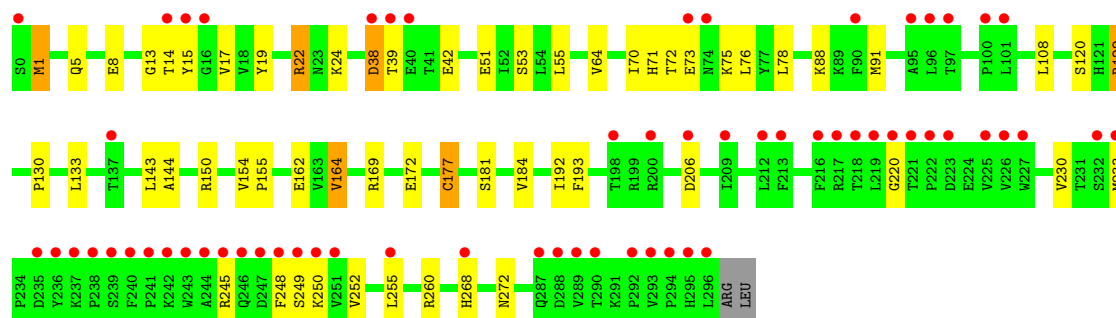
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 



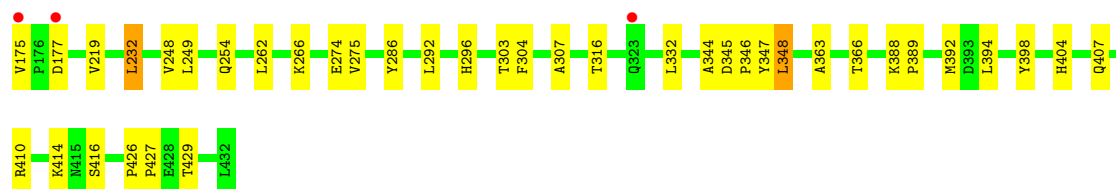
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C: 



#### • Molecule 2: CYCLIN A2

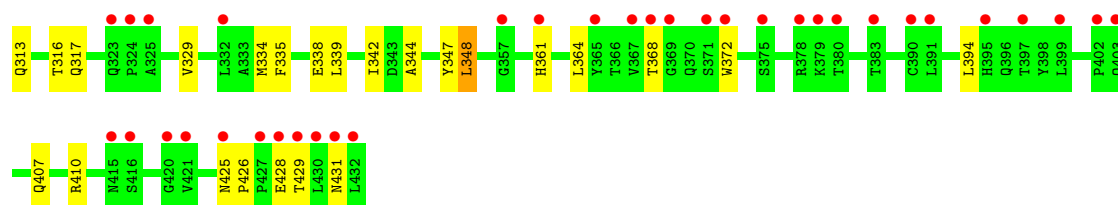
Chain B: 



#### • Molecule 2: CYCLIN A2

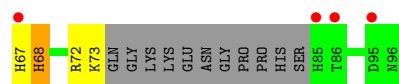
Chain D: 





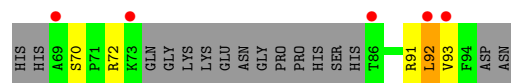
• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG

Chain F:



• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.42Å 114.39Å 170.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 2.70 37.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (94.92-2.70) 97.1 (37.02-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.261 , 0.321 0.264 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 15.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 39591 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	9391	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 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/2438	0.59	1/3308 (0.0%)
1	C	0.39	0/2438	0.55	0/3308
2	B	0.43	0/2133	0.56	0/2897
2	D	0.37	0/2133	0.53	0/2897
3	F	0.37	0/163	0.50	0/215
3	I	0.43	0/114	0.60	0/148
All	All	0.41	0/9419	0.56	1/12773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2430	43	0
1	C	2388	0	2430	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2083	0	2107	24	0
2	D	2083	0	2107	28	0
3	F	160	0	161	2	0
3	I	114	0	130	2	0
4	A	31	0	12	0	0
4	C	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	3	0
6	B	23	0	0	0	0
6	C	22	0	0	0	0
6	D	12	0	0	0	0
6	F	7	0	0	1	0
6	I	3	0	0	1	0
All	All	9391	0	9389	117	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:203:GLN:HE22	2:D:247:SER:HA	1.22	1.05
1:A:154:VAL:O	2:B:316:THR:HG22	1.62	0.97
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.51	0.90
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.54	0.89
1:A:5:GLN:HB2	1:A:24:LYS:HE3	1.66	0.77
2:B:366:THR:HG23	2:B:427:PRO:HD3	1.68	0.75
1:A:177:CYS:HB2	6:A:2023:HOH:O	1.87	0.75
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.54	0.72
1:A:42:GLU:OE1	2:B:275:VAL:HG23	1.89	0.71
3:F:67:HIS:O	3:F:68:HIS:HB2	1.90	0.71
1:A:154:VAL:O	2:B:316:THR:CG2	2.39	0.71
1:C:1:MET:HE2	1:C:1:MET:HA	1.71	0.71
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.72	0.71
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.73	0.71
1:A:51:GLU:O	1:A:55:LEU:HB2	1.91	0.70
2:D:203:GLN:NE2	2:D:247:SER:HA	2.03	0.67
1:C:230:VAL:HA	1:C:233:MET:HE2	1.76	0.67
1:C:1:MET:CE	1:C:1:MET:HA	2.24	0.66
1:C:73:GLU:HG2	2:D:293:ARG:HH22	1.64	0.62
3:F:73:LYS:HA	6:F:2004:HOH:O	2.00	0.62
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:51:GLU:O	1:C:55:LEU:HB2	2.01	0.61
1:A:230:VAL:HG23	1:A:233:MET:HE1	1.82	0.61
2:B:248:VAL:HG12	2:B:249:LEU:O	2.03	0.58
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.57
1:A:252:VAL:HG12	1:A:254:PRO:HD2	1.86	0.57
1:C:64:VAL:HG23	1:C:143:LEU:O	2.04	0.57
1:A:177:CYS:SG	1:A:233:MET:SD	3.02	0.57
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.05	0.57
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.74	0.56
4:C:1297:ATP:O1G	4:C:1297:ATP:O1A	2.22	0.56
1:A:39:THR:HG22	1:A:40:GLU:HG2	1.87	0.56
2:D:347:TYR:OH	2:D:394:LEU:HA	2.06	0.56
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.87	0.55
1:A:1:MET:HA	1:A:1:MET:HE2	1.88	0.55
1:C:72:THR:HB	1:C:75:LYS:H	1.72	0.54
1:C:5:GLN:HB2	1:C:24:LYS:HE3	1.89	0.54
1:A:9:LYS:HD3	1:A:17:VAL:HG11	1.90	0.54
1:C:13:GLY:O	1:C:15:TYR:N	2.40	0.54
1:A:218:THR:HA	1:A:246:GLN:NE2	2.23	0.54
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.88	0.54
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.54
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.44	0.52
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.92	0.52
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.10	0.52
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.92	0.52
2:D:215:VAL:HG12	2:D:342:ILE:HD13	1.91	0.52
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.92	0.52
2:B:303:THR:O	2:B:304:PHE:HB2	2.10	0.51
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.93	0.51
1:C:130:PRO:HD3	1:C:192:ILE:HG12	1.94	0.50
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.93	0.50
1:A:60:HIS:HD2	1:A:62:ASN:H	1.60	0.49
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.95	0.49
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.40	0.49
2:B:416:SER:HB3	1:C:8:GLU:OE2	2.13	0.49
1:A:60:HIS:CD2	1:A:62:ASN:H	2.31	0.48
1:A:71:HIS:CE1	2:B:296:HIS:HD2	2.32	0.48
1:A:249:SER:HA	1:A:260:ARG:HD3	1.94	0.47
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.97	0.47
2:D:329:VAL:HG11	2:D:364:LEU:HD12	1.96	0.47
1:A:252:VAL:HB	1:A:255:LEU:HD22	1.96	0.47
1:C:162:GLU:CD	1:C:162:GLU:H	2.18	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:VAL:HB	1:C:169:ARG:HG3	1.97	0.47
1:A:162:GLU:CD	1:A:162:GLU:H	2.18	0.47
1:A:65:LYS:HE2	6:A:2009:HOH:O	2.14	0.46
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.50	0.46
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.82	0.45
1:A:71:HIS:NE2	2:B:296:HIS:HD2	2.12	0.45
2:B:347:TYR:OH	2:B:394:LEU:HA	2.16	0.45
2:D:277:GLU:O	2:D:281:ILE:HG13	2.16	0.45
1:A:60:HIS:HB3	1:A:63:ILE:HD12	1.98	0.45
2:D:213:ILE:HG22	3:I:92:LEU:HD22	1.99	0.45
1:A:126:ARG:NH2	1:A:150:ARG:HB3	2.31	0.44
1:C:220:GLY:HA3	1:C:245:ARG:HG2	1.99	0.44
1:C:181:SER:O	1:C:184:VAL:HG22	2.17	0.44
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.43
1:A:230:VAL:HA	1:A:233:MET:HE2	2.01	0.43
2:B:388:LYS:O	2:B:392:MET:HG2	2.18	0.43
2:D:250:ARG:HD3	6:I:2003:HOH:O	2.18	0.43
1:A:71:HIS:HA	1:A:76:LEU:HD12	1.99	0.43
1:C:88:LYS:HA	1:C:91:MET:HE2	2.00	0.43
1:C:154:VAL:HA	1:C:155:PRO:HA	1.86	0.43
1:C:5:GLN:HG2	1:C:22:ARG:NH1	2.34	0.43
2:D:190:GLU:N	2:D:309:PRO:HG2	2.33	0.43
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.01	0.43
2:D:254:GLN:HE21	2:D:282:THR:HG22	1.83	0.43
1:C:38:ASP:HB2	1:C:39:THR:H	1.59	0.43
1:A:41:THR:HB	1:A:42:GLU:H	1.73	0.43
1:C:17:VAL:HB	1:C:19:TYR:CE2	2.53	0.43
1:C:172:GLU:O	1:C:177:CYS:HB2	2.19	0.42
1:A:230:VAL:HG23	1:A:233:MET:CE	2.50	0.42
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.96	0.42
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.54	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.54	0.42
2:D:278:PHE:HA	2:D:281:ILE:HD11	2.00	0.42
2:D:210:MET:HE1	2:D:250:ARG:HB3	2.01	0.42
2:B:410:ARG:O	2:B:414:LYS:HG3	2.18	0.42
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.37	0.42
1:C:53:SER:HB3	2:D:304:PHE:O	2.20	0.42
2:D:334:MET:O	2:D:338:GLU:HB2	2.20	0.41
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.55	0.41
2:D:361:HIS:HB2	2:D:372:TRP:HB2	2.01	0.41
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.36	0.41
2:B:404:HIS:O	2:B:407:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:GLU:HG3	6:A:2029:HOH:O	2.19	0.41
1:A:195:GLU:O	1:A:199:ARG:HA	2.21	0.41
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.02	0.41
1:C:249:SER:HA	1:C:260:ARG:HD2	2.02	0.41
1:C:122:ARG:O	1:C:122:ARG:HD2	2.21	0.41
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.86	0.40
1:A:162:GLU:CD	1:A:162:GLU:N	2.75	0.40
1:A:248:PHE:CZ	1:A:264:SER:HA	2.56	0.40
2:D:236:VAL:HA	2:D:239:ILE:HD12	2.03	0.40
3:I:91:ARG:O	3:I:91:ARG:HG2	2.21	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.88	0.40
2:B:254:GLN:HB3	2:B:286:TYR:OH	2.21	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	294/299 (98%)	270 (92%)	18 (6%)	6 (2%)	11	28
1	C	294/299 (98%)	266 (90%)	26 (9%)	2 (1%)	30	62
2	B	256/258 (99%)	246 (96%)	9 (4%)	1 (0%)	43	76
2	D	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	43	76
3	F	15/30 (50%)	13 (87%)	1 (7%)	1 (7%)	2	2
3	I	10/30 (33%)	6 (60%)	3 (30%)	1 (10%)	1	1
All	All	1125/1174 (96%)	1040 (92%)	73 (6%)	12 (1%)	21	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
2	B	177	ASP
1	C	14	THR

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Mol	Chain	Res	Type
1	A	11	GLY
1	A	164	VAL
1	C	164	VAL
3	I	92	LEU
1	A	14	THR
3	F	68	HIS
1	A	38	ASP
1	A	145	ASP
2	D	281	ILE

### 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	261/263 (99%)	250 (96%)	11 (4%)	40	73
1	C	261/263 (99%)	245 (94%)	16 (6%)	26	54
2	B	232/232 (100%)	226 (97%)	6 (3%)	59	88
2	D	232/232 (100%)	223 (96%)	9 (4%)	43	76
3	F	17/26 (65%)	16 (94%)	1 (6%)	28	56
3	I	12/26 (46%)	9 (75%)	3 (25%)	1	2
All	All	1015/1042 (97%)	969 (96%)	46 (4%)	38	70

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	VAL
1	A	55	LEU
1	A	74	ASN
1	A	121	HIS
1	A	122	ARG
1	A	131	GLN
1	A	150	ARG
1	A	163	VAL
1	A	226	VAL

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Mol	Chain	Res	Type
1	A	255	LEU
2	B	175	VAL
2	B	232	LEU
2	B	274	GLU
2	B	292	LEU
2	B	348	LEU
2	B	429	THR
1	C	1	MET
1	C	22	ARG
1	C	38	ASP
1	C	42	GLU
1	C	78	LEU
1	C	120	SER
1	C	122	ARG
1	C	150	ARG
1	C	177	CYS
1	C	206	ASP
1	C	248	PHE
1	C	250	LYS
1	C	252	VAL
1	C	255	LEU
1	C	268	HIS
1	C	272	ASN
2	D	247	SER
2	D	284	ASP
2	D	292	LEU
2	D	293	ARG
2	D	348	LEU
2	D	368	THR
2	D	428	GLU
2	D	429	THR
2	D	431	ASN
3	F	72	ARG
3	I	70	SER
3	I	72	ARG
3	I	93	VAL

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

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	84	HIS
1	A	119	HIS
1	A	246	GLN
1	A	265	GLN
1	A	287	GLN
2	B	183	HIS
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	403	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN
2	D	233	HIS
2	D	317	GLN
2	D	425	ASN
3	F	85	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	A	160	1	10,10,11	6.52	5 (50%)	12,14,16	0.77	1 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	C	160	1	10,10,11	6.34	5 (50%)	12,14,16	1.10	2 (16%)

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	A	160	1	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	18.79	1.24	1.11
1	C	160	TPO	O-C	17.95	1.23	1.11
1	C	160	TPO	P-O1P	5.75	1.70	1.51
1	A	160	TPO	P-O1P	5.54	1.69	1.51
1	C	160	TPO	P-O2P	4.26	1.70	1.54
1	C	160	TPO	P-O3P	4.21	1.70	1.54
1	A	160	TPO	P-O3P	4.17	1.70	1.54
1	A	160	TPO	P-O2P	4.09	1.69	1.54
1	C	160	TPO	CA-C	2.80	1.53	1.48
1	A	160	TPO	CA-C	2.41	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	C-CA-N	-2.22	108.32	111.94
1	C	160	TPO	OG1-CB-CG2	-2.11	106.60	110.13
1	A	160	TPO	C-CA-N	-2.07	108.57	111.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	A	1297	5	33,33,33	1.06	2 (6%)	52,52,52	1.66	8 (15%)
4	ATP	C	1297	5	33,33,33	1.13	2 (6%)	52,52,52	1.57	8 (15%)

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	A	1297	5	-	0/22/38/38	0/1/3/3
4	ATP	C	1297	5	-	0/22/38/38	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1297	ATP	C5-C4	3.32	1.48	1.40
4	A	1297	ATP	C5-C4	3.29	1.47	1.40
4	C	1297	ATP	C4-N9	-2.51	1.34	1.37
4	A	1297	ATP	C4-N9	-2.38	1.34	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297	ATP	N3-C2-N1	-6.05	123.65	128.71
4	A	1297	ATP	N3-C4-N9	5.47	135.30	125.43
4	C	1297	ATP	N3-C4-N9	5.34	135.07	125.43
4	C	1297	ATP	N3-C2-N1	-5.33	124.25	128.71
4	A	1297	ATP	C5-C4-N3	-3.21	118.72	125.70
4	A	1297	ATP	PA-O3A-PB	-3.15	122.44	131.68
4	C	1297	ATP	C5-C4-N3	-3.07	119.02	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1297	ATP	C4-C5-N7	-3.00	106.95	109.52
4	A	1297	ATP	PB-O3B-PG	-2.91	123.14	131.68
4	A	1297	ATP	C4-C5-N7	-2.82	107.10	109.52
4	C	1297	ATP	C3'-C2'-C1'	2.48	104.79	100.91
4	A	1297	ATP	C2-N3-C4	2.41	120.87	114.01
4	A	1297	ATP	C3'-C2'-C1'	2.25	104.43	100.91
4	C	1297	ATP	C2'-C1'-N9	-2.24	107.52	113.27
4	C	1297	ATP	PB-O3B-PG	-2.22	125.19	131.68
4	C	1297	ATP	C2-N3-C4	2.12	120.05	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	297/299 (99%)	0.75	12 (4%) 36 41	30, 35, 46, 51	0
1	C	297/299 (99%)	1.23	63 (21%) 1 2	30, 38, 46, 48	0
2	B	258/258 (100%)	0.47	3 (1%) 75 81	31, 36, 41, 48	0
2	D	258/258 (100%)	1.11	43 (16%) 2 3	30, 37, 44, 49	0
3	F	19/30 (63%)	1.30	4 (21%) 1 2	42, 45, 56, 57	0
3	I	14/30 (46%)	1.70	5 (35%) 1 1	53, 61, 66, 66	0
All	All	1143/1174 (97%)	0.91	130 (11%) 6 6	30, 37, 46, 66	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	7.4
2	D	175	VAL	7.0
1	C	241	PRO	5.8
1	A	39	THR	5.6
1	C	289	VAL	5.0
1	C	213	PHE	5.0
1	C	245	ARG	5.0
1	A	71	HIS	4.8
2	D	367	VAL	4.8
1	A	40	GLU	4.7
2	D	429	THR	4.7
1	C	293	VAL	4.5
1	A	73	GLU	4.5
1	C	296	LEU	4.5
1	C	244	ALA	4.5
1	A	74	ASN	4.4
1	C	247	ASP	4.4
2	D	324	PRO	4.2
2	D	432	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	239	SER	4.0
2	D	425	ASN	3.9
1	C	137	THR	3.8
2	D	281	ILE	3.8
1	C	40	GLU	3.7
1	A	296	LEU	3.7
1	C	101	LEU	3.7
2	D	176	PRO	3.7
1	C	248	PHE	3.7
1	C	95	ALA	3.6
1	C	221	THR	3.6
1	A	295	HIS	3.6
2	D	325	ALA	3.5
2	D	323	GLN	3.5
2	B	175	VAL	3.5
1	C	243	TRP	3.5
2	D	197	VAL	3.4
1	C	295	HIS	3.4
2	D	399	LEU	3.4
1	C	242	LYS	3.4
1	C	74	ASN	3.3
3	I	86	THR	3.3
1	C	294	PRO	3.3
2	D	380	THR	3.3
1	C	288	ASP	3.2
1	C	73	GLU	3.2
1	C	225	VAL	3.2
2	D	383	THR	3.1
2	D	372	TRP	3.1
1	C	287	GLN	3.1
3	F	67	HIS	3.1
1	C	237	LYS	3.1
1	C	16	GLY	3.0
1	C	238	PRO	3.0
1	C	250	LYS	2.9
2	D	365	TYR	2.9
1	C	226	VAL	2.9
1	A	72	THR	2.8
2	D	428	GLU	2.8
2	D	180	GLU	2.8
1	C	198	THR	2.8
2	D	430	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	217	ARG	2.7
1	C	223	ASP	2.7
1	C	251	VAL	2.7
1	C	219	LEU	2.7
1	C	246	GLN	2.7
1	C	236	TYR	2.7
1	C	90	PHE	2.7
2	D	390	CYS	2.7
1	C	96	LEU	2.6
1	C	290	THR	2.6
2	D	395	HIS	2.6
1	C	200	ARG	2.6
1	C	255	LEU	2.6
1	C	218	THR	2.6
1	C	0	SER	2.6
1	C	216	PHE	2.6
3	I	93	VAL	2.6
2	D	379	LYS	2.6
3	F	95	ASP	2.6
1	C	212	LEU	2.5
1	C	209	ILE	2.5
1	A	38	ASP	2.5
2	D	278	PHE	2.5
1	C	235	ASP	2.5
1	C	38	ASP	2.5
1	C	206	ASP	2.4
3	I	73	LYS	2.4
1	C	100	PRO	2.4
1	C	240	PHE	2.4
1	C	249	SER	2.4
2	D	415	ASN	2.4
1	A	77	TYR	2.4
2	D	178	TYR	2.4
1	C	97	THR	2.4
2	D	397	THR	2.4
2	D	378	ARG	2.4
2	B	323	GLN	2.3
1	C	232	SER	2.3
2	D	375	SER	2.3
1	C	268	HIS	2.3
2	D	371	SER	2.3
1	C	222	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	292	PRO	2.2
2	D	391	LEU	2.2
2	D	369	GLY	2.2
2	D	368	THR	2.2
1	A	36	ARG	2.2
1	C	220	GLY	2.2
2	D	403	GLN	2.2
2	D	416	SER	2.2
3	I	92	LEU	2.2
2	D	332	LEU	2.2
3	F	85	HIS	2.2
2	D	427	PRO	2.2
2	B	177	ASP	2.2
2	D	420	GLY	2.2
1	C	15	TYR	2.1
3	F	86	THR	2.1
1	C	227	TRP	2.1
3	I	69	ALA	2.1
1	C	233	MET	2.1
2	D	402	PRO	2.1
2	D	421	VAL	2.1
2	D	280	TYR	2.1
2	D	357	GLY	2.1
2	D	431	ASN	2.1
1	A	97	THR	2.1
2	D	361	HIS	2.0
1	C	14	THR	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.20	-0.58	31,33,33,33	0
1	TPO	C	160	11/12	0.15	-1.33	35,36,36,36	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	C	1298	1/1	0.25	1.76	43,43,43,43	0
4	ATP	A	1297	31/31	0.19	-1.08	35,37,58,58	0
5	MG	A	1298	1/1	0.19	-1.11	38,38,38,38	0
4	ATP	C	1297	31/31	0.15	-1.43	32,36,55,56	0

### 6.5 Other polymers

There are no such residues in this entry.