



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 AM GMT

PDB ID : 2CCH  
Title : THE CRYSTAL STRUCTURE OF CDK2 CYCLIN A IN COMPLEX WITH  
A SUBSTRATE PEPTIDE DERIVED FROM CDC MODIFIED WITH A  
GAMMA-LINKED ATP ANALOGUE  
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togiannis, L.; Shen, K.; Cole, P.A.; Siligardi, G.; Johnson, L.N.  
Deposited on : 2006-01-16  
Resolution : 1.70 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

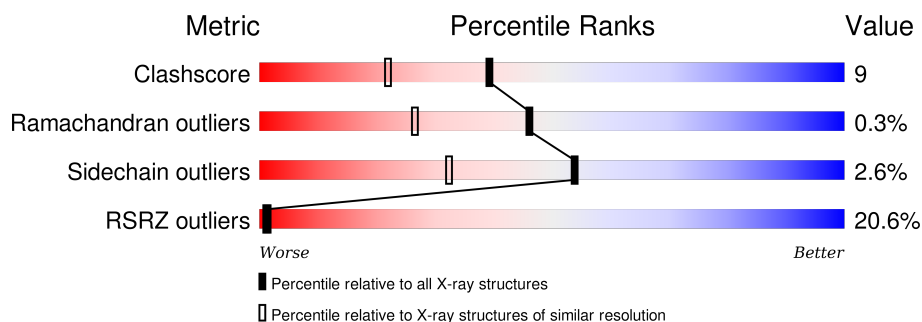
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	299	
1	C	299	
2	B	260	
2	D	260	
3	E	12	
3	F	12	

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
4	ATP	A	1297[A]	-	-	-	X
4	ATP	A	1297[B]	-	-	-	X
4	ATP	C	1297[A]	-	-	-	X
4	ATP	C	1297[B]	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10526 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	9	0
			2460	1592	415	443	1	9			
1	C	297	Total	C	N	O	P	S	0	3	0
			2408	1560	407	431	1	9			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S		0	11	0
			2180	1407	354	405	14				
2	D	256	Total	C	N	O	S		0	3	0
			2088	1351	340	384	13				

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

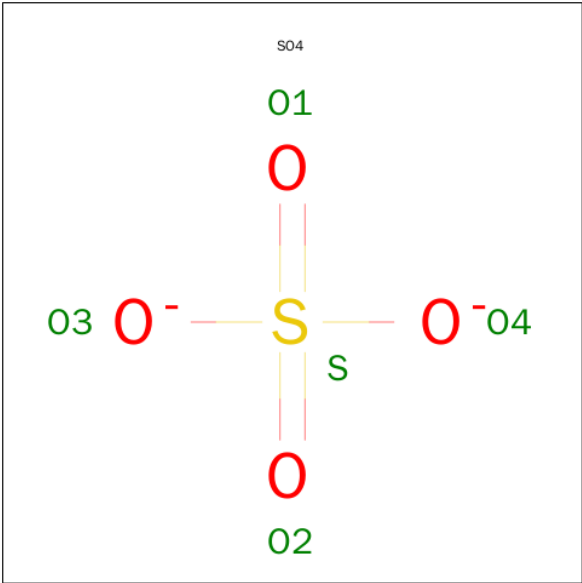
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	12	Total	C	N	O	0	0	0
			102	64	22	16			
3	F	12	Total	C	N	O	0	0	0
			102	64	22	16			

- 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	1
			62	20	10	26	6		
4	C	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

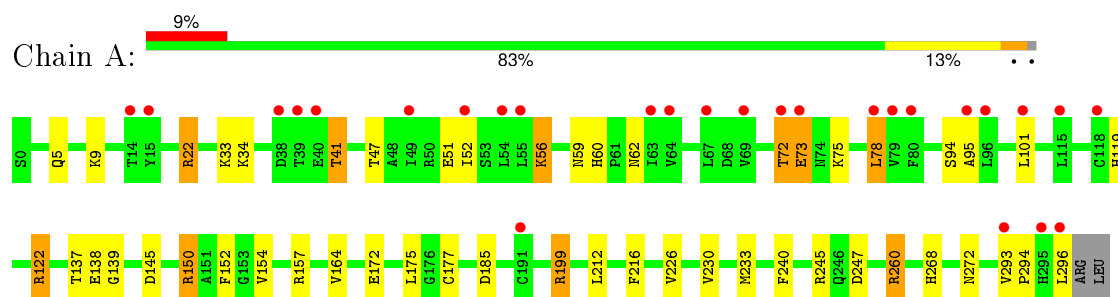
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	390	Total	O	0	0
			390	390		
7	B	327	Total	O	0	0
			327	327		
7	C	144	Total	O	0	0
			144	144		
7	D	160	Total	O	0	0
			160	160		
7	E	17	Total	O	0	0
			17	17		
7	F	7	Total	O	0	0
			7	7		

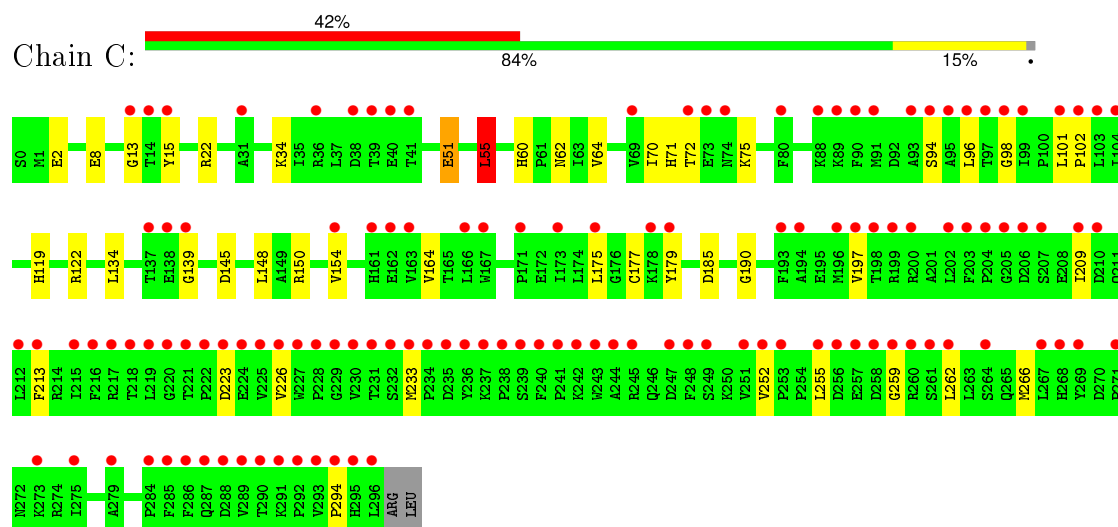
### 3 Residue-property plots [i](#)

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.

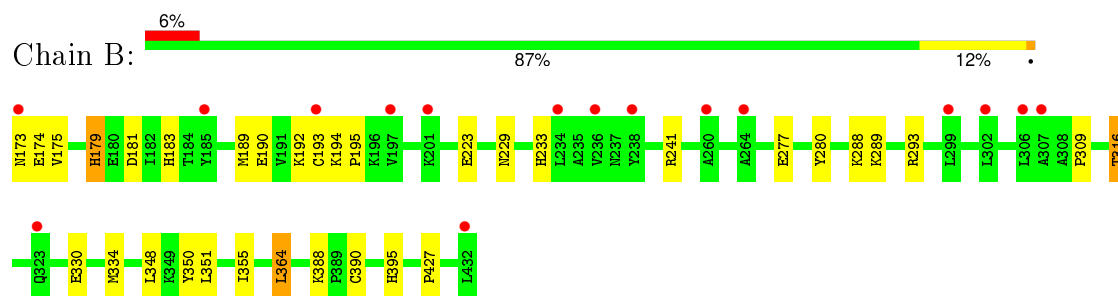
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



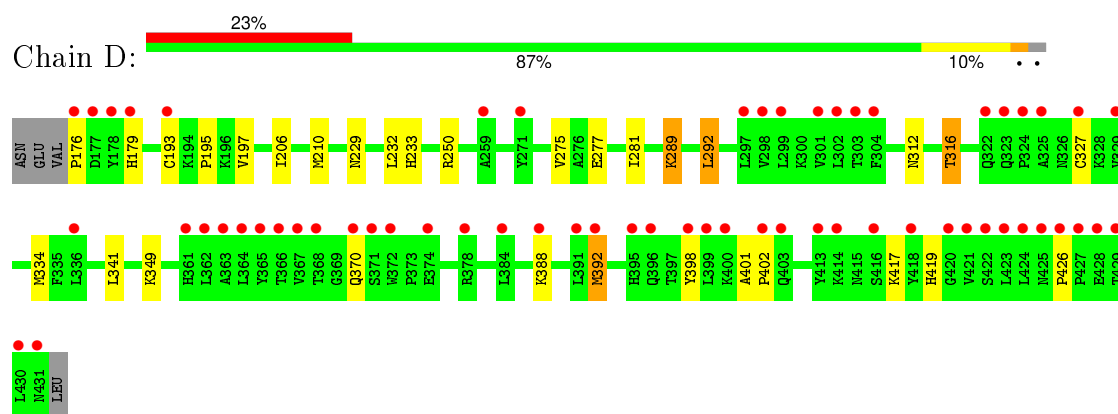
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



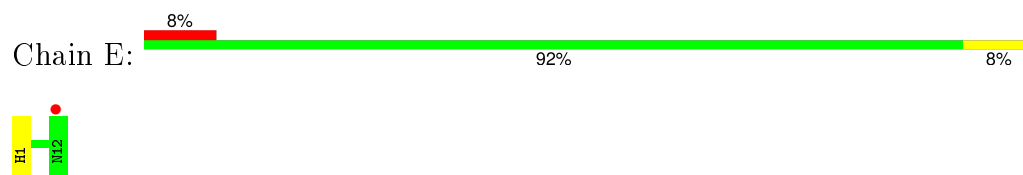
#### • Molecule 2: CYCLIN A2



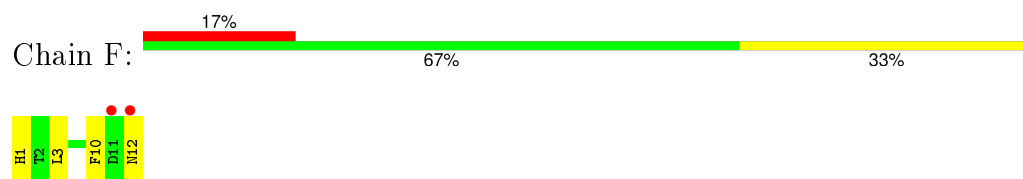
#### • Molecule 2: CYCLIN A2



- Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG



- Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.53Å 114.48Å 181.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.67 – 1.70 57.57 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.67-1.70) 98.0 (57.57-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.148 , 0.182 0.197 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 167293 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, GOL, SO4, 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	0.94	6/2511 (0.2%)	1.12	14/3407 (0.4%)
1	C	0.70	3/2458 (0.1%)	0.72	1/3335 (0.0%)
2	B	0.85	1/2230 (0.0%)	0.82	4/3027 (0.1%)
2	D	0.66	0/2138	0.69	0/2902
3	E	0.85	0/103	0.79	0/136
3	F	0.69	0/103	0.80	0/136
All	All	0.80	10/9543 (0.1%)	0.86	19/12943 (0.1%)

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	C	0	1
2	B	1	0
All	All	1	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ARG	CZ-NH1	7.63	1.43	1.33
1	C	51	GLU	CD-OE2	-7.39	1.17	1.25
2	B	316	THR	CB-CG2	-6.40	1.31	1.52
1	A	150	ARG	CB-CG	-5.95	1.36	1.52
1	C	2	GLU	CG-CD	5.84	1.60	1.51
1	A	157	ARG	CB-CG	-5.65	1.37	1.52
1	C	8	GLU	CB-CG	-5.54	1.41	1.52
1	A	260	ARG	CG-CD	5.31	1.65	1.51
1	A	51	GLU	CD-OE2	-5.19	1.20	1.25
1	A	260	ARG	CB-CG	-5.07	1.38	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	-21.27	109.66	120.30
1	A	260	ARG	NE-CZ-NH2	-20.14	110.23	120.30
1	A	199	ARG	NE-CZ-NH1	16.23	128.41	120.30
1	A	260	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	245	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	B	241	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	22	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	22	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	199	ARG	CG-CD-NE	-6.65	97.83	111.80
2	B	364	LEU	CB-CG-CD1	6.45	121.97	111.00
1	A	199	ARG	CD-NE-CZ	6.24	132.34	123.60
2	B	241	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	55	LEU	CB-CG-CD1	5.77	120.81	111.00
1	A	78	LEU	CB-CG-CD2	5.67	120.64	111.00
1	A	247	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	B	181	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	150	ARG	CA-CB-CG	5.48	125.45	113.40
1	A	150	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	240	PHE	CB-CG-CD1	5.20	124.44	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	316	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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	2460	0	2484	57	0
1	C	2408	0	2441	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2180	0	2189	33	0
2	D	2088	0	2106	46	0
3	E	102	0	108	1	0
3	F	102	0	108	7	0
4	A	62	0	24	7	0
4	C	62	0	24	4	0
5	A	5	0	0	1	0
6	A	12	0	15	0	0
7	A	390	0	0	23	1
7	B	327	0	0	12	0
7	C	144	0	0	5	0
7	D	160	0	0	12	0
7	E	17	0	0	0	0
7	F	7	0	0	0	0
All	All	10526	0	9499	170	1

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 9.

All (170) 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:177[A]:CYS:HB3	7:A:2213:HOH:O	1.35	1.25
1:C:64:VAL:HB	7:C:2065:HOH:O	1.43	1.16
1:A:177[B]:CYS:HB2	7:A:2213:HOH:O	1.54	1.07
1:A:175:LEU:HD13	1:A:233:MET:CE	1.93	0.99
2:D:334:MET:HG2	7:D:2105:HOH:O	1.61	0.99
1:A:101:LEU:HB3	7:A:2143:HOH:O	1.62	0.98
1:A:94:SER:O	1:A:199:ARG:HD3	1.66	0.95
1:A:230:VAL:HG23	1:A:233:MET:HE1	1.53	0.91
2:D:334:MET:HE3	7:D:2105:HOH:O	1.71	0.90
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:C5'	2.19	0.89
1:A:101:LEU:HD12	7:A:2039:HOH:O	1.72	0.89
1:C:190:GLY:HA2	1:C:266:MET:HE3	1.58	0.86
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.58	0.84
1:C:154:VAL:O	2:D:316:THR:HG23	1.77	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.26	0.82
1:A:154:VAL:O	2:B:316:THR:HG23	1.80	0.81
5:A:1298:SO4:O3	7:A:2386:HOH:O	1.98	0.80
1:A:101:LEU:HB3	7:A:2041:HOH:O	1.82	0.79
2:B:193[B]:CYS:HB3	7:B:2130:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:THR:HG21	7:B:2025:HOH:O	1.83	0.78
1:C:190:GLY:HA2	1:C:266:MET:CE	2.14	0.77
2:D:316:THR:HG21	7:D:2008:HOH:O	1.82	0.77
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.66	0.76
2:B:195:PRO:HD3	7:B:2127:HOH:O	1.85	0.76
1:A:172:GLU:O	1:A:177[B]:CYS:SG	2.43	0.75
2:D:197:VAL:N	7:D:2021:HOH:O	2.19	0.74
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.74
1:A:59:ASN:ND2	7:A:2076:HOH:O	2.20	0.73
1:A:230:VAL:HG23	1:A:233:MET:CE	2.17	0.73
2:D:229:ASN:HD22	2:D:334:MET:CE	2.04	0.70
2:B:350:TYR:HB2	2:B:355[B]:ILE:HD11	1.73	0.70
1:C:154:VAL:O	2:D:316:THR:CG2	2.39	0.69
1:A:22:ARG:HD3	7:A:2007:HOH:O	1.92	0.69
2:D:210:MET:CE	2:D:250:ARG:HB2	2.23	0.69
1:C:64:VAL:HG21	1:C:134:LEU:HD12	1.74	0.68
2:B:229:ASN:HD22	2:B:334[A]:MET:CE	2.06	0.68
2:D:232:LEU:C	2:D:232:LEU:HD13	2.14	0.68
1:A:175:LEU:CD1	1:A:233:MET:CE	2.72	0.68
4:A:1297[B]:ATP:H3'	7:A:2379:HOH:O	1.93	0.68
1:C:60:HIS:HD2	1:C:62:ASN:H	1.41	0.67
1:C:190:GLY:CA	1:C:266:MET:HE3	2.24	0.67
1:A:94:SER:O	1:A:199:ARG:CD	2.41	0.66
2:D:210:MET:CE	3:F:10:PHE:HB3	2.25	0.66
2:D:229:ASN:HD22	2:D:334:MET:HE1	1.61	0.64
1:C:51:GLU:OE2	7:C:2052:HOH:O	2.15	0.64
1:A:41:THR:HG22	2:B:288:LYS:HE2	1.80	0.63
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.80	0.63
1:A:268:HIS:ND1	7:A:2338:HOH:O	2.31	0.63
1:C:60:HIS:CD2	1:C:62:ASN:H	2.18	0.62
2:B:229:ASN:HD22	2:B:334[A]:MET:HE2	1.65	0.62
4:A:1297[B]:ATP:O1G	7:A:2380:HOH:O	2.16	0.61
1:A:272[B]:ASN:OD1	2:B:175:VAL:HB	2.00	0.60
1:A:119:HIS:HD2	7:B:2062:HOH:O	1.82	0.60
1:A:175:LEU:CD1	1:A:233:MET:HE1	2.30	0.60
1:A:101:LEU:HD13	7:A:2041:HOH:O	2.02	0.59
2:B:355[B]:ILE:HD13	2:B:390:CYS:SG	2.43	0.59
2:D:210:MET:HE1	2:D:250:ARG:CB	2.33	0.59
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:O5'	2.21	0.59
1:C:34:LYS:HE2	1:C:75:LYS:HD3	1.83	0.59
2:D:388:LYS:O	2:D:392:MET:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:A:233:MET:HE3	2.30	0.59
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:H5'1	2.02	0.58
1:A:33:LYS:NZ	7:A:2037:HOH:O	2.36	0.58
2:D:210:MET:CE	2:D:250:ARG:CB	2.82	0.58
1:A:101:LEU:CB	7:A:2041:HOH:O	2.44	0.57
2:B:395:HIS:HE1	2:B:427:PRO:O	1.87	0.57
2:B:193[B]:CYS:SG	2:B:309:PRO:HD2	2.45	0.57
2:D:232:LEU:CD1	2:D:341:LEU:HD13	2.34	0.57
2:D:232:LEU:HD11	2:D:341:LEU:HD13	1.86	0.57
2:B:189:MET:O	2:B:193[B]:CYS:SG	2.64	0.56
1:C:70:ILE:HG22	1:C:72:THR:OG1	2.06	0.56
1:A:145[B]:ASP:CG	4:A:1297[B]:ATP:O2B	2.45	0.55
2:B:183:HIS:HD2	7:B:2072:HOH:O	1.88	0.55
2:D:277:GLU:OE1	3:F:1:HIS:HE1	1.89	0.55
1:C:22:ARG:HD3	7:C:2030:HOH:O	2.06	0.55
1:A:34:LYS:HZ1	1:A:75:LYS:HE3	1.71	0.55
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.88	0.54
2:D:210:MET:HE3	2:D:250:ARG:HB2	1.90	0.54
4:A:1297[B]:ATP:C3'	7:A:2379:HOH:O	2.51	0.54
2:D:210:MET:HE3	3:F:10:PHE:HB3	1.89	0.54
2:D:289:LYS:HE2	7:D:2080:HOH:O	2.08	0.54
1:A:230:VAL:O	1:A:233:MET:HE2	2.08	0.53
1:C:119:HIS:HD2	7:C:2136:HOH:O	1.90	0.53
1:A:212[B]:LEU:HG	1:A:216:PHE:CZ	2.45	0.53
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:O3B	2.27	0.52
2:D:289:LYS:HD3	7:D:2084:HOH:O	2.10	0.52
2:B:277:GLU:OE1	3:E:1:HIS:HE1	1.91	0.52
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.40	0.52
1:A:73:GLU:N	7:A:2102:HOH:O	2.42	0.52
2:D:210:MET:HE2	3:F:10:PHE:HB3	1.92	0.52
2:B:229:ASN:HD22	2:B:334[B]:MET:CE	2.23	0.51
2:D:176:PRO:HA	2:D:179:HIS:CG	2.47	0.50
2:B:233:HIS:HE1	7:B:2220:HOH:O	1.93	0.50
2:B:233:HIS:HD2	7:B:2193:HOH:O	1.94	0.50
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.94	0.50
1:C:223:ASP:OD1	1:C:226:VAL:HG12	2.11	0.50
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.49
2:B:229:ASN:HD22	2:B:334[A]:MET:HE1	1.75	0.49
1:A:52:ILE:O	1:A:56:LYS:HG3	2.11	0.49
1:C:177[B]:CYS:SG	1:C:179:TYR:O	2.67	0.49
2:D:232:LEU:CD1	2:D:341:LEU:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HG	7:A:2142:HOH:O	2.13	0.49
1:C:94:SER:O	1:C:98:GLY:N	2.44	0.49
2:B:190:GLU:HA	2:B:193[B]:CYS:SG	2.53	0.49
2:B:223:GLU:OE1	7:B:2108:HOH:O	2.20	0.49
1:C:175:LEU:HB3	1:C:233:MET:HE3	1.95	0.48
2:B:194:LYS:HE2	2:B:351:LEU:HD23	1.94	0.48
2:B:289:LYS:HE2	2:B:293:ARG:CZ	2.43	0.48
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:H5'2	2.09	0.48
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:PB	2.72	0.48
1:A:47[B]:THR:HG23	7:A:2054:HOH:O	2.13	0.48
1:C:175:LEU:HD13	1:C:233:MET:CE	2.43	0.48
2:B:192:LYS:O	7:B:2080:HOH:O	2.20	0.47
2:D:327[B]:CYS:HB3	2:D:419:HIS:CE1	2.49	0.47
1:A:175:LEU:HB3	1:A:233:MET:HE3	1.97	0.47
1:A:101:LEU:CD1	7:A:2039:HOH:O	2.46	0.47
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.96	0.47
1:A:101:LEU:CD1	7:A:2041:HOH:O	2.61	0.47
2:B:174:GLU:OE2	2:B:179:HIS:HE1	1.97	0.47
1:A:145[B]:ASP:OD1	4:A:1297[B]:ATP:O2B	2.31	0.47
2:B:229:ASN:HD22	2:B:334[B]:MET:HE3	1.80	0.47
1:A:34:LYS:HE2	1:A:75:LYS:HD3	1.97	0.47
2:D:232:LEU:HD11	2:D:341:LEU:CD1	2.45	0.46
2:D:193[B]:CYS:O	2:D:193[B]:CYS:SG	2.73	0.46
2:D:233:HIS:HE1	7:D:2115:HOH:O	1.98	0.46
2:D:210:MET:HE2	3:F:10:PHE:CG	2.51	0.46
1:A:47[B]:THR:HG22	7:A:2052:HOH:O	2.15	0.46
2:B:330:GLU:O	2:B:334[A]:MET:HG3	2.15	0.45
2:B:174:GLU:OE2	2:B:179:HIS:CE1	2.69	0.45
1:C:175:LEU:HD13	1:C:233:MET:HE1	1.98	0.45
1:C:262:LEU:O	1:C:266:MET:HG3	2.17	0.45
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.99	0.45
2:D:232:LEU:HD13	2:D:232:LEU:O	2.16	0.44
1:A:34:LYS:HZ3	1:A:75:LYS:HG2	1.83	0.44
1:A:5:GLN:HG2	7:A:2007:HOH:O	2.16	0.44
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.33	0.44
1:C:209:ILE:HD11	1:C:213:PHE:CE1	2.52	0.44
1:C:13:GLY:N	1:C:15:TYR:CE2	2.86	0.44
2:D:233:HIS:HD2	7:D:2102:HOH:O	2.00	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
1:A:137:THR:HA	1:A:296:LEU:HD11	2.00	0.43
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:281:ILE:HD11	3:F:3:LEU:HD23	2.00	0.43
1:C:255:LEU:HG	1:C:259:GLY:HA3	2.00	0.43
2:D:334:MET:CE	7:D:2105:HOH:O	2.47	0.43
2:D:210:MET:HE1	2:D:250:ARG:HB3	2.01	0.43
2:D:195:PRO:HD3	7:D:2049:HOH:O	2.18	0.43
1:C:51:GLU:O	1:C:55:LEU:HB2	2.19	0.42
2:D:289:LYS:NZ	7:D:2080:HOH:O	2.52	0.42
1:A:137:THR:HG22	1:A:296:LEU:CD1	2.50	0.42
2:B:388:LYS:NZ	7:B:2273:HOH:O	2.53	0.42
1:C:145[B]:ASP:OD1	7:C:2094:HOH:O	2.22	0.42
1:A:72:THR:O	1:A:73:GLU:HB2	2.20	0.42
2:B:183:HIS:HE1	7:B:2201:HOH:O	2.03	0.41
2:D:206:ILE:HG22	2:D:210:MET:HE1	2.03	0.41
1:A:230:VAL:CG2	1:A:233:MET:CE	2.93	0.41
2:D:206:ILE:HA	2:D:210:MET:SD	2.60	0.41
2:D:401:ALA:N	2:D:402:PRO:CD	2.84	0.41
2:D:349:LYS:NZ	7:D:2126:HOH:O	2.54	0.41
2:D:232:LEU:C	2:D:232:LEU:CD1	2.85	0.41
2:B:194:LYS:HE2	2:B:351:LEU:HA	2.03	0.41
2:B:280:TYR:C	2:B:280:TYR:CD2	2.94	0.41
2:B:334[B]:MET:HE3	7:B:2220:HOH:O	2.19	0.41
1:A:138:GLU:HG3	7:A:2162:HOH:O	2.20	0.41
2:D:312:ASN:O	2:D:316:THR:HB	2.21	0.40
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.56	0.40
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.04	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.40
2:D:210:MET:HE2	3:F:10:PHE:CB	2.51	0.40
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2235:HOH:O	7:A:2386:HOH:O[4_555]	1.99	0.21



## 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	304/299 (102%)	297 (98%)	5 (2%)	2 (1%)	26	9
1	C	297/299 (99%)	287 (97%)	9 (3%)	1 (0%)	46	26
2	B	269/260 (104%)	267 (99%)	2 (1%)	0	100	100
2	D	257/260 (99%)	255 (99%)	2 (1%)	0	100	100
3	E	10/12 (83%)	10 (100%)	0	0	100	100
3	F	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
All	All	1147/1142 (100%)	1125 (98%)	19 (2%)	3 (0%)	46	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	164	VAL
1	C	164	VAL

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/263 (103%)	261 (96%)	10 (4%)	41	18
1	C	264/263 (100%)	259 (98%)	5 (2%)	65	46
2	B	245/234 (105%)	240 (98%)	5 (2%)	63	44
2	D	233/234 (100%)	227 (97%)	6 (3%)	54	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	10 (91%)	1 (9%)	12	2
All	All	1035/1016 (102%)	1008 (97%)	27 (3%)	54	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	41	THR
1	A	56	LYS
1	A	72	THR
1	A	78	LEU
1	A	122	ARG
1	A	150	ARG
1	A	226	VAL
1	A	260	ARG
1	A	293	VAL
2	B	173	ASN
2	B	179	HIS
2	B	348[A]	LEU
2	B	348[B]	LEU
2	B	364	LEU
1	C	55	LEU
1	C	96	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
2	D	289	LYS
2	D	292	LEU
2	D	316	THR
2	D	370	GLN
2	D	392	MET
2	D	417	LYS
3	F	12	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	119	HIS
2	B	173	ASN
2	B	179	HIS
2	B	183	HIS
2	B	229	ASN
2	B	233	HIS
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	113	GLN
1	C	119	HIS
2	D	183	HIS
2	D	233	HIS
2	D	296	HIS
2	D	317	GLN
2	D	395	HIS
2	D	425	ASN
3	E	1	HIS
3	F	1	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	A	160	1	8,10,11	0.66	0	7,14,16	0.85	0
1	TPO	C	160	1	8,10,11	1.01	0	7,14,16	1.35	0

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	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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$
4	ATP	A	1297[A]	-	24,33,33	1.05	2 (8%)	31,52,52	1.82	5 (16%)
4	ATP	A	1297[B]	1	24,33,33	1.14	3 (12%)	31,52,52	2.06	6 (19%)
5	SO4	A	1298	-	4,4,4	0.86	0	6,6,6	0.46	0
6	GOL	A	1299	-	5,5,5	1.17	0	5,5,5	0.50	0
6	GOL	A	1300	-	5,5,5	0.45	0	5,5,5	0.43	0
4	ATP	C	1297[A]	-	24,33,33	1.01	2 (8%)	31,52,52	1.97	6 (19%)
4	ATP	C	1297[B]	-	24,33,33	1.07	2 (8%)	31,52,52	1.88	5 (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
4	ATP	A	1297[A]	-	-	0/18/38/38	0/3/3/3
4	ATP	A	1297[B]	1	-	0/18/38/38	0/3/3/3
5	SO4	A	1298	-	-	0/0/0/0	0/0/0/0
6	GOL	A	1299	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1300	-	-	0/4/4/4	0/0/0/0
4	ATP	C	1297[A]	-	-	0/18/38/38	0/3/3/3
4	ATP	C	1297[B]	-	-	0/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1297[A]	ATP	O4'-C1'	2.01	1.43	1.41
4	A	1297[B]	ATP	C2-N3	2.16	1.36	1.32
4	A	1297[A]	ATP	O4'-C1'	2.30	1.44	1.41
4	C	1297[B]	ATP	O4'-C1'	2.46	1.44	1.41
4	A	1297[B]	ATP	O4'-C1'	2.77	1.44	1.41
4	A	1297[A]	ATP	C5-C4	3.26	1.47	1.40
4	C	1297[A]	ATP	C5-C4	3.27	1.47	1.40
4	C	1297[B]	ATP	C5-C4	3.27	1.47	1.40
4	A	1297[B]	ATP	C5-C4	3.32	1.48	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1297[B]	ATP	N3-C2-N1	-7.00	123.54	128.89
4	C	1297[A]	ATP	N3-C2-N1	-6.96	123.56	128.89
4	A	1297[A]	ATP	N3-C2-N1	-6.62	123.82	128.89
4	A	1297[B]	ATP	N3-C2-N1	-6.30	124.07	128.89
4	A	1297[B]	ATP	PA-O3A-PB	-5.81	116.40	132.73
4	A	1297[B]	ATP	PB-O3B-PG	-4.36	118.06	132.67
4	C	1297[A]	ATP	PA-O3A-PB	-4.10	121.22	132.73
4	A	1297[A]	ATP	C4-C5-N7	-3.58	106.19	109.48
4	A	1297[A]	ATP	PA-O3A-PB	-3.25	123.60	132.73
4	C	1297[B]	ATP	C2'-C1'-N9	-3.24	109.34	114.29
4	C	1297[A]	ATP	PB-O3B-PG	-3.05	122.45	132.67
4	C	1297[A]	ATP	C4-C5-N7	-3.04	106.68	109.48
4	A	1297[A]	ATP	PB-O3B-PG	-3.00	122.62	132.67
4	A	1297[B]	ATP	C4-C5-N7	-2.73	106.97	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1297[A]	ATP	C1'-N9-C4	-2.69	122.88	126.94
4	C	1297[B]	ATP	C4-C5-N7	-2.64	107.05	109.48
4	C	1297[A]	ATP	C2'-C1'-N9	-2.63	110.28	114.29
4	C	1297[B]	ATP	PB-O3B-PG	-2.60	123.94	132.67
4	C	1297[B]	ATP	PA-O3A-PB	-2.49	125.75	132.73
4	A	1297[A]	ATP	C1'-N9-C4	-2.32	123.44	126.94
4	A	1297[B]	ATP	C2'-C1'-N9	-2.03	111.19	114.29
4	A	1297[B]	ATP	C2'-C3'-C4'	2.15	107.04	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1297[B]	ATP	7	0
5	A	1298	SO4	1	0
4	C	1297[B]	ATP	4	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	296/299 (98%)	0.72	27 (9%) 11 13	9, 15, 36, 46	0
1	C	296/299 (98%)	2.25	126 (42%) 0 0	15, 31, 44, 60	0
2	B	260/260 (100%)	0.49	16 (6%) 24 26	11, 14, 26, 44	0
2	D	256/260 (98%)	1.20	61 (23%) 1 1	18, 25, 37, 53	0
3	E	12/12 (100%)	0.37	1 (8%) 14 16	18, 28, 41, 48	0
3	F	12/12 (100%)	1.13	2 (16%) 2 2	32, 41, 49, 54	0
All	All	1132/1142 (99%)	1.18	233 (20%) 1 1	9, 21, 41, 60	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	14.1
1	C	213	PHE	13.1
1	C	236	TYR	9.9
1	C	243	TRP	9.8
1	C	240	PHE	9.6
1	C	248	PHE	9.6
1	C	294	PRO	9.3
1	C	295	HIS	8.9
1	C	96	LEU	8.8
1	C	293	VAL	8.8
1	C	101	LEU	8.1
1	C	216	PHE	8.1
1	C	226	VAL	7.9
1	C	209	ILE	7.8
2	B	173	ASN	7.8
1	C	238	PRO	7.4
1	C	284	PRO	7.2
2	D	365	TYR	7.1
1	C	225	VAL	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	6.9
1	C	175	LEU	6.6
1	C	97	THR	6.4
1	C	15	TYR	6.3
1	C	244	ALA	6.3
1	C	220	GLY	6.2
1	C	242	LYS	6.1
1	C	217	ARG	6.0
2	D	323	GLN	6.0
2	D	364	LEU	6.0
1	C	292	PRO	5.9
2	D	430	LEU	5.9
1	C	198	THR	5.8
1	C	231	THR	5.8
1	C	287	GLN	5.7
2	D	431	ASN	5.6
1	C	221	THR	5.4
1	C	219	LEU	5.3
1	C	215	ILE	5.2
1	C	232	SER	5.2
1	C	251	VAL	5.2
1	C	98	GLY	5.2
1	C	212	LEU	5.1
1	C	290	THR	5.1
1	C	222	PRO	5.1
2	D	324	PRO	5.1
1	C	197	VAL	5.1
1	C	179	TYR	5.0
2	D	422	SER	5.0
1	C	252	VAL	4.9
1	A	295	HIS	4.9
1	C	257	GLU	4.8
1	C	255	LEU	4.8
1	A	72	THR	4.7
1	C	227	TRP	4.7
2	D	427	PRO	4.7
2	D	423	LEU	4.7
1	C	245	ARG	4.6
2	D	428	GLU	4.6
1	C	40	GLU	4.5
1	C	39	THR	4.5
1	A	95	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	239	SER	4.5
1	C	14	THR	4.4
1	C	237	LYS	4.4
1	C	269	TYR	4.4
1	C	235	ASP	4.4
1	A	296	LEU	4.3
2	D	193[A]	CYS	4.2
1	A	101	LEU	4.2
2	D	176	PRO	4.1
1	C	233	MET	4.1
1	C	206	ASP	4.1
1	C	202	LEU	4.1
2	D	177	ASP	4.1
2	D	424	LEU	4.0
2	D	392	MET	3.9
2	D	425	ASN	3.9
1	A	96	LEU	3.9
2	D	384	LEU	3.9
1	A	14	THR	3.9
2	D	366	THR	3.9
2	D	399	LEU	3.9
2	D	329	VAL	3.8
1	C	253	PRO	3.8
2	B	432	LEU	3.8
2	B	197	VAL	3.8
1	C	289	VAL	3.8
3	F	12	ASN	3.8
1	C	223	ASP	3.7
2	D	395	HIS	3.7
2	D	391[A]	LEU	3.6
1	C	200	ARG	3.6
2	D	325	ALA	3.6
2	D	302	LEU	3.6
1	A	73	GLU	3.6
1	C	288	ASP	3.5
1	C	241	PRO	3.5
1	C	73	GLU	3.5
1	C	95	ALA	3.5
2	D	372	TRP	3.5
1	C	161	HIS	3.5
1	C	264	SER	3.5
2	D	378	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	3.4
2	D	370	GLN	3.4
1	C	262	LEU	3.3
1	A	54	LEU	3.3
1	C	285	PHE	3.3
2	D	429	THR	3.3
1	C	205	GLY	3.3
1	A	15	TYR	3.3
2	B	193[A]	CYS	3.3
2	D	367	VAL	3.2
2	D	271	TYR	3.2
2	B	234	LEU	3.2
1	A	38	ASP	3.2
1	C	72	THR	3.2
1	C	218	THR	3.2
1	C	94	SER	3.2
1	C	167	TRP	3.2
1	C	90	PHE	3.2
1	C	13	GLY	3.1
2	D	421	VAL	3.1
1	C	204	PRO	3.1
1	C	178	LYS	3.1
2	D	322	GLN	3.1
1	C	194	ALA	3.1
2	D	361	HIS	3.1
1	C	247	ASP	3.1
1	C	91	MET	3.1
1	C	258	ASP	3.0
2	D	374	GLU	3.0
3	E	12	ASN	3.0
2	B	306	LEU	3.0
1	A	52	ILE	2.9
1	C	267	LEU	2.9
1	C	193	PHE	2.9
1	C	268	HIS	2.9
2	D	403	GLN	2.9
1	C	104	ILE	2.9
1	C	166	LEU	2.9
1	C	199	ARG	2.9
1	A	79	VAL	2.9
2	D	400	LYS	2.8
1	C	93	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	2.8
1	A	69	VAL	2.8
1	A	39	THR	2.8
2	D	416	SER	2.7
2	D	179	HIS	2.7
1	C	286	PHE	2.7
1	C	173	ILE	2.7
1	C	228	PRO	2.7
1	A	55	LEU	2.7
2	D	388	LYS	2.7
2	B	299	LEU	2.7
1	C	36	ARG	2.7
1	C	154	VAL	2.7
1	C	99	ILE	2.7
2	B	323	GLN	2.7
2	D	398	TYR	2.7
2	D	299	LEU	2.7
1	C	41	THR	2.6
2	D	301	VAL	2.6
1	C	279	ALA	2.6
1	C	89	LYS	2.6
1	C	273	LYS	2.6
1	C	74	ASN	2.6
1	C	88	LYS	2.6
1	C	203	PHE	2.6
1	C	229	GLY	2.6
2	D	178	TYR	2.6
1	C	163	VAL	2.6
1	C	291	LYS	2.5
1	C	102	PRO	2.5
2	D	368	THR	2.5
2	D	327[A]	CYS	2.5
2	D	413	TYR	2.5
2	B	307	ALA	2.5
2	D	363	ALA	2.5
2	B	238	TYR	2.5
2	B	236	VAL	2.5
2	D	402	PRO	2.5
1	C	224	GLU	2.5
1	C	171	PRO	2.4
1	C	249	SER	2.4
1	A	67	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	78	LEU	2.4
2	D	362	LEU	2.4
1	C	80	PHE	2.4
2	D	371	SER	2.4
2	D	420	GLY	2.4
2	D	297	LEU	2.3
1	C	138	GLU	2.3
1	C	139	GLY	2.3
2	D	418	TYR	2.3
2	D	303	THR	2.3
1	C	210	ASP	2.3
1	A	49	ILE	2.3
1	C	162	GLU	2.3
2	D	304	PHE	2.3
1	C	259	GLY	2.3
1	C	38	ASP	2.3
1	C	69	VAL	2.3
1	A	118	CYS	2.3
1	C	261	SER	2.2
1	C	260	ARG	2.2
2	D	336	LEU	2.2
2	D	426	PRO	2.2
3	F	11	ASP	2.2
1	A	64	VAL	2.2
2	B	201	LYS	2.2
1	C	207	SER	2.2
1	A	115	LEU	2.2
2	B	185	TYR	2.2
1	C	196	MET	2.2
1	C	230	VAL	2.2
1	C	31	ALA	2.1
2	D	298	VAL	2.1
1	A	80[A]	PHE	2.1
2	D	396	GLN	2.1
1	C	137	THR	2.1
1	A	191	CYS	2.1
2	B	264	ALA	2.1
2	D	259	ALA	2.1
2	B	302	LEU	2.0
1	A	63	ILE	2.0
1	C	275	ILE	2.0
1	A	293	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	260	ALA	2.0
1	C	103	LEU	2.0
1	C	271	PRO	2.0
2	D	414	LYS	2.0

## 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	TPO	A	160	11/12	0.99	0.12	-	9,10,12,12	0
1	TPO	C	160	11/12	0.94	0.11	-	26,28,30,31	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	A	1297[B]	31/31	0.63	0.29	4.51	63,68,79,79	31
4	ATP	C	1297[B]	31/31	0.62	0.37	3.71	65,70,79,79	31
4	ATP	C	1297[A]	31/31	0.62	0.37	3.10	64,68,78,78	31
4	ATP	A	1297[A]	31/31	0.63	0.29	2.91	62,64,74,75	31
6	GOL	A	1299	6/6	0.94	0.10	-0.67	15,17,21,21	0
6	GOL	A	1300	6/6	0.98	0.08	-2.76	11,14,15,16	0
5	SO4	A	1298	5/5	0.98	0.20	-	18,19,20,22	5

## 6.5 Other polymers

There are no such residues in this entry.