



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:36 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

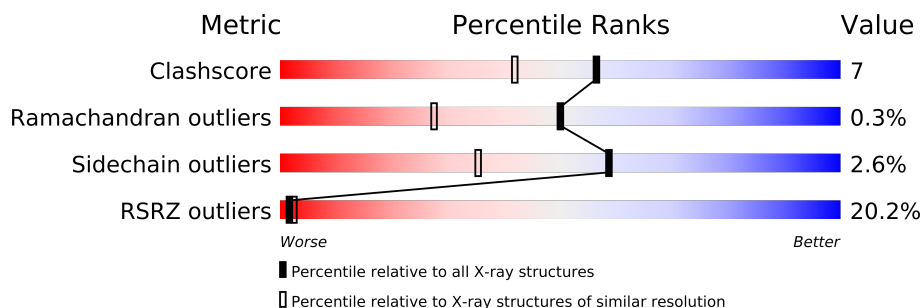
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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 ≥ 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	260	
2	D	260	
3	E	12	
3	F	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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
5	SO4	A	1298	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10526 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	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			

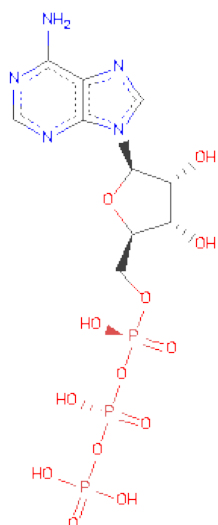
- Molecule 2 is a protein called CYCLIN A2.

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: C₁₀H₁₆N₅O₁₃P₃).



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: O₄S).



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: C₃H₈O₃).



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		

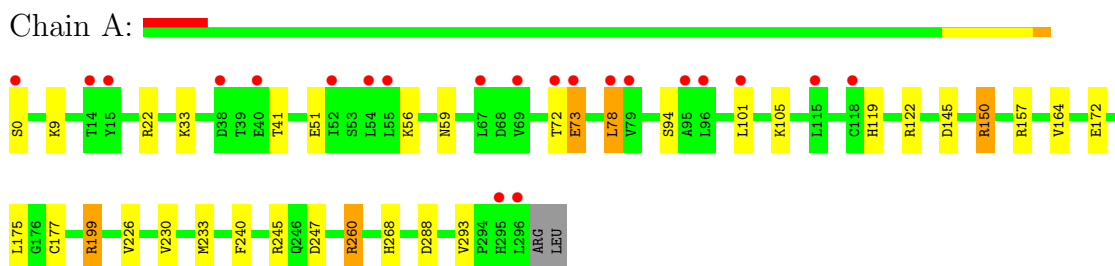
- Molecule 7 is water.

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		

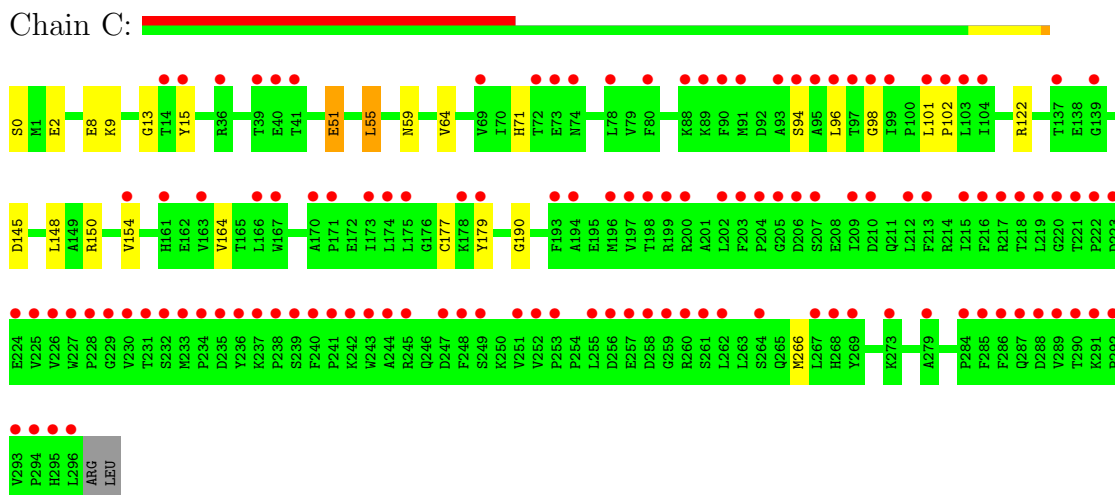
3 Residue-property plots

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.

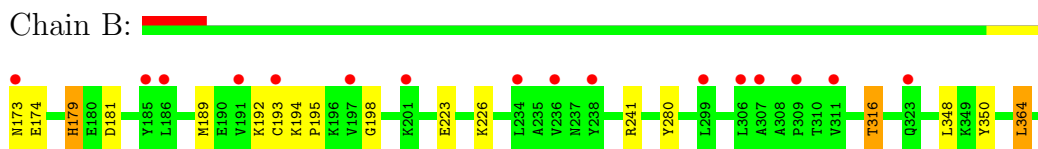
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



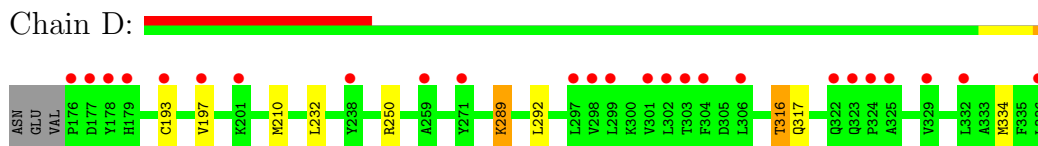
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

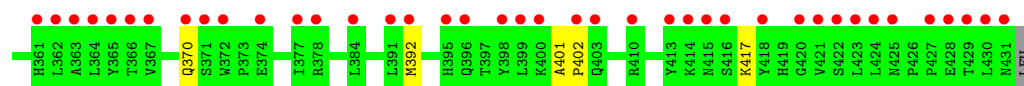


• Molecule 2: CYCLIN A2



• Molecule 2: CYCLIN A2





• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG

Chain E:



• Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.148 , 0.182 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities 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, 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 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	2460	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2408	0	0	14	0
2	B	2180	0	0	12	0
2	D	2088	0	0	13	0
3	E	102	0	0	0	0
3	F	102	0	0	0	0
4	A	62	0	0	6	0
4	C	62	0	0	2	0
5	A	5	0	0	1	0
6	A	12	0	0	0	0
7	A	390	0	0	14	1
7	B	327	0	0	9	0
7	C	144	0	0	6	0
7	D	160	0	0	7	0
7	E	17	0	0	0	0
7	F	7	0	0	0	0
All	All	10526	0	0	62	1

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 7.

All (62) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:C5'	2.19	0.89
1:A:177[A]:CYS:CB	7:A:2213:HOH:O	2.26	0.83
5:A:1298:SO4:O3	7:A:2386:HOH:O	1.98	0.80
2:B:193[B]:CYS:SG	7:B:2191:HOH:O	2.39	0.79
1:C:64:VAL:CB	7:C:2065:HOH:O	2.31	0.79
1:C:0:SER:N	7:C:2003:HOH:O	2.18	0.76
1:A:172:GLU:O	1:A:177[B]:CYS:SG	2.43	0.76
2:D:197:VAL:N	7:D:2021:HOH:O	2.19	0.74
1:A:59:ASN:ND2	7:A:2076:HOH:O	2.20	0.73
1:A:177[B]:CYS:CB	7:A:2213:HOH:O	2.38	0.71
1:C:154:VAL:O	2:D:316:THR:CG2	2.39	0.69
1:A:94:SER:O	1:A:199:ARG:CD	2.41	0.69
1:A:175:LEU:CD1	1:A:233:MET:CE	2.72	0.68
2:D:334:MET:CG	7:D:2105:HOH:O	2.44	0.66
1:A:101:LEU:CB	7:A:2041:HOH:O	2.44	0.66
1:A:101:LEU:CB	7:A:2143:HOH:O	2.45	0.64
1:C:51:GLU:OE2	7:C:2052:HOH:O	2.15	0.64
1:A:101:LEU:CD1	7:A:2039:HOH:O	2.46	0.64
2:B:198:GLY:N	7:B:2089:HOH:O	2.31	0.63
1:A:268:HIS:ND1	7:A:2338:HOH:O	2.31	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:334:MET:CE	7:D:2105:HOH:O	2.47	0.62
4:A:1297[B]:ATP:O1G	7:A:2380:HOH:O	2.16	0.61
1:A:0:SER:N	7:A:2001:HOH:O	2.35	0.60
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:O5'	2.21	0.59
1:C:59:ASN:ND2	7:C:2061:HOH:O	2.36	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
4:A:1297[B]:ATP:C3'	7:A:2379:HOH:O	2.51	0.57
2:B:189:MET:O	2:B:193[B]:CYS:SG	2.64	0.56
1:A:145[B]:ASP:CG	4:A:1297[B]:ATP:O2B	2.45	0.55
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:O3B	2.27	0.52
1:C:177[B]:CYS:SG	1:C:179:TYR:O	2.67	0.52
1:A:73:GLU:N	7:A:2102:HOH:O	2.42	0.52
1:C:94:SER:O	1:C:98:GLY:N	2.44	0.51
1:C:9:LYS:NZ	7:C:2016:HOH:O	2.46	0.49
2:D:232:LEU:CD1	2:D:341:LEU:CD1	2.90	0.49
2:B:223:GLU:OE1	7:B:2108:HOH:O	2.20	0.49
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:PB	2.72	0.48
2:B:192:LYS:O	7:B:2080:HOH:O	2.20	0.47
1:A:101:LEU:CD1	7:A:2041:HOH:O	2.61	0.47
1:A:145[B]:ASP:OD1	4:A:1297[B]:ATP:O2B	2.31	0.47
2:D:317:GLN:NE2	7:D:2110:HOH:O	2.46	0.47
1:A:230:VAL:CG2	1:A:233:MET:CE	2.93	0.47
2:D:193[B]:CYS:O	2:D:193[B]:CYS:SG	2.73	0.46
2:B:174:GLU:OE2	2:B:179:HIS:CE1	2.69	0.45
1:A:105:LYS:NZ	1:A:288:ASP:OD1	2.50	0.45
2:D:232:LEU:C	2:D:232:LEU:CD1	2.85	0.45
1:C:13:GLY:N	1:C:15:TYR:CE2	2.86	0.44
1:A:119:HIS:CD2	7:B:2062:HOH:O	2.71	0.43
2:D:289:LYS:NZ	7:D:2080:HOH:O	2.52	0.42
2:B:195:PRO:CD	7:B:2127:HOH:O	2.66	0.42
2:B:388:LYS:NZ	7:B:2273:HOH:O	2.53	0.42
2:B:316:THR:CG2	7:B:2025:HOH:O	2.67	0.42
1:C:145[B]:ASP:OD1	7:C:2094:HOH:O	2.22	0.42
2:D:401:ALA:N	2:D:402:PRO:CD	2.84	0.41
2:B:226:LYS:NZ	7:B:2114:HOH:O	2.54	0.41
2:D:349:LYS:NZ	7:D:2126:HOH:O	2.54	0.41
2:B:280:TYR:CD2	2:B:280:TYR:C	2.94	0.41
2:B:194:LYS:NZ	2:B:350:TYR:O	2.54	0.41
2:D:289:LYS:CE	7:D:2080:HOH:O	2.69	0.40
1:C:190:GLY:CA	1:C:266:MET:CE	2.99	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	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	Distance(Å)	Clash(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%)	30	10
1	C	297/299 (99%)	287 (97%)	9 (3%)	1 (0%)	50	27
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%)	50	27

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%)	45	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	264/263 (100%)	259 (98%)	5 (2%)	69	50
2	B	245/234 (105%)	240 (98%)	5 (2%)	68	47
2	D	233/234 (100%)	227 (97%)	6 (3%)	59	35
3	E	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	10 (91%)	1 (9%)	14	3
All	All	1035/1016 (102%)	1008 (97%)	27 (3%)	59	35

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. There are no such sidechains identified.

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	5.12	1 (10%)	12,14,16	0.74	0
1	TPO	C	160	1	10,10,11	6.16	2 (20%)	12,14,16	0.96	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	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	19.17	1.24	1.11
1	A	160	TPO	O-C	15.93	1.22	1.11
1	C	160	TPO	CA-C	2.20	1.52	1.48

There are no bond angle outliers.

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 ⓘ

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]	-	33,33,33	1.09	2 (6%)	52,52,52	1.66	8 (15%)
4	ATP	A	1297[B]	1	33,33,33	1.09	3 (9%)	52,52,52	1.98	11 (21%)
5	SO4	A	1298	-	4,4,4	0.88	0	6,6,6	0.47	0
6	GOL	A	1299	-	5,5,5	1.13	0	5,5,5	0.50	0
6	GOL	A	1300	-	5,5,5	0.44	0	5,5,5	0.44	0
4	ATP	C	1297[A]	-	33,33,33	1.07	2 (6%)	52,52,52	1.76	11 (21%)
4	ATP	C	1297[B]	-	33,33,33	1.10	2 (6%)	52,52,52	1.75	9 (17%)

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]	-	-	0/22/38/38	0/1/3/3
4	ATP	A	1297[B]	1	-	0/22/38/38	0/1/3/3
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]	-	-	0/22/38/38	0/1/3/3
4	ATP	C	1297[B]	-	-	0/22/38/38	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297[B]	ATP	C5-C4	3.32	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1297[B]	ATP	C5-C4	3.27	1.47	1.40
4	C	1297[A]	ATP	C5-C4	3.27	1.47	1.40
4	A	1297[A]	ATP	C5-C4	3.26	1.47	1.40
4	C	1297[A]	ATP	C4-N9	-3.23	1.33	1.37
4	A	1297[A]	ATP	C4-N9	-3.09	1.33	1.37
4	C	1297[B]	ATP	C4-N9	-2.26	1.34	1.37
4	A	1297[B]	ATP	O4'-C1'	2.18	1.44	1.41
4	A	1297[B]	ATP	C4-N9	-2.02	1.34	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297[B]	ATP	N3-C4-N9	6.21	136.65	125.43
4	C	1297[B]	ATP	N3-C2-N1	-6.18	123.54	128.71
4	C	1297[A]	ATP	N3-C2-N1	-6.15	123.56	128.71
4	A	1297[A]	ATP	N3-C2-N1	-5.84	123.82	128.71
4	A	1297[B]	ATP	N3-C2-N1	-5.55	124.07	128.71
4	C	1297[B]	ATP	N3-C4-N9	5.29	134.99	125.43
4	A	1297[B]	ATP	PA-O3A-PB	-5.21	116.40	131.68
4	A	1297[A]	ATP	N3-C4-N9	4.80	134.09	125.43
4	C	1297[A]	ATP	N3-C4-N9	4.67	133.86	125.43
4	A	1297[B]	ATP	PB-O3B-PG	-4.64	118.06	131.68
4	A	1297[A]	ATP	C4-C5-N7	-3.89	106.19	109.52
4	A	1297[B]	ATP	C5-C4-N3	-3.58	117.90	125.70
4	C	1297[A]	ATP	PA-O3A-PB	-3.57	121.22	131.68
4	C	1297[A]	ATP	C4-C5-N7	-3.32	106.68	109.52
4	C	1297[B]	ATP	C5-C4-N3	-3.18	118.78	125.70
4	C	1297[A]	ATP	PB-O3B-PG	-3.15	122.45	131.68
4	A	1297[A]	ATP	PB-O3B-PG	-3.09	122.62	131.68
4	C	1297[B]	ATP	O4'-C1'-N9	3.09	111.31	108.44
4	A	1297[A]	ATP	C5-C4-N3	-3.01	119.15	125.70
4	A	1297[B]	ATP	C4-C5-N7	-2.99	106.97	109.52
4	C	1297[B]	ATP	C4-C5-N7	-2.89	107.05	109.52
4	A	1297[A]	ATP	PA-O3A-PB	-2.76	123.60	131.68
4	C	1297[A]	ATP	C5-C4-N3	-2.73	119.75	125.70
4	C	1297[B]	ATP	C3'-C2'-C1'	2.70	105.14	100.91
4	C	1297[B]	ATP	PB-O3B-PG	-2.64	123.94	131.68
4	A	1297[B]	ATP	O4'-C1'-N9	2.59	110.85	108.44
4	C	1297[A]	ATP	O4'-C1'-N9	2.59	110.85	108.44
4	C	1297[A]	ATP	C8-N9-C4	2.59	108.88	106.90
4	C	1297[A]	ATP	C3'-C2'-C1'	2.58	104.95	100.91
4	A	1297[B]	ATP	O3A-PB-O3B	2.52	106.79	101.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1297[B]	ATP	C2-N3-C4	2.49	121.09	114.01
4	A	1297[B]	ATP	C2-N3-C4	2.46	121.01	114.01
4	A	1297[B]	ATP	C8-N9-C4	2.39	108.73	106.90
4	A	1297[A]	ATP	C2-N3-C4	2.39	120.82	114.01
4	C	1297[A]	ATP	C2-N3-C4	2.28	120.51	114.01
4	A	1297[A]	ATP	C8-N9-C4	2.27	108.63	106.90
4	A	1297[B]	ATP	C2'-C3'-C4'	2.20	107.04	102.65
4	C	1297[A]	ATP	C1'-N9-C4	-2.17	122.88	126.64
4	C	1297[B]	ATP	PA-O3A-PB	-2.02	125.75	131.68

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/299 (99%)	0.62	21 (7%) 16 19	9, 14, 36, 46	0
1	C	297/299 (99%)	2.22	122 (41%) 1 2	15, 31, 44, 60	0
2	B	260/260 (100%)	0.45	17 (6%) 18 23	11, 14, 26, 44	0
2	D	256/260 (98%)	1.27	65 (25%) 1 2	18, 25, 37, 53	0
3	E	12/12 (100%)	0.46	1 (8%) 11 14	18, 28, 41, 48	0
3	F	12/12 (100%)	1.09	2 (16%) 2 3	32, 41, 49, 54	0
All	All	1134/1142 (99%)	1.15	228 (20%) 2 2	9, 21, 41, 60	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	16.0
1	C	213	PHE	10.8
1	C	240	PHE	10.6
1	C	236	TYR	10.6
1	C	248	PHE	10.5
1	C	294	PRO	10.2
1	C	295	HIS	9.7
1	C	243	TRP	8.8
1	C	293	VAL	8.5
1	C	216	PHE	7.9
1	C	226	VAL	7.9
1	C	209	ILE	7.8
1	C	96	LEU	7.7
2	B	173	ASN	7.6
1	C	238	PRO	7.6
2	D	365	TYR	7.0
1	C	101	LEU	7.0
2	D	430	LEU	6.9
1	C	225	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	175	LEU	6.6
1	C	252	VAL	6.4
1	C	251	VAL	6.2
1	C	242	LYS	6.1
1	C	284	PRO	6.1
1	C	292	PRO	6.1
2	D	422	SER	6.0
1	C	198	THR	6.0
1	C	244	ALA	6.0
1	C	220	GLY	5.9
2	D	431	ASN	5.8
2	D	323	GLN	5.8
1	C	234	PRO	5.7
1	C	197	VAL	5.7
2	D	364	LEU	5.7
1	C	222	PRO	5.5
1	C	97	THR	5.4
1	C	221	THR	5.4
1	C	287	GLN	5.3
1	C	239	SER	5.3
1	C	219	LEU	5.3
2	D	423	LEU	5.2
1	C	212	LEU	5.2
1	C	255	LEU	5.1
1	C	217	ARG	5.1
1	C	245	ARG	5.0
1	C	231	THR	5.0
1	C	98	GLY	4.9
1	A	72	THR	4.9
1	C	215	ILE	4.8
1	C	237	LYS	4.8
2	D	372	TRP	4.7
1	C	269	TYR	4.6
2	D	384	LEU	4.5
1	C	90	PHE	4.5
1	C	227	TRP	4.4
2	D	176	PRO	4.4
1	C	73	GLU	4.4
1	C	206	ASP	4.4
2	B	432	LEU	4.4
1	C	15	TYR	4.3
2	D	427	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	202	LEU	4.3
1	A	95	ALA	4.3
1	C	257	GLU	4.3
1	C	232	SER	4.3
2	D	391[A]	LEU	4.2
2	D	302	LEU	4.2
2	D	324	PRO	4.2
3	F	12	ASN	4.2
1	C	235	ASP	4.2
2	D	193[A]	CYS	4.1
1	A	96	LEU	4.1
2	D	424	LEU	4.1
1	C	241	PRO	4.1
2	D	428	GLU	4.1
1	C	253	PRO	4.0
2	D	329	VAL	4.0
1	C	179	TYR	4.0
1	C	290	THR	4.0
2	D	399	LEU	3.9
2	D	177	ASP	3.9
1	A	101	LEU	3.8
1	C	40	GLU	3.8
1	C	194	ALA	3.8
1	A	73	GLU	3.7
1	A	295	HIS	3.6
2	D	374	GLU	3.6
1	C	233	MET	3.6
2	D	429	THR	3.6
1	A	296	LEU	3.6
2	D	378	ARG	3.5
2	D	366	THR	3.5
1	C	262	LEU	3.5
1	C	161	HIS	3.5
2	D	395	HIS	3.5
1	C	14	THR	3.5
1	A	14	THR	3.4
1	C	39	THR	3.4
1	C	264	SER	3.4
1	C	223	ASP	3.3
1	C	205	GLY	3.3
2	D	361	HIS	3.3
1	C	93	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	88	LYS	3.3
2	D	392	MET	3.3
2	D	367	VAL	3.3
1	A	38	ASP	3.3
1	C	72	THR	3.2
1	C	163	VAL	3.2
1	C	89	LYS	3.2
1	C	95	ALA	3.2
1	C	267	LEU	3.2
2	D	398	TYR	3.1
1	C	99	ILE	3.1
2	D	425	ASN	3.1
1	C	200	ARG	3.1
1	A	54	LEU	3.1
2	D	303	THR	3.1
2	B	193[A]	CYS	3.1
1	C	94	SER	3.1
1	C	258	ASP	3.1
2	D	400	LYS	3.1
1	C	173	ILE	3.1
3	E	12	ASN	3.1
1	C	167	TRP	3.1
2	D	299	LEU	3.1
1	C	218	THR	3.1
1	C	204	PRO	3.1
2	B	197	VAL	3.0
1	C	256	ASP	3.0
2	D	301	VAL	3.0
1	C	288	ASP	3.0
1	C	268	HIS	3.0
2	D	336	LEU	2.9
1	C	247	ASP	2.9
1	A	40	GLU	2.9
2	D	403	GLN	2.9
2	D	421	VAL	2.9
1	C	228	PRO	2.9
1	C	166	LEU	2.8
2	D	377	ILE	2.8
2	D	304	PHE	2.8
1	C	91	MET	2.8
1	A	15	TYR	2.8
2	B	234	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	199	ARG	2.8
2	D	322	GLN	2.8
2	D	362	LEU	2.8
2	D	325	ALA	2.8
1	C	178	LYS	2.8
2	D	402	PRO	2.8
2	D	370	GLN	2.7
1	C	193	PHE	2.7
1	A	55	LEU	2.7
1	C	273	LYS	2.7
1	C	289	VAL	2.7
2	D	420	GLY	2.7
1	A	52	ILE	2.7
2	D	259	ALA	2.7
2	D	271	TYR	2.6
1	C	69	VAL	2.6
2	D	298	VAL	2.6
1	C	285	PHE	2.6
1	C	104	ILE	2.6
1	C	80	PHE	2.6
1	C	229	GLY	2.6
2	D	371	SER	2.5
2	D	414	LYS	2.5
2	B	323	GLN	2.5
1	C	103	LEU	2.5
2	D	396	GLN	2.5
2	D	363	ALA	2.5
2	D	416	SER	2.4
1	C	286	PHE	2.4
2	B	306	LEU	2.4
1	C	203	PHE	2.4
1	C	224	GLU	2.4
1	C	260	ARG	2.4
1	C	279	ALA	2.4
2	B	238	TYR	2.3
1	C	230	VAL	2.3
1	C	139	GLY	2.3
1	A	0	SER	2.3
1	C	249	SER	2.3
1	C	137	THR	2.3
2	D	197	VAL	2.3
1	C	74	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	297	LEU	2.3
2	D	410	ARG	2.3
1	C	259	GLY	2.3
2	B	236	VAL	2.3
1	C	174	LEU	2.3
2	B	299	LEU	2.3
2	B	201	LYS	2.2
2	B	185	TYR	2.2
1	A	69	VAL	2.2
1	C	36	ARG	2.2
1	C	261	SER	2.2
2	D	306	LEU	2.2
2	D	332	LEU	2.2
2	D	413	TYR	2.2
1	C	78	LEU	2.2
1	C	102	PRO	2.2
1	C	171	PRO	2.2
1	C	210	ASP	2.2
1	C	41	THR	2.2
1	A	79	VAL	2.2
2	D	201	LYS	2.2
1	A	118	CYS	2.2
2	B	307	ALA	2.2
2	D	179	HIS	2.1
1	C	291	LYS	2.1
2	D	238	TYR	2.1
1	A	67	LEU	2.1
2	B	186	LEU	2.1
2	B	309	PRO	2.1
2	D	415	ASN	2.1
1	C	207	SER	2.1
1	A	78	LEU	2.1
1	A	115	LEU	2.1
2	D	178	TYR	2.0
3	F	11	ASP	2.0
1	C	196	MET	2.0
1	C	170	ALA	2.0
1	C	154	VAL	2.0
2	B	191	VAL	2.0
2	B	311	VAL	2.0
2	D	418	TYR	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, 95th 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 ²)	Q<0.9
1	TPO	A	160	11/12	0.11	-0.20	9,10,12,12	0
1	TPO	C	160	11/12	0.10	-0.73	26,28,30,31	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, 95th 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 ²)	Q<0.9
5	SO4	A	1298	5/5	0.21	4.42	18,19,20,22	5
4	ATP	A	1297[B]	31/31	0.27	4.29	63,68,79,79	31
4	ATP	C	1297[B]	31/31	0.37	3.74	65,70,79,79	31
4	ATP	C	1297[A]	31/31	0.37	3.34	64,68,78,78	31
4	ATP	A	1297[A]	31/31	0.27	2.35	62,64,74,75	31
6	GOL	A	1299	6/6	0.10	-0.23	15,17,21,21	0
6	GOL	A	1300	6/6	0.08	-2.40	11,14,15,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.