



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:35 pm GMT

PDB ID : 2B53
Title : Human cyclin dependent kinase 2 (CDK2) complexed with DIN-234325
Authors : Muckelbauer, J.
Deposited on : 2005-09-27
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

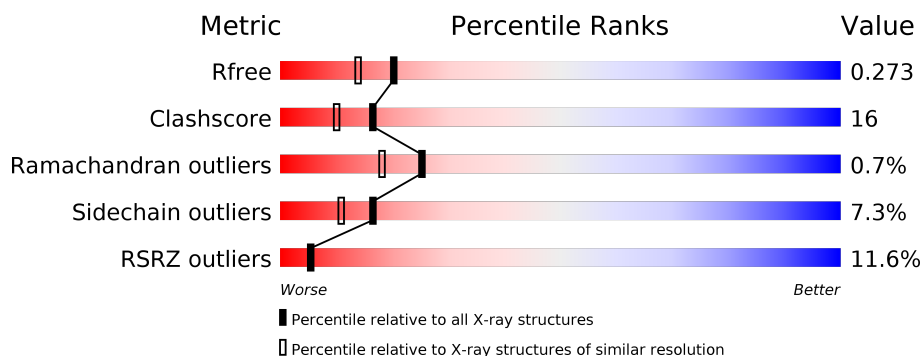
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	298	

2 Entry composition [i](#)

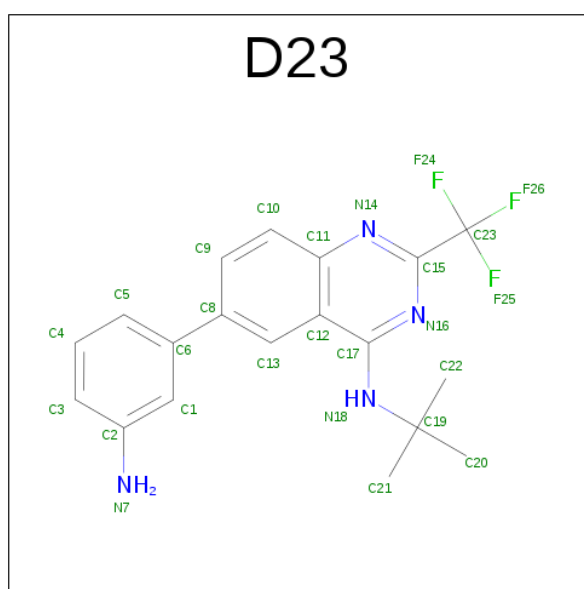
There are 3 unique types of molecules in this entry. The entry contains 2465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	294	Total	C	N	O	S	0	0	0
			2366	1540	404	414	8			

- Molecule 2 is 6-(3-AMINOPHENYL)-N-(TERT-BUTYL)-2-(TRIFLUOROMETHYL)QUINAZOLIN-4-AMINE (three-letter code: D23) (formula: C₁₉H₁₉F₃N₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			26	19	3	4		

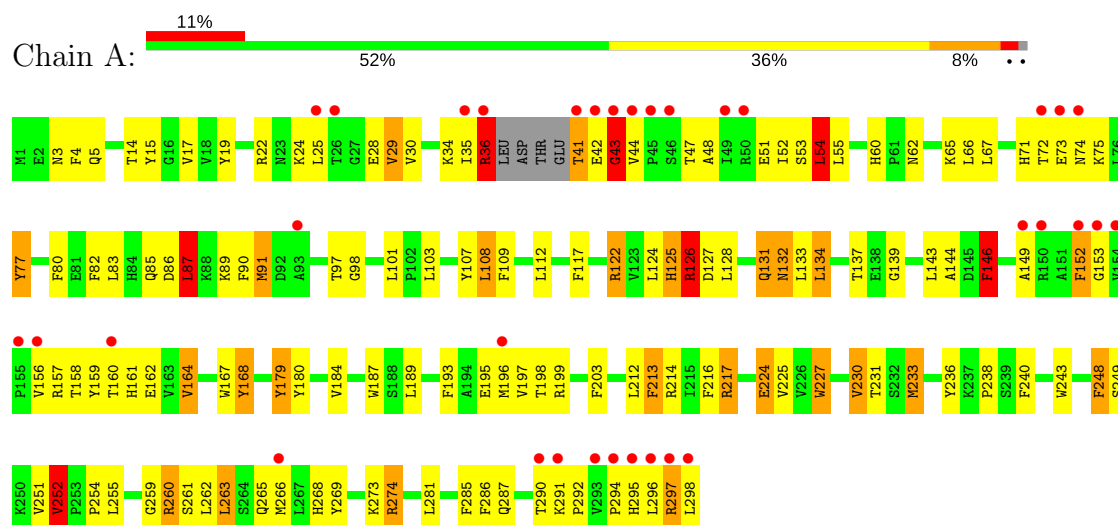
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total 73 O 73	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Cell division protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.96Å 73.51Å 54.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.98 – 2.00 24.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (18.98-2.00) 96.1 (24.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 1.99Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.223 , 0.273 0.230 , 0.273	Depositor DCC
R_{free} test set	1896 reflections (10.93%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2465	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D23

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	1.50	80/2428 (3.3%)	1.86	69/3294 (2.1%)

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	A	0	12

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	TRP	CD2-CE2	7.11	1.49	1.41
1	A	216	PHE	CG-CD1	7.07	1.49	1.38
1	A	243	TRP	CD2-CE2	7.05	1.49	1.41
1	A	187	TRP	CD2-CE2	6.73	1.49	1.41
1	A	77	TYR	CE1-CZ	6.45	1.47	1.38
1	A	159	TYR	CE2-CZ	6.31	1.46	1.38
1	A	236	TYR	CE1-CZ	6.31	1.46	1.38
1	A	107	TYR	CG-CD1	6.27	1.47	1.39
1	A	15	TYR	CE2-CZ	6.27	1.46	1.38
1	A	179	TYR	CE2-CZ	6.13	1.46	1.38
1	A	107	TYR	CE2-CZ	6.10	1.46	1.38
1	A	236	TYR	CG-CD2	6.08	1.47	1.39
1	A	193	PHE	CG-CD2	6.07	1.47	1.38
1	A	15	TYR	CG-CD1	6.00	1.47	1.39
1	A	77	TYR	CE2-CZ	5.97	1.46	1.38
1	A	107	TYR	CG-CD2	5.96	1.46	1.39
1	A	168	TYR	CE1-CZ	5.93	1.46	1.38
1	A	19	TYR	CE2-CZ	5.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	TRP	CZ2-CH2	5.87	1.48	1.37
1	A	179	TYR	CE1-CZ	5.83	1.46	1.38
1	A	269	TYR	CG-CD1	5.73	1.46	1.39
1	A	82	PHE	CG-CD1	5.73	1.47	1.38
1	A	117	PHE	CG-CD2	5.65	1.47	1.38
1	A	213	PHE	CG-CD1	5.64	1.47	1.38
1	A	19	TYR	CE1-CZ	5.63	1.45	1.38
1	A	167	TRP	CE3-CZ3	5.63	1.48	1.38
1	A	4	PHE	CG-CD2	5.63	1.47	1.38
1	A	236	TYR	CE2-CZ	5.61	1.45	1.38
1	A	180	TYR	CE2-CZ	5.60	1.45	1.38
1	A	80	PHE	CG-CD2	5.57	1.47	1.38
1	A	15	TYR	CG-CD2	5.56	1.46	1.39
1	A	152	PHE	CG-CD2	5.56	1.47	1.38
1	A	187	TRP	CE3-CZ3	5.54	1.47	1.38
1	A	203	PHE	CG-CD1	5.54	1.47	1.38
1	A	227	TRP	CZ2-CH2	5.54	1.47	1.37
1	A	179	TYR	CG-CD1	5.54	1.46	1.39
1	A	240	PHE	CG-CD1	5.53	1.47	1.38
1	A	269	TYR	CE2-CZ	5.52	1.45	1.38
1	A	152	PHE	CG-CD1	5.50	1.47	1.38
1	A	168	TYR	CG-CD1	5.50	1.46	1.39
1	A	80	PHE	CG-CD1	5.49	1.47	1.38
1	A	227	TRP	CE3-CZ3	5.47	1.47	1.38
1	A	91	MET	CG-SD	5.47	1.95	1.81
1	A	107	TYR	CE1-CZ	5.47	1.45	1.38
1	A	179	TYR	CG-CD2	5.46	1.46	1.39
1	A	167	TRP	CZ2-CH2	5.44	1.47	1.37
1	A	227	TRP	CD2-CE2	5.44	1.47	1.41
1	A	159	TYR	CG-CD1	5.43	1.46	1.39
1	A	77	TYR	CG-CD2	5.43	1.46	1.39
1	A	15	TYR	CE1-CZ	5.38	1.45	1.38
1	A	243	TRP	CZ2-CH2	5.37	1.47	1.37
1	A	243	TRP	CE3-CZ3	5.37	1.47	1.38
1	A	159	TYR	CE1-CZ	5.35	1.45	1.38
1	A	248	PHE	CG-CD1	5.34	1.46	1.38
1	A	19	TYR	CG-CD2	5.33	1.46	1.39
1	A	168	TYR	CG-CD2	5.33	1.46	1.39
1	A	196	MET	CG-SD	5.31	1.95	1.81
1	A	117	PHE	CG-CD1	5.29	1.46	1.38
1	A	233	MET	CG-SD	5.29	1.94	1.81
1	A	213	PHE	CG-CD2	5.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	PHE	CE2-CZ	5.26	1.47	1.37
1	A	286	PHE	CG-CD1	5.25	1.46	1.38
1	A	269	TYR	CG-CD2	5.24	1.46	1.39
1	A	285	PHE	CG-CD1	5.23	1.46	1.38
1	A	286	PHE	CE1-CZ	5.20	1.47	1.37
1	A	90	PHE	CG-CD1	5.19	1.46	1.38
1	A	180	TYR	CE1-CZ	5.19	1.45	1.38
1	A	240	PHE	CE1-CZ	5.19	1.47	1.37
1	A	152	PHE	CE2-CZ	5.17	1.47	1.37
1	A	203	PHE	CE2-CZ	5.14	1.47	1.37
1	A	248	PHE	CE2-CZ	5.14	1.47	1.37
1	A	180	TYR	CG-CD2	5.11	1.45	1.39
1	A	168	TYR	CE2-CZ	5.08	1.45	1.38
1	A	236	TYR	CG-CD1	5.08	1.45	1.39
1	A	109	PHE	CG-CD2	5.08	1.46	1.38
1	A	266	MET	CG-SD	5.08	1.94	1.81
1	A	285	PHE	CG-CD2	5.08	1.46	1.38
1	A	4	PHE	CE1-CZ	5.03	1.47	1.37
1	A	19	TYR	CG-CD1	5.03	1.45	1.39
1	A	82	PHE	CG-CD2	5.02	1.46	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	TYR	CB-CG-CD1	-16.54	111.08	121.00
1	A	180	TYR	CB-CG-CD1	-14.22	112.47	121.00
1	A	107	TYR	CB-CG-CD2	-12.72	113.37	121.00
1	A	159	TYR	CB-CG-CD2	-11.62	114.03	121.00
1	A	252	VAL	CA-CB-CG2	-11.25	94.03	110.90
1	A	248	PHE	CB-CG-CD1	-11.22	112.95	120.80
1	A	269	TYR	CB-CG-CD1	-10.99	114.41	121.00
1	A	184	VAL	CA-CB-CG2	-10.09	95.76	110.90
1	A	152	PHE	CB-CG-CD1	-9.11	114.42	120.80
1	A	252	VAL	CA-CB-CG1	9.01	124.41	110.90
1	A	216	PHE	CB-CG-CD2	-8.83	114.62	120.80
1	A	146	PHE	CB-CG-CD2	-8.60	114.78	120.80
1	A	230	VAL	CA-CB-CG1	-8.29	98.46	110.90
1	A	273	LYS	C-N-CA	-8.21	101.18	121.70
1	A	168	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	193	PHE	CB-CG-CD1	-8.08	115.14	120.80
1	A	179	TYR	CB-CG-CD2	-8.06	116.16	121.00
1	A	240	PHE	CB-CG-CD2	-8.05	115.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	TYR	CB-CG-CD1	-7.67	116.40	121.00
1	A	77	TYR	CD1-CG-CD2	7.14	125.76	117.90
1	A	19	TYR	CD1-CG-CD2	7.14	125.75	117.90
1	A	184	VAL	CA-CB-CG1	7.12	121.57	110.90
1	A	236	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	A	91	MET	CG-SD-CE	-7.07	88.90	100.20
1	A	15	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	125	HIS	C-N-CA	6.87	138.87	121.70
1	A	179	TYR	CD1-CG-CD2	6.75	125.32	117.90
1	A	203	PHE	CB-CG-CD2	-6.73	116.09	120.80
1	A	213	PHE	CB-CG-CD2	-6.67	116.13	120.80
1	A	43	GLY	C-N-CA	-6.65	105.08	121.70
1	A	15	TYR	CD1-CG-CD2	6.63	125.19	117.90
1	A	230	VAL	CA-CB-CG2	6.56	120.74	110.90
1	A	36	ARG	CD-NE-CZ	-6.38	114.66	123.60
1	A	281	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	A	30	VAL	CA-CB-CG2	-6.31	101.43	110.90
1	A	82	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	A	117	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	A	180	TYR	CD1-CG-CD2	6.27	124.79	117.90
1	A	168	TYR	CD1-CG-CD2	6.23	124.75	117.90
1	A	224	GLU	C-N-CA	-6.19	106.22	121.70
1	A	77	TYR	CG-CD1-CE1	-6.15	116.38	121.30
1	A	236	TYR	CD1-CG-CD2	6.08	124.59	117.90
1	A	159	TYR	CD1-CG-CD2	6.07	124.58	117.90
1	A	260	ARG	CD-NE-CZ	-5.99	115.21	123.60
1	A	19	TYR	CG-CD2-CE2	-5.93	116.56	121.30
1	A	249	SER	C-N-CA	-5.87	107.03	121.70
1	A	29	VAL	CA-CB-CG2	-5.85	102.12	110.90
1	A	269	TYR	CD1-CG-CD2	5.81	124.29	117.90
1	A	107	TYR	CD1-CG-CD2	5.79	124.26	117.90
1	A	214	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	153	GLY	C-N-CA	5.61	135.72	121.70
1	A	199	ARG	CD-NE-CZ	-5.57	115.80	123.60
1	A	168	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	A	274	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	15	TYR	CG-CD2-CE2	-5.53	116.88	121.30
1	A	77	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	A	212	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	A	274	ARG	CB-CG-CD	-5.35	97.69	111.60
1	A	180	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	A	87	LEU	CB-CG-CD1	-5.22	102.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	263	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	A	269	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	A	15	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	17	VAL	O-C-N	5.09	130.85	122.70
1	A	164	VAL	C-N-CA	-5.06	109.04	121.70
1	A	217	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	A	179	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	A	53	SER	C-N-CA	-5.01	109.16	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain
1	A	126	ARG	Sidechain
1	A	152	PHE	Peptide
1	A	168	TYR	Sidechain
1	A	179	TYR	Sidechain
1	A	22	ARG	Sidechain
1	A	260	ARG	Sidechain
1	A	295	HIS	Peptide
1	A	36	ARG	Sidechain
1	A	43	GLY	Peptide
1	A	54	LEU	Peptide
1	A	72	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2366	0	2422	77	0
2	A	26	0	19	2	0
3	A	73	0	0	1	0
All	All	2465	0	2441	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 16.

All (77) 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:51:GLU:O	1:A:54:LEU:HD22	1.78	0.83
1:A:89:LYS:HG2	2:A:299:D23:HN72	1.45	0.81
1:A:125:HIS:HD2	1:A:127:ASP:H	1.32	0.75
1:A:139:GLY:HA2	1:A:294:PRO:HD2	1.67	0.75
1:A:14:THR:HG23	1:A:158:THR:HG22	1.69	0.75
1:A:44:VAL:HG22	1:A:71:HIS:CE1	2.22	0.73
1:A:290:THR:OG1	1:A:292:PRO:HD3	1.92	0.69
1:A:108:LEU:O	1:A:112:LEU:HB2	1.94	0.67
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.24	0.67
1:A:227:TRP:O	1:A:230:VAL:HG23	1.94	0.67
1:A:34:LYS:HE3	1:A:77:TYR:HE1	1.60	0.66
1:A:224:GLU:OE1	1:A:231:THR:HB	2.00	0.62
1:A:3:ASN:HD22	1:A:25:LEU:HD13	1.65	0.62
1:A:137:THR:OG1	1:A:298:LEU:HD11	2.00	0.61
1:A:227:TRP:CG	1:A:230:VAL:HG22	2.36	0.60
1:A:297:ARG:NE	1:A:297:ARG:HA	2.18	0.59
1:A:125:HIS:HE1	1:A:144:ALA:O	1.87	0.57
1:A:139:GLY:HA2	1:A:294:PRO:CD	2.35	0.57
1:A:34:LYS:HE3	1:A:77:TYR:CE1	2.40	0.56
1:A:86:ASP:OD1	1:A:89:LYS:HD3	2.07	0.55
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.89	0.55
1:A:73:GLU:N	1:A:74:ASN:HA	2.22	0.55
1:A:297:ARG:HA	1:A:297:ARG:HE	1.72	0.55
1:A:252:VAL:CG1	1:A:255:LEU:HD12	2.37	0.55
1:A:43:GLY:HA2	1:A:74:ASN:OD1	2.07	0.54
1:A:85:GLN:HG2	1:A:86:ASP:N	2.23	0.54
1:A:87:LEU:HD22	1:A:91:MET:HG3	1.90	0.53
1:A:125:HIS:O	1:A:149:ALA:HB3	2.09	0.53
1:A:197:VAL:HG23	1:A:198:THR:HG23	1.89	0.53
1:A:268:HIS:HB2	1:A:274:ARG:HB3	1.91	0.53
1:A:54:LEU:HD23	1:A:55:LEU:N	2.24	0.53
1:A:60:HIS:HD2	1:A:62:ASN:H	1.57	0.53
1:A:255:LEU:HD22	1:A:259:GLY:HA3	1.92	0.52
1:A:157:ARG:HD2	1:A:161:HIS:O	2.11	0.51
1:A:227:TRP:CD2	1:A:230:VAL:HG22	2.46	0.51
1:A:143:LEU:HD13	1:A:146:PHE:HE2	1.76	0.50
1:A:132:ASN:HD22	1:A:132:ASN:C	2.15	0.50
1:A:124:LEU:N	1:A:124:LEU:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HA	1:A:158:THR:CG2	2.42	0.50
1:A:230:VAL:O	1:A:233:MET:HG2	2.12	0.49
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.95	0.49
1:A:125:HIS:HB2	1:A:146:PHE:CZ	2.47	0.49
1:A:103:LEU:HD13	1:A:292:PRO:HB2	1.94	0.49
1:A:139:GLY:CA	1:A:294:PRO:HD2	2.40	0.49
1:A:60:HIS:CD2	1:A:62:ASN:H	2.31	0.48
1:A:108:LEU:HD22	1:A:112:LEU:HD22	1.95	0.48
1:A:156:VAL:HA	1:A:164:VAL:HG22	1.96	0.48
1:A:97:THR:HG22	1:A:98:GLY:O	2.14	0.48
1:A:48:ALA:O	1:A:52:ILE:HG12	2.14	0.48
1:A:51:GLU:O	1:A:54:LEU:CD2	2.56	0.48
1:A:5:GLN:HB2	1:A:24:LYS:HD3	1.97	0.47
1:A:44:VAL:HG22	1:A:71:HIS:NE2	2.29	0.47
1:A:47:THR:O	1:A:51:GLU:HG2	2.14	0.47
1:A:42:GLU:HA	1:A:43:GLY:HA2	1.64	0.47
1:A:248:PHE:O	1:A:251:VAL:HG22	2.14	0.47
1:A:261:SER:O	1:A:265:GLN:HG3	2.14	0.47
1:A:131:GLN:CD	1:A:131:GLN:H	2.18	0.47
1:A:28:GLU:HG3	1:A:29:VAL:O	2.13	0.46
1:A:3:ASN:ND2	1:A:25:LEU:HD13	2.30	0.46
1:A:83:LEU:HG	1:A:134:LEU:HB3	1.96	0.46
1:A:252:VAL:HG13	1:A:255:LEU:HD12	1.98	0.45
1:A:35:ILE:HG22	1:A:36:ARG:HG3	1.98	0.45
1:A:89:LYS:CG	2:A:299:D23:HN72	2.22	0.44
1:A:87:LEU:HD12	1:A:133:LEU:HD12	1.97	0.44
1:A:36:ARG:HB3	1:A:41:THR:H	1.55	0.44
1:A:65:LYS:HG2	1:A:67:LEU:HD12	1.99	0.44
1:A:252:VAL:CG1	1:A:252:VAL:O	2.67	0.43
1:A:134:LEU:HD22	1:A:144:ALA:HB2	2.00	0.42
1:A:213:PHE:O	1:A:217:ARG:HG3	2.18	0.42
1:A:125:HIS:O	1:A:126:ARG:HG3	2.20	0.42
1:A:41:THR:OG1	1:A:42:GLU:N	2.50	0.41
1:A:227:TRP:CB	1:A:230:VAL:HG22	2.50	0.41
1:A:75:LYS:HD2	1:A:75:LYS:N	2.35	0.41
1:A:291:LYS:HB2	1:A:291:LYS:HE2	1.86	0.41
1:A:128:LEU:HB2	3:A:300:HOH:O	2.21	0.41
1:A:91:MET:CE	1:A:195:GLU:HG2	2.51	0.40
1:A:160:THR:HB	1:A:162:GLU:HG3	2.03	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	292/298 (98%)	270 (92%)	20 (7%)	2 (1%)	25	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	238	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/263 (98%)	240 (93%)	19 (7%)	16	11

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	66	LEU
1	A	87	LEU
1	A	101	LEU
1	A	108	LEU
1	A	122	ARG
1	A	126	ARG
1	A	131	GLN
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	134	LEU
1	A	146	PHE
1	A	189	LEU
1	A	225	VAL
1	A	252	VAL
1	A	254	PRO
1	A	262	LEU
1	A	263	LEU
1	A	287	GLN
1	A	297	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	59	ASN
1	A	60	HIS
1	A	125	HIS
1	A	132	ASN
1	A	287	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	D23	A	299	-	28,28,28	3.14	17 (60%)	40,43,43	2.90	13 (32%)

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
2	D23	A	299	-	-	0/15/15/15	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	299	D23	C15-N14	2.09	1.36	1.33
2	A	299	D23	C15-N16	2.26	1.37	1.33
2	A	299	D23	C17-C12	2.81	1.48	1.44
2	A	299	D23	C10-C11	2.83	1.46	1.41
2	A	299	D23	C13-C12	2.85	1.47	1.42
2	A	299	D23	C3-C2	2.99	1.46	1.39
2	A	299	D23	C4-C3	3.41	1.45	1.38
2	A	299	D23	C1-C6	3.53	1.46	1.39
2	A	299	D23	C4-C5	3.79	1.46	1.38
2	A	299	D23	C17-N16	3.88	1.38	1.33
2	A	299	D23	C10-C9	3.90	1.44	1.36
2	A	299	D23	C1-C2	4.13	1.45	1.39
2	A	299	D23	C9-C8	4.46	1.48	1.39
2	A	299	D23	C5-C6	4.55	1.49	1.39
2	A	299	D23	C17-N18	5.30	1.44	1.35
2	A	299	D23	C13-C8	5.44	1.51	1.38
2	A	299	D23	C12-C11	6.38	1.52	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D23	C12-C11-N14	-5.33	117.33	122.84
2	A	299	D23	N14-C15-N16	-4.11	122.72	129.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D23	C1-C2-N7	-2.78	116.13	120.54
2	A	299	D23	F26-C23-C15	-2.60	105.35	112.72
2	A	299	D23	C5-C6-C1	-2.49	114.93	118.16
2	A	299	D23	C13-C12-C11	-2.31	116.09	118.92
2	A	299	D23	C10-C11-C12	2.32	121.84	119.11
2	A	299	D23	C23-C15-N16	3.11	119.72	115.27
2	A	299	D23	C4-C5-C6	4.19	125.88	120.57
2	A	299	D23	C3-C2-C1	4.34	124.39	118.65
2	A	299	D23	C15-N14-C11	7.08	123.49	115.61
2	A	299	D23	C13-C12-C17	7.67	129.15	124.85
2	A	299	D23	C12-C17-N18	8.11	129.08	120.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	299	D23	2	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, 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	294/298 (98%)	0.68	34 (11%) 5 5	12, 29, 67, 95	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	THR	12.7
1	A	44	VAL	11.9
1	A	296	LEU	10.6
1	A	298	LEU	9.3
1	A	297	ARG	7.2
1	A	42	GLU	4.8
1	A	74	ASN	4.7
1	A	43	GLY	4.6
1	A	153	GLY	4.6
1	A	25	LEU	4.3
1	A	46	SER	4.3
1	A	45	PRO	4.2
1	A	36	ARG	4.1
1	A	295	HIS	3.9
1	A	152	PHE	3.9
1	A	290	THR	3.8
1	A	149	ALA	3.6
1	A	294	PRO	3.5
1	A	73	GLU	3.4
1	A	150	ARG	3.0
1	A	156	VAL	3.0
1	A	291	LYS	3.0
1	A	93	ALA	3.0
1	A	50	ARG	2.7
1	A	154	VAL	2.7
1	A	72	THR	2.6
1	A	160	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	49	ILE	2.5
1	A	266	MET	2.4
1	A	155	PRO	2.3
1	A	293	VAL	2.2
1	A	35	ILE	2.2
1	A	26	THR	2.2
1	A	196	MET	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	D23	A	299	26/26	0.83	0.17	0.24	35,42,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.