



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:40 AM UTC

PDB ID : 4YC6 / pdb_00004yc6
Title : CDK1/CKS1
Authors : Brown, N.R.; Korolchuk, S.; Martin, M.P.; Stanley, W.; Moukhametzianov, R.; Noble, M.E.M.; Endicott, J.A.
Deposited on : 2015-02-19
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

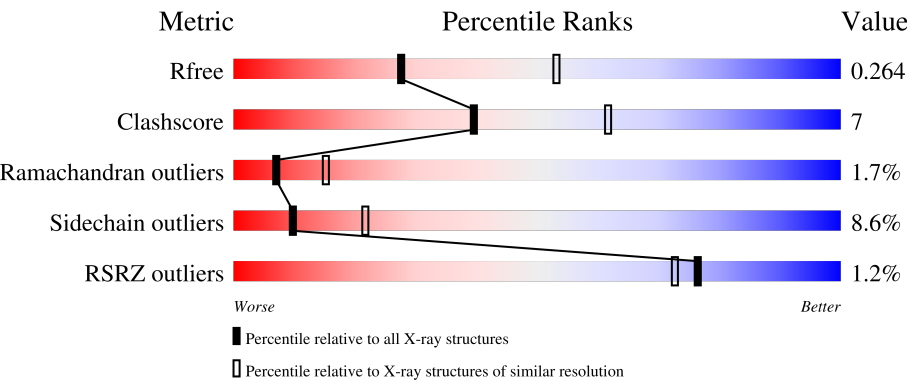
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	297	79%13% . .
1	C	297	2% 78%14% . .
1	E	297	% 77%15% . .
1	G	297	2% 74%17%5% .
2	B	85	% 61%14%6% .18%

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Mol	Chain	Length	Quality of chain
2	D	85	60%15%6%•18%
2	F	85	60%16%5%•18%
2	H	85	% 59%19%••18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12339 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 Cyclin-dependent kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	C	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	E	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	G	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			

- Molecule 2 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	D	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	F	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	H	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	HIS	-	expression tag	UNP P61024
B	81	HIS	-	expression tag	UNP P61024
B	82	HIS	-	expression tag	UNP P61024
B	83	HIS	-	expression tag	UNP P61024
B	84	HIS	-	expression tag	UNP P61024
B	85	HIS	-	expression tag	UNP P61024
D	80	HIS	-	expression tag	UNP P61024
D	81	HIS	-	expression tag	UNP P61024

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Chain	Residue	Modelled	Actual	Comment	Reference
D	82	HIS	-	expression tag	UNP P61024
D	83	HIS	-	expression tag	UNP P61024
D	84	HIS	-	expression tag	UNP P61024
D	85	HIS	-	expression tag	UNP P61024
F	80	HIS	-	expression tag	UNP P61024
F	81	HIS	-	expression tag	UNP P61024
F	82	HIS	-	expression tag	UNP P61024
F	83	HIS	-	expression tag	UNP P61024
F	84	HIS	-	expression tag	UNP P61024
F	85	HIS	-	expression tag	UNP P61024
H	80	HIS	-	expression tag	UNP P61024
H	81	HIS	-	expression tag	UNP P61024
H	82	HIS	-	expression tag	UNP P61024
H	83	HIS	-	expression tag	UNP P61024
H	84	HIS	-	expression tag	UNP P61024
H	85	HIS	-	expression tag	UNP P61024

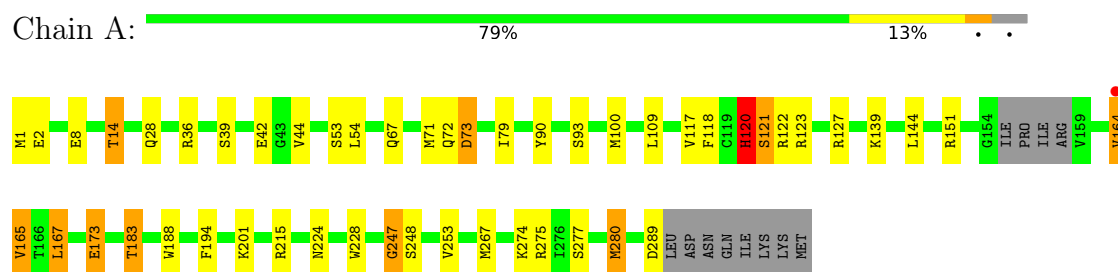
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	147	Total O 147 147	0	0
3	B	42	Total O 42 42	0	0
3	C	118	Total O 118 118	0	0
3	D	48	Total O 48 48	0	0
3	E	128	Total O 128 128	0	0
3	F	16	Total O 16 16	0	0
3	G	115	Total O 115 115	0	0
3	H	25	Total O 25 25	0	0

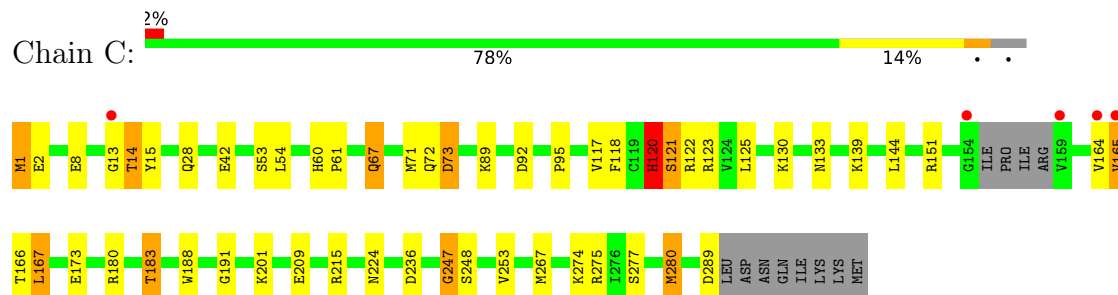
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

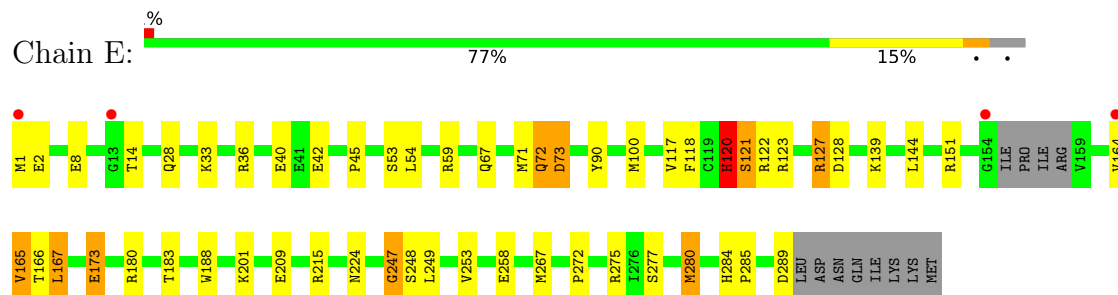
• Molecule 1: Cyclin-dependent kinase 1



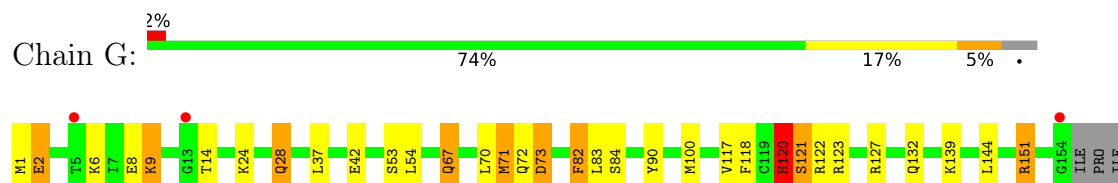
• Molecule 1: Cyclin-dependent kinase 1

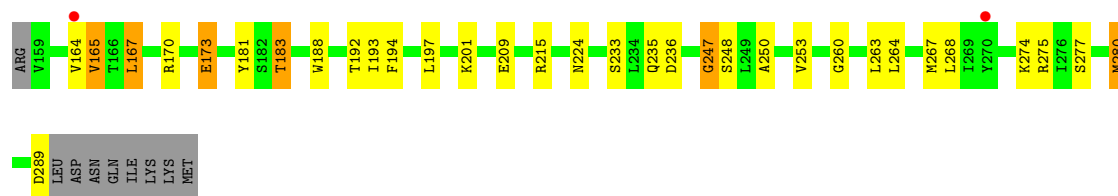


• Molecule 1: Cyclin-dependent kinase 1



• Molecule 1: Cyclin-dependent kinase 1

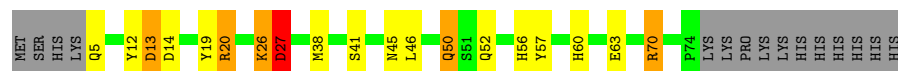




- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



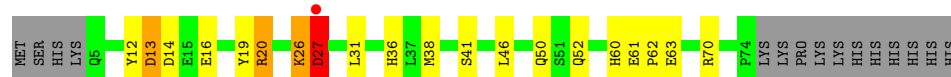
- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.82Å 147.53Å 87.30Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	75.09 – 2.60 75.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (75.09-2.60) 97.0 (75.09-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.225 , 0.267 0.228 , 0.264	Depositor DCC
R_{free} test set	1787 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12339	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

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	1.09	3/2364 (0.1%)	1.16	9/3194 (0.3%)
1	C	1.06	3/2364 (0.1%)	1.15	7/3194 (0.2%)
1	E	1.04	1/2364 (0.0%)	1.15	4/3194 (0.1%)
1	G	0.99	0/2362	1.13	9/3188 (0.3%)
2	B	1.03	0/634	1.09	2/860 (0.2%)
2	D	1.14	1/634 (0.2%)	1.14	3/860 (0.3%)
2	F	0.88	0/634	1.06	2/860 (0.2%)
2	H	0.94	0/634	1.08	3/860 (0.3%)
All	All	1.04	8/11990 (0.1%)	1.13	39/16210 (0.2%)

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	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	16

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	33	LYS	C-O	-6.91	1.15	1.24
1	C	89	LYS	C-O	-6.45	1.16	1.24
1	A	79	ILE	C-O	-5.92	1.17	1.24
1	A	14	THR	N-CA	5.41	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	LEU	N-CA	5.16	1.51	1.45
2	D	60	HIS	N-CA	-5.11	1.40	1.46
1	A	164	VAL	N-CA	5.09	1.52	1.46
1	C	14	THR	N-CA	5.08	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	HIS	N-CA-C	12.01	124.36	111.03
1	G	120	HIS	N-CA-C	8.20	121.82	111.24
1	A	120	HIS	N-CA-C	7.89	121.42	111.24
1	C	120	HIS	N-CA-C	7.68	121.15	111.24
1	C	167	LEU	N-CA-C	7.13	119.91	111.71
1	A	67	GLN	N-CA-C	7.02	119.01	111.36
1	G	167	LEU	N-CA-C	6.86	119.60	111.71
2	H	13	ASP	N-CA-C	6.64	119.26	108.76
1	E	67	GLN	N-CA-C	6.60	118.48	111.28
2	F	13	ASP	N-CA-C	6.52	119.07	108.76
2	B	13	ASP	N-CA-C	6.45	119.12	108.99
1	E	8	GLU	N-CA-C	6.45	118.95	108.76
1	G	67	GLN	N-CA-C	6.39	118.25	111.28
2	F	16	GLU	N-CA-C	6.20	119.24	111.24
1	A	183	THR	CA-C-N	-6.01	113.43	119.56
1	A	183	THR	C-N-CA	-6.01	113.43	119.56
2	D	13	ASP	N-CA-C	5.83	117.96	108.76
1	G	82	PHE	N-CA-C	5.81	123.17	110.80
2	D	14	ASP	CB-CA-C	-5.78	100.28	113.33
1	A	167	LEU	N-CA-C	5.68	119.02	111.75
2	D	50	GLN	N-CA-CB	-5.58	103.07	111.56
2	B	14	ASP	CB-CA-C	-5.57	100.75	113.33
1	G	183	THR	CA-C-N	-5.56	113.89	119.56
1	G	183	THR	C-N-CA	-5.56	113.89	119.56
1	A	8	GLU	N-CA-C	5.51	117.46	108.76
1	C	67	GLN	N-CA-C	5.51	117.36	111.36
1	G	9	LYS	N-CA-C	-5.50	101.57	110.32
1	E	167	LEU	N-CA-C	5.49	118.78	111.75
1	C	8	GLU	N-CA-C	5.48	117.42	108.76
1	A	228	TRP	CA-C-N	-5.45	114.14	119.76
1	A	228	TRP	C-N-CA	-5.45	114.14	119.76
1	G	6	LYS	N-CA-C	-5.41	101.84	109.96
2	H	16	GLU	N-CA-C	5.21	117.97	111.24
2	H	14	ASP	CB-CA-C	-5.17	101.63	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	PRO	O-C-N	5.14	123.56	121.15
1	A	173	GLU	CB-CA-C	-5.04	102.74	110.81
1	G	173	GLU	CB-CA-C	-5.03	102.76	110.81
1	C	183	THR	CA-C-N	-5.01	114.45	119.56
1	C	183	THR	C-N-CA	-5.01	114.45	119.56

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	HIS	Peptide
1	A	247	GLY	Peptide
2	B	26	LYS	Peptide
2	B	27[B]	ASP	Peptide
1	C	120	HIS	Peptide
1	C	247	GLY	Peptide
2	D	26	LYS	Peptide
2	D	27[B]	ASP	Peptide
1	E	120	HIS	Peptide
1	E	247	GLY	Peptide
2	F	26	LYS	Peptide
2	F	27[B]	ASP	Peptide
1	G	120	HIS	Peptide
1	G	247	GLY	Peptide
2	H	26	LYS	Peptide
2	H	27[B]	ASP	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	2312	0	2334	27	0
1	C	2312	0	2334	25	0
1	E	2312	0	2334	30	0
1	G	2312	0	2332	56	0
2	B	613	0	584	9	0
2	D	613	0	584	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	613	0	584	13	0
2	H	613	0	584	8	0
3	A	147	0	0	1	0
3	B	42	0	0	0	0
3	C	118	0	0	6	0
3	D	48	0	0	3	0
3	E	128	0	0	7	0
3	F	16	0	0	5	0
3	G	115	0	0	24	0
3	H	25	0	0	1	0
All	All	12339	0	11670	157	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 7.

All (157) 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:G:193:ILE:O	3:G:301:HOH:O	1.68	1.08
1:G:8:GLU:C	1:G:9:LYS:N	2.13	1.07
1:G:188:TRP:O	3:G:302:HOH:O	1.75	1.04
2:F:17:PHE:O	3:F:101:HOH:O	1.92	0.86
1:C:1:MET:N	3:C:301:HOH:O	2.00	0.85
1:G:260:GLY:HA2	3:G:397:HOH:O	1.77	0.84
1:E:277:SER:OG	1:E:280:MET:SD	2.35	0.83
1:G:83:LEU:C	1:G:84:SER:N	2.40	0.80
2:F:19:TYR:CE2	3:F:101:HOH:O	2.35	0.79
1:A:73:ASP:HB2	1:G:235:GLN:HB3	1.67	0.75
1:G:197:LEU:CB	3:G:301:HOH:O	2.35	0.75
1:G:197:LEU:HB2	3:G:301:HOH:O	1.85	0.75
1:G:24:LYS:O	3:G:303:HOH:O	2.08	0.71
1:A:247:GLY:HA2	1:A:248:SER:HB3	1.73	0.71
1:G:194:PHE:O	3:G:301:HOH:O	2.08	0.70
1:E:247:GLY:HA2	1:E:248:SER:HB3	1.73	0.70
1:A:73:ASP:OD2	1:G:233:SER:O	2.10	0.70
1:G:132[B]:GLN:OE1	1:G:132[B]:GLN:N	2.22	0.69
1:C:247:GLY:HA2	1:C:248:SER:HB3	1.74	0.69
1:G:247:GLY:HA2	1:G:248:SER:HB3	1.74	0.68
1:G:268:LEU:HD21	3:G:302:HOH:O	1.93	0.68
1:G:192:THR:HG23	3:G:302:HOH:O	1.95	0.66
1:G:192:THR:N	3:G:302:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:LEU:HG	3:G:319:HOH:O	1.96	0.66
1:A:164:VAL:C	1:A:165:VAL:N	2.56	0.64
1:E:164:VAL:C	1:E:165:VAL:N	2.57	0.62
1:G:194:PHE:C	3:G:301:HOH:O	2.42	0.62
2:F:19:TYR:HE2	3:F:101:HOH:O	1.77	0.62
1:C:120:HIS:CE1	1:C:183:THR:HB	2.37	0.59
1:G:277:SER:OG	1:G:280:MET:HG2	2.02	0.59
1:G:28:GLN:OE1	1:G:67:GLN:NE2	2.36	0.58
1:A:117:VAL:O	1:A:121:SER:CB	2.52	0.58
1:E:117:VAL:O	1:E:121:SER:CB	2.52	0.58
1:G:117:VAL:O	1:G:121:SER:CB	2.51	0.58
1:C:117:VAL:O	1:C:121:SER:CB	2.53	0.57
1:E:128:ASP:HB2	3:E:413:HOH:O	2.05	0.57
1:G:24:LYS:NZ	3:G:307:HOH:O	2.35	0.56
1:G:37:LEU:HB2	3:G:340:HOH:O	2.03	0.56
1:A:117:VAL:O	1:A:121:SER:HB2	2.06	0.56
1:A:277:SER:OG	1:A:280:MET:HG2	2.06	0.56
1:G:120:HIS:CE1	1:G:183:THR:HB	2.40	0.55
1:E:117:VAL:O	1:E:121:SER:HB2	2.07	0.55
1:C:164:VAL:C	1:C:165:VAL:N	2.65	0.55
1:E:120:HIS:CE1	1:E:183:THR:HB	2.42	0.55
1:G:117:VAL:O	1:G:121:SER:HB2	2.07	0.55
1:G:274:LYS:NZ	3:G:308:HOH:O	2.40	0.55
1:A:73:ASP:HB2	1:G:235:GLN:CB	2.34	0.54
1:G:83:LEU:C	1:G:84:SER:CA	2.80	0.54
1:C:191:GLY:HA3	3:C:313:HOH:O	2.07	0.54
1:A:73:ASP:CB	1:G:235:GLN:HB3	2.36	0.54
2:D:20:ARG:HE	2:D:50:GLN:HE21	1.56	0.54
1:A:120:HIS:CE1	1:A:183:THR:HB	2.44	0.53
1:G:2:GLU:HG2	3:G:407:HOH:O	2.08	0.53
1:E:127:ARG:HD3	3:E:340:HOH:O	2.08	0.53
1:E:277:SER:OG	1:E:280:MET:HG2	2.09	0.52
1:E:280:MET:N	1:E:280:MET:HE3	2.25	0.52
1:C:277:SER:OG	1:C:280:MET:HG2	2.09	0.52
1:G:197:LEU:N	3:G:301:HOH:O	2.09	0.52
1:C:117:VAL:O	1:C:121:SER:HB2	2.09	0.52
1:C:188:TRP:HA	3:C:313:HOH:O	2.10	0.51
1:G:117:VAL:O	1:G:121:SER:HB3	2.11	0.51
1:A:73:ASP:O	1:G:235:GLN:HB3	2.11	0.51
1:A:36:ARG:NH2	1:G:236:ASP:OD1	2.42	0.51
2:B:20:ARG:HE	2:B:50:GLN:HE21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:VAL:O	1:C:121:SER:HB3	2.11	0.50
2:F:20:ARG:HE	2:F:50:GLN:HE21	1.59	0.50
1:C:267:MET:HB3	3:C:313:HOH:O	2.11	0.50
1:E:277:SER:OG	1:E:280:MET:CG	2.60	0.49
1:G:164:VAL:C	1:G:165:VAL:N	2.70	0.49
1:A:36:ARG:NH2	1:G:236:ASP:OD2	2.44	0.49
1:E:73:ASP:OD1	1:E:73:ASP:N	2.45	0.49
2:H:12:TYR:CD1	2:H:19:TYR:HB2	2.48	0.49
1:A:118:PHE:O	1:A:121:SER:HB3	2.13	0.49
2:B:31:LEU:HD12	2:F:31:LEU:HD12	1.94	0.49
2:D:56:HIS:HE1	3:D:107:HOH:O	1.96	0.49
1:E:117:VAL:O	1:E:121:SER:HB3	2.13	0.48
1:A:73:ASP:OD1	1:A:73:ASP:N	2.46	0.48
1:A:117:VAL:O	1:A:121:SER:HB3	2.13	0.48
2:B:12:TYR:CD1	2:B:19:TYR:HB2	2.49	0.48
2:F:12:TYR:CD1	2:F:19:TYR:HB2	2.48	0.48
1:C:188:TRP:C	1:C:188:TRP:CD1	2.92	0.48
1:C:73:ASP:N	1:C:73:ASP:OD1	2.46	0.47
1:E:45:PRO:HD2	3:E:334:HOH:O	2.12	0.47
1:C:236:ASP:OD1	1:E:36:ARG:NH2	2.47	0.47
1:G:188:TRP:C	1:G:188:TRP:CD1	2.92	0.47
1:G:209:GLU:HB2	2:H:63:GLU:CD	2.39	0.47
1:G:264:LEU:HA	3:G:319:HOH:O	2.14	0.47
1:E:118:PHE:O	1:E:121:SER:HB3	2.14	0.47
2:D:12:TYR:CD1	2:D:19:TYR:HB2	2.49	0.47
1:G:170:ARG:O	3:G:304:HOH:O	2.20	0.47
1:A:188:TRP:CD1	1:A:188:TRP:C	2.93	0.47
1:G:73:ASP:N	1:G:73:ASP:OD1	2.48	0.47
1:G:132[B]:GLN:H	1:G:132[B]:GLN:CD	2.18	0.47
1:G:118:PHE:O	1:G:121:SER:HB3	2.15	0.46
1:G:247:GLY:CA	1:G:248:SER:HB3	2.45	0.46
1:C:280:MET:CE	3:C:320:HOH:O	2.64	0.46
1:E:59:ARG:NH1	3:E:304:HOH:O	2.49	0.46
2:B:57:TYR:CD1	2:B:70:ARG:HB3	2.52	0.45
2:H:36:HIS:ND1	3:H:101:HOH:O	2.36	0.45
1:C:118:PHE:O	1:C:121:SER:HB3	2.17	0.45
1:A:164:VAL:HG12	3:A:356:HOH:O	2.17	0.45
1:G:197:LEU:CG	3:G:301:HOH:O	2.64	0.44
1:G:83:LEU:C	1:G:84:SER:HA	2.41	0.44
1:A:247:GLY:CA	1:A:248:SER:HB3	2.46	0.44
1:E:188:TRP:CD1	1:E:188:TRP:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:GLN:N	3:D:101:HOH:O	2.50	0.44
1:G:268:LEU:CD2	3:G:302:HOH:O	2.58	0.44
2:H:20:ARG:HE	2:H:50:GLN:HE21	1.65	0.44
1:C:166:THR:HG21	3:C:327:HOH:O	2.18	0.44
1:A:93:SER:HB2	3:D:142:HOH:O	2.18	0.43
1:C:209:GLU:HB2	2:D:63:GLU:CD	2.43	0.43
2:F:57:TYR:CD1	2:F:70:ARG:HB3	2.53	0.43
1:G:71:MET:HE1	3:G:340:HOH:O	2.17	0.43
1:E:90:TYR:CE2	1:E:100:MET:HE2	2.54	0.43
2:H:61:GLU:N	2:H:62:PRO:CD	2.81	0.43
2:D:38:MET:HE1	2:D:46:LEU:HD11	2.01	0.42
1:G:224:ASN:OD1	1:G:224:ASN:C	2.62	0.42
1:E:173:GLU:CG	1:E:272:PRO:HG3	2.49	0.42
1:A:44:VAL:HG21	1:G:151:ARG:CD	2.50	0.42
2:H:38:MET:HE1	2:H:46:LEU:HD11	2.02	0.42
1:E:180:ARG:NH1	3:E:310:HOH:O	2.53	0.42
1:A:36:ARG:NH2	1:G:236:ASP:CG	2.78	0.41
1:A:224:ASN:OD1	1:A:224:ASN:C	2.63	0.41
1:E:209:GLU:HB2	2:F:63:GLU:CD	2.44	0.41
2:F:8:TYR:HD1	2:F:22:VAL:HG22	1.85	0.41
1:G:194:PHE:CA	3:G:301:HOH:O	2.69	0.41
1:C:267:MET:O	1:C:275:ARG:HD3	2.21	0.41
2:F:38:MET:HE1	2:F:46:LEU:HD11	2.03	0.41
2:B:31:LEU:HD12	2:F:31:LEU:CD1	2.50	0.41
1:C:224:ASN:OD1	1:C:224:ASN:C	2.64	0.41
1:E:164:VAL:O	1:E:165:VAL:N	2.54	0.41
1:E:267:MET:O	1:E:275:ARG:HD3	2.21	0.41
1:E:284:HIS:CG	1:E:285:PRO:HD2	2.56	0.41
1:G:90:TYR:CE2	1:G:100:MET:HE2	2.56	0.41
1:A:90:TYR:CE2	1:A:100:MET:HE2	2.56	0.41
1:E:165:VAL:O	1:E:166:THR:C	2.63	0.41
2:H:60:HIS:C	2:H:62:PRO:HD2	2.46	0.41
1:C:180:ARG:HA	1:E:40:GLU:O	2.21	0.41
2:F:19:TYR:CD2	3:F:101:HOH:O	2.69	0.41
2:B:14:ASP:HB3	2:B:16:GLU:H	1.86	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.41
2:D:45:ASN:O	2:H:31:LEU:HD22	2.21	0.41
2:D:57:TYR:CD1	2:D:70:ARG:HB3	2.55	0.41
1:E:249:LEU:N	3:E:303:HOH:O	2.48	0.41
1:A:267:MET:O	1:A:275:ARG:HD3	2.21	0.40
1:E:224:ASN:OD1	1:E:224:ASN:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:LYS:NZ	3:F:103:HOH:O	2.54	0.40
1:G:250:ALA:N	3:G:315:HOH:O	2.55	0.40
1:A:39:SER:OG	1:G:181:TYR:HD1	2.04	0.40
2:B:51:SER:OG	1:C:92:ASP:OD2	2.39	0.40
1:C:13:GLY:O	1:C:15:TYR:N	2.46	0.40
1:A:109:LEU:HD22	1:A:194:PHE:CD1	2.56	0.40
2:B:38:MET:HE1	2:B:46:LEU:HD11	2.02	0.40
2:B:61:GLU:N	2:B:62:PRO:CD	2.85	0.40
1:C:130:LYS:HG2	1:C:133:ASN:ND2	2.36	0.40
1:E:72:GLN:HA	3:E:377:HOH:O	2.21	0.40
1:G:267:MET:O	1:G:275:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	280/297 (94%)	246 (88%)	30 (11%)	4 (1%)	9	19
1	C	280/297 (94%)	246 (88%)	31 (11%)	3 (1%)	11	25
1	E	280/297 (94%)	244 (87%)	32 (11%)	4 (1%)	9	19
1	G	276/297 (93%)	239 (87%)	32 (12%)	5 (2%)	6	14
2	B	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	2	2
2	D	69/85 (81%)	65 (94%)	1 (1%)	3 (4%)	2	2
2	F	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	2	2
2	H	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	2	2
All	All	1392/1528 (91%)	1232 (88%)	132 (10%)	28 (2%)	7	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	C	121	SER
1	E	121	SER
1	G	14	THR
1	G	82	PHE
1	G	121	SER
1	A	14	THR
2	B	26	LYS
1	C	14	THR
2	D	26	LYS
1	E	14	THR
2	F	26	LYS
2	H	26	LYS
1	A	127	ARG
2	F	27[A]	ASP
2	F	27[B]	ASP
2	H	27[A]	ASP
2	H	27[B]	ASP
2	B	27[A]	ASP
2	B	27[B]	ASP
2	D	27[A]	ASP
2	D	27[B]	ASP
1	C	42	GLU
1	E	42	GLU
1	E	127	ARG
1	G	42	GLU
1	A	42	GLU
1	G	127	ARG

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	256/267 (96%)	234 (91%)	22 (9%)	10	22
1	C	256/267 (96%)	233 (91%)	23 (9%)	9	20
1	E	256/267 (96%)	234 (91%)	22 (9%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	256/267 (96%)	234 (91%)	22 (9%)	10	22
2	B	68/82 (83%)	62 (91%)	6 (9%)	9	21
2	D	68/82 (83%)	61 (90%)	7 (10%)	7	15
2	F	68/82 (83%)	62 (91%)	6 (9%)	9	21
2	H	68/82 (83%)	61 (90%)	7 (10%)	7	15
All	All	1296/1396 (93%)	1181 (91%)	115 (9%)	10	20

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	28	GLN
1	A	53	SER
1	A	54	LEU
1	A	71	MET
1	A	72	GLN
1	A	73	ASP
1	A	122	ARG
1	A	123	ARG
1	A	139	LYS
1	A	144	LEU
1	A	151	ARG
1	A	165	VAL
1	A	167	LEU
1	A	173	GLU
1	A	201	LYS
1	A	215	ARG
1	A	253	VAL
1	A	274	LYS
1	A	280	MET
1	A	289	ASP
2	B	13	ASP
2	B	20	ARG
2	B	27[A]	ASP
2	B	27[B]	ASP
2	B	52	GLN
2	B	70	ARG
1	C	1	MET
1	C	2	GLU

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Mol	Chain	Res	Type
1	C	28	GLN
1	C	53	SER
1	C	54	LEU
1	C	67	GLN
1	C	71	MET
1	C	72	GLN
1	C	73	ASP
1	C	122	ARG
1	C	123	ARG
1	C	139	LYS
1	C	144	LEU
1	C	151	ARG
1	C	165	VAL
1	C	167	LEU
1	C	173	GLU
1	C	201	LYS
1	C	215	ARG
1	C	253	VAL
1	C	274	LYS
1	C	280	MET
1	C	289	ASP
2	D	13	ASP
2	D	20	ARG
2	D	27[A]	ASP
2	D	27[B]	ASP
2	D	41	SER
2	D	52	GLN
2	D	70	ARG
1	E	1	MET
1	E	2	GLU
1	E	28	GLN
1	E	53	SER
1	E	54	LEU
1	E	71	MET
1	E	72	GLN
1	E	73	ASP
1	E	122	ARG
1	E	123	ARG
1	E	139	LYS
1	E	144	LEU
1	E	151	ARG
1	E	165	VAL

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Mol	Chain	Res	Type
1	E	167	LEU
1	E	173	GLU
1	E	201	LYS
1	E	215	ARG
1	E	253	VAL
1	E	258	GLU
1	E	280	MET
1	E	289	ASP
2	F	13	ASP
2	F	20	ARG
2	F	27[A]	ASP
2	F	27[B]	ASP
2	F	52	GLN
2	F	70	ARG
1	G	1	MET
1	G	2	GLU
1	G	28	GLN
1	G	53	SER
1	G	54	LEU
1	G	70	LEU
1	G	71	MET
1	G	72	GLN
1	G	73	ASP
1	G	122	ARG
1	G	123	ARG
1	G	139	LYS
1	G	144	LEU
1	G	151	ARG
1	G	165	VAL
1	G	167	LEU
1	G	173	GLU
1	G	201	LYS
1	G	215	ARG
1	G	253	VAL
1	G	280	MET
1	G	289	ASP
2	H	13	ASP
2	H	20	ARG
2	H	27[A]	ASP
2	H	27[B]	ASP
2	H	41	SER
2	H	52	GLN

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Mol	Chain	Res	Type
2	H	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	114	GLN
1	A	255	ASN
2	B	36	HIS
2	B	50	GLN
1	C	111	GLN
1	C	114	GLN
1	C	255	ASN
2	D	36	HIS
2	D	50	GLN
1	E	111	GLN
1	E	114	GLN
1	E	133	ASN
1	E	239	ASN
1	E	255	ASN
2	F	36	HIS
2	F	50	GLN
1	G	111	GLN
1	G	114	GLN
1	G	255	ASN
2	H	36	HIS
2	H	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	3
1	C	1
1	E	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	164:VAL	C	165:VAL	N	2.70
1	C	164:VAL	C	165:VAL	N	2.65
1	E	164:VAL	C	165:VAL	N	2.57
1	A	164:VAL	C	165:VAL	N	2.56
1	G	83:LEU	C	84:SER	N	2.40
1	G	8:GLU	C	9:LYS	N	2.13

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	285/297 (95%)	-0.14	1 (0%) 88 86	23, 77, 121, 179	1 (0%)
1	C	285/297 (95%)	-0.04	5 (1%) 67 63	29, 80, 136, 187	1 (0%)
1	E	285/297 (95%)	0.16	4 (1%) 73 69	30, 96, 137, 212	1 (0%)
1	G	285/297 (95%)	0.35	5 (1%) 67 63	47, 120, 167, 188	1 (0%)
2	B	70/85 (82%)	-0.10	1 (1%) 73 69	52, 77, 119, 152	1 (1%)
2	D	70/85 (82%)	-0.18	0 100 100	44, 65, 100, 118	1 (1%)
2	F	70/85 (82%)	0.48	0 100 100	90, 127, 170, 187	1 (1%)
2	H	70/85 (82%)	-0.01	1 (1%) 73 69	66, 91, 131, 144	1 (1%)
All	All	1420/1528 (92%)	0.08	17 (1%) 76 73	23, 94, 152, 212	8 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	GLY	5.7
1	E	164	VAL	3.0
1	G	164	VAL	3.0
1	C	165	VAL	2.9
1	C	13	GLY	2.7
1	A	164	VAL	2.7
1	C	164	VAL	2.7
1	E	1	MET	2.4
1	G	154	GLY	2.3
1	C	159	VAL	2.3
1	C	154	GLY	2.3
2	B	27[A]	ASP	2.2
1	E	13	GLY	2.1
2	H	27[A]	ASP	2.1
1	G	5	THR	2.0
1	E	154	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	270	TYR	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.