



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:02 PM UTC

PDB ID : 1VYJ / pdb_00001vyj
Title : Structural and biochemical studies of human PCNA complexes provide the basis for association with CDK/cyclin and rationale for inhibitor design
Authors : Kontopidis, G.; Wu, S.; Zheleva, D.; Taylor, P.; McInnes, C.; Lane, D.; Fischer, P.; Walkinshaw, M.D.
Deposited on : 2004-04-30
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

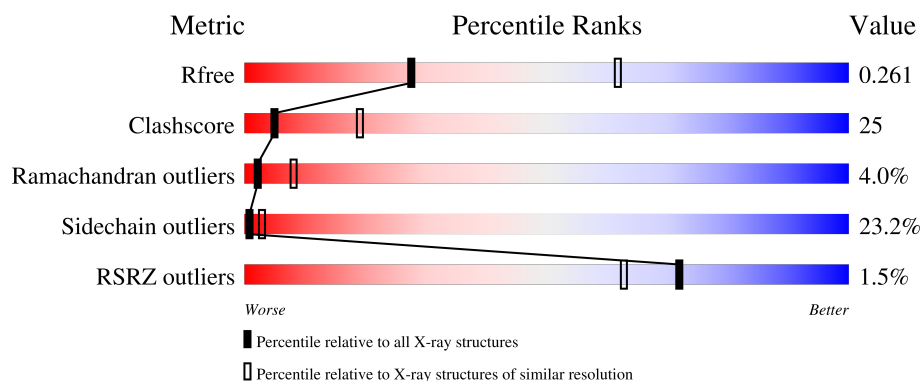
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	261	% 54% 35% 8% ..
1	C	261	% 52% 34% 10% ..
1	E	261	2% 51% 35% 11% ..
1	G	261	% 50% 34% 13% .
1	I	261	% 52% 36% 9% ..

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Mol	Chain	Length	Quality of chain
1	K	261	% 44% 38% 13%
2	B	16	6% 25% 31% 44%
2	D	16	12% 50% 25% 19% 6%
2	F	16	6% 38% 50% 12%
2	H	16	56% 19% 12% 12%
2	J	16	6% 38% 44% 12% 6%
2	L	16	31% 38% 31%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13057 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 PROLIFERATING CELL NUCLEAR ANTIGEN.

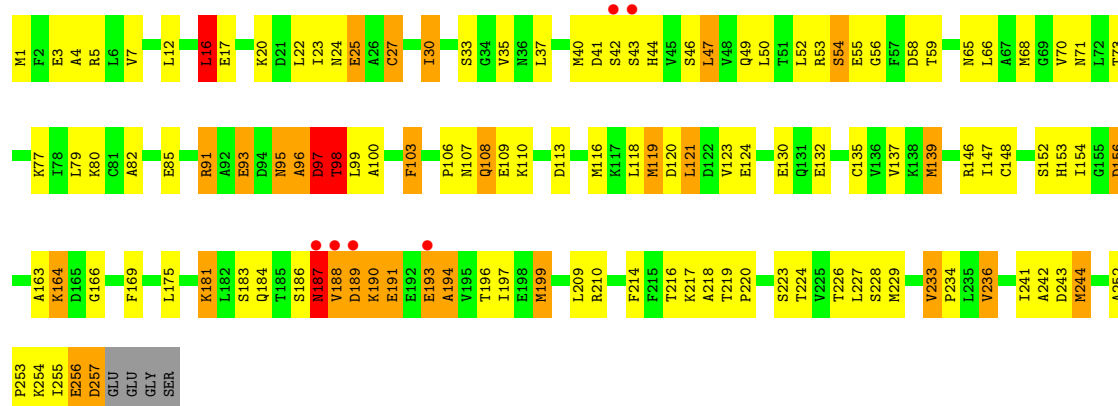
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	C	257	Total	C	N	O	S	0	3	0
			2005	1257	328	404	16			
1	E	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	G	260	Total	C	N	O	S	0	0	0
			2002	1254	327	405	16			
1	I	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			
1	K	257	Total	C	N	O	S	0	0	0
			1980	1242	324	398	16			

- Molecule 2 is a protein called SMALL PEPTIDE SAVLQKKITDYFHPKK.

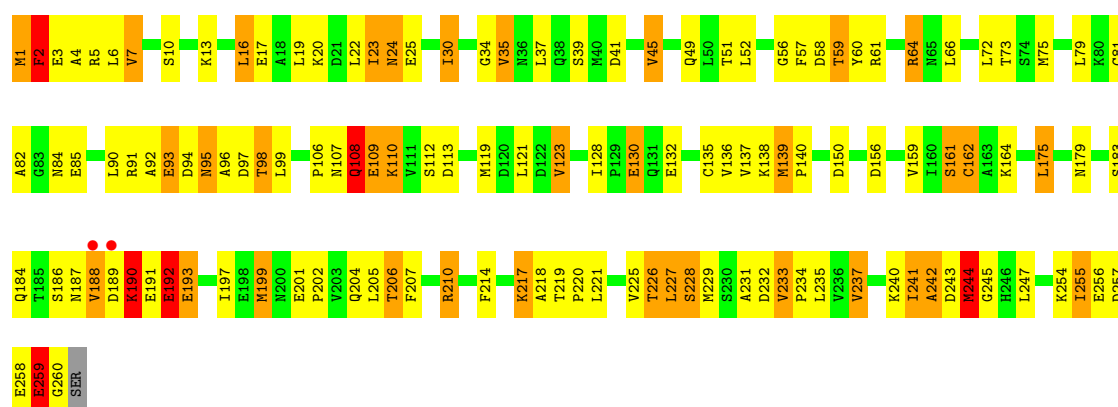
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	D	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	F	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	H	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	J	16	Total	C	N	O	0	0	0
			135	89	23	23			
2	L	16	Total	C	N	O	0	0	0
			135	89	23	23			

- Molecule 3 is water.

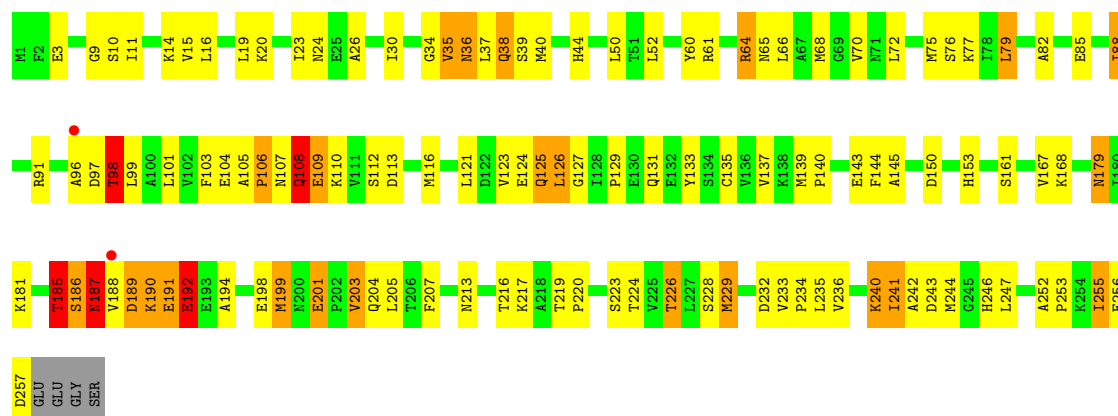
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	3	Total 3	O 3	0	0
3	C	50	Total 50	O 50	0	0
3	D	3	Total 3	O 3	0	0
3	E	59	Total 59	O 59	0	0
3	G	51	Total 51	O 51	0	0
3	H	5	Total 5	O 5	0	0
3	I	56	Total 56	O 56	0	0
3	J	5	Total 5	O 5	0	0
3	K	45	Total 45	O 45	0	0
3	L	2	Total 2	O 2	0	0



• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

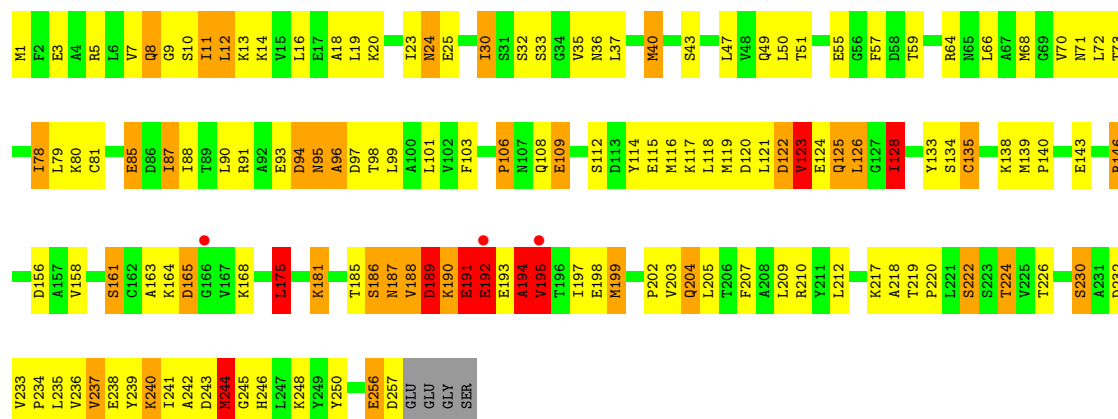


• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

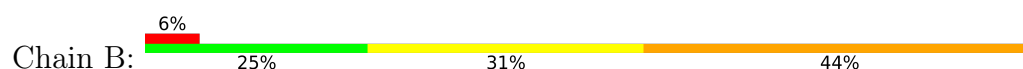


• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN





● Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK



● Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK



● Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK



● Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK



● Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK



- Molecule 2: SMALL PEPTIDE SAVLQKKITDYFHPKK

Chain L: 31% 38% 31%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.10Å 119.10Å 305.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.00 – 2.80 14.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.00-2.80) 98.6 (14.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.256 0.191 , 0.261	Depositor DCC
R_{free} test set	1917 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13057	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.83	2/2006 (0.1%)	1.36	9/2710 (0.3%)
1	C	1.20	3/2031 (0.1%)	1.46	17/2744 (0.6%)
1	E	0.88	3/2006 (0.1%)	1.47	20/2710 (0.7%)
1	G	0.87	1/2028 (0.0%)	1.39	13/2739 (0.5%)
1	I	0.85	1/2006 (0.0%)	1.40	11/2710 (0.4%)
1	K	0.82	1/2006 (0.0%)	1.35	15/2710 (0.6%)
2	B	0.95	1/138 (0.7%)	1.36	0/182
2	D	0.61	0/138	1.09	1/182 (0.5%)
2	F	0.75	0/138	1.35	2/182 (1.1%)
2	H	0.75	0/138	1.42	2/182 (1.1%)
2	J	0.72	0/138	1.01	0/182
2	L	0.98	0/138	1.36	1/182 (0.5%)
All	All	0.91	12/12911 (0.1%)	1.40	91/17415 (0.5%)

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	3
1	E	0	4
1	G	0	1
1	I	0	2
1	K	0	4
All	All	0	14

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	ILE	C-N	35.48	1.82	1.33
1	G	255	ILE	C-N	12.38	1.49	1.33
1	E	253	PRO	C-N	9.46	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ILE	C-N	8.69	1.47	1.33
1	C	139	MET	SD-CE	-7.63	1.60	1.79

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ILE	O-C-N	-16.19	104.50	122.95
1	I	192	GLU	O-C-N	12.72	139.51	122.59
1	E	97	ASP	O-C-N	11.37	135.98	122.34
1	E	103	PHE	CA-C-N	-11.11	107.33	122.99
1	E	103	PHE	C-N-CA	-11.11	107.33	122.99

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	ASN	Peptide
1	C	180	ILE	Mainchain
1	C	193	GLU	Mainchain
1	E	110	LYS	Mainchain
1	E	98	THR	Mainchain

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	1980	0	1983	93	0
1	C	2005	0	2001	77	2
1	E	1980	0	1981	104	1
1	G	2002	0	1996	112	3
1	I	1980	0	1981	92	0
1	K	1980	0	1981	125	0
2	B	135	0	146	23	0
2	D	135	0	146	12	0
2	F	135	0	146	10	0
2	H	135	0	146	10	0
2	J	135	0	146	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	135	0	146	10	0
3	A	41	0	0	9	0
3	B	3	0	0	0	0
3	C	50	0	0	5	0
3	D	3	0	0	0	0
3	E	59	0	0	4	0
3	G	51	0	0	3	0
3	H	5	0	0	0	0
3	I	56	0	0	1	0
3	J	5	0	0	0	0
3	K	45	0	0	5	0
3	L	2	0	0	0	0
All	All	13057	0	12799	640	3

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 25.

The worst 5 of 640 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:C:255:ILE:C	1:C:256:GLU:N	1.82	1.37
1:G:108:GLN:O	1:G:109:GLU:CG	1.82	1.24
1:E:189:ASP:OD1	1:E:189:ASP:O	1.55	1.22
2:F:2:ALA:O	2:F:3:VAL:HG13	1.08	1.20
1:G:108:GLN:O	1:G:109:GLU:HG2	1.01	1.16

All (3) 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)
1:C:77:LYS:NZ	1:G:130:GLU:OE2[6_555]	1.42	0.78
1:E:42:SER:OG	1:G:243:ASP:OD1[6_555]	1.94	0.26
1:C:77:LYS:CE	1:G:130:GLU:OE2[6_555]	2.08	0.12

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	255/261 (98%)	236 (92%)	15 (6%)	4 (2%)	7	27
1	C	258/261 (99%)	233 (90%)	14 (5%)	11 (4%)	2	7
1	E	255/261 (98%)	229 (90%)	16 (6%)	10 (4%)	2	8
1	G	258/261 (99%)	237 (92%)	12 (5%)	9 (4%)	3	10
1	I	255/261 (98%)	236 (92%)	13 (5%)	6 (2%)	4	17
1	K	255/261 (98%)	224 (88%)	17 (7%)	14 (6%)	1	4
2	B	14/16 (88%)	9 (64%)	2 (14%)	3 (21%)	0	0
2	D	14/16 (88%)	11 (79%)	1 (7%)	2 (14%)	0	0
2	F	14/16 (88%)	10 (71%)	3 (21%)	1 (7%)	1	2
2	H	14/16 (88%)	11 (79%)	2 (14%)	1 (7%)	1	2
2	J	14/16 (88%)	11 (79%)	1 (7%)	2 (14%)	0	0
2	L	14/16 (88%)	12 (86%)	0	2 (14%)	0	0
All	All	1620/1662 (98%)	1459 (90%)	96 (6%)	65 (4%)	2	8

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	A	188	VAL
2	B	2	ALA
1	C	24[A]	ASN
1	C	24[B]	ASN

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	225/228 (99%)	175 (78%)	50 (22%)	1	3
1	C	228/228 (100%)	170 (75%)	58 (25%)	0	2
1	E	225/228 (99%)	177 (79%)	48 (21%)	1	4
1	G	227/228 (100%)	179 (79%)	48 (21%)	1	4
1	I	225/228 (99%)	174 (77%)	51 (23%)	1	3
1	K	225/228 (99%)	173 (77%)	52 (23%)	1	3
2	B	15/15 (100%)	10 (67%)	5 (33%)	0	1
2	D	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	F	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	H	15/15 (100%)	11 (73%)	4 (27%)	0	1
2	J	15/15 (100%)	9 (60%)	6 (40%)	0	0
2	L	15/15 (100%)	9 (60%)	6 (40%)	0	0
All	All	1445/1458 (99%)	1109 (77%)	336 (23%)	1	3

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	88	ILE
1	K	25	GLU
1	I	121	LEU
1	I	226	THR
1	K	98	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	8	GLN
1	K	8	GLN
1	I	24	ASN
1	I	84	ASN
1	K	65	ASN

5.3.3 RNA ⓘ

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 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	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	255:ILE	C	256:GLU	N	1.82

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	257/261 (98%)	-0.52	3 (1%) 76 68	32, 52, 102, 162	0
1	C	257/261 (98%)	-0.65	3 (1%) 76 68	20, 44, 88, 146	3 (1%)
1	E	257/261 (98%)	-0.46	6 (2%) 61 51	28, 49, 95, 151	0
1	G	260/261 (99%)	-0.50	2 (0%) 82 75	33, 54, 105, 158	0
1	I	257/261 (98%)	-0.57	2 (0%) 82 75	29, 49, 95, 156	0
1	K	257/261 (98%)	-0.51	3 (1%) 76 68	38, 55, 96, 132	0
2	B	16/16 (100%)	0.36	1 (6%) 26 19	55, 68, 151, 153	0
2	D	16/16 (100%)	0.12	2 (12%) 8 6	44, 56, 119, 120	0
2	F	16/16 (100%)	0.07	1 (6%) 26 19	50, 64, 121, 124	0
2	H	16/16 (100%)	-0.23	0 100 100	44, 63, 114, 128	0
2	J	16/16 (100%)	0.13	1 (6%) 26 19	50, 67, 125, 129	0
2	L	16/16 (100%)	-0.09	0 100 100	47, 57, 114, 121	0
All	All	1641/1662 (98%)	-0.50	24 (1%) 72 63	20, 52, 104, 162	3 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	188	VAL	6.6
1	E	188	VAL	5.5
1	A	188	VAL	5.1
1	E	189	ASP	4.7
1	G	189	ASP	4.2

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

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.