



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 3I6W / pdb_00003i6w
Title : Structure and Activation Mechanism of the CHK2 DNA-Damage Checkpoint Kinase
Authors : Pavletich, N.P.
Deposited on : 2009-07-07
Resolution : 3.25 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

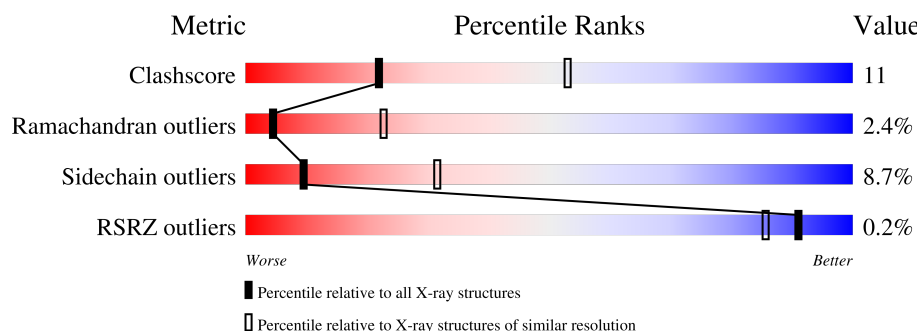
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	443	
1	B	443	
1	C	443	
1	D	443	
1	E	443	
1	F	443	

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Mol	Chain	Length	Quality of chain
1	G	443	 59% 20% • 17%
1	H	443	 62% 21% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24560 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 Serine/threonine-protein kinase Chk2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	B	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	C	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	D	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	E	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	F	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	G	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	H	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			

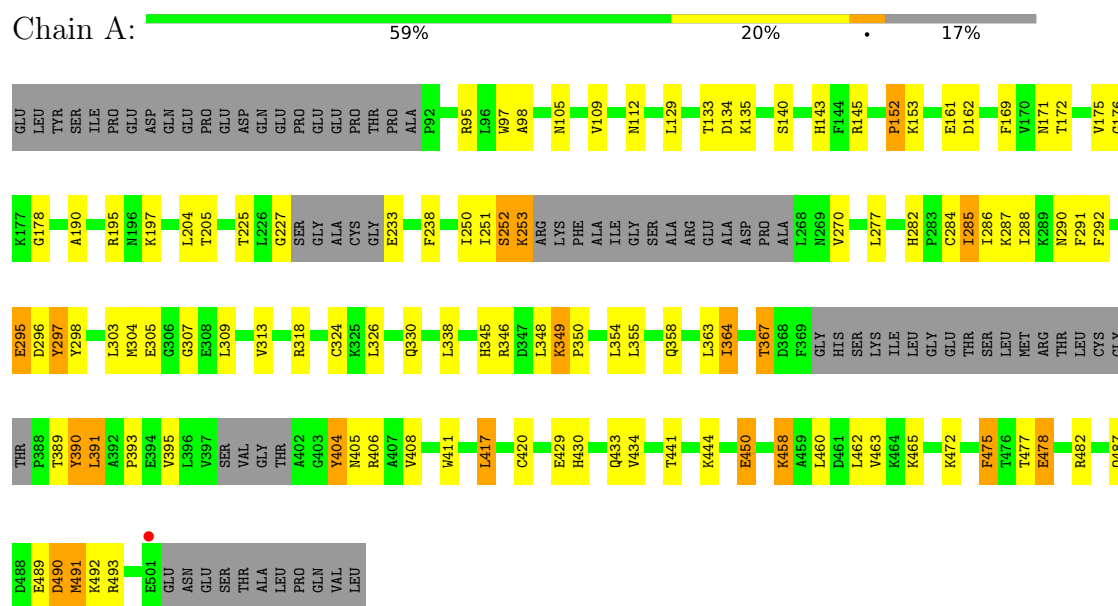
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ARG	LYS	engineered mutation	UNP O96017
B	249	ARG	LYS	engineered mutation	UNP O96017
C	249	ARG	LYS	engineered mutation	UNP O96017
D	249	ARG	LYS	engineered mutation	UNP O96017
E	249	ARG	LYS	engineered mutation	UNP O96017
F	249	ARG	LYS	engineered mutation	UNP O96017
G	249	ARG	LYS	engineered mutation	UNP O96017
H	249	ARG	LYS	engineered mutation	UNP O96017

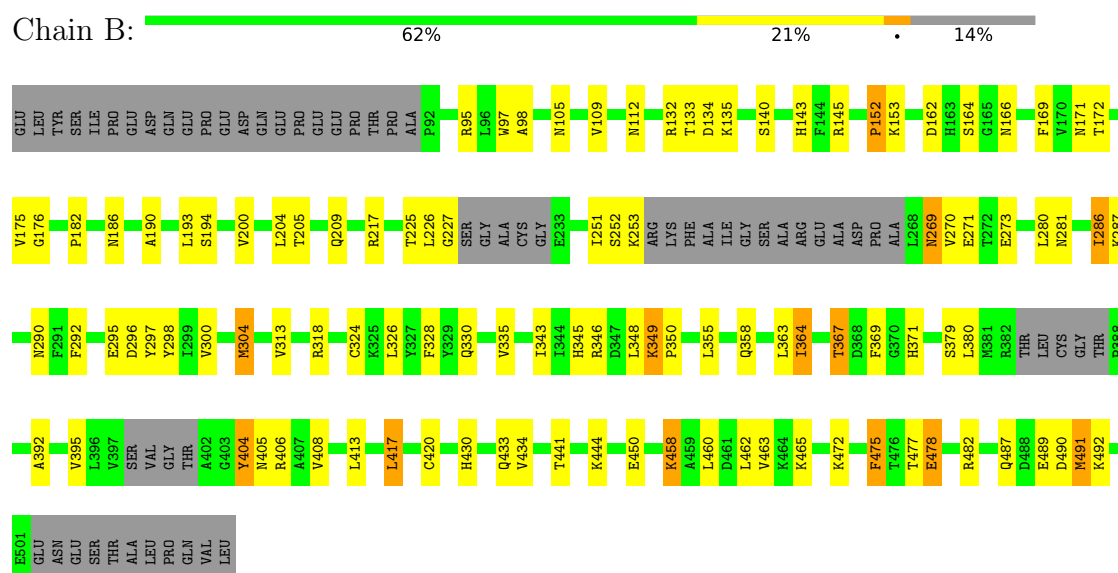
3 Residue-property plots

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.

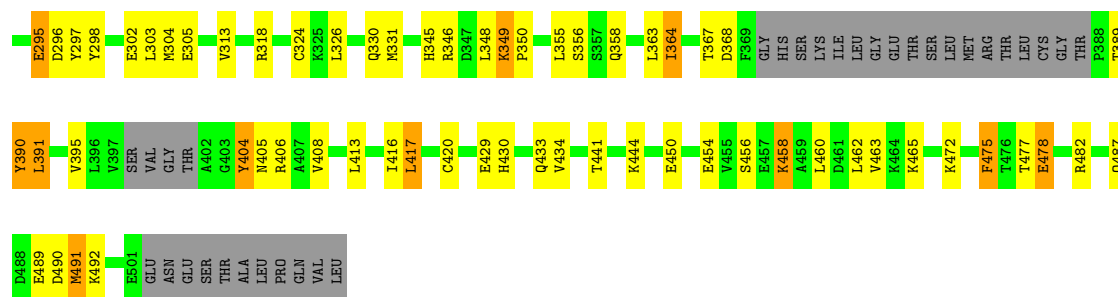
• Molecule 1: Serine/threonine-protein kinase Chk2



• Molecule 1: Serine/threonine-protein kinase Chk2

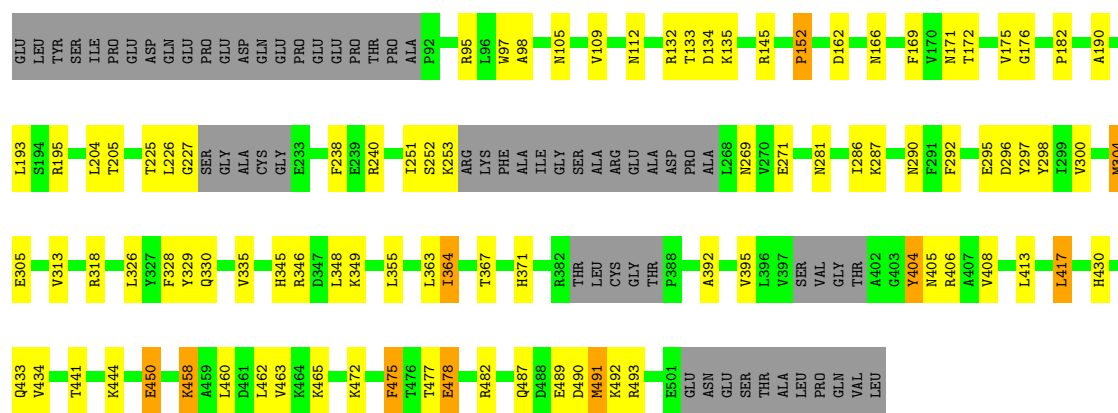


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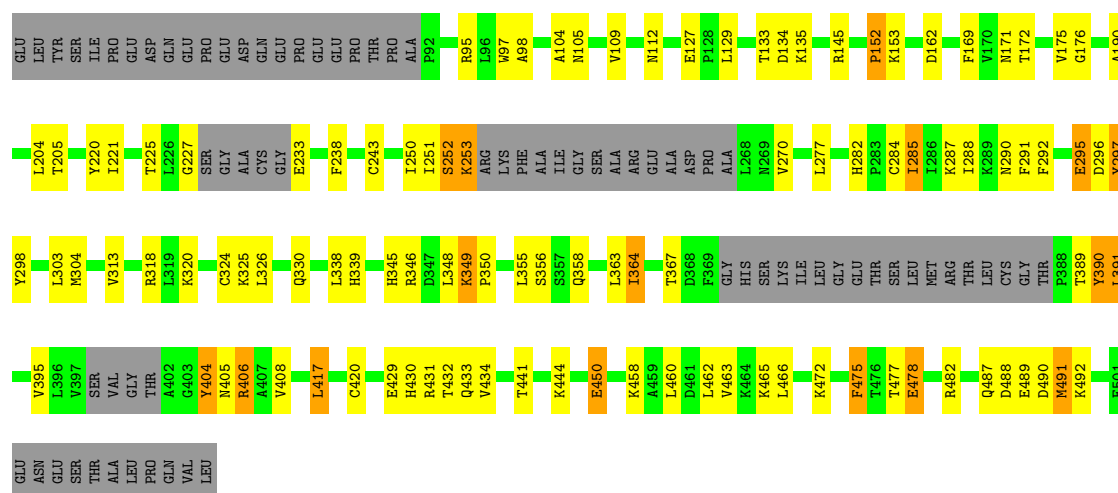
• Molecule 1: Serine/threonine-protein kinase Chk2

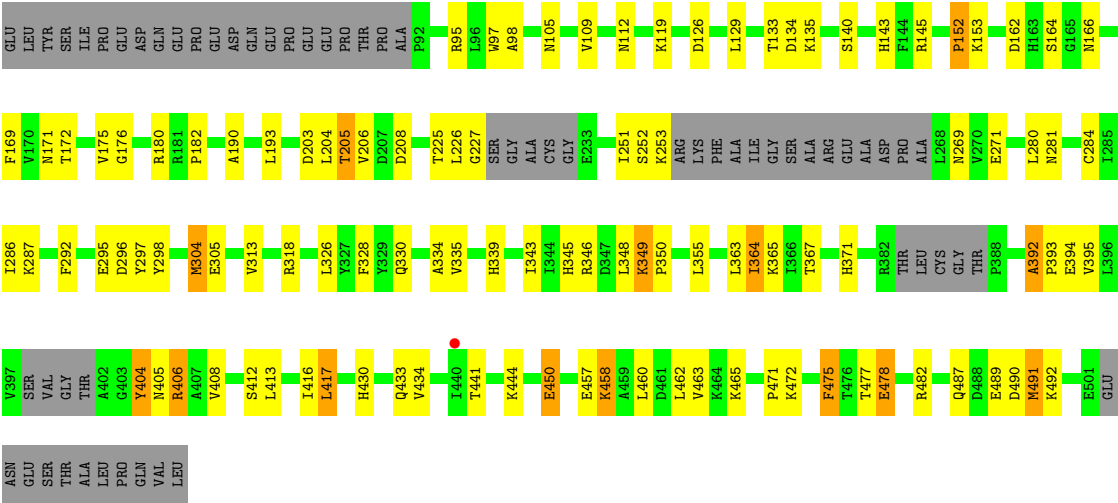
Chain F: 65% 19% 14%



• Molecule 1: Serine/threonine-protein kinase Chk2

Chain G: 59% 20% 17%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.20Å 114.70Å 123.00Å 84.10° 81.20° 80.70°	Depositor
Resolution (Å)	30.00 – 3.25 30.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.00-3.25) 90.8 (30.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.251 , 0.287 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	119.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 180.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24560	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.57	0/3087	0.87	5/4163 (0.1%)
1	B	0.58	0/3186	0.88	6/4294 (0.1%)
1	C	0.69	2/3083 (0.1%)	0.89	4/4158 (0.1%)
1	D	0.56	0/3186	0.88	8/4294 (0.2%)
1	E	0.53	0/3083	0.85	6/4158 (0.1%)
1	F	0.50	0/3186	0.85	5/4294 (0.1%)
1	G	0.51	0/3087	0.85	5/4163 (0.1%)
1	H	0.48	0/3186	0.84	5/4294 (0.1%)
All	All	0.56	2/25084 (0.0%)	0.86	44/33818 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	VAL	N-CA	-5.93	1.39	1.46
1	C	205	THR	C-N	-5.72	1.25	1.33

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LYS	N-CA-C	6.92	116.28	108.25
1	D	205	THR	O-C-N	-6.80	114.87	122.55
1	C	282	HIS	CA-C-N	6.44	126.12	119.56
1	C	282	HIS	C-N-CA	6.44	126.12	119.56
1	D	369	PHE	N-CA-C	-6.43	106.15	112.97

There are no chirality outliers.

There are no planarity outliers.

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	3022	0	3026	84	6
1	B	3120	0	3130	84	0
1	C	3018	0	3023	74	5
1	D	3120	0	3130	73	0
1	E	3018	0	3023	83	6
1	F	3120	0	3130	69	8
1	G	3022	0	3026	69	5
1	H	3120	0	3130	84	4
All	All	24560	0	24618	524	20

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 11.

The worst 5 of 524 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:129:LEU:HD23	1:D:193:LEU:CD2	1.47	1.44
1:A:129:LEU:CD2	1:D:193:LEU:HD21	1.52	1.40
1:F:132:ARG:CD	1:H:129:LEU:HD13	1.74	1.16
1:B:166:ASN:HD22	1:C:129:LEU:HB2	1.15	1.09
1:F:132:ARG:HD2	1:H:129:LEU:CD1	1.84	1.07

The worst 5 of 20 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:G:320:LYS:CD	1:H:457:GLU:OE2[1_455]	0.80	1.40
1:C:138:THR:CG2	1:C:496:GLN:NE2[1_655]	1.64	0.56
1:E:137:ARG:CD	1:F:450:GLU:CG[1_455]	1.64	0.56
1:G:320:LYS:CE	1:H:457:GLU:OE2[1_455]	1.71	0.49
1:A:195:ARG:O	1:F:493:ARG:NH1[1_456]	1.73	0.47

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	359/443 (81%)	326 (91%)	23 (6%)	10 (3%)	4	20
1	B	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	6	28
1	C	358/443 (81%)	326 (91%)	21 (6%)	11 (3%)	3	19
1	D	372/443 (84%)	334 (90%)	31 (8%)	7 (2%)	6	28
1	E	358/443 (81%)	327 (91%)	21 (6%)	10 (3%)	4	20
1	F	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	6	28
1	G	359/443 (81%)	328 (91%)	21 (6%)	10 (3%)	4	20
1	H	372/443 (84%)	335 (90%)	30 (8%)	7 (2%)	6	28
All	All	2922/3544 (82%)	2650 (91%)	203 (7%)	69 (2%)	4	23

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	390	TYR
1	A	433	GLN
1	B	134	ASP
1	B	433	GLN

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	333/395 (84%)	303 (91%)	30 (9%)	9	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	344/395 (87%)	314 (91%)	30 (9%)	9	31
1	C	333/395 (84%)	299 (90%)	34 (10%)	7	25
1	D	344/395 (87%)	315 (92%)	29 (8%)	10	33
1	E	333/395 (84%)	305 (92%)	28 (8%)	10	33
1	F	344/395 (87%)	316 (92%)	28 (8%)	11	35
1	G	333/395 (84%)	304 (91%)	29 (9%)	9	31
1	H	344/395 (87%)	316 (92%)	28 (8%)	11	35
All	All	2708/3160 (86%)	2472 (91%)	236 (9%)	9	31

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	462	LEU
1	H	406	ARG
1	E	462	LEU
1	H	367	THR
1	G	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	196	ASN
1	G	358	GLN
1	F	330	GLN
1	G	112	ASN
1	H	105	ASN

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 [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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	369/443 (83%)	-0.26	1 (0%) 90 82	118, 136, 157, 175	0
1	B	382/443 (86%)	-0.27	0 100 100	115, 136, 154, 182	0
1	C	368/443 (83%)	-0.14	3 (0%) 82 68	119, 134, 158, 178	0
1	D	382/443 (86%)	-0.35	0 100 100	118, 136, 154, 182	0
1	E	368/443 (83%)	-0.26	0 100 100	118, 136, 157, 180	0
1	F	382/443 (86%)	-0.38	0 100 100	118, 137, 153, 182	0
1	G	369/443 (83%)	-0.26	0 100 100	115, 137, 156, 178	0
1	H	382/443 (86%)	-0.39	1 (0%) 90 82	119, 136, 153, 181	0
All	All	3002/3544 (84%)	-0.29	5 (0%) 91 85	115, 136, 156, 182	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	GLU	2.9
1	C	443	GLY	2.8
1	C	444	LYS	2.4
1	H	440	ILE	2.1
1	C	129	LEU	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.