



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 10:55 PM UTC

PDB ID : 2J04 / pdb_00002j04
Title : The tau60-tau91 subcomplex of yeast transcription factor IIIC
Authors : Mylona, A.; Fernandez-Tornero, C.; Legrand, P.; Muller, C.W.
Deposited on : 2006-07-31
Resolution : 3.20 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

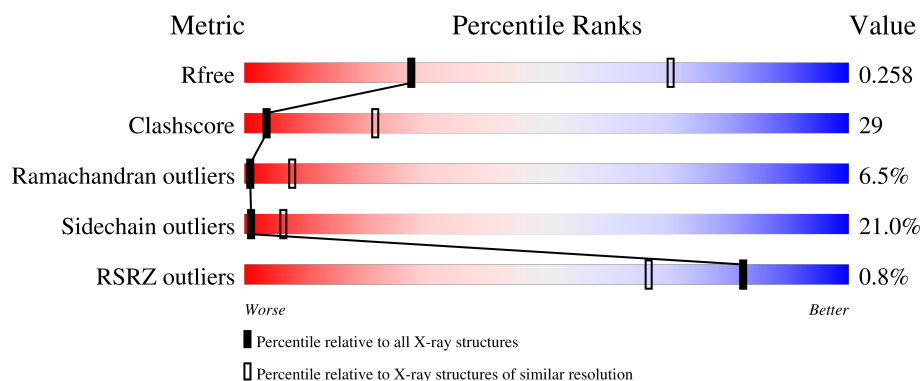
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	588	% 52% 35% 12% .
1	C	588	% 45% 39% 13% .
2	B	524	% 40% 34% 13% . 10%
2	D	524	% 41% 33% 12% . 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16935 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 HYPOTHETICAL PROTEIN YPL007C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4760	3058	777	902	23			
1	C	586	Total	C	N	O	S	0	0	0
			4751	3052	775	901	23			

- Molecule 2 is a protein called YDR362CP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	472	Total	C	N	O	S	0	0	1
			3715	2384	613	703	15			
2	D	469	Total	C	N	O	S	0	0	1
			3704	2379	609	701	15			

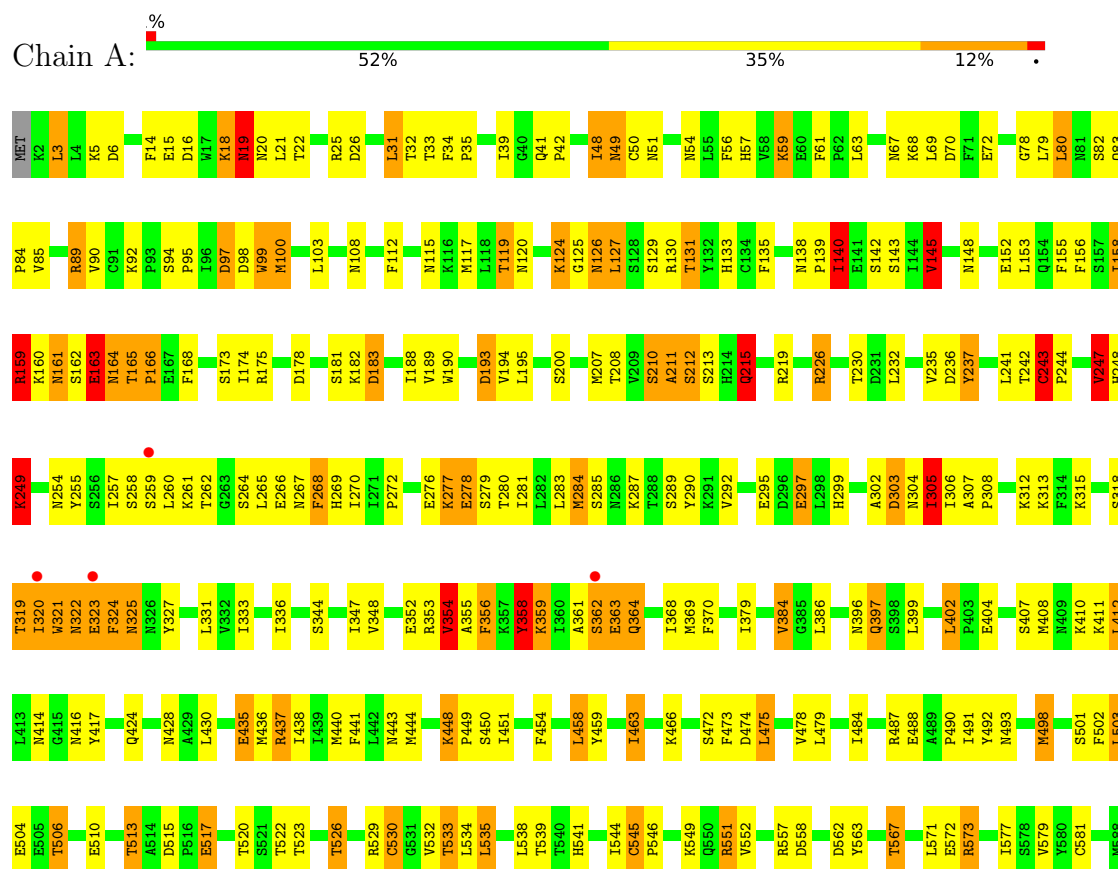
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

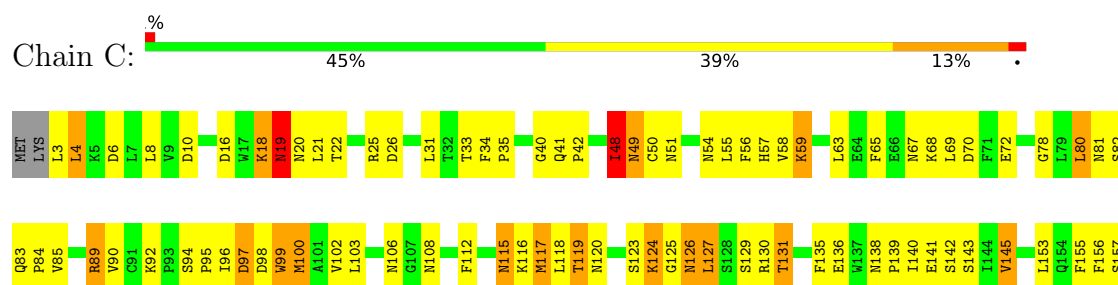
3 Residue-property plots

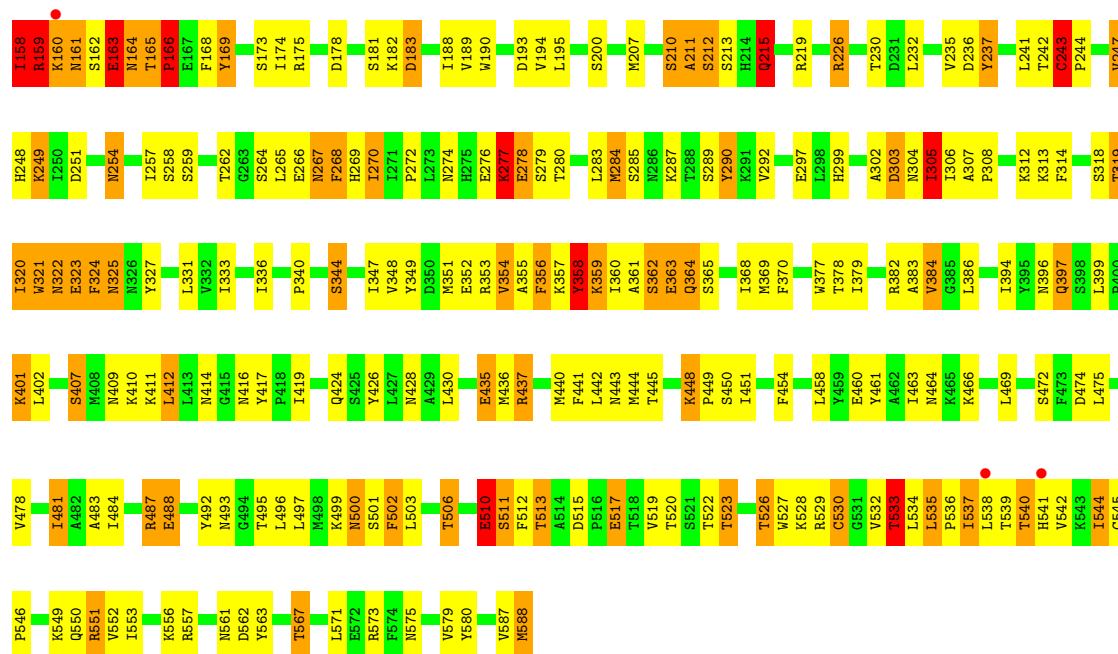
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HYPOTHETICAL PROTEIN YPL007C

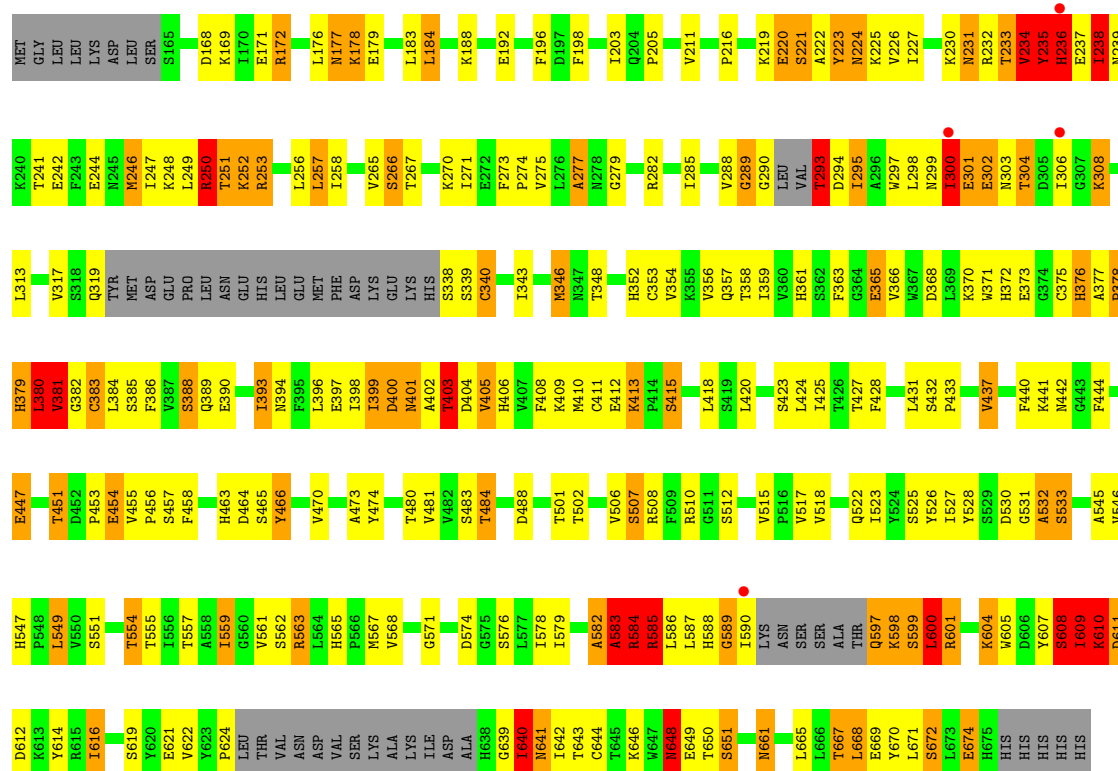
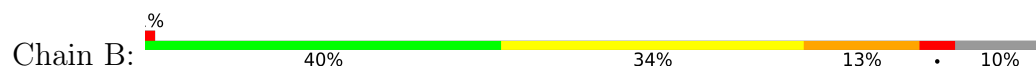


• Molecule 1: HYPOTHETICAL PROTEIN YPL007C





• Molecule 2: YDR362CP



• Molecule 2: YDR362CP





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.42Å 125.80Å 210.47Å 90.00° 94.49° 90.00°	Depositor
Resolution (Å)	208.51 – 3.20 208.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (208.51-3.20) 98.7 (208.51-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.257 (Not available) , 0.258	Depositor DCC
R_{free} test set	2619 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 128.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16935	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.96	4/4872 (0.1%)	1.17	19/6610 (0.3%)
1	C	0.93	3/4863 (0.1%)	1.15	25/6599 (0.4%)
2	B	0.94	6/3798 (0.2%)	1.21	27/5153 (0.5%)
2	D	0.91	7/3788 (0.2%)	1.17	24/5140 (0.5%)
All	All	0.94	20/17321 (0.1%)	1.17	95/23502 (0.4%)

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	3
2	B	0	8
2	D	0	7
All	All	0	20

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	413	LYS	CD-CE	15.06	1.97	1.52
2	B	300	ILE	CA-CB	13.18	1.69	1.53
2	B	413	LYS	CD-CE	11.78	1.87	1.52
1	A	249	LYS	CD-CE	10.98	1.85	1.52
2	D	300	ILE	CA-CB	9.79	1.65	1.53

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	599	SER	N-CA-C	12.14	128.04	109.23
2	D	599	SER	N-CA-C	11.12	126.04	109.24
2	D	413	LYS	CG-CD-CE	-9.59	89.24	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	340	CYS	N-CA-C	9.19	120.03	108.45
1	C	532	VAL	N-CA-C	-9.15	103.94	111.81

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	CYS	Peptide
1	A	98	ASP	Peptide
2	B	277	ALA	Peptide
2	B	293	THR	Peptide
2	B	379	HIS	Peptide

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	4760	0	4722	235	0
1	C	4751	0	4709	258	0
2	B	3715	0	3674	265	0
2	D	3704	0	3660	242	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	16935	0	16765	983	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 29.

The worst 5 of 983 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:249:LYS:CE	1:C:249:LYS:CD	1.79	1.60
2:B:413:LYS:CE	2:B:413:LYS:CD	1.87	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:CE	1:A:249:LYS:CD	1.85	1.50
2:B:413:LYS:CE	2:B:413:LYS:NZ	1.74	1.47
2:D:413:LYS:NZ	2:D:413:LYS:CE	1.76	1.45

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	585/588 (100%)	475 (81%)	74 (13%)	36 (6%)	1	9
1	C	584/588 (99%)	475 (81%)	69 (12%)	40 (7%)	1	7
2	B	462/524 (88%)	362 (78%)	68 (15%)	32 (7%)	1	7
2	D	459/524 (88%)	356 (78%)	76 (17%)	27 (6%)	1	10
All	All	2090/2224 (94%)	1668 (80%)	287 (14%)	135 (6%)	1	8

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	124	LYS
1	A	159	ARG
1	A	164	ASN
1	A	166	PRO

5.3.2 Protein sidechains [i](#)

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	543/544 (100%)	437 (80%)	106 (20%)	1	8
1	C	542/544 (100%)	432 (80%)	110 (20%)	1	7
2	B	415/465 (89%)	323 (78%)	92 (22%)	1	5
2	D	414/465 (89%)	320 (77%)	94 (23%)	1	5
All	All	1914/2018 (95%)	1512 (79%)	402 (21%)	1	6

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	189	VAL
1	C	497	LEU
2	D	667	THR
1	C	237	TYR
1	C	358	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	311	GLN
2	D	361	HIS
2	D	565	HIS
2	B	357	GLN
2	B	342	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](#)

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	587/588 (99%)	0.09	4 (0%) 84 69	61, 71, 71, 81	0
1	C	586/588 (99%)	0.19	3 (0%) 87 76	60, 71, 71, 87	0
2	B	472/524 (90%)	0.16	4 (0%) 82 67	70, 71, 71, 72	0
2	D	469/524 (89%)	0.06	5 (1%) 78 61	71, 71, 71, 75	0
All	All	2114/2224 (95%)	0.13	16 (0%) 82 67	60, 71, 71, 87	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	300	ILE	3.3
2	B	590	ILE	2.8
2	D	300	ILE	2.6
1	A	362	SER	2.4
2	D	306	ILE	2.4

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.