W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2023 – 08:10 AM EDT

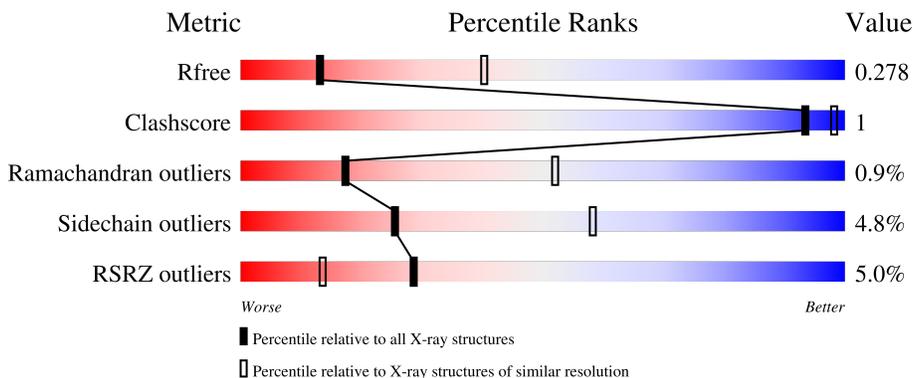|		
PDB ID	:	5WBY
Title	:	Crystal structure of mTOR(deltaN)-mLST8-PRAS40(beta-strand) complex
Authors	:	Pavletich, N.P.; Yang, H.
Deposited on	:	2017-06-29
Resolution	:	3.10 Å(reported)

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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 3.10 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		1
Ramachandran outliers		0.9%
Sidechain outliers		4.8%
RSRZ outliers		5.0%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	1177	6% · 83% · 6% · 11%
1	B	1177	4% · 83% · 6% · 10%
2	C	328	3% · 86% · 10% · ·
2	D	328	% · 85% · 11% · ·
3	O	98	6% · 10% · 90%

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Mol	Chain	Length	Quality of chain
3	P	98	
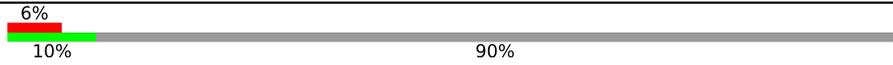
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22243 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 mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	63			
1	A	1052	Total	C	N	O	S	0	0	0
			8557	5439	1511	1544	63			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1373	GLY	-	expression tag	UNP P42345
B	1374	THR	-	expression tag	UNP P42345
B	1375	GLY	-	expression tag	UNP P42345
A	1373	GLY	-	expression tag	UNP P42345
A	1374	THR	-	expression tag	UNP P42345
A	1375	GLY	-	expression tag	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9BVC4
D	0	SER	-	expression tag	UNP Q9BVC4
C	-1	GLY	-	expression tag	UNP Q9BVC4
C	0	SER	-	expression tag	UNP Q9BVC4

- Molecule 3 is a protein called Proline-rich AKT1 substrate 1.

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total 83	C 57	N 13	O 13	0	0	0
3	O	10	Total 83	C 57	N 13	O 13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
P	110	GLY	-	expression tag	UNP Q96B36
P	111	SER	-	expression tag	UNP Q96B36
P	112	GLY	-	expression tag	UNP Q96B36
P	113	ARG	-	expression tag	UNP Q96B36
O	110	GLY	-	expression tag	UNP Q96B36
O	111	SER	-	expression tag	UNP Q96B36
O	112	GLY	-	expression tag	UNP Q96B36
O	113	ARG	-	expression tag	UNP Q96B36

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.
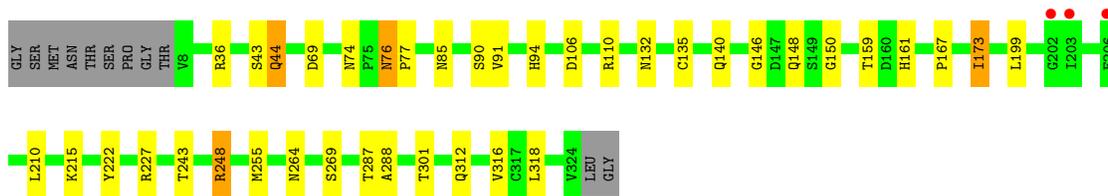
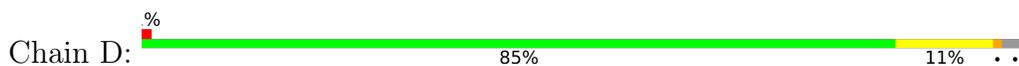- Molecule 1: Serine/threonine-protein kinase mTOR
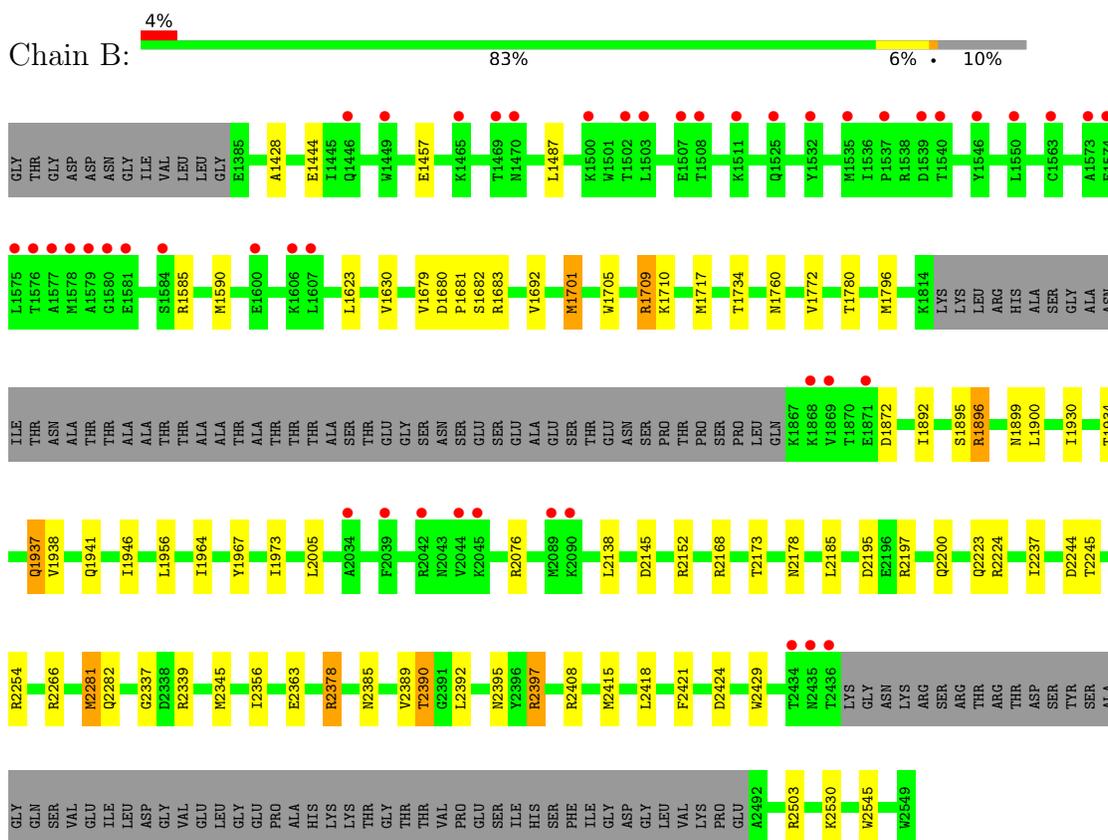
- Molecule 1: Serine/threonine-protein kinase mTOR
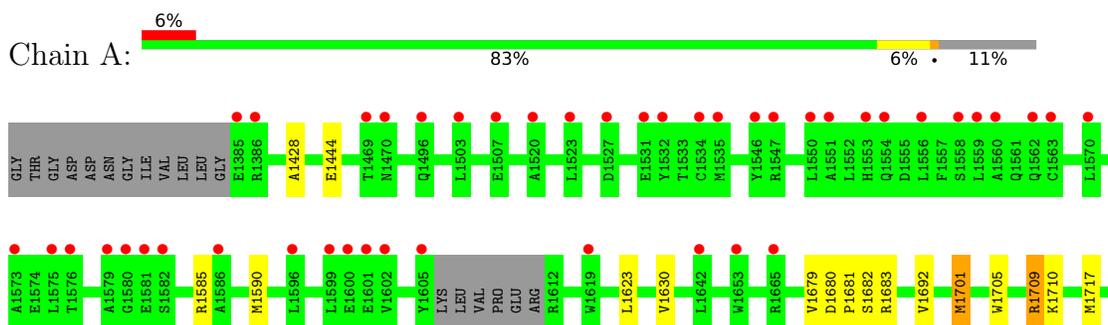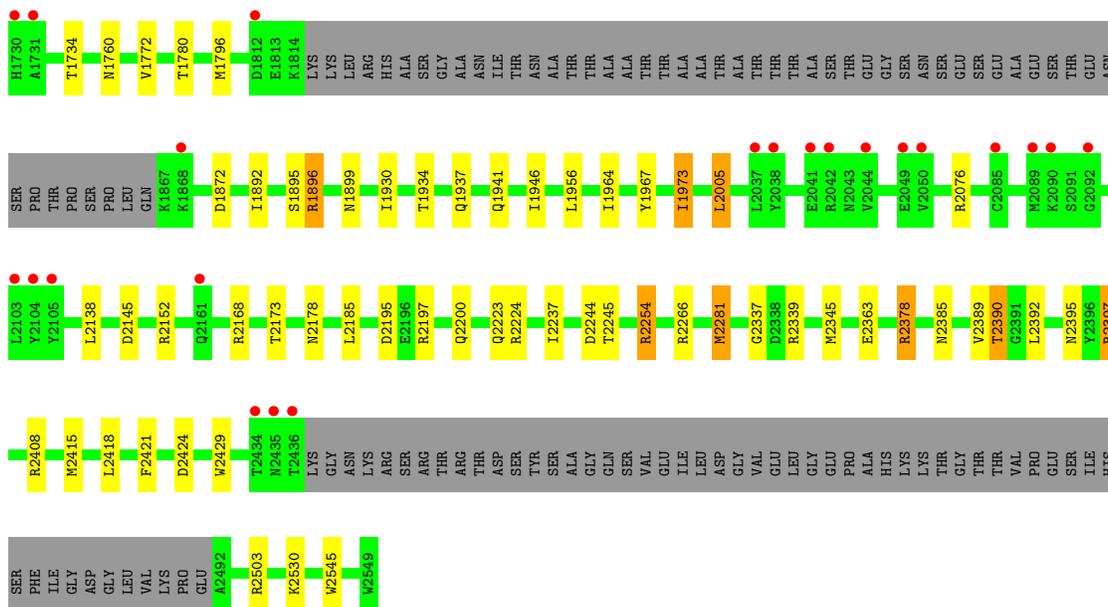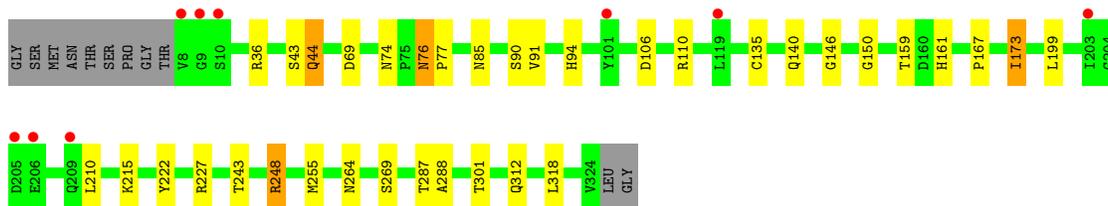
• Molecule 2: Target of rapamycin complex subunit LST8

Chain D:

• Molecule 2: Target of rapamycin complex subunit LST8

Chain C:

• Molecule 3: Proline-rich AKT1 substrate 1

Chain P:

• Molecule 3: Proline-rich AKT1 substrate 1

Chain O:

6%

10%

90%
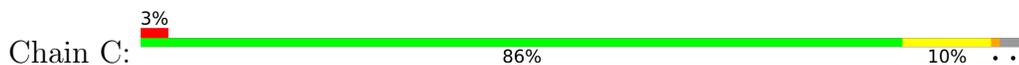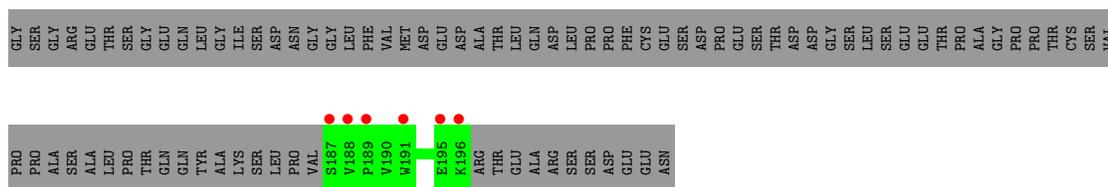
GLY SER GLY ARG GLU THR SER GLY GLU GLN LEU GLY ILE SER ASP ASN GLY GLY LEU PHE VAL MET ASP GLU ASP ALA THR LEU GLN ASP LEU PRO PRO PHE CYS GLU SER ASP PRO GLU SER THR ASP ASP GLY SER LEU SER GLU GLU THR PRO ALA GLY PRO PRO THR CYS SER VAL

PRO PRO ALA SER ALA LEU PRO THR GLN GLN TYR ALA LYS SER LEU PRO VAL S187 V188 P189 V190 W191 E195 K196 ARG THR GLU ALA ARG SER SER ASP GLU GLU ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.93Å 163.04Å 206.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.10 82.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.5 (50.01-3.10) 82.3 (82.91-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.233 , 0.276 0.235 , 0.278	Depositor DCC
R_{free} test set	1912 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22243	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4698e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/8752	0.58	1/11847 (0.0%)
1	B	0.38	0/8805	0.58	0/11920
2	C	0.37	0/2514	0.65	0/3426
2	D	0.37	0/2514	0.66	0/3426
3	O	0.48	0/86	0.51	0/115
3	P	0.48	0/86	0.52	0/115
All	All	0.38	0/22757	0.60	1/30849 (0.0%)

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	B	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2254	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	A	1680	ASP	Peptide
1	B	1444	GLU	Peptide
1	B	1680	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	8557	0	8533	19	0
1	B	8608	0	8593	23	0
2	C	2456	0	2341	11	0
2	D	2456	0	2341	13	0
3	O	83	0	83	0	0
3	P	83	0	83	0	0
All	All	22243	0	21974	63	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 1.

The worst 5 of 63 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:1941:GLN:HE22	1:A:2200:GLN:HE22	1.50	0.59
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.50	0.59
1:A:1681:PRO:O	1:A:1683:ARG:N	2.36	0.59
1:B:1681:PRO:O	1:B:1683:ARG:N	2.37	0.58
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.72	0.55

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	1044/1177 (89%)	993 (95%)	44 (4%)	7 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1052/1177 (89%)	997 (95%)	48 (5%)	7 (1%)	22	57
2	C	315/328 (96%)	289 (92%)	21 (7%)	5 (2%)	9	37
2	D	315/328 (96%)	290 (92%)	20 (6%)	5 (2%)	9	37
3	O	8/98 (8%)	8 (100%)	0	0	100	100
3	P	8/98 (8%)	8 (100%)	0	0	100	100
All	All	2742/3206 (86%)	2585 (94%)	133 (5%)	24 (1%)	17	52

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1682	SER
1	B	1692	VAL
2	D	74	ASN
1	A	1682	SER
1	A	1692	VAL

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	925/1025 (90%)	883 (96%)	42 (4%)	27	60
1	B	931/1025 (91%)	888 (95%)	43 (5%)	27	59
2	C	269/277 (97%)	254 (94%)	15 (6%)	21	52
2	D	269/277 (97%)	254 (94%)	15 (6%)	21	52
3	O	9/83 (11%)	9 (100%)	0	100	100
3	P	9/83 (11%)	9 (100%)	0	100	100
All	All	2412/2770 (87%)	2297 (95%)	115 (5%)	25	58

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	312	GLN

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Mol	Chain	Res	Type
2	C	243	THR
1	A	1956	LEU
2	C	227	ARG
1	A	2530	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	85	ASN
2	C	132	ASN
2	D	132	ASN
2	D	85	ASN
2	C	140	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1052/1177 (89%)	0.30	67 (6%)	19	8	46, 94, 188, 223	0
1	B	1058/1177 (89%)	0.17	46 (4%)	35	17	38, 83, 170, 211	0
2	C	317/328 (96%)	0.10	9 (2%)	53	30	50, 88, 147, 215	0
2	D	317/328 (96%)	-0.01	3 (0%)	84	69	34, 63, 126, 208	0
3	O	10/98 (10%)	3.01	6 (60%)	0	0	134, 170, 189, 196	0
3	P	10/98 (10%)	2.98	6 (60%)	0	0	101, 150, 187, 194	0
All	All	2764/3206 (86%)	0.21	137 (4%)	28	13	34, 85, 177, 223	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1579	ALA	8.3
1	A	1503	LEU	7.1
1	B	1580	GLY	6.5
1	B	1469	THR	6.4
1	A	1559	LEU	6.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.