



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:44 PM EDT

PDB ID : 5WBY / pdb_00005wby
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)

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

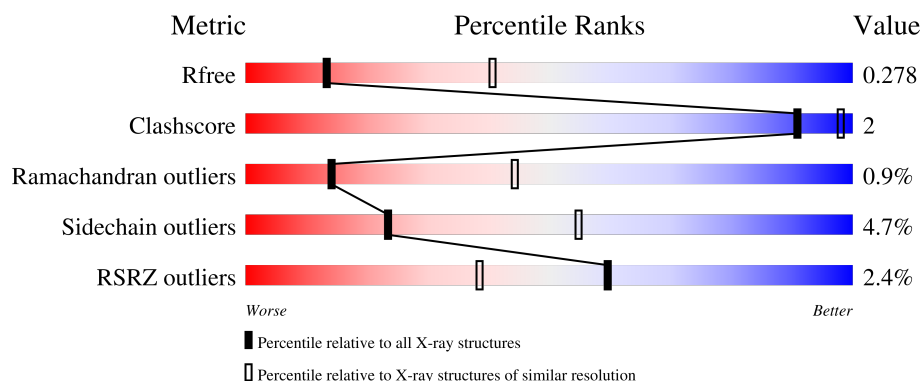
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	1177	
1	B	1177	
2	C	328	
2	D	328	
3	O	98	

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Mol	Chain	Length	Quality of chain
3	P	98	2% 10% 90%

2 Entry composition

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	C	N	O	0	0	0
			83	57	13	13			
3	O	10	Total	C	N	O	0	0	0
			83	57	13	13			

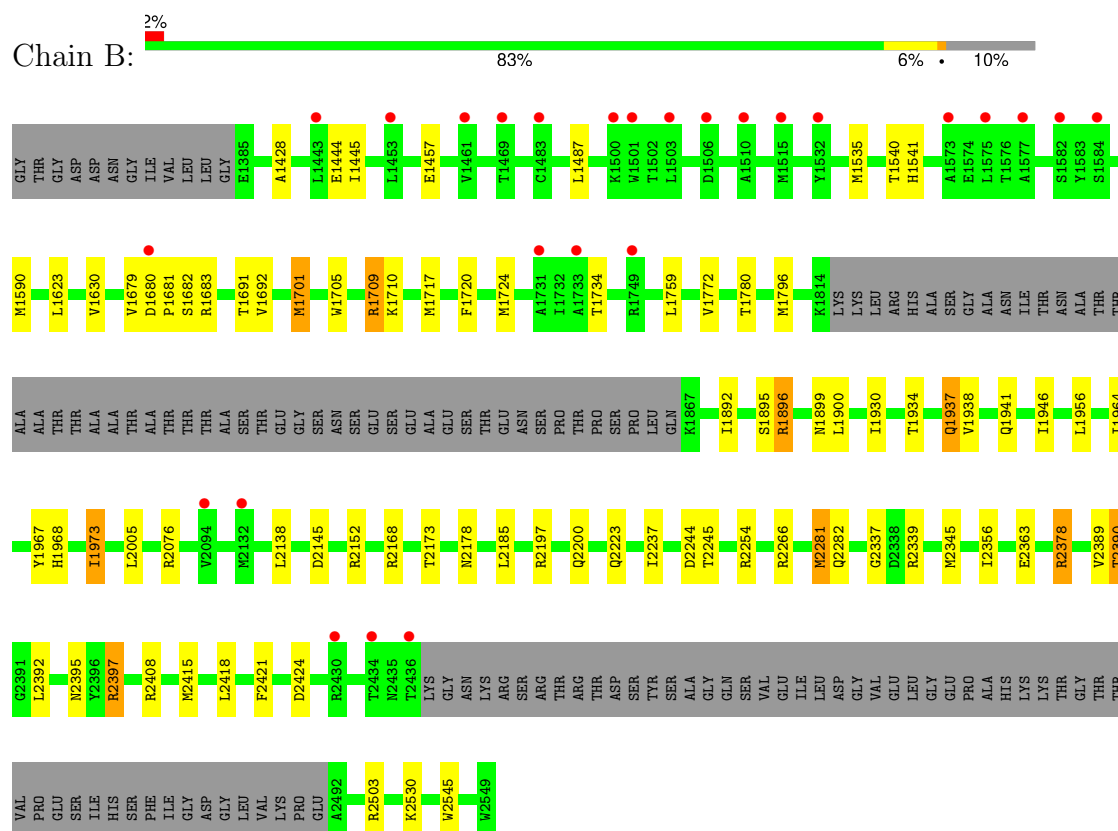
There are 8 discrepancies between the modelled and reference sequences:

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

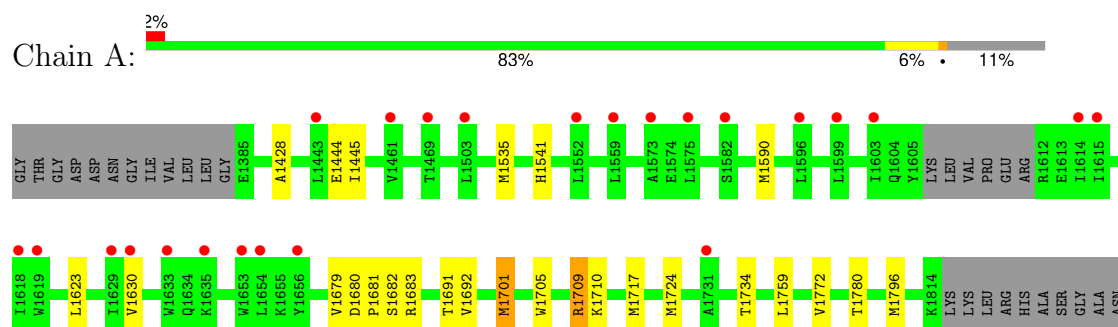
3 Residue-property plots [i](#)

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.

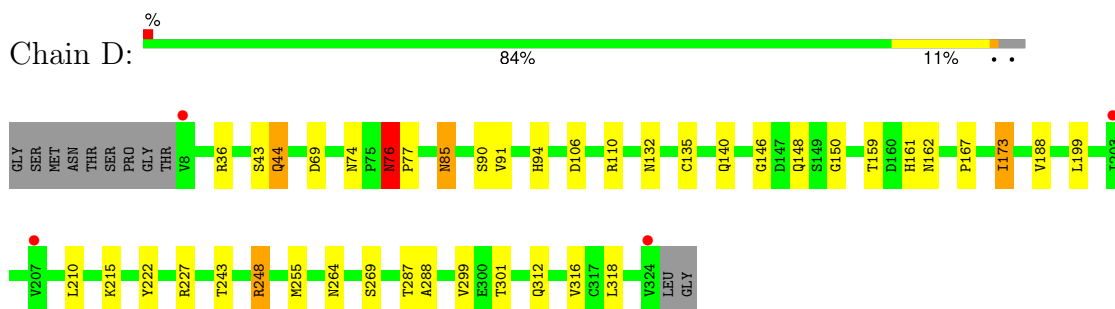
- Molecule 1: Serine/threonine-protein kinase mTOR



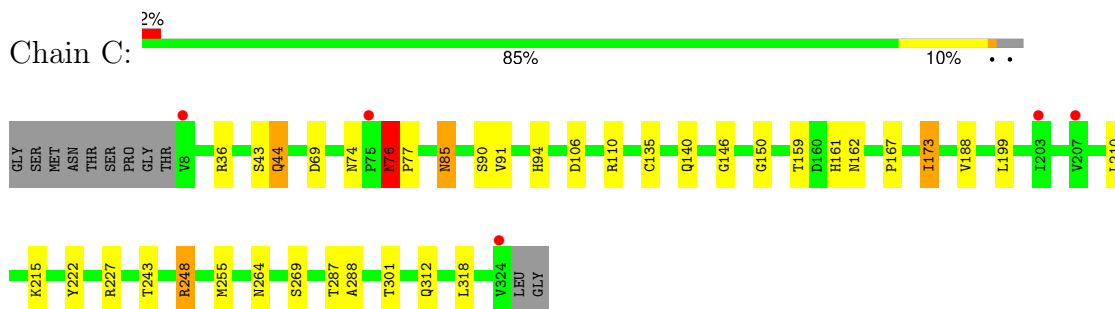
- Molecule 1: Serine/threonine-protein kinase mTOR



- Molecule 2: Target of rapamycin complex subunit LST8



- Molecule 2: Target of rapamycin complex subunit LST8



- Molecule 3: Proline-rich AKT1 substrate 1



- Molecule 3: Proline-rich AKT1 substrate 1



GLY SER GLY GLY ARG GLU THR SER GLY GLN GLN LEU GLY TLE SER ASP ASN GLY GLY LEU PHE VAL MET ASP GLU ASP ALA THR LEU GLN ASP LEU PRO PHE CYS GLU SER ASP PRO GLU SER THR ASP ASP GLY SER LEU SER GLU THR PRO PRO GLY ALA GLY PRO THR CYS SER VAL

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.5 (50.01-3.10) 82.5 (50.01-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (2.22%)	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)	0.31 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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	0.56	0/8752	0.87	3/11847 (0.0%)
1	B	0.56	0/8805	0.87	3/11920 (0.0%)
2	C	0.54	0/2514	0.79	2/3426 (0.1%)
2	D	0.55	0/2514	0.79	2/3426 (0.1%)
3	O	0.64	0/86	0.78	0/115
3	P	0.65	0/86	0.79	0/115
All	All	0.56	0/22757	0.85	10/30849 (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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1445	ILE	N-CA-C	-6.14	99.02	107.99
1	B	1445	ILE	N-CA-C	-5.99	99.25	107.99
2	C	76	ASN	CA-C-N	-5.34	114.46	119.85
2	C	76	ASN	C-N-CA	-5.34	114.46	119.85
1	B	1973	ILE	N-CA-CB	5.29	117.35	110.57
1	B	1973	ILE	CB-CA-C	-5.29	105.10	112.02
2	D	76	ASN	CA-C-N	-5.27	114.53	119.85
2	D	76	ASN	C-N-CA	-5.27	114.53	119.85
1	A	1973	ILE	N-CA-CB	5.26	117.30	110.57
1	A	1973	ILE	CB-CA-C	-5.13	105.30	112.02

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	24	0
1	B	8608	0	8593	27	0
2	C	2456	0	2341	13	0
2	D	2456	0	2341	16	0
3	O	83	0	83	0	0
3	P	83	0	83	0	0
All	All	22243	0	21974	75	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 2.

All (75) 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:B:2281:MET:HE1	2:D:222:TYR:CG	2.33	0.64
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
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.42	0.53
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.42	0.52
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.44	0.52
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.45	0.51
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1701:MET:HE1	1:B:1717:MET:N	2.26	0.50
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.93	0.50
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.93	0.50
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.93	0.50
1:B:1964:ILE:O	1:B:1967:TYR:O	2.29	0.50
1:A:1701:MET:HE1	1:A:1717:MET:N	2.27	0.49
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.46	0.49
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.95	0.49
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.95	0.48
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.95	0.48
1:A:1964:ILE:O	1:A:1967:TYR:O	2.31	0.47
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.48	0.47
2:D:36:ARG:NH2	2:D:69:ASP:O	2.47	0.47
2:D:43:SER:OG	2:D:44:GLN:N	2.48	0.47
2:C:36:ARG:NH2	2:C:69:ASP:O	2.47	0.46
2:D:248:ARG:NH1	2:D:255:MET:SD	2.88	0.46
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.97	0.46
1:A:1691:THR:HG23	1:A:1724:MET:HE1	1.97	0.46
1:B:1691:THR:HG23	1:B:1724:MET:HE1	1.97	0.46
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.97	0.46
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.49	0.45
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.82	0.45
2:C:43:SER:OG	2:C:44:GLN:N	2.50	0.45
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.17	0.45
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.50	0.44
2:C:248:ARG:NH1	2:C:255:MET:SD	2.90	0.44
1:B:1772:VAL:HG23	1:B:1796:MET:HG2	2.00	0.44
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.18	0.44
2:D:150:GLY:HA2	2:D:173:ILE:HG23	2.00	0.44
1:A:1772:VAL:HG23	1:A:1796:MET:HG2	2.00	0.44
2:C:150:GLY:HA2	2:C:173:ILE:HG23	2.00	0.44
1:B:1900:LEU:HD13	1:B:1937:GLN:HG2	2.01	0.43
2:D:85:ASN:C	2:D:85:ASN:HD22	2.26	0.43
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	1.99	0.43
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.99	0.43
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.84	0.43
2:C:85:ASN:HD22	2:C:85:ASN:C	2.27	0.43
2:D:106:ASP:OD1	2:D:110:ARG:NH1	2.52	0.42
1:B:1705:TRP:CE3	1:B:1710:LYS:HB2	2.54	0.42
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.19	0.42
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:HIS:CD2	2:D:140:GLN:HE21	2.36	0.42
1:A:1705:TRP:CE3	1:A:1710:LYS:HB2	2.55	0.42
1:A:2197:ARG:NH1	1:A:2424:ASP:OD2	2.53	0.42
2:C:106:ASP:OD1	2:C:110:ARG:NH1	2.53	0.42
1:B:2390:THR:HG23	1:B:2390:THR:O	2.20	0.41
2:D:76:ASN:CB	2:D:77:PRO:CD	2.98	0.41
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	2.02	0.41
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	2.02	0.41
2:C:76:ASN:CB	2:C:77:PRO:CD	2.98	0.41
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	2.02	0.41
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	2.01	0.41
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.20	0.41
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.54	0.41
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.55	0.41
2:C:94:HIS:CD2	2:C:140:GLN:HE21	2.37	0.41
2:C:146:GLY:HA3	2:C:173:ILE:HD11	2.03	0.41
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	2.03	0.41
1:B:1720:PHE:CZ	1:B:1724:MET:HE3	2.56	0.41
1:A:1701:MET:HB3	1:A:1701:MET:HE2	1.87	0.41
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.87	0.40
2:D:146:GLY:HA3	2:D:173:ILE:HD11	2.03	0.40
2:D:255:MET:HE1	2:D:299:VAL:HG12	2.02	0.40
1:A:1899:ASN:HD22	1:A:1899:ASN:C	2.29	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	1044/1177 (89%)	993 (95%)	44 (4%)	7 (1%)	18 49
1	B	1052/1177 (89%)	997 (95%)	48 (5%)	7 (1%)	18 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	315/328 (96%)	289 (92%)	21 (7%)	5 (2%)	7	30
2	D	315/328 (96%)	290 (92%)	20 (6%)	5 (2%)	7	30
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%)	14	44

All (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
2	C	74	ASN
1	B	1630	VAL
1	B	1709	ARG
1	B	1937	GLN
1	A	1630	VAL
1	A	1709	ARG
1	A	1937	GLN
1	B	1623	LEU
1	B	1896	ARG
2	D	76	ASN
2	D	269	SER
1	A	1623	LEU
2	C	76	ASN
2	C	269	SER
1	A	1896	ARG
2	D	167	PRO
2	C	167	PRO
2	D	264	ASN
2	C	264	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	925/1025 (90%)	885 (96%)	40 (4%)	26	57
1	B	931/1025 (91%)	891 (96%)	40 (4%)	26	57
2	C	269/277 (97%)	252 (94%)	17 (6%)	16	45
2	D	269/277 (97%)	252 (94%)	17 (6%)	16	45
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%)	2298 (95%)	114 (5%)	23	55

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1535	MET
1	B	1540	THR
1	B	1541	HIS
1	B	1590	MET
1	B	1679	VAL
1	B	1701	MET
1	B	1709	ARG
1	B	1734	THR
1	B	1780	THR
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1938	VAL
1	B	1946	ILE
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	2005	LEU
1	B	2076	ARG
1	B	2138	LEU
1	B	2145	ASP
1	B	2152	ARG
1	B	2168	ARG
1	B	2173	THR
1	B	2178	ASN
1	B	2185	LEU
1	B	2223	GLN
1	B	2237	ILE

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Mol	Chain	Res	Type
1	B	2244	ASP
1	B	2254	ARG
1	B	2266	ARG
1	B	2281	MET
1	B	2363	GLU
1	B	2378	ARG
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2415	MET
1	B	2503	ARG
1	B	2530	LYS
2	D	44	GLN
2	D	85	ASN
2	D	90	SER
2	D	91	VAL
2	D	135	CYS
2	D	159	THR
2	D	161	HIS
2	D	162	ASN
2	D	173	ILE
2	D	188	VAL
2	D	215	LYS
2	D	227	ARG
2	D	243	THR
2	D	248	ARG
2	D	287	THR
2	D	301	THR
2	D	312	GLN
1	A	1535	MET
1	A	1541	HIS
1	A	1590	MET
1	A	1679	VAL
1	A	1701	MET
1	A	1709	ARG
1	A	1734	THR
1	A	1780	THR
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1938	VAL
1	A	1946	ILE

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Mol	Chain	Res	Type
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	2005	LEU
1	A	2076	ARG
1	A	2138	LEU
1	A	2145	ASP
1	A	2152	ARG
1	A	2168	ARG
1	A	2173	THR
1	A	2178	ASN
1	A	2185	LEU
1	A	2223	GLN
1	A	2237	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2266	ARG
1	A	2281	MET
1	A	2344	LEU
1	A	2363	GLU
1	A	2378	ARG
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2415	MET
1	A	2503	ARG
1	A	2530	LYS
2	C	44	GLN
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
2	C	135	CYS
2	C	159	THR
2	C	161	HIS
2	C	162	ASN
2	C	173	ILE
2	C	188	VAL
2	C	215	LYS
2	C	227	ARG
2	C	243	THR
2	C	248	ARG
2	C	287	THR

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Mol	Chain	Res	Type
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1670	HIS
1	B	1695	GLN
1	B	1803	HIS
1	B	1899	ASN
1	B	1941	GLN
1	B	2003	ASN
1	B	2082	GLN
1	B	2124	GLN
1	B	2178	ASN
1	B	2265	HIS
1	B	2343	ASN
1	B	2395	ASN
1	B	2428	ASN
2	D	28	GLN
2	D	85	ASN
2	D	132	ASN
2	D	140	GLN
2	D	162	ASN
2	D	177	HIS
2	D	198	ASN
2	D	209	GLN
1	A	1525	GLN
1	A	1541	HIS
1	A	1561	GLN
1	A	1695	GLN
1	A	1703	ASN
1	A	1727	GLN
1	A	1808	ASN
1	A	1899	ASN
1	A	2003	ASN
1	A	2082	GLN
1	A	2124	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2200	GLN

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Mol	Chain	Res	Type
1	A	2343	ASN
1	A	2395	ASN
1	A	2428	ASN
1	A	2435	ASN
2	C	28	GLN
2	C	85	ASN
2	C	132	ASN
2	C	140	GLN
2	C	162	ASN
2	C	177	HIS
2	C	198	ASN
2	C	209	GLN

5.3.3 RNA [i](#)

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](#)

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%)	0.25	29 (2%) 55 34	46, 94, 188, 223	0
1	B	1058/1177 (89%)	0.15	26 (2%) 58 37	38, 83, 170, 211	0
2	C	317/328 (96%)	0.12	5 (1%) 70 49	50, 88, 147, 215	0
2	D	317/328 (96%)	-0.10	4 (1%) 75 56	34, 63, 126, 208	0
3	O	10/98 (10%)	1.43	1 (10%) 12 6	134, 170, 189, 196	0
3	P	10/98 (10%)	1.25	2 (20%) 3 1	101, 150, 187, 194	0
All	All	2764/3206 (86%)	0.16	67 (2%) 59 38	34, 85, 177, 223	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1503	LEU	4.1
1	A	1619	TRP	4.1
2	C	203	ILE	3.8
1	B	1469	THR	3.7
1	A	1443	LEU	3.4
2	D	203	ILE	3.3
1	A	1503	LEU	3.3
1	A	2434	THR	3.2
1	B	1582	SER	3.2
1	A	1573	ALA	3.1
2	C	324	VAL	3.1
1	A	1614	ILE	3.1
1	B	1575	LEU	3.0
1	A	1552	LEU	3.0
1	B	2434	THR	3.0
1	A	1629	ILE	3.0
1	A	1559	LEU	2.9
1	A	1599	LEU	2.8
1	B	1461	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1443	LEU	2.7
1	A	1654	LEU	2.7
1	A	1615	ILE	2.7
2	D	207	VAL	2.7
2	C	8	VAL	2.6
1	B	1532	TYR	2.6
1	A	1656	TYR	2.6
1	B	1500	LYS	2.6
1	A	1596	LEU	2.5
3	P	189	PRO	2.5
1	A	1461	VAL	2.5
3	P	188	VAL	2.5
1	A	1603	ILE	2.5
1	B	1501	TRP	2.4
1	A	1635	LYS	2.4
1	A	1653	TRP	2.4
1	B	1506	ASP	2.4
1	B	1453	LEU	2.4
2	D	8	VAL	2.3
1	B	1510	ALA	2.3
1	B	2094	VAL	2.3
1	B	2436	THR	2.3
2	C	207	VAL	2.2
1	B	1731	ALA	2.2
1	A	1575	LEU	2.2
1	A	1582	SER	2.2
2	D	324	VAL	2.2
3	O	188	VAL	2.2
1	A	2430	ARG	2.2
2	C	75	PRO	2.2
1	A	1618	ILE	2.2
1	A	1469	THR	2.1
1	B	2132	MET	2.1
1	A	1731	ALA	2.1
1	A	2514	SER	2.1
1	A	1633	TRP	2.1
1	A	1630	VAL	2.1
1	A	2119	THR	2.1
1	B	1584	SER	2.1
1	B	1515	MET	2.1
1	B	1680	ASP	2.1
1	A	2436	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1573	ALA	2.1
1	B	1749	ARG	2.0
1	B	1483	CYS	2.0
1	B	1577	ALA	2.0
1	B	1733	ALA	2.0
1	B	2430	ARG	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.