



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:19 PM UTC

PDB ID : 5WBU / pdb_00005wbu
Title : Crystal structure of mTOR(deltaN)-mLST8-PRAS40(alpha-helix & beta-strand) complex
Authors : Pavletich, N.P.; Yang, H.
Deposited on : 2017-06-29
Resolution : 3.42 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

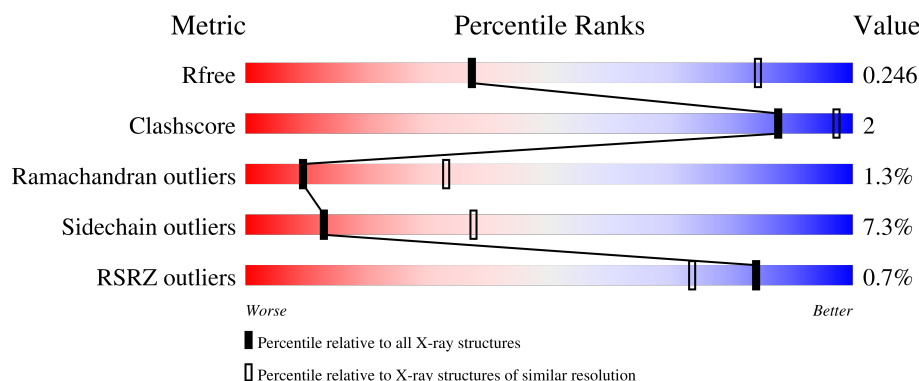
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	78% 10% 11%
1	B	1177	79% 10% 10%
2	C	328	84% 11% 5%
2	D	328	84% 11% 5%
3	O	88	9% 90%

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Mol	Chain	Length	Quality of chain
3	P	88	9% .90%
3	Q	88	24%76%
3	R	88	24%76%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22553 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	9	Total C N O 77 54 12 11	0	0	0
3	R	21	Total C N O S 161 97 30 33 1	0	0	0
3	O	9	Total C N O 77 54 12 11	0	0	0
3	Q	21	Total C N O S 161 97 30 33 1	0	0	0

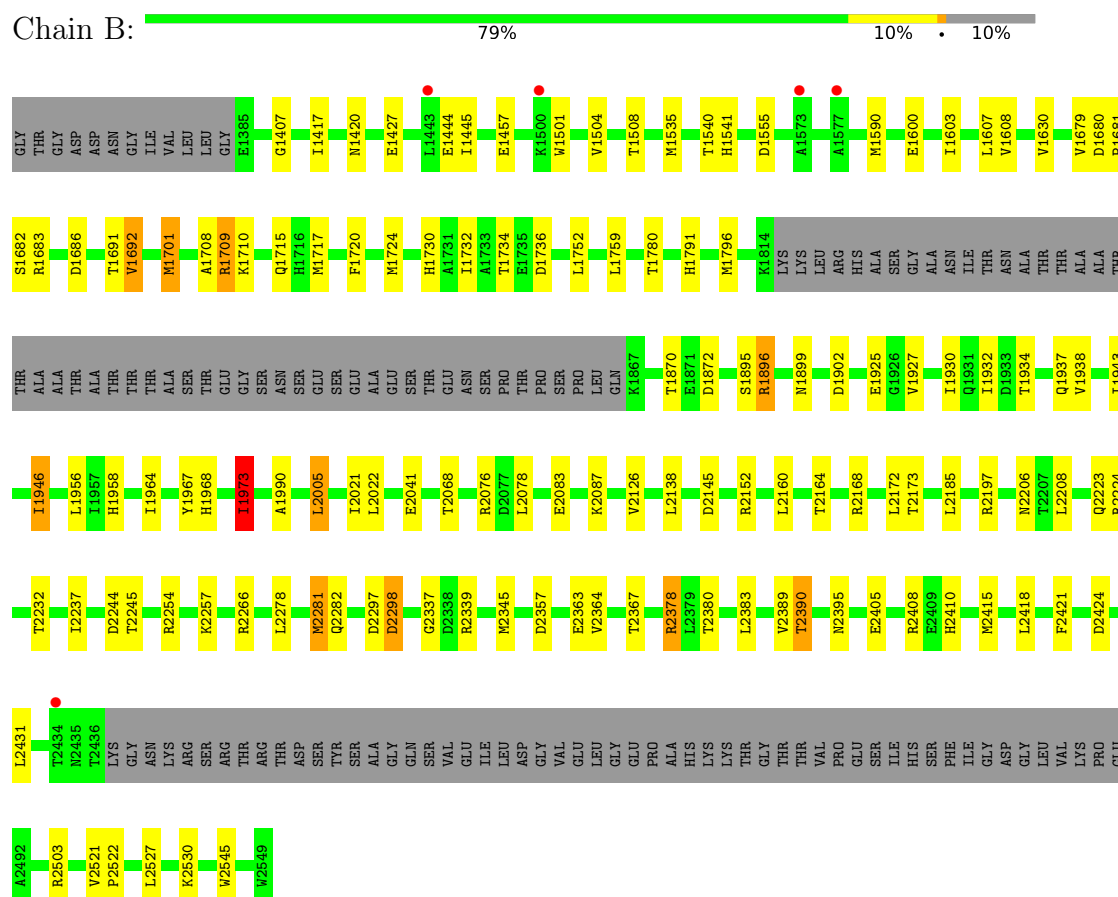
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	169	GLY	-	expression tag	UNP Q96B36
P	170	SER	-	expression tag	UNP Q96B36
P	171	GLY	-	expression tag	UNP Q96B36
P	172	ARG	-	expression tag	UNP Q96B36
R	169	GLY	-	expression tag	UNP Q96B36
R	170	SER	-	expression tag	UNP Q96B36
R	171	GLY	-	expression tag	UNP Q96B36
R	172	ARG	-	expression tag	UNP Q96B36
O	169	GLY	-	expression tag	UNP Q96B36
O	170	SER	-	expression tag	UNP Q96B36
O	171	GLY	-	expression tag	UNP Q96B36
O	172	ARG	-	expression tag	UNP Q96B36
Q	169	GLY	-	expression tag	UNP Q96B36
Q	170	SER	-	expression tag	UNP Q96B36
Q	171	GLY	-	expression tag	UNP Q96B36
Q	172	ARG	-	expression tag	UNP Q96B36

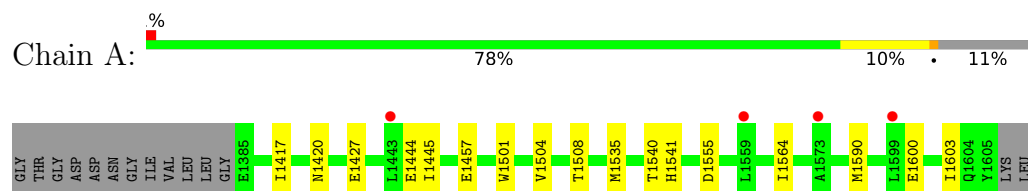
3 Residue-property plots

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



THR
GLN
VAL
PHE
GLY
ASP
LEU
PRO
ARG
PRO
GLN
ARG
LEU
ASN
THR
SER
SER
ASP
PHE
GLN
LYS
LEU
LEU
ARG
LYS
TYR

● Molecule 3: Proline-rich AKT1 substrate 1



GLY
SER
GLY
ARG
GLN
PHE
LYS
SER
ALA
LEU
LEU
PRO
THR
THR
GLN
PRO
GLN
TYR
ALA
LYS
SER
SER
LEU
LEU
PRO
PHE
VAL
SER
SER
VAL
PRO
VAL
TRP
GLY
PHE
GLY
LYS
GLU
LYS
LYS
ARG
THR
THR
GLU
ALA
ARG
SER
SER
ASP
GLU
GLU
ASN
GLY
PRO
PRO
PRO
SER
SER
SER
SER
S212
D232
THR
GLN
VAL
PHE
GLY
ASP
LEU
PRO
ARG
PRO
ARG
LEU
ASN
THR

SER
ASP
PHE
GLN
LYS
LEU
LYS
ARG
TYR

● Molecule 3: Proline-rich AKT1 substrate 1



GLY
SER
GLY
ARG
SER
ALA
LEU
PRO
THR
THR
GLN
PRO
GLN
TYR
ALA
LYS
SER
SER
LEU
LEU
PRO
PHE
VAL
SER
SER
VAL
M188
M191
K196
ARG
THR
GLU
ALA
ALA
ARG
SER
SER
SER
ASP
GLU
GLU
ASN
SER
GLY
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LEU
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ARG
ALA
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GLU
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GLU
ASP

THR
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ASN
THR
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ASP
PHE
GLN
LYS
LEU
LEU
ARG
LYS
TYR

● Molecule 3: Proline-rich AKT1 substrate 1



GLY
SER
GLY
ARG
GLN
PHE
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ALA
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LEU
PRO
THR
THR
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ALA
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GLU
ALA
ARG
SER
SER
ASP
GLU
GLU
ASN
GLY
PRO
PRO
PRO
SER
SER
SER
SER
S212
D232
THR
GLN
VAL
PHE
GLY
ASP
LEU
PRO
ARG
PRO
ARG
LEU
ASN
THR

SER
ASP
PHE
GLN
LYS
LEU
LYS
ARG
TYR

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	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.42 50.01 – 3.42	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.01-3.42) 83.8 (50.01-3.42)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.235 , 0.266 0.236 , 0.246	Depositor DCC
R_{free} test set	1812 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22553	wwPDB-VP
Average B, all atoms (Å ²)	117.0	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 44.21 % 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 1.5768e-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	0.66	1/8752 (0.0%)	0.95	3/11847 (0.0%)
1	B	0.67	0/8805	0.95	2/11920 (0.0%)
2	C	0.60	0/2514	0.87	0/3426
2	D	0.62	0/2514	0.88	1/3426 (0.0%)
3	O	0.60	0/80	0.70	0/107
3	P	0.58	0/80	0.72	0/107
3	Q	0.78	0/161	1.13	0/216
3	R	0.75	0/161	1.12	0/216
All	All	0.65	1/23067 (0.0%)	0.94	6/31265 (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	3
1	B	0	3
2	C	0	1
2	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	ILE	CA-CB	5.08	1.56	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1445	ILE	N-CA-C	-7.09	98.37	108.58
1	A	1445	ILE	N-CA-C	-7.07	98.40	108.58
1	B	1973	ILE	CB-CA-C	-6.09	104.06	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1973	ILE	CB-CA-C	-5.67	104.61	112.04
1	A	1973	ILE	N-CA-C	5.27	116.63	110.62
2	D	78	ILE	N-CA-C	-5.19	106.02	110.74

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	A	1680	ASP	Peptide
1	A	1732	ILE	Peptide
1	B	1444	GLU	Peptide
1	B	1680	ASP	Peptide
1	B	1732	ILE	Peptide
2	C	76	ASN	Peptide
2	D	76	ASN	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	39	0
1	B	8608	0	8593	38	0
2	C	2456	0	2341	11	0
2	D	2456	0	2341	11	0
3	O	77	0	78	0	0
3	P	77	0	78	0	0
3	Q	161	0	161	0	0
3	R	161	0	161	0	0
All	All	22553	0	22286	91	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 (91) 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:CD2	2.25	0.72
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.76	0.66
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.77	0.66
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.31	0.65
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.79	0.65
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.79	0.64
1:B:1681:PRO:O	1:B:1683:ARG:N	2.31	0.64
1:A:1681:PRO:O	1:A:1683:ARG:N	2.32	0.63
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.80	0.61
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.81	0.60
1:A:2390:THR:HG23	1:A:2390:THR:O	2.03	0.58
1:B:2390:THR:HG23	1:B:2390:THR:O	2.04	0.57
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.38	0.56
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.39	0.56
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.40	0.55
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.39	0.55
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.89	0.53
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.43	0.52
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.44	0.52
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.91	0.52
1:B:1701:MET:HE1	1:B:1717:MET:N	2.25	0.51
1:A:1701:MET:HE1	1:A:1717:MET:N	2.26	0.51
1:B:1964:ILE:O	1:B:1967:TYR:O	2.29	0.51
1:B:1691:THR:O	1:B:1692:VAL:C	2.53	0.51
1:A:2278:LEU:HD22	1:A:2282:GLN:HB3	1.92	0.50
1:A:1964:ILE:O	1:A:1967:TYR:O	2.30	0.50
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.94	0.50
1:B:2278:LEU:HD22	1:B:2282:GLN:HB3	1.92	0.50
2:D:231:ASP:HB3	2:D:233:THR:OG1	2.12	0.49
1:A:2206:ASN:ND2	1:A:2224:ARG:HD2	2.27	0.49
2:C:231:ASP:HB3	2:C:233:THR:OG1	2.13	0.49
1:B:2245:THR:HA	1:B:2345:MET:HB3	1.96	0.47
1:A:1691:THR:O	1:A:1692:VAL:C	2.58	0.47
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.98	0.46
1:B:2297:ASP:O	1:B:2298:ASP:C	2.58	0.46
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.25	0.46
2:D:233:THR:C	2:D:249:THR:HG1	2.23	0.46
1:A:1600:GLU:HA	1:A:1603:ILE:HG22	1.96	0.46
1:A:2245:THR:HA	1:A:2345:MET:HB3	1.97	0.46
1:B:1600:GLU:HA	1:B:1603:ILE:HG22	1.97	0.46
1:A:2297:ASP:O	1:A:2298:ASP:C	2.59	0.46
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2197:ARG:NH1	1:A:2424:ASP:OD2	2.49	0.45
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.97	0.45
1:A:1973:ILE:HD13	1:A:2005:LEU:HD22	1.98	0.45
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.97	0.45
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.51	0.45
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.99	0.45
1:B:1427:GLU:OE2	1:B:2395:ASN:ND2	2.50	0.45
1:A:1427:GLU:OE2	1:A:2395:ASN:ND2	2.49	0.45
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.99	0.44
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.18	0.44
2:D:171:VAL:O	2:D:171:VAL:HG23	2.16	0.44
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.98	0.44
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.53	0.44
1:B:1730:HIS:HE1	2:C:293:LEU:HD21	1.82	0.43
1:B:1501:TRP:O	1:B:1504:VAL:HG22	2.18	0.43
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.51	0.43
1:A:1501:TRP:O	1:A:1504:VAL:HG22	2.17	0.43
1:B:1973:ILE:HD13	1:B:2005:LEU:HD22	2.00	0.43
2:C:233:THR:C	2:C:249:THR:HG1	2.25	0.43
1:A:1882:VAL:HG12	1:A:1886:GLN:HE21	1.84	0.43
1:A:1943:ILE:HG23	1:A:1946:ILE:HD12	2.00	0.43
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.29	0.42
1:A:1564:ILE:HG21	1:A:1600:GLU:HG3	2.01	0.42
1:A:2389:VAL:O	1:A:2390:THR:HG22	2.19	0.42
1:B:1943:ILE:HG23	1:B:1946:ILE:HD12	2.01	0.42
1:B:1759:LEU:HD11	1:B:1796:MET:HE3	2.01	0.42
1:B:2208:LEU:HD22	1:B:2410:HIS:CG	2.54	0.42
2:D:43:SER:OG	2:D:44:GLN:N	2.51	0.42
1:A:1708:ALA:O	1:A:1710:LYS:N	2.52	0.42
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	2.01	0.41
1:B:2281:MET:HE3	1:B:2281:MET:HA	2.02	0.41
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	2.01	0.41
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.53	0.41
1:A:2390:THR:O	1:A:2390:THR:CG2	2.69	0.41
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.56	0.41
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	2.02	0.41
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.56	0.41
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.20	0.41
1:B:1720:PHE:CZ	1:B:1724:MET:HE3	2.56	0.41
1:A:2380:THR:HG22	1:A:2383:LEU:HG	2.02	0.41
2:C:133:CYS:SG	2:C:175:SER:HA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:VAL:HG23	2:C:171:VAL:O	2.19	0.41
2:D:248:ARG:HH11	2:D:248:ARG:HB3	1.85	0.41
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	2.02	0.41
1:B:1708:ALA:O	1:B:1710:LYS:N	2.53	0.40
1:B:2390:THR:O	1:B:2390:THR:CG2	2.70	0.40
1:A:2321:THR:HG23	1:A:2387:MET:HG2	2.04	0.40
1:B:1791:HIS:ND1	1:B:1902:ASP:OD1	2.55	0.40
1:A:1720:PHE:CZ	1:A:1724:MET:HE3	2.57	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%)	982 (94%)	53 (5%)	9 (1%)	14	41
1	B	1052/1177 (89%)	984 (94%)	56 (5%)	12 (1%)	11	37
2	C	315/328 (96%)	285 (90%)	23 (7%)	7 (2%)	5	23
2	D	315/328 (96%)	284 (90%)	24 (8%)	7 (2%)	5	23
3	O	7/88 (8%)	6 (86%)	1 (14%)	0	100	100
3	P	7/88 (8%)	6 (86%)	1 (14%)	0	100	100
3	Q	19/88 (22%)	18 (95%)	1 (5%)	0	100	100
3	R	19/88 (22%)	18 (95%)	1 (5%)	0	100	100
All	All	2778/3362 (83%)	2583 (93%)	160 (6%)	35 (1%)	9	33

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1630	VAL
1	B	1682	SER

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Mol	Chain	Res	Type
1	B	1692	VAL
1	B	1709	ARG
2	D	74	ASN
1	A	1630	VAL
1	A	1682	SER
1	A	1692	VAL
1	A	1709	ARG
2	C	74	ASN
1	B	1896	ARG
1	B	1937	GLN
1	B	2298	ASP
1	A	1896	ARG
1	A	1937	GLN
1	B	2364	VAL
2	D	167	PRO
2	D	269	SER
2	D	310	GLY
1	A	2298	ASP
2	C	167	PRO
2	C	269	SER
2	C	310	GLY
2	D	206	GLU
1	A	2364	VAL
2	C	106	ASP
2	C	206	GLU
1	B	1607	LEU
1	B	2357	ASP
2	D	106	ASP
1	B	1555	ASP
1	A	1555	ASP
2	D	264	ASN
2	C	264	ASN
1	B	1407	GLY

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%)	860 (93%)	65 (7%)	14	39
1	B	931/1025 (91%)	867 (93%)	64 (7%)	14	39
2	C	269/277 (97%)	245 (91%)	24 (9%)	9	30
2	D	269/277 (97%)	245 (91%)	24 (9%)	9	30
3	O	8/76 (10%)	7 (88%)	1 (12%)	4	17
3	P	8/76 (10%)	7 (88%)	1 (12%)	4	17
3	Q	17/76 (22%)	17 (100%)	0	100	100
3	R	17/76 (22%)	17 (100%)	0	100	100
All	All	2444/2908 (84%)	2265 (93%)	179 (7%)	13	37

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1457	GLU
1	B	1508	THR
1	B	1535	MET
1	B	1540	THR
1	B	1541	HIS
1	B	1590	MET
1	B	1608	VAL
1	B	1679	VAL
1	B	1701	MET
1	B	1709	ARG
1	B	1715	GLN
1	B	1734	THR
1	B	1736	ASP
1	B	1752	LEU
1	B	1780	THR
1	B	1870	THR
1	B	1872	ASP
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1925	GLU
1	B	1927	VAL
1	B	1932	ILE
1	B	1938	VAL
1	B	1946	ILE

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Mol	Chain	Res	Type
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	2005	LEU
1	B	2021	ILE
1	B	2041	GLU
1	B	2068	THR
1	B	2076	ARG
1	B	2078	LEU
1	B	2083	GLU
1	B	2087	LYS
1	B	2138	LEU
1	B	2145	ASP
1	B	2152	ARG
1	B	2164	THR
1	B	2168	ARG
1	B	2173	THR
1	B	2185	LEU
1	B	2223	GLN
1	B	2232	THR
1	B	2237	ILE
1	B	2244	ASP
1	B	2254	ARG
1	B	2257	LYS
1	B	2266	ARG
1	B	2281	MET
1	B	2363	GLU
1	B	2367	THR
1	B	2378	ARG
1	B	2390	THR
1	B	2405	GLU
1	B	2408	ARG
1	B	2415	MET
1	B	2431	LEU
1	B	2503	ARG
1	B	2527	LEU
1	B	2530	LYS
2	D	13	VAL
2	D	44	GLN
2	D	84	VAL
2	D	85	ASN
2	D	90	SER

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Mol	Chain	Res	Type
2	D	91	VAL
2	D	159	THR
2	D	161	HIS
2	D	162	ASN
2	D	173	ILE
2	D	175	SER
2	D	188	VAL
2	D	214	THR
2	D	215	LYS
2	D	227	ARG
2	D	243	THR
2	D	248	ARG
2	D	249	THR
2	D	250	SER
2	D	251	ASN
2	D	287	THR
2	D	301	THR
2	D	304	ILE
2	D	312	GLN
3	P	191	TRP
1	A	1417	ILE
1	A	1420	ASN
1	A	1457	GLU
1	A	1508	THR
1	A	1535	MET
1	A	1540	THR
1	A	1541	HIS
1	A	1590	MET
1	A	1679	VAL
1	A	1701	MET
1	A	1709	ARG
1	A	1715	GLN
1	A	1734	THR
1	A	1736	ASP
1	A	1752	LEU
1	A	1780	THR
1	A	1870	THR
1	A	1872	ASP
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1925	GLU

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Mol	Chain	Res	Type
1	A	1927	VAL
1	A	1932	ILE
1	A	1938	VAL
1	A	1946	ILE
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	2005	LEU
1	A	2021	ILE
1	A	2041	GLU
1	A	2063	GLN
1	A	2068	THR
1	A	2076	ARG
1	A	2078	LEU
1	A	2083	GLU
1	A	2087	LYS
1	A	2138	LEU
1	A	2145	ASP
1	A	2152	ARG
1	A	2164	THR
1	A	2168	ARG
1	A	2173	THR
1	A	2185	LEU
1	A	2223	GLN
1	A	2228	ILE
1	A	2232	THR
1	A	2237	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2257	LYS
1	A	2266	ARG
1	A	2281	MET
1	A	2363	GLU
1	A	2367	THR
1	A	2378	ARG
1	A	2390	THR
1	A	2405	GLU
1	A	2408	ARG
1	A	2415	MET
1	A	2431	LEU
1	A	2503	ARG
1	A	2527	LEU

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Mol	Chain	Res	Type
1	A	2530	LYS
2	C	13	VAL
2	C	44	GLN
2	C	84	VAL
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
2	C	128	ASN
2	C	159	THR
2	C	161	HIS
2	C	162	ASN
2	C	173	ILE
2	C	175	SER
2	C	188	VAL
2	C	214	THR
2	C	215	LYS
2	C	227	ARG
2	C	243	THR
2	C	248	ARG
2	C	249	THR
2	C	251	ASN
2	C	287	THR
2	C	301	THR
2	C	304	ILE
2	C	312	GLN
3	O	191	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1421	ASN
1	B	1425	GLN
1	B	1492	GLN
1	B	1496	GLN
1	B	1624	GLN
1	B	1730	HIS
1	B	1797	ASN
1	B	1886	GLN
1	B	1920	ASN
1	B	1941	GLN
1	B	2148	GLN
1	B	2200	GLN

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Mol	Chain	Res	Type
1	B	2265	HIS
1	B	2435	ASN
1	B	2502	ASN
2	D	73	ASN
2	D	132	ASN
2	D	148	GLN
2	D	162	ASN
2	D	209	GLN
1	A	1425	GLN
1	A	1492	GLN
1	A	1496	GLN
1	A	1561	GLN
1	A	1624	GLN
1	A	1797	ASN
1	A	1808	ASN
1	A	1886	GLN
1	A	1941	GLN
1	A	2148	GLN
1	A	2167	GLN
1	A	2200	GLN
1	A	2223	GLN
1	A	2265	HIS
1	A	2435	ASN
1	A	2502	ASN
2	C	132	ASN
2	C	148	GLN
2	C	162	ASN
2	C	209	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

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%)	-0.07	8 (0%) 82 71	55, 112, 215, 261	0
1	B	1058/1177 (89%)	-0.14	5 (0%) 87 78	46, 97, 204, 227	0
2	C	317/328 (96%)	-0.11	4 (1%) 75 61	60, 107, 177, 221	0
2	D	317/328 (96%)	-0.28	2 (0%) 85 75	41, 77, 143, 228	0
3	O	9/88 (10%)	0.72	0 100 100	128, 166, 178, 184	0
3	P	9/88 (10%)	0.28	0 100 100	102, 151, 168, 171	0
3	Q	21/88 (23%)	0.52	0 100 100	175, 203, 244, 261	0
3	R	21/88 (23%)	0.15	0 100 100	160, 174, 191, 196	0
All	All	2804/3362 (83%)	-0.12	19 (0%) 84 73	41, 101, 207, 261	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	203	ILE	3.5
1	A	1619	TRP	3.1
2	C	203	ILE	3.1
2	C	8	VAL	2.8
1	A	1614	ILE	2.7
1	B	1573	ALA	2.6
1	A	1443	LEU	2.5
2	D	8	VAL	2.5
1	A	1615	ILE	2.5
1	A	1629	ILE	2.3
1	A	1559	LEU	2.3
1	B	2434	THR	2.3
1	B	1443	LEU	2.2
1	B	1500	LYS	2.2
2	C	207	VAL	2.2
1	B	1577	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1573	ALA	2.1
1	A	1599	LEU	2.1
2	C	324	VAL	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.