Full wwPDB X-ray Structure Validation 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)

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:

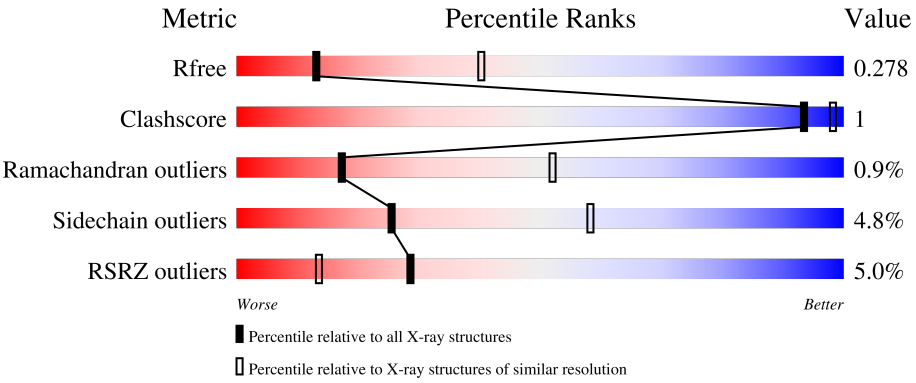
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	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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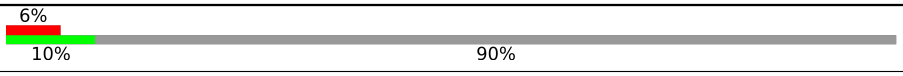
Mol	Chain	Length	Quality of chain
3	P	98	

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:

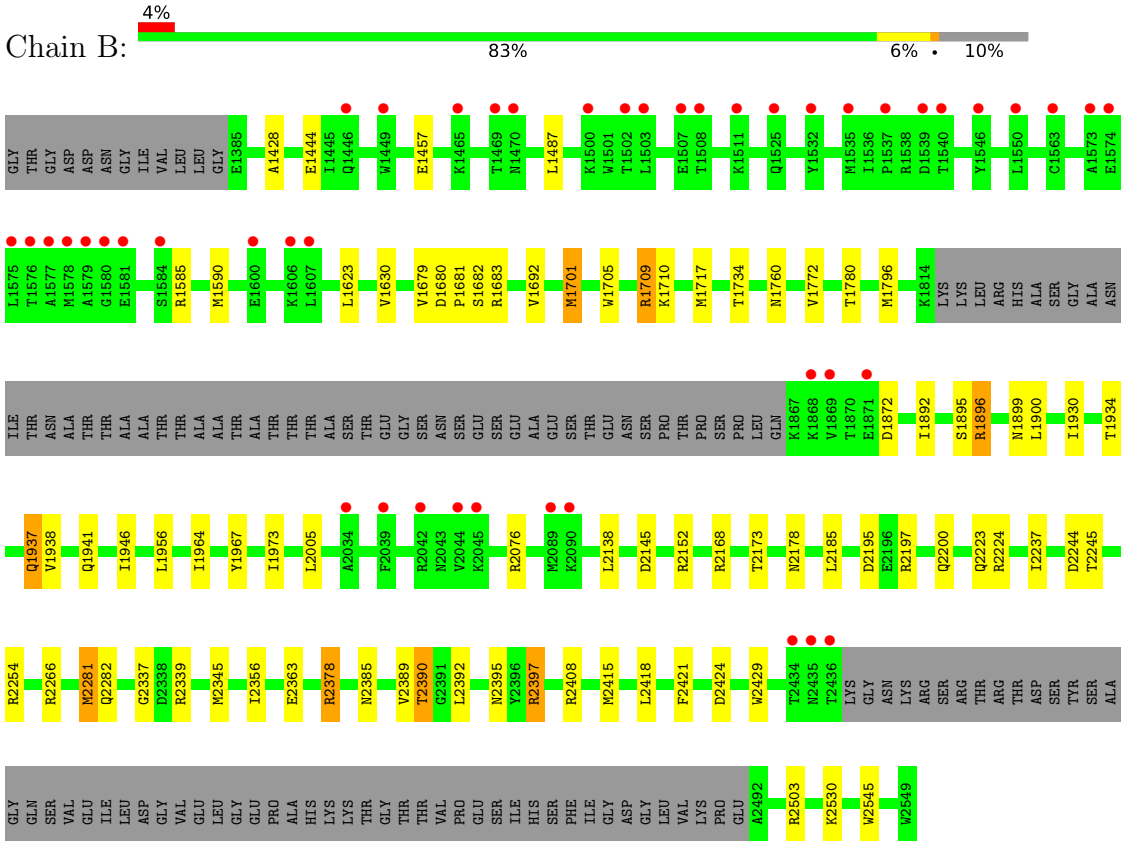
Chain	Residue	Modelled	Actual	Comment	Reference
P	110	GLY	-	expression tag	UNP Q96B36
P	111	SER	-	expression tag	UNP Q96B36
P	112	GLY	-	expression tag	UNP Q96B36
P	113	ARG	-	expression tag	UNP Q96B36
O	110	GLY	-	expression tag	UNP Q96B36
O	111	SER	-	expression tag	UNP Q96B36
O	112	GLY	-	expression tag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

3 Residue-property plots (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.

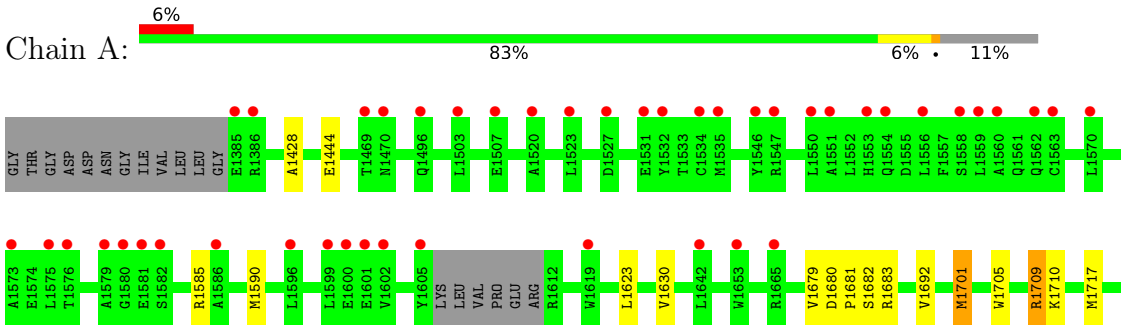
• Molecule 1: Serine/threonine-protein kinase mTOR

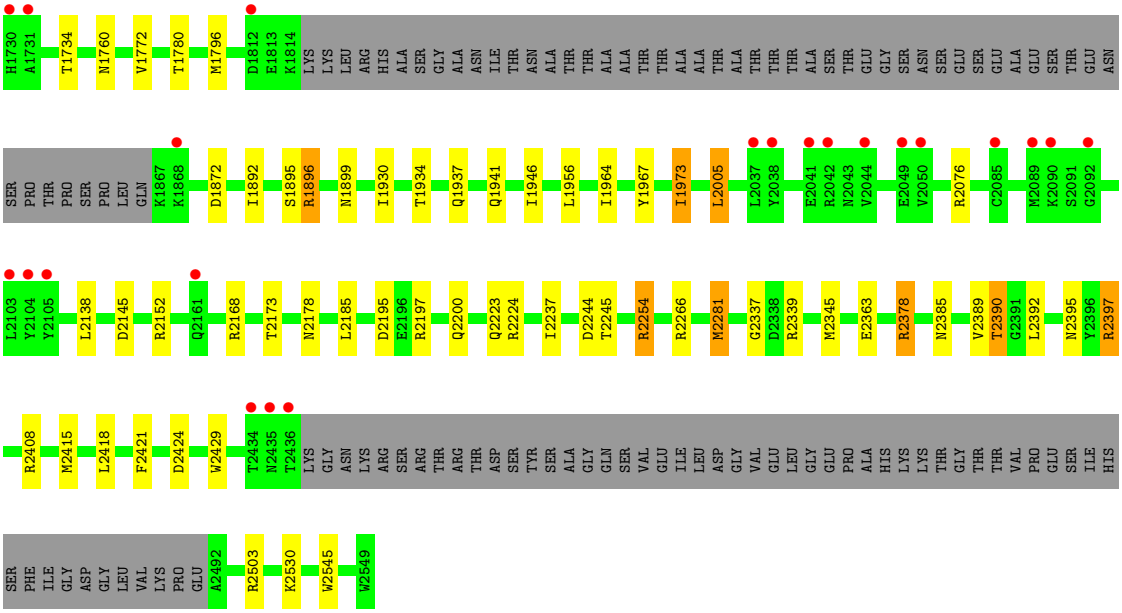
Chain B:



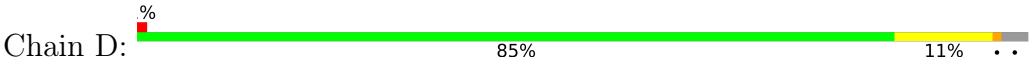
• Molecule 1: Serine/threonine-protein kinase mTOR

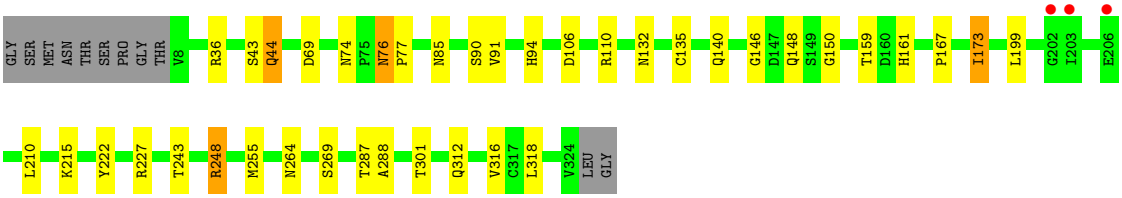
Chain A:



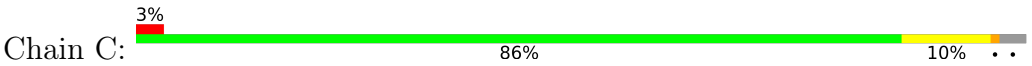


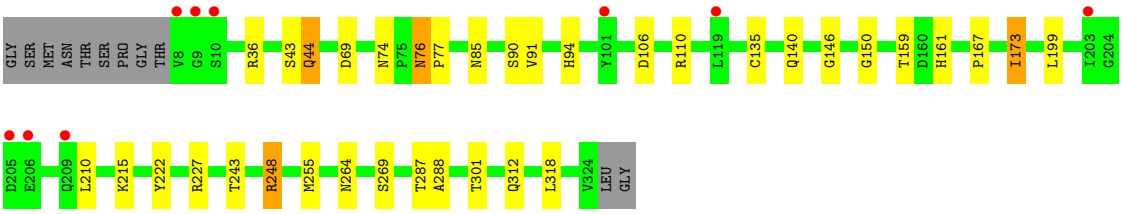
• Molecule 2: Target of rapamycin complex subunit LST8



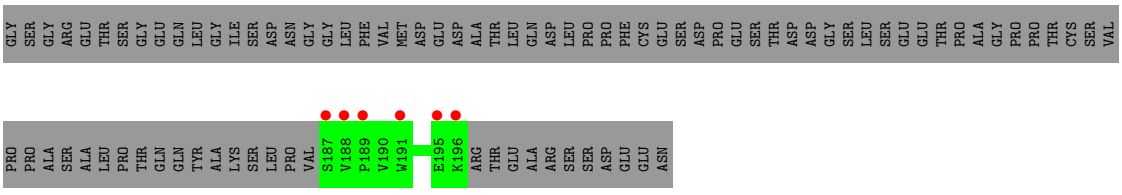


• Molecule 2: Target of rapamycin complex subunit LST8





• Molecule 3: Proline-rich AKT1 substrate 1

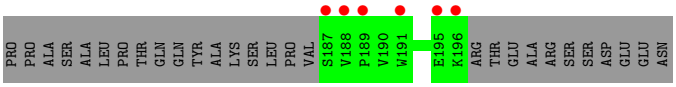


• Molecule 3: Proline-rich AKT1 substrate 1

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 (i)

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.*

[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 (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	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.

All (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
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.43	0.53
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
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.93	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: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:B:1701:MET:HE1	1:B:1717:MET:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:2281:MET:HE1	2:C:222:TYR:CG	2.53	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
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
1:A:1701:MET:HE1	1:A:1717:MET:N	2.34	0.42
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
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: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: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:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:GLY:HA3	2:D:173:ILE:HD11	2.03	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%)	22	57
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

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

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Mol	Chain	Res	Type
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 (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	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

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1585	ARG
1	B	1590	MET
1	B	1679	VAL
1	B	1701	MET
1	B	1709	ARG

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Mol	Chain	Res	Type
1	B	1734	THR
1	B	1760	ASN
1	B	1780	THR
1	B	1872	ASP
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	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	2195	ASP
1	B	2223	GLN
1	B	2224	ARG
1	B	2237	ILE
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	2385	ASN
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2415	MET
1	B	2429	TRP
1	B	2503	ARG
1	B	2530	LYS
2	D	44	GLN
2	D	85	ASN
2	D	90	SER
2	D	91	VAL

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Mol	Chain	Res	Type
2	D	135	CYS
2	D	159	THR
2	D	161	HIS
2	D	173	ILE
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	1585	ARG
1	A	1590	MET
1	A	1679	VAL
1	A	1701	MET
1	A	1709	ARG
1	A	1734	THR
1	A	1760	ASN
1	A	1780	THR
1	A	1872	ASP
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1946	ILE
1	A	1956	LEU
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	2195	ASP
1	A	2223	GLN
1	A	2224	ARG
1	A	2237	ILE
1	A	2244	ASP
1	A	2254	ARG
1	A	2266	ARG

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Mol	Chain	Res	Type
1	A	2281	MET
1	A	2363	GLU
1	A	2378	ARG
1	A	2385	ASN
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2415	MET
1	A	2429	TRP
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	173	ILE
2	C	215	LYS
2	C	227	ARG
2	C	243	THR
2	C	248	ARG
2	C	287	THR
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1760	ASN
1	B	1899	ASN
1	B	1937	GLN
1	B	1941	GLN
1	B	2082	GLN
1	B	2178	ASN
1	B	2343	ASN
1	B	2385	ASN
1	B	2395	ASN
2	D	41	GLN
2	D	44	GLN
2	D	85	ASN

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Mol	Chain	Res	Type
2	D	132	ASN
2	D	140	GLN
2	D	209	GLN
1	A	1760	ASN
1	A	1899	ASN
1	A	1937	GLN
1	A	1941	GLN
1	A	2082	GLN
1	A	2178	ASN
1	A	2189	HIS
1	A	2233	ASN
1	A	2343	ASN
1	A	2385	ASN
1	A	2395	ASN
2	C	41	GLN
2	C	44	GLN
2	C	85	ASN
2	C	132	ASN
2	C	140	GLN
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 monosaccharides 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, 95^{th} 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

All (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
3	P	187	SER	6.0
3	O	187	SER	5.9
1	A	1599	LEU	5.0
3	P	189	PRO	4.8
3	O	196	LYS	4.7
3	P	188	VAL	4.6
1	A	1596	LEU	4.5
1	A	1546	TYR	4.4
1	B	1578	MET	4.4
3	P	191	TRP	4.4
1	B	1503	LEU	4.4
1	A	2038	TYR	4.3
1	B	1546	TYR	4.3
1	B	1581	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1619	TRP	4.1
1	A	1600	GLU	4.1
3	O	191	TRP	4.1
2	C	205	ASP	4.1
1	B	1577	ALA	4.0
3	O	188	VAL	3.9
1	A	1469	THR	3.9
1	A	1554	GLN	3.9
3	O	195	GLU	3.9
1	B	1508	THR	3.8
1	A	1582	SER	3.7
1	A	1558	SER	3.7
1	A	1730	HIS	3.7
1	A	2042	ARG	3.7
1	A	1579	ALA	3.6
2	C	10	SER	3.6
3	P	196	LYS	3.6
1	A	1642	LEU	3.6
1	A	1576	THR	3.6
1	A	1527	ASP	3.5
1	A	1470	ASN	3.5
1	A	1653	TRP	3.5
1	B	1465	LYS	3.4
1	A	1385	GLU	3.4
1	B	1575	LEU	3.4
1	A	1580	GLY	3.3
2	D	202	GLY	3.3
1	A	1547	ARG	3.3
1	A	2044	VAL	3.3
1	B	1507	GLU	3.3
1	A	2434	THR	3.2
1	B	1607	LEU	3.2
1	B	2039	PHE	3.2
1	B	1500	LYS	3.1
1	B	1540	THR	3.1
1	A	1562	GLN	3.1
1	B	1584	SER	3.1
1	B	2090	LYS	3.1
1	A	1531	GLU	3.0
3	P	195	GLU	3.0
1	B	2089	MET	3.0
1	B	2436	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1553	HIS	2.9
2	D	203	ILE	2.9
1	A	2104	TYR	2.9
1	B	1606	LYS	2.9
1	A	2092	GLY	2.9
1	B	1563	CYS	2.9
1	A	1570	LEU	2.9
1	A	2050	VAL	2.9
2	C	8	VAL	2.9
1	A	2436	THR	2.9
1	A	2090	LYS	2.8
1	A	1523	LEU	2.8
1	B	2434	THR	2.8
1	A	1573	ALA	2.8
1	A	1586	ALA	2.7
1	A	1496	GLN	2.7
1	A	1550	LEU	2.7
1	A	1551	ALA	2.7
2	C	206	GLU	2.7
1	B	1539	ASP	2.7
1	A	2089	MET	2.7
1	B	1446	GLN	2.6
1	B	1573	ALA	2.6
1	A	1563	CYS	2.6
1	B	2044	VAL	2.6
2	D	206	GLU	2.6
1	A	1602	VAL	2.6
2	C	119	LEU	2.5
1	A	1868	LYS	2.5
1	B	1868	LYS	2.5
1	B	1869	VAL	2.5
1	A	1520	ALA	2.5
1	A	2103	LEU	2.5
1	A	1731	ALA	2.4
1	B	1532	TYR	2.4
1	B	1535	MET	2.4
1	A	1535	MET	2.4
1	B	2042	ARG	2.4
1	A	2435	ASN	2.4
1	B	1449	TRP	2.4
1	A	1581	GLU	2.4
1	A	2161	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1537	PRO	2.3
2	C	9	GLY	2.3
1	A	1556	LEU	2.3
1	B	1470	ASN	2.3
1	B	1574	GLU	2.3
1	B	1502	THR	2.3
1	A	2105	TYR	2.3
1	B	2045	LYS	2.2
1	A	1507	GLU	2.2
2	C	203	ILE	2.2
1	B	1871	GLU	2.2
2	C	101	TYR	2.2
2	C	209	GLN	2.2
1	A	1575	LEU	2.2
1	A	2049	GLU	2.2
1	B	2034	ALA	2.2
3	O	189	PRO	2.1
1	B	1511	LYS	2.1
1	B	1525	GLN	2.1
1	A	1812	ASP	2.1
1	A	1601	GLU	2.1
1	A	2085	CYS	2.1
1	B	1576	THR	2.1
1	A	1560	ALA	2.1
1	A	1605	TYR	2.1
1	B	2435	ASN	2.1
1	A	1534	CYS	2.1
1	A	1532	TYR	2.1
1	A	2037	LEU	2.0
1	B	1600	GLU	2.0
1	A	1665	ARG	2.0
1	B	1550	LEU	2.0
1	A	2041	GLU	2.0
1	A	1386	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 monosaccharides 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.