



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:39 am BST

PDB ID : 5WBU
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 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	:	2.11
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)	:	2.11

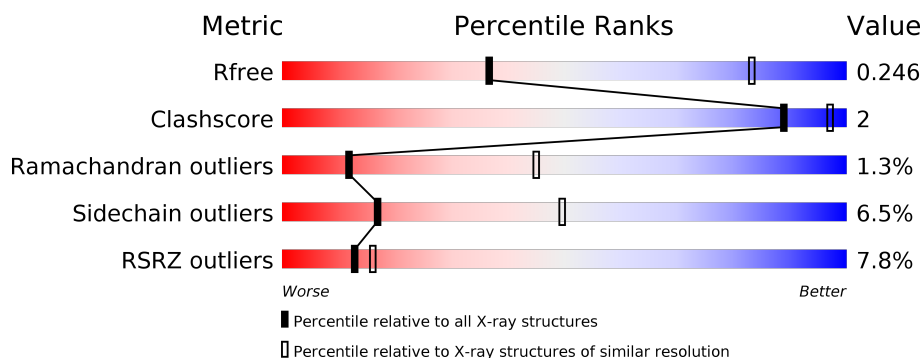
1 Overall quality at a glance

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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 on 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	<div> <div>9%</div> <div>79%</div> <div>9%</div> <div>11%</div> </div>
1	B	1177	<div> <div>6%</div> <div>80%</div> <div>9%</div> <div>10%</div> </div>
2	C	328	<div> <div>5%</div> <div>85%</div> <div>10%</div> <div>•</div> </div>
2	D	328	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>•</div> </div>
3	O	88	<div> <div>3%</div> <div>9%</div> <div>90%</div> </div>
3	P	88	<div> <div>3%</div> <div>9%</div> <div>90%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	88	<div><div><div></div><div></div><div></div></div><div>10%23%76%</div></div>
3	R	88	<div><div><div></div><div></div><div></div></div><div>3%23%76%</div></div>

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:

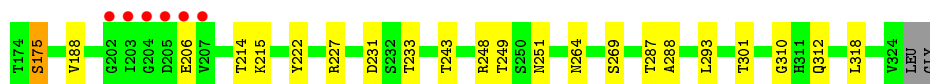
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9BVC4
D	0	SER	-	expression tag	UNP Q9BVC4
C	-1	GLY	-	expression tag	UNP Q9BVC4
C	0	SER	-	expression tag	UNP Q9BVC4

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

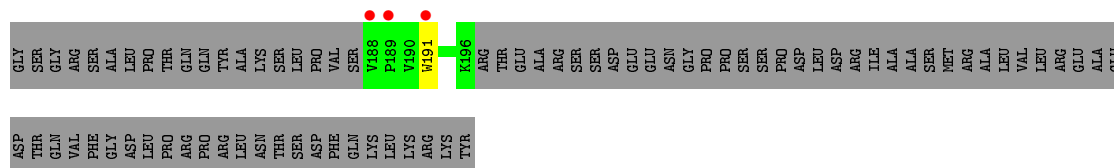
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	R	21	Total	C	N	O	0	0	0
			161	97	30	33			
3	O	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	Q	21	Total	C	N	O	0	0	0
			161	97	30	33			

There are 16 discrepancies between the modelled and reference sequences:

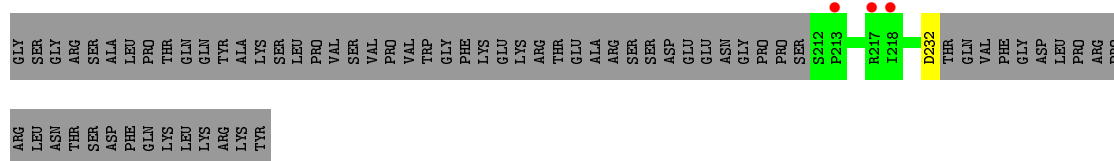
Chain	Residue	Modelled	Actual	Comment	Reference
P	169	GLY	-	expression tag	UNP Q96B36
P	170	SER	-	expression tag	UNP Q96B36
P	171	GLY	-	expression tag	UNP Q96B36
P	172	ARG	-	expression tag	UNP Q96B36
R	169	GLY	-	expression tag	UNP Q96B36
R	170	SER	-	expression tag	UNP Q96B36
R	171	GLY	-	expression tag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



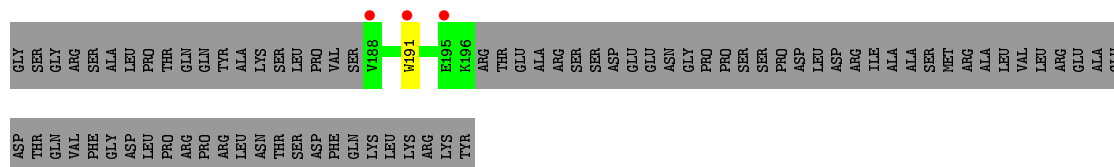
• Molecule 3: Proline-rich AKT1 substrate 1



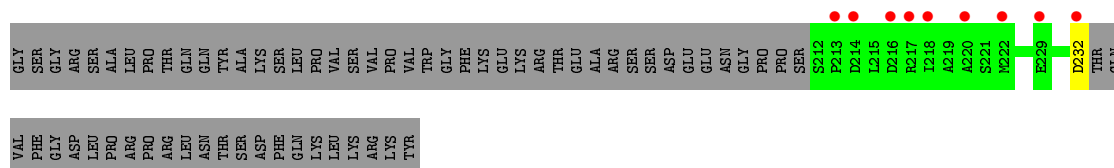
• Molecule 3: Proline-rich AKT1 substrate 1



• Molecule 3: Proline-rich AKT1 substrate 1



• Molecule 3: Proline-rich AKT1 substrate 1



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	139.40 Å 163.20 Å 207.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.42 75.95 – 3.22	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.01-3.42) 78.7 (75.95-3.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.19 Å)	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 (2.49%)	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 , 63.0	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	0.92	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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/8752	0.66	1/11847 (0.0%)
1	B	0.46	0/8805	0.67	1/11920 (0.0%)
2	C	0.42	0/2514	0.73	0/3426
2	D	0.45	0/2514	0.74	1/3426 (0.0%)
3	O	0.51	0/80	0.56	0/107
3	P	0.48	0/80	0.56	0/107
3	Q	0.50	0/161	0.67	0/216
3	R	0.51	0/161	0.67	0/216
All	All	0.45	0/23067	0.68	3/31265 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2254	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	2254	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	D	248	ARG	NE-CZ-NH1	5.38	122.99	120.30

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 [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	36	0
1	B	8608	0	8593	35	0
2	C	2456	0	2341	9	0
2	D	2456	0	2341	10	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	83	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 (83) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1964:ILE:O	1:B:1967:TYR:O	2.29	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
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.47	0.49
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:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.98	0.46
2:D:106:ASP:OD1	2:D:108:THR:OG1	2.25	0.46
1:B:1691:THR:O	1:B:1692:VAL:C	2.53	0.46
2:D:171:VAL:HG23	2:D:171:VAL:O	2.16	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:2197:ARG:NH1	1:A:2424:ASP:OD2	2.49	0.45
1:B:2206:ASN:ND2	1:B:2224:ARG:HD2	2.31	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:2521:VAL:HB	1:A:2522:PRO:HD3	1.99	0.45
1:A:1427:GLU:OE2	1:A:2395:ASN:ND2	2.49	0.45
1:B:1427:GLU:OE2	1:B:2395:ASN:ND2	2.50	0.45
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.99	0.44
1:B:2281:MET:CE	2:D:222:TYR:CD2	3.00	0.44
1:B:2389:VAL:O	1:B:2390:THR:HG22	2.18	0.44
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.98	0.44
2:C:106:ASP:OD1	2:C:108:THR:OG1	2.29	0.44
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.53	0.44
1:A:1701:MET:HE1	1:A:1717:MET:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1501:TRP:O	1:A:1504:VAL:HG22	2.17	0.43
1:B:1701:MET:HE1	1:B:1717:MET:N	2.34	0.43
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.51	0.43
1:B:1973:ILE:HD13	1:B:2005:LEU:HD22	2.00	0.43
2:C:171:VAL:O	2:C:171:VAL:HG23	2.19	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
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: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:A:1691:THR:O	1:A:1692:VAL:C	2.58	0.42
1:B:2297:ASP:O	1:B:2298:ASP:C	2.58	0.41
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.55	0.41
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	2.01	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:CG2	1:A:2390:THR:O	2.69	0.41
1:A:2297:ASP:O	1:A:2298:ASP:C	2.59	0.41
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.56	0.41
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.56	0.41
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.20	0.41
2:C:133:CYS:SG	2:C:175:SER:HA	2.61	0.41
1:A:2380:THR:HG22	1:A:2383:LEU:HG	2.02	0.41
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	2.02	0.41
2:D:248:ARG:HH11	2:D:248:ARG:HB3	1.85	0.41
1:B:1708:ALA:O	1:B:1710:LYS:N	2.53	0.40
1:A:2321:THR:HG23	1:A:2387:MET:HG2	2.04	0.40
1:B:2390:THR:CG2	1:B:2390:THR:O	2.70	0.40
1:B:1791:HIS:ND1	1:B:1902:ASP:OD1	2.55	0.40

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%)	982 (94%)	53 (5%)	9 (1%)	17	53
1	B	1052/1177 (89%)	984 (94%)	56 (5%)	12 (1%)	14	49
2	C	315/328 (96%)	285 (90%)	23 (7%)	7 (2%)	6	35
2	D	315/328 (96%)	284 (90%)	24 (8%)	7 (2%)	6	35
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%)	12	45

All (35) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	868 (94%)	57 (6%)	18	51
1	B	931/1025 (91%)	872 (94%)	59 (6%)	18	51
2	C	269/277 (97%)	249 (93%)	20 (7%)	13	44
2	D	269/277 (97%)	249 (93%)	20 (7%)	13	44
3	O	8/76 (10%)	7 (88%)	1 (12%)	4	21
3	P	8/76 (10%)	7 (88%)	1 (12%)	4	21
3	Q	17/76 (22%)	16 (94%)	1 (6%)	19	52
3	R	17/76 (22%)	16 (94%)	1 (6%)	19	52
All	All	2444/2908 (84%)	2284 (94%)	160 (6%)	17	49

All (160) 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	1480	ARG
1	B	1539	ASP
1	B	1540	THR
1	B	1541	HIS
1	B	1585	ARG
1	B	1590	MET
1	B	1594	HIS
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	1780	THR
1	B	1870	THR
1	B	1872	ASP
1	B	1895	SER
1	B	1896	ARG
1	B	1899	ASN
1	B	1918	ASP
1	B	1938	VAL
1	B	1956	LEU
1	B	1968	HIS
1	B	1973	ILE
1	B	2005	LEU
1	B	2068	THR
1	B	2076	ARG
1	B	2077	ASP
1	B	2083	GLU
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	2224	ARG
1	B	2232	THR
1	B	2244	ASP

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Mol	Chain	Res	Type
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	2429	TRP
1	B	2431	LEU
1	B	2503	ARG
1	B	2515	HIS
1	B	2530	LYS
2	D	44	GLN
2	D	85	ASN
2	D	90	SER
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	251	ASN
2	D	287	THR
2	D	301	THR
2	D	312	GLN
3	P	191	TRP
3	R	232	ASP
1	A	1417	ILE
1	A	1420	ASN
1	A	1457	GLU
1	A	1480	ARG

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Mol	Chain	Res	Type
1	A	1539	ASP
1	A	1540	THR
1	A	1541	HIS
1	A	1585	ARG
1	A	1590	MET
1	A	1594	HIS
1	A	1679	VAL
1	A	1701	MET
1	A	1709	ARG
1	A	1715	GLN
1	A	1734	THR
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	1918	ASP
1	A	1938	VAL
1	A	1956	LEU
1	A	1968	HIS
1	A	1973	ILE
1	A	2005	LEU
1	A	2068	THR
1	A	2076	ARG
1	A	2083	GLU
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	2224	ARG
1	A	2232	THR
1	A	2244	ASP
1	A	2254	ARG
1	A	2257	LYS
1	A	2266	ARG
1	A	2281	MET
1	A	2363	GLU

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Mol	Chain	Res	Type
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	2429	TRP
1	A	2431	LEU
1	A	2503	ARG
1	A	2515	HIS
1	A	2530	LYS
2	C	44	GLN
2	C	85	ASN
2	C	90	SER
2	C	91	VAL
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	312	GLN
3	O	191	TRP
3	Q	232	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1492	GLN
1	B	1496	GLN
1	B	1730	HIS
1	B	1886	GLN
1	B	2001	HIS

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Mol	Chain	Res	Type
1	B	2148	GLN
2	D	209	GLN
1	A	1492	GLN
1	A	1496	GLN
1	A	1886	GLN
1	A	2001	HIS
1	A	2148	GLN
1	A	2189	HIS
1	A	2233	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 carbohydrates 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%)	0.50	105 (9%) 7 9	55, 112, 215, 261	0
1	B	1058/1177 (89%)	0.36	68 (6%) 19 21	46, 97, 204, 227	0
2	C	317/328 (96%)	0.36	18 (5%) 23 25	60, 107, 177, 221	0
2	D	317/328 (96%)	0.16	11 (3%) 44 44	41, 77, 143, 228	0
3	O	9/88 (10%)	1.63	3 (33%) 0 0	128, 166, 178, 184	0
3	P	9/88 (10%)	1.26	3 (33%) 0 0	102, 151, 168, 171	0
3	Q	21/88 (23%)	1.91	9 (42%) 0 0	175, 203, 244, 261	0
3	R	21/88 (23%)	0.81	3 (14%) 2 4	160, 174, 191, 196	0
All	All	2804/3362 (83%)	0.41	220 (7%) 13 16	41, 101, 207, 261	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1503	LEU	8.0
1	B	1500	LYS	7.7
1	B	1607	LEU	7.1
1	B	1579	ALA	7.1
2	C	205	ASP	6.9
1	A	1559	LEU	6.6
1	A	1599	LEU	6.5
1	A	1553	HIS	6.1
1	A	1596	LEU	6.1
1	A	1619	TRP	6.1
1	A	1600	GLU	6.0
1	A	1573	ALA	6.0
1	B	1507	GLU	5.6
1	B	1573	ALA	5.5
1	A	1576	THR	5.4
1	B	1581	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	2094	VAL	5.4
1	A	1586	ALA	5.3
3	Q	218	ILE	5.1
1	A	1579	ALA	5.1
1	B	1446	GLN	5.0
1	A	1583	TYR	4.9
1	B	1577	ALA	4.9
1	A	1580	GLY	4.9
1	B	1503	LEU	4.9
1	B	1540	THR	4.8
1	A	1603	ILE	4.8
1	A	1642	LEU	4.7
1	A	2435	ASN	4.6
3	Q	214	ASP	4.4
1	A	1532	TYR	4.4
1	A	1507	GLU	4.4
1	A	1537	PRO	4.3
1	B	1578	MET	4.3
2	D	203	ILE	4.3
1	A	1469	THR	4.2
1	B	1575	LEU	4.2
1	B	1449	TRP	4.2
1	A	1549	VAL	4.1
1	B	1580	GLY	4.0
1	B	1869	VAL	4.0
1	A	1535	MET	4.0
2	D	206	GLU	4.0
1	B	2434	THR	3.9
1	A	1496	GLN	3.9
1	A	1470	ASN	3.9
2	D	10	SER	3.8
1	B	1546	TYR	3.8
1	B	1469	THR	3.8
1	A	1558	SER	3.8
1	B	1502	THR	3.8
1	A	1500	LYS	3.7
1	B	1563	CYS	3.7
1	A	1385	GLU	3.7
1	A	1595	MET	3.7
1	A	1577	ALA	3.7
1	B	1539	ASP	3.7
2	C	207	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1564	ILE	3.7
2	D	205	ASP	3.6
1	A	2434	THR	3.6
1	A	2038	TYR	3.6
1	A	1504	VAL	3.6
1	B	1537	PRO	3.5
1	B	1584	SER	3.5
1	A	2101	TRP	3.5
2	C	112	TRP	3.5
1	A	1522	GLY	3.5
2	C	119	LEU	3.5
1	B	1576	THR	3.5
1	B	1535	MET	3.5
1	A	1575	LEU	3.5
1	A	1653	TRP	3.5
1	A	1528	SER	3.4
2	C	10	SER	3.4
1	A	1578	MET	3.4
1	B	1606	LYS	3.4
1	B	1571	LEU	3.4
1	A	1563	CYS	3.4
1	B	1508	THR	3.4
2	C	8	VAL	3.4
2	C	67	MET	3.4
3	Q	232	ASP	3.4
1	A	1554	GLN	3.3
1	B	1393	TYR	3.3
2	C	81	TYR	3.3
1	B	1549	VAL	3.3
1	A	1550	LEU	3.3
1	B	1541	HIS	3.3
1	A	1584	SER	3.2
1	A	1581	GLU	3.2
1	A	1602	VAL	3.2
1	A	1520	ALA	3.2
1	B	1511	LYS	3.2
1	A	1525	GLN	3.2
2	C	79	ILE	3.2
1	B	1585	ARG	3.1
1	A	2050	VAL	3.1
1	B	1574	GLU	3.1
3	Q	217	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	2104	TYR	3.1
1	A	1582	SER	3.1
1	A	1536	ILE	3.1
1	A	1393	TYR	3.1
1	A	1647	HIS	3.1
1	A	2055	HIS	3.0
1	B	1550	LEU	3.0
1	A	1386	ARG	3.0
1	A	1526	TRP	3.0
3	O	188	VAL	3.0
1	A	1869	VAL	3.0
3	P	189	PRO	3.0
1	A	1551	ALA	3.0
1	B	1605	TYR	3.0
1	B	1525	GLN	2.9
2	C	206	GLU	2.9
1	B	1868	LYS	2.9
1	B	1496	GLN	2.9
1	A	1546	TYR	2.8
1	B	1564	ILE	2.8
1	B	2435	ASN	2.8
1	B	1570	LEU	2.8
3	P	188	VAL	2.8
3	Q	216	ASP	2.8
1	A	1508	THR	2.8
1	A	1539	ASP	2.8
1	A	1388	ALA	2.8
1	A	1390	CYS	2.8
1	B	1559	LEU	2.7
1	A	1547	ARG	2.7
2	C	101	TYR	2.7
1	B	1515	MET	2.7
1	B	1532	TYR	2.7
1	B	1603	ILE	2.7
1	A	2436	THR	2.7
1	A	2104	TYR	2.7
1	B	1385	GLU	2.7
1	B	1453	LEU	2.7
2	C	155	TRP	2.7
2	D	9	GLY	2.7
1	B	1599	LEU	2.6
3	R	218	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1512	MET	2.6
1	A	1523	LEU	2.6
1	B	1477	MET	2.6
1	A	1566	LYS	2.6
1	A	1521	TRP	2.6
3	Q	213	PRO	2.6
1	A	1646	PRO	2.5
1	A	1605	TYR	2.5
1	A	1527	ASP	2.5
1	A	1486	ALA	2.5
1	A	2047	MET	2.5
1	B	1602	VAL	2.5
3	Q	229	GLU	2.5
1	A	1543	GLY	2.5
1	A	1562	GLN	2.5
2	D	8	VAL	2.5
2	C	143	LEU	2.5
1	A	1468	ASP	2.5
1	A	1730	HIS	2.5
1	B	2098	THR	2.5
1	A	1569	ASP	2.5
3	P	191	TRP	2.5
2	D	202	GLY	2.5
1	A	1560	ALA	2.5
1	B	1495	GLN	2.4
1	A	1531	GLU	2.4
2	C	124	ILE	2.4
2	C	9	GLY	2.4
2	C	204	GLY	2.4
1	B	1456	TRP	2.4
1	A	1604	GLN	2.4
2	C	202	GLY	2.4
3	R	213	PRO	2.4
1	B	1520	ALA	2.4
1	B	1534	CYS	2.4
1	A	1574	GLU	2.4
1	B	1483	CYS	2.4
1	A	1616	ARG	2.4
1	A	1541	HIS	2.3
1	A	1868	LYS	2.3
1	B	1595	MET	2.3
1	A	1516	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	191	TRP	2.3
1	A	2044	VAL	2.3
1	A	1524	GLY	2.3
1	B	1556	LEU	2.3
1	B	1512	MET	2.2
2	D	207	VAL	2.2
1	B	1451	GLU	2.2
1	B	1562	GLN	2.2
2	C	203	ILE	2.2
3	Q	222	MET	2.2
1	A	1542	ASP	2.2
1	A	1656	TYR	2.2
1	A	1407	GLY	2.2
3	O	195	GLU	2.2
2	D	81	TYR	2.1
1	B	1569	ASP	2.1
1	B	1498	CYS	2.1
1	A	1530	GLU	2.1
1	A	1628	ARG	2.1
1	A	1446	GLN	2.1
1	A	1545	PHE	2.1
3	Q	220	ALA	2.1
1	A	1477	MET	2.1
3	R	217	ARG	2.1
1	A	1518	ALA	2.1
1	A	1639	VAL	2.1
1	B	1499	GLU	2.1
1	A	1572	ASP	2.1
1	B	1542	ASP	2.1
1	B	1386	ARG	2.0
2	D	201	GLY	2.0
1	A	1587	TYR	2.0
1	A	1620	TRP	2.0
2	D	70	LEU	2.0
1	A	1734	THR	2.0
1	A	2090	LYS	2.0

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 [i](#)

There are no carbohydrates 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.