



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 AM UTC

PDB ID : 6DLO / pdb_00006dlo
Title : Crystal structure of LRRK2 WD40 domain dimer
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Deposited on : 2018-06-02
Resolution : 2.70 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

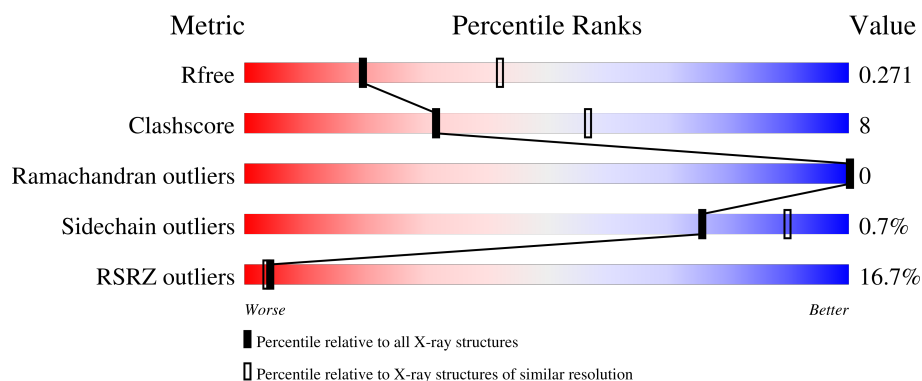
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	389	10% 65% 14% • 20%
1	B	389	16% 63% 16% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4891 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	310	Total	C	N	O	S	0	0	0
			2404	1535	405	444	20			
1	A	311	Total	C	N	O	S	0	0	0
			2421	1542	410	449	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2139	GLY	-	expression tag	UNP Q5S007
B	2140	GLY	-	expression tag	UNP Q5S007
B	2141	SER	-	expression tag	UNP Q5S007
A	2139	GLY	-	expression tag	UNP Q5S007
A	2140	GLY	-	expression tag	UNP Q5S007
A	2141	SER	-	expression tag	UNP Q5S007

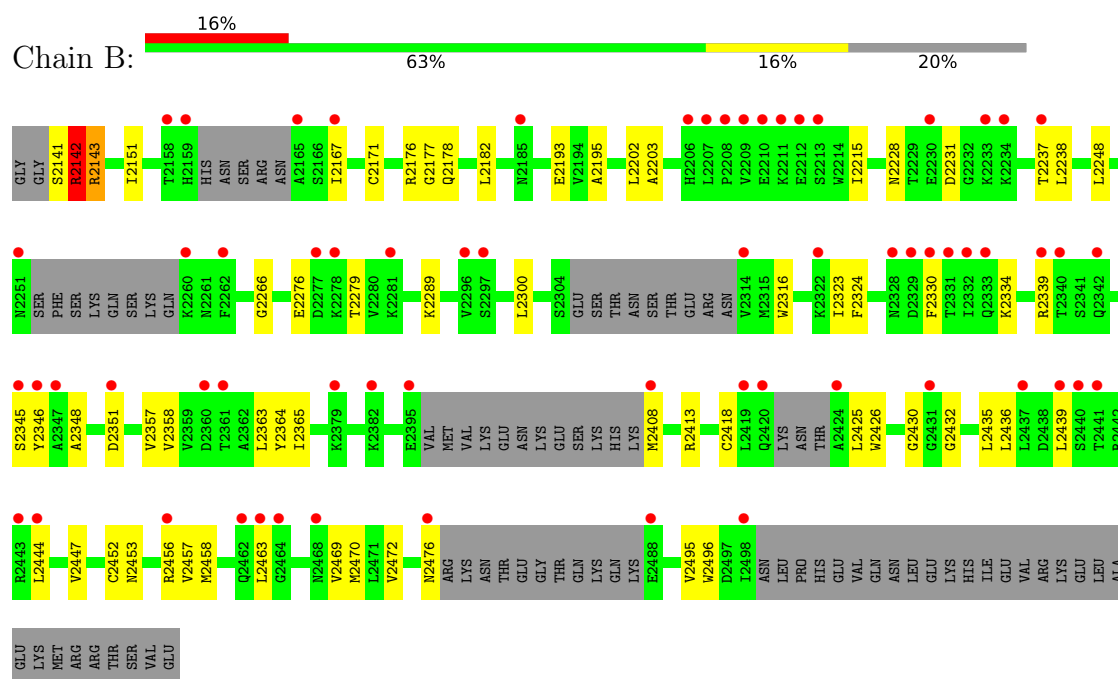
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	32	Total	O	0	0
			32	32		
2	A	34	Total	O	0	0
			34	34		

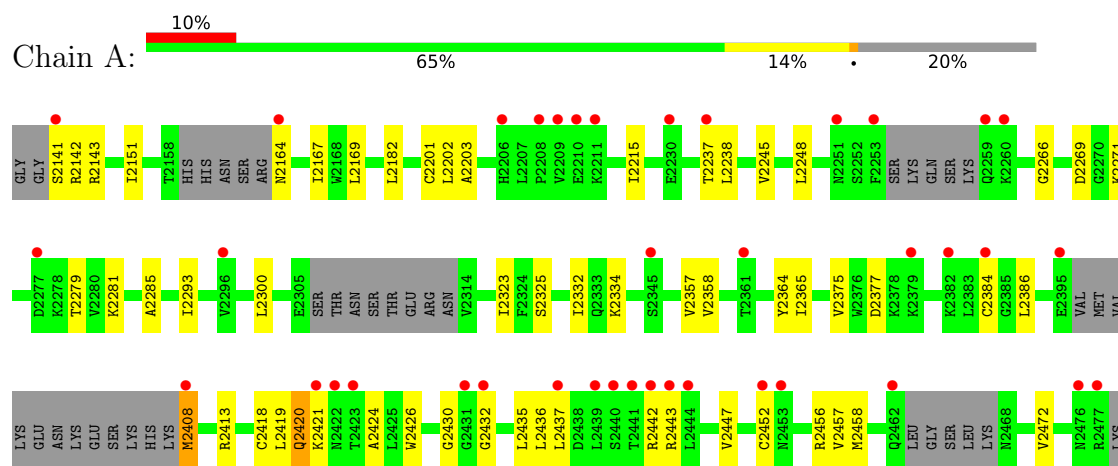
3 Residue-property plots

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: Leucine-rich repeat serine/threonine-protein kinase 2



- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



ASN	THR	GLY	THR	GLN	LYS	GLN	LYS	E2488	V2495	V2496	ASP	ILE	ASN	LEU	PRO	HIS	GLU	VAL	GLN	ASN	LEU	GLU	LYS	HIS	ILE	GLU	VAL	ARG	LYS	GLU	LEU	ALA	GLU	LYS	MET	ARG	ARG	THR	SER	VAL	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.29Å 103.59Å 112.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.26 – 2.70 76.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.5 (76.26-2.70) 92.5 (76.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.234 , 0.275 0.235 , 0.271	Depositor DCC
R_{free} test set	2004 reflections (7.67%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4891	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.22	0/2454	0.40	0/3313
1	B	0.19	0/2437	0.43	0/3291
All	All	0.21	0/4891	0.41	0/6604

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.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2142	ARG	Sidechain
1	A	2143	ARG	Sidechain
1	B	2142	ARG	Sidechain
1	B	2143	ARG	Sidechain

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	2421	0	2481	41	0
1	B	2404	0	2473	39	0
2	A	34	0	0	1	0
2	B	32	0	0	3	0
All	All	4891	0	4954	79	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 8.

All (79) 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:2470:MET:SD	2:B:2630:HOH:O	2.29	0.90
1:B:2151:ILE:HG23	1:B:2456:ARG:HH12	1.42	0.84
1:A:2419:LEU:HD12	1:A:2424:ALA:O	1.85	0.77
1:A:2424:ALA:HB1	1:A:2436:LEU:HD11	1.72	0.70
1:B:2418:CYS:SG	2:B:2630:HOH:O	2.31	0.69
1:A:2293:ILE:HG12	1:A:2332:ILE:HD11	1.76	0.67
1:A:2420:GLN:HB2	1:A:2424:ALA:HB3	1.77	0.67
1:B:2408:MET:N	2:B:2601:HOH:O	2.31	0.63
1:B:2453:ASN:HB2	1:B:2476:ASN:HA	1.80	0.63
1:B:2339:ARG:NE	1:B:2351:ASP:OD1	2.27	0.63
1:B:2458:MET:HG3	1:B:2472:VAL:HG22	1.80	0.63
1:A:2151:ILE:HG23	1:A:2456:ARG:HH12	1.64	0.62
1:A:2203:ALA:HB2	1:A:2248:LEU:HB3	1.81	0.62
1:B:2413:ARG:O	1:B:2430:GLY:N	2.33	0.61
1:B:2357:VAL:HG22	1:B:2365:ILE:HG22	1.82	0.61
1:B:2202:LEU:HD22	1:B:2215:ILE:HD11	1.84	0.60
1:A:2279:THR:HG22	1:A:2285:ALA:HB1	1.84	0.59
1:A:2408:MET:O	1:A:2408:MET:HG3	2.01	0.59
1:A:2458:MET:HG3	1:A:2472:VAL:HG22	1.85	0.59
1:A:2357:VAL:HG22	1:A:2365:ILE:HG22	1.86	0.58
1:B:2167:ILE:HG22	1:B:2182:LEU:HB3	1.85	0.58
1:A:2413:ARG:O	1:A:2430:GLY:N	2.37	0.57
1:B:2176:ARG:NH1	1:B:2193:GLU:OE1	2.38	0.57
1:A:2420:GLN:HG3	1:A:2424:ALA:HB3	1.87	0.57
1:A:2420:GLN:CB	1:A:2424:ALA:HB3	2.35	0.56
1:B:2151:ILE:HG23	1:B:2456:ARG:NH1	2.16	0.55
1:A:2167:ILE:HD11	1:A:2182:LEU:HD23	1.87	0.55
1:B:2444:LEU:HD21	1:B:2447:VAL:HG23	1.87	0.54
1:B:2203:ALA:HB2	1:B:2248:LEU:HB3	1.90	0.54
1:B:2171:CYS:HB2	1:B:2178:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2167:ILE:HD12	1:A:2169:LEU:HD21	1.91	0.52
1:B:2316:TRP:HH2	1:B:2334:LYS:HD2	1.74	0.52
1:B:2456:ARG:HG2	1:B:2457:VAL:HG23	1.91	0.52
1:A:2164:ASN:N	2:A:2606:HOH:O	2.43	0.52
1:B:2432:GLY:HA3	1:B:2452:CYS:O	2.10	0.51
1:A:2266:GLY:HA3	1:A:2300:LEU:HD22	1.93	0.51
1:B:2345:SER:H	1:A:2386:LEU:HB2	1.76	0.51
1:A:2323:ILE:HD11	1:A:2365:ILE:HD13	1.94	0.50
1:B:2289:LYS:HD2	1:B:2330:PHE:CD2	2.47	0.50
1:A:2432:GLY:HA3	1:A:2452:CYS:O	2.11	0.50
1:A:2358:VAL:HG23	1:A:2364:TYR:HB2	1.94	0.50
1:B:2358:VAL:HG23	1:B:2364:TYR:HB2	1.93	0.49
1:A:2269:ASP:OD2	1:A:2271:LYS:HE2	2.13	0.49
1:B:2266:GLY:HA3	1:B:2300:LEU:HD22	1.95	0.48
1:A:2420:GLN:CG	1:A:2424:ALA:HB3	2.44	0.48
1:B:2228:ASN:HB3	1:B:2231:ASP:O	2.14	0.47
1:B:2177:GLY:HA3	1:B:2195:ALA:HB3	1.95	0.47
1:A:2408:MET:HE3	1:A:2408:MET:HB2	1.67	0.47
1:A:2437:LEU:HD23	1:A:2443:ARG:HB3	1.96	0.47
1:A:2141:SER:HA	1:A:2495:VAL:O	2.15	0.46
1:A:2426:TRP:CE2	1:A:2436:LEU:HD13	2.51	0.46
1:B:2316:TRP:CH2	1:B:2334:LYS:HD2	2.51	0.46
1:B:2346:TYR:CE2	1:B:2348:ALA:HB3	2.51	0.46
1:B:2324:PHE:HA	1:B:2334:LYS:O	2.17	0.45
1:B:2425:LEU:HB2	1:B:2439:LEU:HD11	1.98	0.45
1:A:2237:THR:HG22	1:A:2238:LEU:O	2.17	0.45
1:A:2202:LEU:HD22	1:A:2215:ILE:HD11	1.99	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.57	0.44
1:A:2456:ARG:HG2	1:A:2457:VAL:HG23	1.99	0.44
1:B:2141:SER:CB	1:B:2496:TRP:HB3	2.48	0.43
1:B:2142:ARG:HG2	1:B:2495:VAL:HG13	1.99	0.43
1:A:2201:CYS:SG	1:A:2245:VAL:HG12	2.57	0.43
1:A:2238:LEU:HD22	1:A:2285:ALA:HB3	2.01	0.43
1:A:2435:LEU:HD22	1:A:2447:VAL:HG22	2.00	0.43
1:B:2463:LEU:HD12	1:B:2469:VAL:HG21	2.01	0.43
1:B:2323:ILE:HG21	1:B:2363:LEU:HD13	1.99	0.43
1:A:2281:LYS:HE3	1:A:2281:LYS:HB2	1.85	0.43
1:A:2418:CYS:HB3	1:A:2426:TRP:HB2	1.99	0.43
1:B:2141:SER:HB2	1:B:2496:TRP:HB3	2.00	0.42
1:B:2276:GLU:O	1:B:2279:THR:HG22	2.18	0.42
1:B:2237:THR:HG22	1:B:2238:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2442:ARG:HG2	1:A:2443:ARG:H	1.84	0.42
1:B:2426:TRP:CE2	1:B:2436:LEU:HD13	2.56	0.41
1:A:2325:SER:HB3	1:A:2334:LYS:HB2	2.03	0.41
1:A:2420:GLN:O	1:A:2421:LYS:C	2.63	0.41
1:B:2323:ILE:HD11	1:B:2365:ILE:HD13	2.03	0.41
1:B:2435:LEU:HD22	1:B:2447:VAL:HG22	2.03	0.40
1:A:2151:ILE:HG23	1:A:2456:ARG:NH1	2.31	0.40
1:A:2375:VAL:O	1:A:2384:CYS:N	2.45	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	297/389 (76%)	283 (95%)	14 (5%)	0	100	100
1	B	296/389 (76%)	284 (96%)	12 (4%)	0	100	100
All	All	593/778 (76%)	567 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	276/349 (79%)	274 (99%)	2 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	274/349 (78%)	272 (99%)	2 (1%)	76	90
All	All	550/698 (79%)	546 (99%)	4 (1%)	76	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2142	ARG
1	B	2143	ARG
1	A	2408	MET
1	A	2420	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2328	ASN

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 ⓘ

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	311/389 (79%)	0.65	40 (12%) 7 6	10, 28, 68, 111	0
1	B	310/389 (79%)	1.07	64 (20%) 2 2	13, 37, 78, 107	0
All	All	621/778 (79%)	0.86	104 (16%) 4 3	10, 32, 73, 111	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2441	THR	9.9
1	B	2345	SER	9.0
1	B	2330	PHE	6.4
1	B	2395	GLU	5.9
1	A	2395	GLU	5.6
1	B	2331	THR	5.2
1	B	2443	ARG	5.2
1	A	2442	ARG	5.1
1	B	2329	ASP	4.9
1	B	2212	GLU	4.9
1	B	2408	MET	4.7
1	A	2443	ARG	4.6
1	B	2431	GLY	4.6
1	B	2420	GLN	4.5
1	B	2209	VAL	4.4
1	B	2360	ASP	4.4
1	A	2422	ASN	4.3
1	B	2159	HIS	4.3
1	B	2462	GLN	4.3
1	A	2277	ASP	4.2
1	B	2440	SER	4.2
1	B	2351	ASP	4.1
1	A	2462	GLN	4.1
1	B	2441	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	2211	LYS	4.0
1	A	2431	GLY	3.9
1	A	2210	GLU	3.8
1	B	2314	VAL	3.8
1	A	2259	GLN	3.8
1	B	2277	ASP	3.7
1	A	2440	SER	3.7
1	B	2208	PRO	3.7
1	B	2328	ASN	3.6
1	A	2421	LYS	3.6
1	A	2477	ARG	3.5
1	B	2361	THR	3.5
1	A	2439	LEU	3.5
1	B	2379	LYS	3.5
1	A	2209	VAL	3.4
1	B	2206	HIS	3.4
1	A	2423	THR	3.4
1	B	2332	ILE	3.3
1	B	2437	LEU	3.3
1	A	2230	GLU	3.3
1	B	2439	LEU	3.3
1	B	2340	THR	3.2
1	B	2488	GLU	3.2
1	B	2165	ALA	3.1
1	A	2361	THR	3.1
1	A	2382	LYS	3.1
1	A	2141	SER	3.1
1	A	2408	MET	3.0
1	B	2207	LEU	3.0
1	B	2464	GLY	3.0
1	A	2444	LEU	2.9
1	B	2210	GLU	2.9
1	A	2384	CYS	2.9
1	B	2281	LYS	2.9
1	A	2432	GLY	2.9
1	B	2498	ILE	2.8
1	A	2437	LEU	2.8
1	A	2476	ASN	2.7
1	A	2452	CYS	2.7
1	B	2230	GLU	2.7
1	B	2260	LYS	2.6
1	A	2251	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2347	ALA	2.6
1	B	2346	TYR	2.6
1	B	2185	ASN	2.6
1	B	2296	VAL	2.6
1	A	2379	LYS	2.5
1	B	2213	SER	2.5
1	A	2488	GLU	2.5
1	B	2322	LYS	2.5
1	B	2382	LYS	2.5
1	B	2444	LEU	2.5
1	B	2339	ARG	2.4
1	A	2208	PRO	2.4
1	B	2278	LYS	2.4
1	B	2419	LEU	2.3
1	B	2251	ASN	2.3
1	A	2211	LYS	2.3
1	A	2237	THR	2.3
1	A	2164	ASN	2.2
1	B	2456	ARG	2.2
1	B	2476	ASN	2.2
1	B	2234	LYS	2.2
1	B	2158	THR	2.1
1	A	2260	LYS	2.1
1	B	2167	ILE	2.1
1	B	2237	THR	2.1
1	A	2345	SER	2.1
1	B	2468	ASN	2.1
1	A	2253	PHE	2.1
1	B	2297	SER	2.1
1	B	2233	LYS	2.1
1	B	2342	GLN	2.1
1	A	2206	HIS	2.1
1	B	2262	PHE	2.1
1	A	2453	ASN	2.0
1	A	2296	VAL	2.0
1	B	2424	ALA	2.0
1	B	2333	GLN	2.0
1	B	2463	LEU	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 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.