



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:31 PM UTC

PDB ID : 2CKD / pdb_00002ckd
Title : Crystal structure of ML2640 from Mycobacterium leprae
Authors : Grana, M.; Buschiazzo, A.; Wehenkel, A.; Haouz, A.; Alzari, P.M.
Deposited on : 2006-04-17
Resolution : 2.80 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

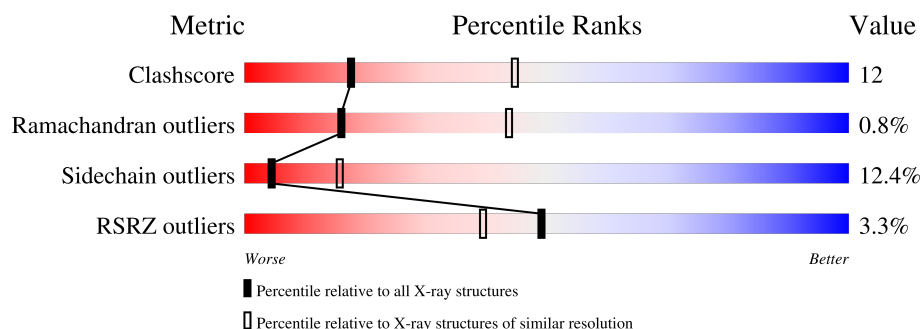
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	310	 5% 67% 25% 5% ..
1	B	310	 5% 65% 26% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4692 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.

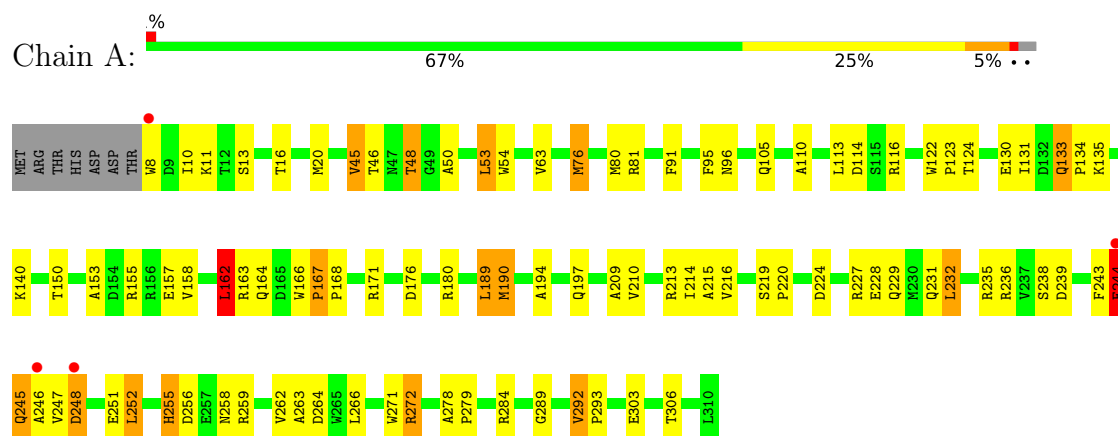
- Molecule 1 is a protein called PUTATIVE S-ADENOSYL-L-METHIONINE-DEPENDENT METHYLTRANSFERASE ML2640.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2369	1489	421	450	9			
1	B	298	Total	C	N	O	S	0	0	0
			2323	1458	414	442	9			

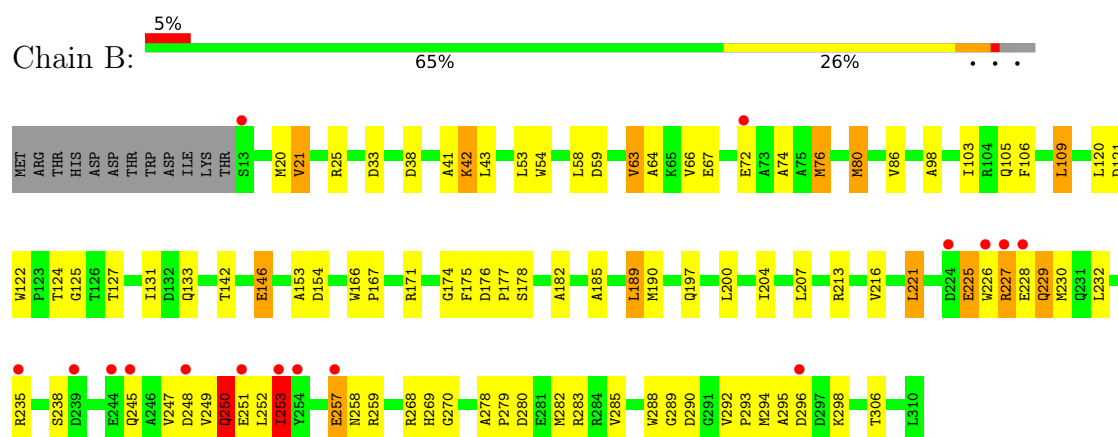
3 Residue-property plots [i](#)

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: PUTATIVE S-ADENOSYL-L-METHIONINE-DEPENDENT METHYLTRANSFERASE ML2640



- Molecule 1: PUTATIVE S-ADENOSYL-L-METHIONINE-DEPENDENT METHYLTRANSFERASE ML2640



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.78Å 96.78Å 169.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.92 – 2.80 83.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (83.92-2.80) 99.3 (83.92-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.255 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 12.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4692	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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	1.05	3/2424 (0.1%)	1.21	13/3302 (0.4%)
1	B	1.05	3/2376 (0.1%)	1.19	7/3236 (0.2%)
All	All	1.05	6/4800 (0.1%)	1.20	20/6538 (0.3%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ASN	CB-CG	5.76	1.66	1.52
1	B	270	GLY	CA-C	5.72	1.59	1.51
1	B	253	ILE	CA-CB	5.56	1.62	1.54
1	A	167	PRO	CA-C	5.44	1.57	1.52
1	A	45	VAL	CA-CB	-5.43	1.48	1.54
1	B	121	ASP	CA-C	-5.30	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	GLY	N-CA-C	-9.67	90.26	113.18
1	A	292	VAL	CA-C-N	-8.53	111.95	120.31
1	A	292	VAL	C-N-CA	-8.53	111.95	120.31
1	A	255	HIS	CA-C-N	-7.40	111.54	122.86
1	A	255	HIS	C-N-CA	-7.40	111.54	122.86
1	B	245	GLN	N-CA-C	6.94	119.72	108.41
1	A	245	GLN	N-CA-C	6.58	119.18	107.80
1	A	166	TRP	CA-C-N	-6.55	113.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	TRP	C-N-CA	-6.55	113.63	120.38
1	A	247	VAL	CB-CA-C	-5.94	103.08	111.28
1	A	262	VAL	N-CA-C	5.71	116.44	110.62
1	A	284	ARG	N-CA-CB	5.66	119.05	110.28
1	B	125	GLY	N-CA-C	-5.62	107.34	115.27
1	B	124	THR	N-CA-CB	5.38	118.05	110.36
1	A	189	LEU	N-CA-C	5.30	117.06	111.28
1	A	167	PRO	N-CA-C	5.20	117.05	110.70
1	B	189	LEU	N-CA-C	5.19	117.68	111.71
1	A	162	LEU	N-CA-C	5.05	117.52	111.71
1	B	38	ASP	CA-C-N	-5.04	114.62	119.87
1	B	38	ASP	C-N-CA	-5.04	114.62	119.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	HIS	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	2369	0	2293	61	0
1	B	2323	0	2248	57	0
All	All	4692	0	4541	114	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 12.

All (114) 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:227:ARG:HH11	1:B:227:ARG:HG2	1.14	1.13
1:A:48:THR:HG22	1:A:50:ALA:H	1.01	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:HG22	1:A:50:ALA:N	1.83	0.92
1:A:272:ARG:HH11	1:A:272:ARG:HG2	1.38	0.88
1:A:227:ARG:HD3	1:A:251:GLU:HA	1.55	0.87
1:B:226:TRP:HZ3	1:B:293:PRO:O	1.60	0.85
1:B:227:ARG:HG2	1:B:227:ARG:NH1	1.90	0.84
1:B:227:ARG:HH11	1:B:227:ARG:CG	1.90	0.82
1:B:280:ASP:OD1	1:B:283:ARG:NH1	2.18	0.76
1:B:105:GLN:HE22	1:B:176:ASP:H	1.33	0.74
1:A:16:THR:HG21	1:A:248:ASP:OD2	1.87	0.73
1:B:226:TRP:CZ3	1:B:293:PRO:O	2.42	0.73
1:A:232:LEU:HD11	1:A:236:ARG:HH21	1.53	0.71
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.04	0.70
1:A:8:TRP:HB2	1:A:48:THR:O	1.93	0.69
1:A:292:VAL:HG12	1:A:293:PRO:HD2	1.74	0.68
1:A:45:VAL:O	1:A:48:THR:HB	1.95	0.66
1:A:114:ASP:OD2	1:A:116:ARG:NH1	2.28	0.66
1:A:289:GLY:O	1:A:292:VAL:HG23	1.95	0.66
1:A:227:ARG:CD	1:A:251:GLU:HA	2.26	0.64
1:A:190:MET:HB3	1:A:252:LEU:HD13	1.81	0.61
1:B:189:LEU:HD11	1:B:216:VAL:HG11	1.83	0.59
1:B:227:ARG:O	1:B:230:MET:HB2	2.03	0.58
1:B:109:LEU:HD23	1:B:131:ILE:HD12	1.85	0.58
1:A:105:GLN:HE22	1:A:176:ASP:H	1.53	0.56
1:B:76:MET:HE3	1:B:226:TRP:CZ2	2.41	0.56
1:A:122:TRP:CD1	1:A:153:ALA:HB2	2.41	0.55
1:A:232:LEU:CD1	1:A:236:ARG:HH21	2.18	0.55
1:B:20:MET:HG3	1:B:54:TRP:CE3	2.43	0.54
1:B:292:VAL:HG22	1:B:293:PRO:CD	2.38	0.53
1:A:292:VAL:HG12	1:A:293:PRO:CD	2.38	0.53
1:B:106:PHE:CD1	1:B:182:ALA:HB3	2.44	0.53
1:A:53:LEU:HD13	1:A:238:SER:HB3	1.91	0.53
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.16	0.52
1:B:66:VAL:HG12	1:B:74:ALA:HB2	1.91	0.52
1:A:180:ARG:HD2	1:B:289:GLY:CA	2.39	0.52
1:A:10:ILE:HD11	1:A:135:LYS:HB3	1.92	0.52
1:A:130:GLU:CD	1:A:155:ARG:HH11	2.17	0.51
1:B:59:ASP:OD1	1:B:59:ASP:C	2.52	0.51
1:B:227:ARG:NH1	1:B:227:ARG:CG	2.61	0.51
1:A:133:GLN:HG3	1:A:134:PRO:HD2	1.91	0.51
1:B:225:GLU:HB3	1:B:294:MET:HE1	1.93	0.50
1:A:91:PHE:HE2	1:A:215:ALA:HB1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:C	1:A:232:LEU:HD12	2.37	0.50
1:B:185:ALA:HB3	1:B:216:VAL:HG22	1.94	0.50
1:A:130:GLU:OE2	1:A:155:ARG:HD2	2.12	0.49
1:A:197:GLN:NE2	1:A:259:ARG:HH11	2.11	0.49
1:A:131:ILE:HG12	1:A:158:VAL:HB	1.94	0.49
1:A:209:ALA:O	1:A:210:VAL:C	2.56	0.49
1:B:122:TRP:CD1	1:B:153:ALA:HB2	2.48	0.48
1:B:251:GLU:O	1:B:253:ILE:HG12	2.13	0.48
1:B:292:VAL:HG22	1:B:293:PRO:HD2	1.95	0.48
1:A:167:PRO:HB2	1:A:168:PRO:HD3	1.96	0.47
1:B:142:THR:O	1:B:146:GLU:HB2	2.13	0.47
1:B:189:LEU:HD11	1:B:216:VAL:CG1	2.44	0.47
1:B:127:THR:HG22	1:B:154:ASP:CG	2.39	0.47
1:B:250:GLN:O	1:B:251:GLU:C	2.57	0.47
1:A:180:ARG:HD2	1:B:289:GLY:HA2	1.97	0.46
1:B:174:GLY:O	1:B:175:PHE:C	2.58	0.46
1:A:110:ALA:H	1:A:162:LEU:CD1	2.29	0.46
1:A:194:ALA:O	1:A:197:GLN:HB3	2.15	0.46
1:B:197:GLN:NE2	1:B:259:ARG:HH11	2.13	0.46
1:B:76:MET:CE	1:B:226:TRP:CZ2	2.98	0.46
1:A:53:LEU:CD1	1:A:238:SER:HB3	2.46	0.45
1:A:197:GLN:HE22	1:A:259:ARG:HD3	1.82	0.45
1:B:292:VAL:O	1:B:295:ALA:HB2	2.16	0.45
1:A:76:MET:HE1	1:A:229:GLN:HB2	1.98	0.45
1:A:244:GLU:OE1	1:A:245:GLN:HB2	2.15	0.45
1:B:221:LEU:HD21	1:B:257:GLU:HB3	1.99	0.45
1:B:21:VAL:HG12	1:B:25:ARG:HH21	1.80	0.45
1:A:76:MET:HE1	1:A:229:GLN:CB	2.47	0.45
1:A:189:LEU:HD11	1:A:216:VAL:HG11	1.99	0.45
1:B:80:MET:HE3	1:B:80:MET:HB3	1.85	0.45
1:A:105:GLN:HE22	1:A:176:ASP:HB3	1.82	0.45
1:B:288:TRP:HE1	1:B:290:ASP:HB3	1.82	0.45
1:A:20:MET:HG3	1:A:54:TRP:CE3	2.52	0.44
1:B:229:GLN:HE21	1:B:229:GLN:HB2	1.49	0.44
1:A:91:PHE:CE2	1:A:215:ALA:HB1	2.53	0.44
1:A:105:GLN:NE2	1:A:176:ASP:H	2.15	0.44
1:B:278:ALA:HB3	1:B:279:PRO:HD3	2.00	0.43
1:B:86:VAL:HG21	1:B:282:MET:HG2	2.00	0.43
1:A:266:LEU:HB3	1:A:271:TRP:HB2	2.01	0.43
1:A:292:VAL:CG1	1:A:293:PRO:HD2	2.44	0.43
1:B:58:LEU:HD21	1:B:80:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HA	1:A:140:LYS:HD3	2.01	0.43
1:A:155:ARG:NH2	1:A:157:GLU:OE2	2.50	0.43
1:B:76:MET:HB3	1:B:76:MET:HE2	1.68	0.43
1:B:175:PHE:CE2	1:B:207:LEU:HB3	2.54	0.43
1:A:224:ASP:O	1:A:228:GLU:HG3	2.18	0.43
1:A:227:ARG:NH1	1:A:231:GLN:HG3	2.34	0.42
1:B:171:ARG:HH11	1:B:171:ARG:HG2	1.84	0.42
1:B:176:ASP:C	1:B:178:SER:H	2.27	0.42
1:A:238:SER:HB2	1:A:243:PHE:HB2	2.01	0.42
1:A:180:ARG:HD2	1:B:289:GLY:HA3	2.00	0.42
1:B:292:VAL:CG2	1:B:293:PRO:CD	2.97	0.42
1:B:175:PHE:O	1:B:177:PRO:HD3	2.19	0.41
1:A:219:SER:HA	1:A:220:PRO:HD3	1.91	0.41
1:A:278:ALA:HB3	1:A:279:PRO:HD3	2.02	0.41
1:B:200:LEU:O	1:B:204:ILE:HG13	2.20	0.41
1:A:190:MET:HA	1:A:219:SER:HB2	2.02	0.41
1:B:53:LEU:HD11	1:B:238:SER:HB3	2.02	0.41
1:B:166:TRP:N	1:B:167:PRO:CD	2.84	0.41
1:A:190:MET:HA	1:A:219:SER:CB	2.50	0.41
1:A:255:HIS:NE2	1:A:256:ASP:OD2	2.54	0.41
1:B:20:MET:HG3	1:B:54:TRP:CZ3	2.56	0.41
1:B:278:ALA:N	1:B:279:PRO:CD	2.84	0.41
1:B:41:ALA:O	1:B:42:LYS:C	2.64	0.40
1:A:45:VAL:O	1:A:46:THR:C	2.64	0.40
1:A:123:PRO:HB2	1:B:67:GLU:HG3	2.04	0.40
1:A:263:ALA:O	1:A:264:ASP:C	2.65	0.40
1:B:98:ALA:HB1	1:B:103:ILE:HD12	2.03	0.40
1:A:80:MET:O	1:A:81:ARG:C	2.63	0.40
1:B:63:VAL:HG12	1:B:64:ALA:N	2.35	0.40
1:B:296:ASP:OD2	1:B:296:ASP:N	2.49	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	301/310 (97%)	280 (93%)	19 (6%)	2 (1%)	18	47
1	B	296/310 (96%)	270 (91%)	23 (8%)	3 (1%)	12	38
All	All	597/620 (96%)	550 (92%)	42 (7%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	B	253	ILE
1	A	246	ALA
1	B	247	VAL
1	B	250	GLN

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	240/247 (97%)	213 (89%)	27 (11%)	5	19
1	B	235/247 (95%)	203 (86%)	32 (14%)	3	13
All	All	475/494 (96%)	416 (88%)	59 (12%)	4	16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	13	SER
1	A	48	THR
1	A	53	LEU
1	A	63	VAL
1	A	76	MET
1	A	95	PHE
1	A	124	THR

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Mol	Chain	Res	Type
1	A	133	GLN
1	A	150	THR
1	A	162	LEU
1	A	163	ARG
1	A	164	GLN
1	A	171	ARG
1	A	190	MET
1	A	213	ARG
1	A	214	ILE
1	A	232	LEU
1	A	235	ARG
1	A	239	ASP
1	A	244	GLU
1	A	248	ASP
1	A	252	LEU
1	A	258	ASN
1	A	272	ARG
1	A	303	GLU
1	A	306	THR
1	B	21	VAL
1	B	33	ASP
1	B	42	LYS
1	B	43	LEU
1	B	63	VAL
1	B	72	GLU
1	B	76	MET
1	B	80	MET
1	B	109	LEU
1	B	120	LEU
1	B	133	GLN
1	B	146	GLU
1	B	190	MET
1	B	213	ARG
1	B	221	LEU
1	B	225	GLU
1	B	227	ARG
1	B	228	GLU
1	B	229	GLN
1	B	232	LEU
1	B	235	ARG
1	B	248	ASP
1	B	249	VAL

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	252	LEU
1	B	253	ILE
1	B	257	GLU
1	B	258	ASN
1	B	268	ARG
1	B	285	VAL
1	B	298	LYS
1	B	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	105	GLN
1	A	133	GLN
1	A	197	GLN
1	B	105	GLN
1	B	133	GLN
1	B	197	GLN
1	B	229	GLN
1	B	258	ASN

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 [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	303/310 (97%)	0.01	4 (1%) 75 66	2, 10, 26, 36	0
1	B	298/310 (96%)	0.15	16 (5%) 31 24	2, 10, 34, 51	0
All	All	601/620 (96%)	0.08	20 (3%) 49 39	2, 10, 28, 51	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	GLN	4.5
1	B	228	GLU	4.4
1	B	253	ILE	3.6
1	B	254	TYR	3.3
1	B	257	GLU	3.2
1	A	246	ALA	3.1
1	B	244	GLU	3.0
1	B	239	ASP	2.9
1	B	248	ASP	2.8
1	B	251	GLU	2.7
1	B	13	SER	2.7
1	B	72	GLU	2.6
1	B	226	TRP	2.6
1	B	235	ARG	2.5
1	A	8	TRP	2.4
1	A	248	ASP	2.3
1	B	224	ASP	2.1
1	B	296	ASP	2.1
1	A	244	GLU	2.1
1	B	227	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.