W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID	:	2B0L
Title	:	C-terminal DNA binding domain of transcriptional pleiotropic repressor CodY.
Authors	:	Levdikov, V.M.; Blagova, E.; Joseph, P.; Sonenshein, A.L.; Wilkinson, A.J.
Deposited on	:	2005-09-14
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		24
Ramachandran outliers		5.0%
Sidechain outliers		21.4%
RSRZ outliers		66.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
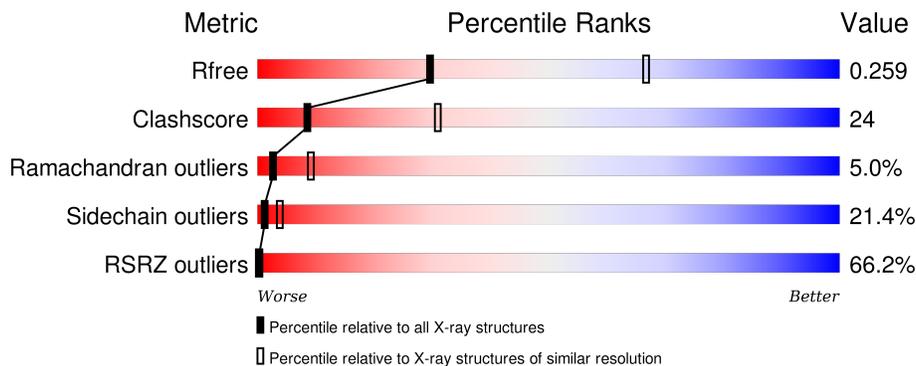
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	102	32% ▬ 55% / 30% / 9% / · ·
1	B	102	69% ▬ 50% / 33% / 10% / 7%
1	C	102	85% ▬ 46% / 35% / 10% / · / 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2300 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 GTP-sensing transcriptional pleiotropic repressor codY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	2	0
			783	493	141	145	4			
1	B	95	Total	C	N	O	S	4	4	0
			768	485	135	143	5			
1	C	94	Total	C	N	O	S	107	0	0
			730	461	128	138	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	CLONING ARTIFACT	UNP P39779
A	159	SER	-	CLONING ARTIFACT	UNP P39779
A	160	SER	-	CLONING ARTIFACT	UNP P39779
A	161	HIS	-	EXPRESSION TAG	UNP P39779
A	162	HIS	-	EXPRESSION TAG	UNP P39779
A	163	HIS	-	EXPRESSION TAG	UNP P39779
A	164	HIS	-	EXPRESSION TAG	UNP P39779
A	165	HIS	-	EXPRESSION TAG	UNP P39779
A	166	HIS	-	EXPRESSION TAG	UNP P39779
A	167	MET	-	INITIATING METHIONINE	UNP P39779
B	158	GLY	-	CLONING ARTIFACT	UNP P39779
B	159	SER	-	CLONING ARTIFACT	UNP P39779
B	160	SER	-	CLONING ARTIFACT	UNP P39779
B	161	HIS	-	EXPRESSION TAG	UNP P39779
B	162	HIS	-	EXPRESSION TAG	UNP P39779
B	163	HIS	-	EXPRESSION TAG	UNP P39779
B	164	HIS	-	EXPRESSION TAG	UNP P39779
B	165	HIS	-	EXPRESSION TAG	UNP P39779
B	166	HIS	-	EXPRESSION TAG	UNP P39779
B	167	MET	-	INITIATING METHIONINE	UNP P39779
C	158	GLY	-	CLONING ARTIFACT	UNP P39779
C	159	SER	-	CLONING ARTIFACT	UNP P39779
C	160	SER	-	CLONING ARTIFACT	UNP P39779

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Chain	Residue	Modelled	Actual	Comment	Reference
C	161	HIS	-	EXPRESSION TAG	UNP P39779
C	162	HIS	-	EXPRESSION TAG	UNP P39779
C	163	HIS	-	EXPRESSION TAG	UNP P39779
C	164	HIS	-	EXPRESSION TAG	UNP P39779
C	165	HIS	-	EXPRESSION TAG	UNP P39779
C	166	HIS	-	EXPRESSION TAG	UNP P39779
C	167	MET	-	INITIATING METHIONINE	UNP P39779

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	1	Total O 1 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: GTP-sensing transcriptional pleiotropic repressor codY
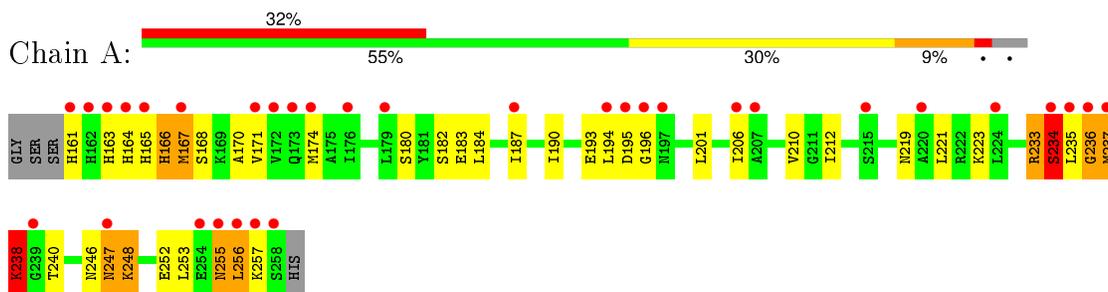
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor codY
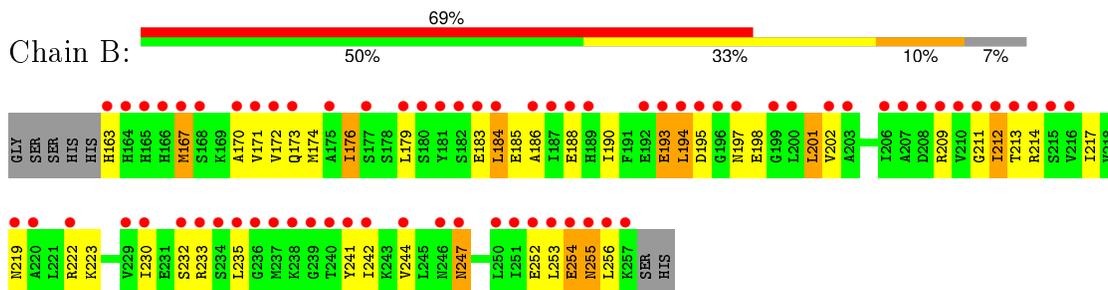
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor codY
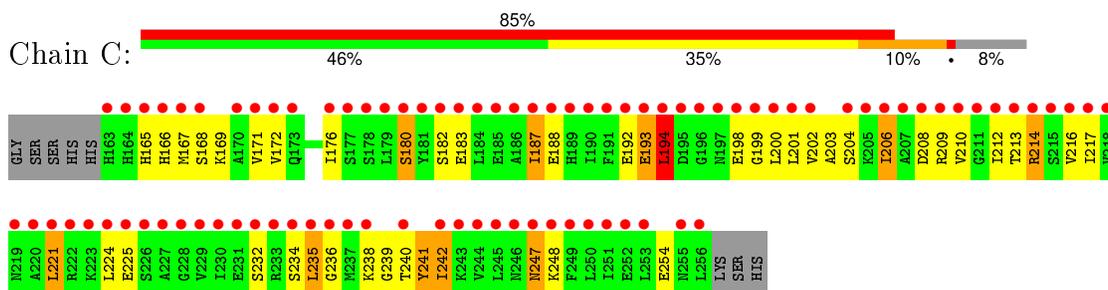
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	68.13Å 68.13Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 9.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.90) 93.8 (9.99-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.250 0.212 , 0.259	Depositor DCC
R_{free} test set	393 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 142.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 8411 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2300	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/794	0.70	0/1065
1	B	0.47	0/780	0.70	0/1045
1	C	0.24	0/738	0.43	1/991 (0.1%)
All	All	0.44	0/2312	0.63	1/3101 (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	1
1	C	0	2
All	All	0	6

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	C	208	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	HIS	Peptide
1	A	233	ARG	Peptide
1	A	234	SER	Peptide
1	B	193	GLU	Peptide
1	C	210	VAL	Peptide
1	C	236	GLY	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	783	0	799	48	0
1	B	768	0	795	44	0
1	C	730	0	753	23	0
2	A	18	0	0	0	0
2	B	1	0	0	0	0
All	All	2300	0	2347	103	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 24.

All (103) 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:174[B]:MET:HE1	1:B:174[B]:MET:CA	1.62	1.28
1:A:174[B]:MET:CE	1:B:174[B]:MET:HA	1.70	1.19
1:A:174[B]:MET:CE	1:B:174[B]:MET:CA	2.28	1.07
1:A:174[B]:MET:HE1	1:B:174[B]:MET:CB	1.86	1.04
1:A:170:ALA:O	1:A:174[A]:MET:HG3	1.59	1.01
1:C:206:ILE:HD13	1:C:206:ILE:N	1.74	1.00
1:A:174[B]:MET:CE	1:B:174[B]:MET:CB	2.44	0.96
1:A:256:LEU:C	1:A:256:LEU:HD23	1.85	0.94
1:A:190:ILE:HG23	1:A:201:LEU:HD13	1.47	0.94
1:A:174[B]:MET:HE1	1:B:174[B]:MET:HB3	1.50	0.94
1:A:174[B]:MET:CE	1:B:174[B]:MET:HB3	2.02	0.89
1:A:237:MET:CG	1:A:238:LYS:H	1.88	0.85
1:A:174[B]:MET:HE2	1:B:174[B]:MET:HA	1.61	0.83
1:A:247:ASN:HD22	1:A:247:ASN:H	1.22	0.83
1:A:235:LEU:O	1:A:237:MET:HG2	1.80	0.81
1:A:237:MET:HG3	1:A:238:LYS:H	1.46	0.79
1:A:247:ASN:HD22	1:A:247:ASN:N	1.81	0.79
1:A:237:MET:HG3	1:A:238:LYS:HG2	1.68	0.75
1:B:172:VAL:O	1:B:176:ILE:HG22	1.85	0.75
1:C:247:ASN:H	1:C:247:ASN:HD22	1.34	0.74
1:B:170:ALA:O	1:B:174[B]:MET:HG3	1.92	0.69
1:B:186:ALA:O	1:B:190:ILE:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:GLU:O	1:C:192:GLU:HG2	1.94	0.67
1:C:206:ILE:HD13	1:C:206:ILE:H	1.57	0.66
1:B:190:ILE:HD11	1:B:217:ILE:HG23	1.79	0.64
1:B:214:ARG:HG2	1:B:214:ARG:O	1.97	0.63
1:C:167:MET:O	1:C:171:VAL:HG23	1.98	0.63
1:A:237:MET:HG3	1:A:238:LYS:CG	2.28	0.63
1:C:187:ILE:HG13	1:C:224:LEU:HD11	1.79	0.63
1:A:164[B]:HIS:CE1	1:A:167:MET:HB2	2.35	0.61
1:A:247:ASN:H	1:A:247:ASN:ND2	1.96	0.61
1:C:200:LEU:HA	1:C:241:TYR:HA	1.82	0.60
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CB	2.31	0.60
1:A:235:LEU:O	1:A:236:GLY:C	2.41	0.59
1:C:172:VAL:O	1:C:176:ILE:HG13	2.03	0.59
1:A:164[B]:HIS:CG	1:A:164[B]:HIS:O	2.57	0.58
1:B:232:SER:HB3	1:B:242:ILE:HD13	1.85	0.57
1:B:185:GLU:O	1:B:188:GLU:HB3	2.04	0.57
1:A:190:ILE:HG23	1:A:201:LEU:CD1	2.30	0.57
1:A:237:MET:CG	1:A:238:LYS:N	2.62	0.57
1:C:206:ILE:N	1:C:206:ILE:CD1	2.48	0.57
1:C:247:ASN:N	1:C:247:ASN:HD22	2.02	0.57
1:B:230:ILE:HG22	1:B:244:VAL:HA	1.86	0.56
1:A:256:LEU:C	1:A:256:LEU:CD2	2.60	0.56
1:B:253:LEU:O	1:B:256:LEU:HG	2.05	0.56
1:B:253:LEU:HD12	1:B:256:LEU:CD1	2.37	0.55
1:B:201:LEU:HD12	1:B:202:VAL:H	1.72	0.55
1:C:193:GLU:O	1:C:194:LEU:C	2.46	0.54
1:A:256:LEU:O	1:A:256:LEU:HD23	2.07	0.54
1:A:165:HIS:O	1:A:166:HIS:C	2.46	0.54
1:A:180:SER:N	1:A:183:GLU:OE2	2.31	0.54
1:C:209:ARG:HG2	1:C:209:ARG:O	2.07	0.54
1:A:165:HIS:O	1:A:167:MET:N	2.42	0.53
1:A:165:HIS:O	1:A:168:SER:N	2.41	0.53
1:B:183:GLU:OE1	1:B:223:LYS:NZ	2.39	0.53
1:B:253:LEU:O	1:B:255:ASN:N	2.42	0.52
1:B:172:VAL:HG11	1:B:252:GLU:HB3	1.91	0.52
1:A:246:ASN:OD1	1:A:246:ASN:C	2.49	0.51
1:B:170:ALA:O	1:B:174[A]:MET:HG3	2.12	0.50
1:B:167[A]:MET:O	1:B:170:ALA:HB3	2.11	0.49
1:A:165:HIS:HB3	1:A:248:LYS:HD3	1.95	0.49
1:A:252:GLU:O	1:A:255:ASN:HB3	2.13	0.48
1:A:174[B]:MET:SD	1:B:174[B]:MET:HB3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:HA	1:B:242:ILE:O	2.13	0.48
1:C:206:ILE:CD1	1:C:206:ILE:H	2.21	0.47
1:B:171:VAL:HA	1:B:174[A]:MET:SD	2.54	0.47
1:B:194:LEU:HG	1:B:195:ASP:H	1.79	0.47
1:C:232:SER:HA	1:C:241:TYR:O	2.15	0.47
1:C:168:SER:O	1:C:172:VAL:HG23	2.15	0.47
1:B:179:LEU:HD23	1:B:223:LYS:HD3	1.98	0.46
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.82	0.46
1:B:253:LEU:HD12	1:B:256:LEU:HD11	1.98	0.46
1:B:194:LEU:HG	1:B:195:ASP:N	2.31	0.46
1:A:256:LEU:HD23	1:A:257:LYS:N	2.31	0.46
1:C:203:ALA:HB3	1:C:214:ARG:NE	2.31	0.45
1:B:214:ARG:CG	1:B:214:ARG:O	2.65	0.45
1:A:187:ILE:HD13	1:A:190:ILE:HD12	1.98	0.45
1:A:194:LEU:HD23	1:A:196:GLY:O	2.17	0.45
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CG	2.47	0.44
1:B:253:LEU:HD12	1:B:256:LEU:HD12	1.99	0.44
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CA	2.27	0.44
1:C:241:TYR:C	1:C:241:TYR:CD2	2.91	0.44
1:B:184:LEU:HD22	1:B:256:LEU:HD13	2.00	0.44
1:A:206:ILE:O	1:A:210:VAL:HG23	2.18	0.43
1:B:184:LEU:CD2	1:B:256:LEU:HD13	2.49	0.43
1:C:234:SER:O	1:C:235:LEU:C	2.57	0.42
1:C:199:GLY:O	1:C:242:ILE:N	2.51	0.42
1:C:234:SER:O	1:C:235:LEU:O	2.38	0.42
1:B:253:LEU:O	1:B:254:GLU:C	2.58	0.42
1:A:183:GLU:OE2	1:A:223:LYS:NZ	2.53	0.42
1:A:246:ASN:OD1	1:A:248:LYS:N	2.53	0.42
1:B:233:ARG:C	1:B:235:LEU:H	2.23	0.41
1:B:211:GLY:C	1:B:212:ILE:HG13	2.34	0.41
1:A:171:VAL:HA	1:A:174[A]:MET:SD	2.60	0.41
1:C:202:VAL:HG22	1:C:239:GLY:CA	2.51	0.41
1:A:233:ARG:O	1:A:234:SER:C	2.59	0.41
1:C:180:SER:H	1:C:183:GLU:HB2	1.85	0.41
1:B:232:SER:HA	1:B:241:TYR:O	2.20	0.40
1:A:247:ASN:N	1:A:247:ASN:ND2	2.53	0.40
1:B:176:ILE:HD13	1:B:176:ILE:C	2.42	0.40
1:C:221:LEU:O	1:C:225:GLU:HB2	2.21	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	98/102 (96%)	79 (81%)	13 (13%)	6 (6%)	2	5
1	B	97/102 (95%)	81 (84%)	12 (12%)	4 (4%)	3	14
1	C	92/102 (90%)	73 (79%)	15 (16%)	4 (4%)	3	13
All	All	287/306 (94%)	233 (81%)	40 (14%)	14 (5%)	3	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	237	MET
1	B	254	GLU
1	A	234	SER
1	A	236	GLY
1	A	255	ASN
1	B	194	LEU
1	B	247	ASN
1	C	194	LEU
1	C	235	LEU
1	A	238	LYS
1	B	197	ASN
1	C	193	GLU
1	C	180	SER

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	87/88 (99%)	71 (82%)	16 (18%)	2	6
1	B	86/88 (98%)	71 (83%)	15 (17%)	2	7
1	C	81/88 (92%)	58 (72%)	23 (28%)	0	1
All	All	254/264 (96%)	200 (79%)	54 (21%)	1	4

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	167	MET
1	A	182	SER
1	A	184	LEU
1	A	193	GLU
1	A	195	ASP
1	A	212	ILE
1	A	219	ASN
1	A	221	LEU
1	A	234	SER
1	A	238	LYS
1	A	240	THR
1	A	247	ASN
1	A	248	LYS
1	A	253	LEU
1	A	256	LEU
1	B	163	HIS
1	B	167[A]	MET
1	B	167[B]	MET
1	B	173	GLN
1	B	176	ILE
1	B	184	LEU
1	B	193	GLU
1	B	201	LEU
1	B	209	ARG
1	B	212	ILE
1	B	213	THR
1	B	219	ASN
1	B	222	ARG
1	B	247	ASN
1	B	255	ASN
1	C	165	HIS
1	C	166	HIS
1	C	169	LYS

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
1	C	182	SER
1	C	187	ILE
1	C	194	LEU
1	C	198	GLU
1	C	201	LEU
1	C	204	SER
1	C	206	ILE
1	C	212	ILE
1	C	213	THR
1	C	214	ARG
1	C	216	VAL
1	C	217	ILE
1	C	221	LEU
1	C	238	LYS
1	C	240	THR
1	C	241	TYR
1	C	242	ILE
1	C	247	ASN
1	C	248	LYS
1	C	254	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	B	247	ASN
1	C	247	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	98/102 (96%)	2.02	33 (33%)	0	0	10, 32, 79, 93	0
1	B	95/102 (93%)	3.31	70 (73%)	0	0	41, 75, 111, 116	1 (1%)
1	C	94/102 (92%)	5.59	87 (92%)	0	0	103, 127, 152, 154	37 (39%)
All	All	287/306 (93%)	3.62	190 (66%)	0	0	10, 79, 148, 154	38 (13%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	LYS	23.7
1	C	246	ASN	16.2
1	C	251	ILE	15.5
1	C	211	GLY	11.3
1	B	206	ILE	10.7
1	C	250	LEU	10.3
1	C	163	HIS	10.3
1	C	256	LEU	10.2
1	C	237	MET	10.0
1	A	258	SER	10.0
1	C	187	ILE	9.6
1	B	234	SER	9.6
1	C	164	HIS	9.4
1	C	232	SER	9.0
1	C	216	VAL	8.9
1	B	235	LEU	8.8
1	B	255	ASN	8.6
1	C	197	ASN	8.5
1	B	241	TYR	8.4
1	C	247	ASN	8.4
1	C	210	VAL	8.3
1	B	207	ALA	8.2
1	C	242	ILE	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	255	ASN	7.9
1	C	185	GLU	7.9
1	C	215	SER	7.8
1	C	180	SER	7.7
1	C	193	GLU	7.6
1	C	182	SER	7.6
1	C	202	VAL	7.5
1	C	235	LEU	7.3
1	A	161	HIS	7.2
1	C	178	SER	7.1
1	C	244	VAL	7.0
1	C	168	SER	6.8
1	B	250	LEU	6.8
1	C	252	GLU	6.7
1	C	234	SER	6.5
1	A	164[A]	HIS	6.3
1	B	236	GLY	6.3
1	C	225	GLU	6.2
1	A	194	LEU	6.2
1	B	256	LEU	6.2
1	C	177	SER	6.1
1	C	188	GLU	6.1
1	A	196	GLY	6.0
1	C	181	TYR	6.0
1	A	162	HIS	6.0
1	B	163	HIS	5.9
1	B	165	HIS	5.9
1	C	200	LEU	5.8
1	C	194	LEU	5.8
1	C	230	ILE	5.8
1	C	184	LEU	5.8
1	A	234	SER	5.6
1	B	194	LEU	5.6
1	B	164	HIS	5.5
1	C	186	ALA	5.5
1	C	248	LYS	5.4
1	B	210	VAL	5.4
1	A	165	HIS	5.4
1	C	183	GLU	5.3
1	C	219	ASN	5.3
1	A	207	ALA	5.2
1	B	195	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	5.1
1	C	165	HIS	5.1
1	C	207	ALA	5.0
1	C	208	ASP	5.0
1	B	240	THR	5.0
1	C	209	ARG	4.9
1	C	236	GLY	4.9
1	A	256	LEU	4.8
1	C	221	LEU	4.8
1	C	220	ALA	4.8
1	A	163	HIS	4.8
1	C	240	THR	4.7
1	B	253	LEU	4.7
1	C	206	ILE	4.7
1	C	204	SER	4.7
1	B	167[A]	MET	4.7
1	C	176	ILE	4.6
1	C	212	ILE	4.6
1	C	171	VAL	4.6
1	A	237	MET	4.6
1	C	218	VAL	4.6
1	B	257	LYS	4.5
1	C	198	GLU	4.5
1	B	239	GLY	4.5
1	C	217	ILE	4.5
1	C	249	PHE	4.5
1	A	235	LEU	4.4
1	C	214	ARG	4.3
1	C	229	VAL	4.2
1	C	201	LEU	4.2
1	B	232	SER	4.2
1	B	187	ILE	4.1
1	C	222	ARG	4.1
1	C	227	ALA	4.1
1	B	172	VAL	4.1
1	B	216	VAL	4.0
1	B	215	SER	4.0
1	B	180	SER	3.9
1	B	220	ALA	3.8
1	B	212	ILE	3.7
1	A	174[A]	MET	3.7
1	C	196	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	245	LEU	3.7
1	C	189	HIS	3.7
1	C	223	LYS	3.6
1	B	238	LYS	3.6
1	B	209	ARG	3.6
1	B	254	GLU	3.5
1	C	195	ASP	3.5
1	C	170	ALA	3.5
1	C	228	GLY	3.5
1	B	193	GLU	3.4
1	B	208	ASP	3.4
1	A	236	GLY	3.4
1	B	233	ARG	3.4
1	C	226	SER	3.4
1	A	257	LYS	3.4
1	B	251	ILE	3.3
1	C	224	LEU	3.3
1	B	202	VAL	3.2
1	B	173	GLN	3.2
1	B	230	ILE	3.2
1	A	247	ASN	3.1
1	C	231	GLU	3.1
1	C	238	LYS	3.1
1	A	167	MET	3.1
1	A	172	VAL	3.1
1	B	183	GLU	3.0
1	C	253	LEU	3.0
1	B	181	TYR	3.0
1	B	184	LEU	2.9
1	B	179	LEU	2.9
1	B	188	GLU	2.9
1	B	222	ARG	2.9
1	B	197	ASN	2.9
1	C	190	ILE	2.8
1	B	192	GLU	2.8
1	C	205	LYS	2.8
1	B	211	GLY	2.8
1	B	229	VAL	2.8
1	C	179	LEU	2.7
1	C	166	HIS	2.7
1	A	254	GLU	2.7
1	C	199	GLY	2.7

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Full wwPDB X-ray Structure Validation Report 2B0L

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Mol	Chain	Res	Type	RSRZ
1	C	167	MET	2.6
1	A	215	SER	2.6
1	B	242	ILE	2.6
1	C	213	THR	2.6
1	B	189	HIS	2.6
1	A	224	LEU	2.5
1	A	239	GLY	2.5
1	B	244	VAL	2.5
1	C	172	VAL	2.5
1	B	196	GLY	2.5
1	B	199	GLY	2.5
1	A	255	ASN	2.5
1	B	186	ALA	2.5
1	A	187	ILE	2.5
1	C	173	GLN	2.4
1	C	191	PHE	2.4
1	B	171	VAL	2.4
1	B	175	ALA	2.4
1	B	246	ASN	2.4
1	C	192	GLU	2.4
1	B	252	GLU	2.4
1	B	166[A]	HIS	2.4
1	B	213	THR	2.3
1	A	220	ALA	2.3
1	B	237	MET	2.3
1	B	170	ALA	2.2
1	B	203	ALA	2.2
1	B	168[A]	SER	2.2
1	A	173	GLN	2.2
1	B	219	ASN	2.2
1	A	179	LEU	2.2
1	B	200	LEU	2.2
1	A	206	ILE	2.2
1	B	214	ARG	2.2
1	A	197	ASN	2.1
1	B	177	SER	2.1
1	A	195	ASP	2.1
1	A	176	ILE	2.0
1	A	171	VAL	2.0
1	C	233	ARG	2.0
1	B	182	SER	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 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.