



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 11:27 pm GMT

PDB ID : 2B0L
Title : C-terminal DNA binding domain of transcriptional pleiotropic repressor CodY.
Authors : Levnikov, V.M.; Blagova, E.; Joseph, P.; Sonenshein, A.L.; Wilkinson, A.J.
Deposited on : 2005-09-14
Resolution : 2.90 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	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

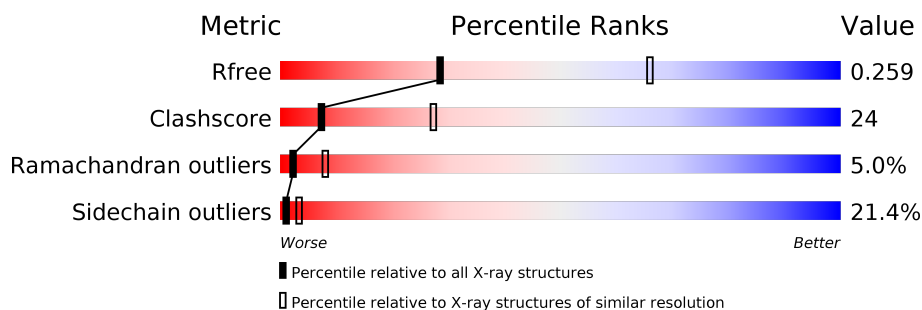
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	102	
1	B	102	
1	C	102	

2 Entry composition

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

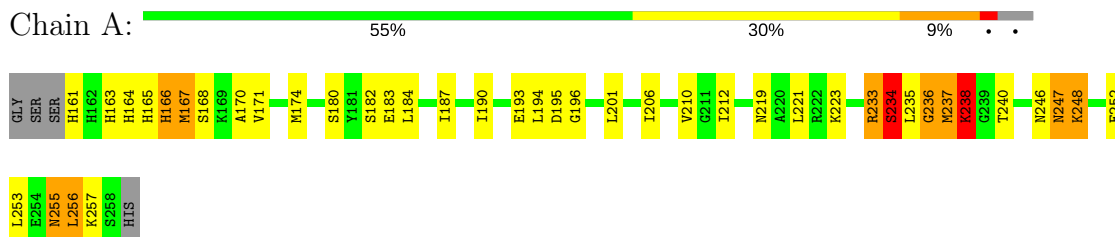
- Molecule 2 is water.

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

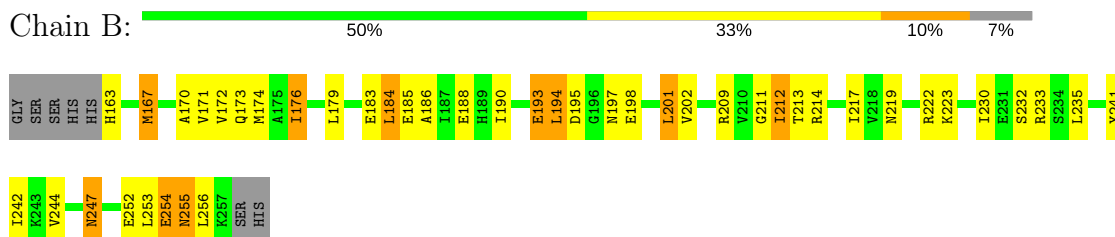
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

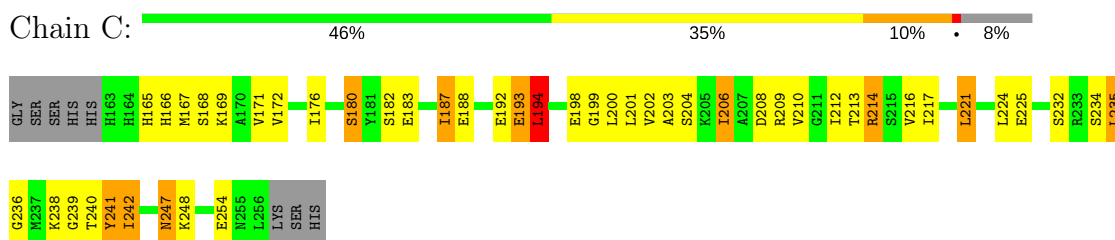
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor codY



- Molecule 1: GTP-sensing transcriptional pleiotropic repressor codY



- Molecule 1: GTP-sensing transcriptional pleiotropic repressor codY



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.67%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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	0.55	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(°)	Ideal(°)
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 ⓘ

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:190:ILE:HG23	1:A:201:LEU:HD13	1.47	0.94
1:A:256:LEU:C	1:A:256:LEU:HD23	1.85	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:185:GLU:O	1:B:188:GLU:HB3	2.04	0.57
1:B:232:SER:HB3	1:B:242:ILE:HD13	1.85	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:165:HIS:O	1:A:166:HIS:C	2.46	0.54
1:A:256:LEU:HD23	1:A:256:LEU:O	2.07	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:A:165:HIS:HB3	1:A:248:LYS:HD3	1.95	0.49
1:B:167[A]:MET:O	1:B:170:ALA:HB3	2.11	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:A:183:GLU:OE2	1:A:223:LYS:NZ	2.53	0.42
1:B:253:LEU:O	1:B:254:GLU:C	2.58	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%)	1	5
1	B	97/102 (95%)	81 (84%)	12 (12%)	4 (4%)	3	12
1	C	92/102 (90%)	73 (79%)	15 (16%)	4 (4%)	3	11
All	All	287/306 (94%)	233 (81%)	40 (14%)	14 (5%)	2	9

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	5
1	B	86/88 (98%)	71 (83%)	15 (17%)	2	6
1	C	81/88 (92%)	58 (72%)	23 (28%)	0	1
All	All	254/264 (96%)	200 (79%)	54 (21%)	1	3

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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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

There are no ligands in this entry.

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.