WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2022 – 06:07 PM JST

PDB ID	:	8H8H
Title	:	Crystal structure of the N-terminal domain of H-NS family protein TurB (TurB_nt50)
Authors	:	Vasileva, D.; Suzuki-Minakuchi, C.; Arakawa, T.; Nojiri, H.
Deposited on	:	2022-10-22
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 (i) symbol.

The types of validation reports are described at
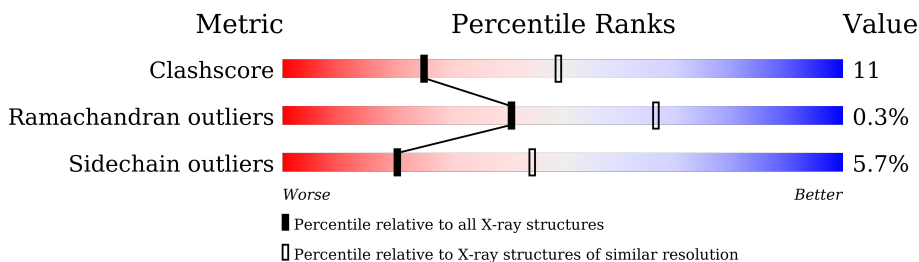http://www.wwpdb.org/validation/2017/FAQs#types.

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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		5.7%

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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	58	66% 21% • 12%
1	B	58	64% 21% • 12%
1	C	58	57% 29% • 12%
1	D	58	66% 21% • 12%
1	E	58	66% 22% 12%
1	F	58	64% 24% 12%
1	G	58	57% 24% • 16%
1	H	58	60% 24% 16%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3255 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 H-NS family protein MvaT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	51	Total	C	N	O	S	0	0	0
			410	258	71	79	2			
1	B	51	Total	C	N	O	S	0	0	0
			410	258	71	79	2			
1	C	51	Total	C	N	O	S	0	0	0
			410	258	71	79	2			
1	D	51	Total	C	N	O	S	0	0	0
			410	258	71	79	2			
1	E	51	Total	C	N	O	S	0	0	0
			406	256	71	77	2			
1	F	51	Total	C	N	O	S	0	0	0
			410	258	71	79	2			
1	G	49	Total	C	N	O	S	0	0	0
			393	247	69	75	2			
1	H	49	Total	C	N	O	S	0	0	0
			393	247	69	75	2			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LEU	-	expression tag	UNP Q88GF9
A	52	GLU	-	expression tag	UNP Q88GF9
A	53	HIS	-	expression tag	UNP Q88GF9
A	54	HIS	-	expression tag	UNP Q88GF9
A	55	HIS	-	expression tag	UNP Q88GF9
A	56	HIS	-	expression tag	UNP Q88GF9
A	57	HIS	-	expression tag	UNP Q88GF9
A	58	HIS	-	expression tag	UNP Q88GF9
B	51	LEU	-	expression tag	UNP Q88GF9
B	52	GLU	-	expression tag	UNP Q88GF9
B	53	HIS	-	expression tag	UNP Q88GF9
B	54	HIS	-	expression tag	UNP Q88GF9
B	55	HIS	-	expression tag	UNP Q88GF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	56	HIS	-	expression tag	UNP Q88GF9
B	57	HIS	-	expression tag	UNP Q88GF9
B	58	HIS	-	expression tag	UNP Q88GF9
C	51	LEU	-	expression tag	UNP Q88GF9
C	52	GLU	-	expression tag	UNP Q88GF9
C	53	HIS	-	expression tag	UNP Q88GF9
C	54	HIS	-	expression tag	UNP Q88GF9
C	55	HIS	-	expression tag	UNP Q88GF9
C	56	HIS	-	expression tag	UNP Q88GF9
C	57	HIS	-	expression tag	UNP Q88GF9
C	58	HIS	-	expression tag	UNP Q88GF9
D	51	LEU	-	expression tag	UNP Q88GF9
D	52	GLU	-	expression tag	UNP Q88GF9
D	53	HIS	-	expression tag	UNP Q88GF9
D	54	HIS	-	expression tag	UNP Q88GF9
D	55	HIS	-	expression tag	UNP Q88GF9
D	56	HIS	-	expression tag	UNP Q88GF9
D	57	HIS	-	expression tag	UNP Q88GF9
D	58	HIS	-	expression tag	UNP Q88GF9
E	51	LEU	-	expression tag	UNP Q88GF9
E	52	GLU	-	expression tag	UNP Q88GF9
E	53	HIS	-	expression tag	UNP Q88GF9
E	54	HIS	-	expression tag	UNP Q88GF9
E	55	HIS	-	expression tag	UNP Q88GF9
E	56	HIS	-	expression tag	UNP Q88GF9
E	57	HIS	-	expression tag	UNP Q88GF9
E	58	HIS	-	expression tag	UNP Q88GF9
F	51	LEU	-	expression tag	UNP Q88GF9
F	52	GLU	-	expression tag	UNP Q88GF9
F	53	HIS	-	expression tag	UNP Q88GF9
F	54	HIS	-	expression tag	UNP Q88GF9
F	55	HIS	-	expression tag	UNP Q88GF9
F	56	HIS	-	expression tag	UNP Q88GF9
F	57	HIS	-	expression tag	UNP Q88GF9
F	58	HIS	-	expression tag	UNP Q88GF9
G	51	LEU	-	expression tag	UNP Q88GF9
G	52	GLU	-	expression tag	UNP Q88GF9
G	53	HIS	-	expression tag	UNP Q88GF9
G	54	HIS	-	expression tag	UNP Q88GF9
G	55	HIS	-	expression tag	UNP Q88GF9
G	56	HIS	-	expression tag	UNP Q88GF9
G	57	HIS	-	expression tag	UNP Q88GF9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	58	HIS	-	expression tag	UNP Q88GF9
H	51	LEU	-	expression tag	UNP Q88GF9
H	52	GLU	-	expression tag	UNP Q88GF9
H	53	HIS	-	expression tag	UNP Q88GF9
H	54	HIS	-	expression tag	UNP Q88GF9
H	55	HIS	-	expression tag	UNP Q88GF9
H	56	HIS	-	expression tag	UNP Q88GF9
H	57	HIS	-	expression tag	UNP Q88GF9
H	58	HIS	-	expression tag	UNP Q88GF9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	O 3	0	0
2	B	2	Total 2	O 2	0	0
2	C	3	Total 3	O 3	0	0
2	D	1	Total 1	O 1	0	0
2	E	1	Total 1	O 1	0	0
2	G	1	Total 1	O 1	0	0
2	H	2	Total 2	O 2	0	0

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. 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.

Note EDS failed to run properly.

• Molecule 1: H-NS family protein MvaT

Chain A:

• Molecule 1: H-NS family protein MvaT

Chain B:

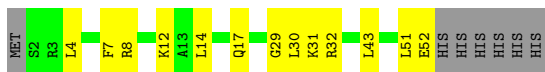• Molecule 1: H-NS family protein MvaT

Chain C:

• Molecule 1: H-NS family protein MvaT

Chain D:

• Molecule 1: H-NS family protein MvaT

Chain E:

• Molecule 1: H-NS family protein MvaT

Chain F: 64% 24% 12%

MET S2 F7 K12 Q15 E16 Q17 M18 A19 Q20 A28 R32 E33 I34 Q38 S46 L51 E52 HIS HIS HIS HIS HIS

• Molecule 1: H-NS family protein MvaT

Chain G: 57% 24% • 16%

MET S2 R3 L4 A5 E6 K12 Q15 E16 Q17 M18 A19 Q20 G29 L30 K31 R32 E33 I34 L40 Y47 S50 LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: H-NS family protein MvaT

Chain H: 60% 24% 16%

MET S2 R3 L4 R8 E11 L14 Q15 E16 Q17 M18 A19 Q20 K39 L43 Y47 D48 K49 S50 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.69Å 63.30Å 275.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 2.70	Depositor
% Data completeness (in resolution range)	99.0 (40.92-2.70)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.246 , 0.285	Depositor
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	1.038	Xtriage
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3255	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.19% 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, 0.333 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	0.42	0/412	0.62	0/544
1	B	0.46	0/412	0.61	0/544
1	C	0.42	0/412	0.70	0/544
1	D	0.45	0/412	0.67	0/544
1	E	0.42	0/408	0.60	0/539
1	F	0.44	0/412	0.63	0/544
1	G	0.44	0/395	0.72	0/521
1	H	0.40	0/395	0.65	1/521 (0.2%)
All	All	0.43	0/3258	0.65	1/4301 (0.0%)

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	H	43	LEU	CB-CG-CD1	-5.12	102.29	111.00

There are no chirality outliers.

There are no planarity outliers.

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	410	0	426	10	0
1	B	410	0	426	12	0
1	C	410	0	426	11	0
1	D	410	0	426	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	406	0	422	13	0
1	F	410	0	426	13	0
1	G	393	0	409	13	0
1	H	393	0	409	6	1
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
All	All	3255	0	3370	71	1

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 11.

All (71) 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:17:GLN:HG3	1:G:17:GLN:HE22	1.28	0.96
1:G:3:ARG:HD2	1:G:5:ALA:H	1.48	0.78
1:C:17:GLN:HE22	1:E:17:GLN:HG2	1.48	0.77
1:C:18:MET:HG2	1:E:14:LEU:HD21	1.74	0.70
1:E:31:LYS:O	1:E:31:LYS:HD3	1.92	0.69
1:C:17:GLN:NE2	1:E:17:GLN:HG2	2.09	0.68
1:B:25:LYS:HG2	1:F:7:PHE:HE2	1.59	0.67
1:E:4:LEU:HD21	1:E:8:ARG:HH11	1.61	0.65
1:B:17:GLN:NE2	1:F:17:GLN:OE1	2.32	0.62
1:C:3:ARG:HG3	1:C:5:ALA:H	1.65	0.62
1:G:30:LEU:O	1:G:34:ILE:HG13	2.00	0.61
1:B:14:LEU:O	1:B:18:MET:HG2	2.01	0.61
1:E:52:GLU:N	1:E:52:GLU:OE1	2.34	0.60
1:G:12:LYS:O	1:G:16:GLU:HG2	2.02	0.60
1:E:29:GLY:HA2	1:E:32:ARG:HE	1.66	0.58
1:H:11:GLU:O	1:H:15:GLN:HG3	2.04	0.58
1:G:15:GLN:HA	1:G:18:MET:HE3	1.86	0.57
1:H:16:GLU:O	1:H:20:GLN:HG3	2.05	0.57
1:F:16:GLU:O	1:F:20:GLN:HG3	2.06	0.56
1:B:3:ARG:HB3	1:B:6:GLU:HG3	1.88	0.56
1:A:29:GLY:O	1:A:33:GLU:HG3	2.05	0.55
1:B:16:GLU:O	1:B:20:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ALA:O	1:C:32:ARG:HG3	2.07	0.55
1:A:4:LEU:O	1:A:8:ARG:HG3	2.07	0.55
1:A:13:ALA:O	1:A:17:GLN:HG2	2.07	0.54
1:A:16:GLU:O	1:A:20:GLN:HG3	2.07	0.54
1:D:3:ARG:HB3	1:D:3:ARG:CZ	2.38	0.54
1:B:14:LEU:HD11	1:F:18:MET:HG2	1.90	0.52
1:D:14:LEU:O	1:D:18:MET:HG3	2.09	0.52
1:C:28:ALA:HA	1:C:31:LYS:HB2	1.92	0.52
1:B:17:GLN:NE2	1:F:17:GLN:CD	2.64	0.50
1:D:11:GLU:O	1:D:15:GLN:HG2	2.11	0.50
1:C:4:LEU:HA	1:E:30:LEU:HD12	1.95	0.49
1:G:47:TYR:O	1:G:47:TYR:HD1	1.96	0.48
1:D:35:GLU:HA	1:D:38:GLN:HG3	1.95	0.48
1:B:17:GLN:HE22	1:F:17:GLN:CD	2.15	0.48
1:F:12:LYS:O	1:F:16:GLU:HG3	2.14	0.48
1:A:40:LEU:O	1:A:44:MET:HG3	2.15	0.47
1:G:12:LYS:HA	1:G:15:GLN:HG2	1.96	0.47
1:A:17:GLN:HA	1:A:17:GLN:OE1	2.15	0.47
1:C:22:GLU:O	1:C:26:LYS:HD3	2.14	0.47
1:B:27:ASP:OD2	1:F:2:SER:N	2.47	0.47
1:D:12:LYS:O	1:D:16:GLU:HG2	2.15	0.47
1:G:16:GLU:O	1:G:20:GLN:HG2	2.15	0.46
1:D:33:GLU:OE1	1:H:2:SER:HB2	2.15	0.46
1:C:12:LYS:O	1:C:16:GLU:HG2	2.15	0.46
1:B:28:ALA:HA	1:B:31:LYS:HE3	1.98	0.45
1:E:14:LEU:HA	1:E:14:LEU:HD12	1.71	0.45
1:G:3:ARG:O	1:G:6:GLU:HG2	2.17	0.45
1:B:14:LEU:HD12	1:F:17:GLN:HB3	1.99	0.45
1:E:4:LEU:HD21	1:E:8:ARG:NH1	2.30	0.44
1:F:34:ILE:O	1:F:38:GLN:HG2	2.17	0.44
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.85	0.44
1:A:17:GLN:HG3	1:G:17:GLN:NE2	2.12	0.44
1:D:20:GLN:HA	1:D:20:GLN:OE1	2.18	0.43
1:H:14:LEU:O	1:H:18:MET:HG3	2.19	0.43
1:A:14:LEU:HD11	1:G:18:MET:HB2	2.00	0.42
1:B:45:LYS:O	1:B:49:LYS:HE2	2.19	0.42
1:G:40:LEU:HD23	1:G:40:LEU:HA	1.76	0.42
1:F:28:ALA:O	1:F:32:ARG:HG3	2.20	0.42
1:D:16:GLU:HG2	1:D:16:GLU:H	1.68	0.41
1:F:15:GLN:HA	1:F:15:GLN:OE1	2.20	0.41
1:D:40:LEU:HD12	1:D:40:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LEU:HD23	1:E:51:LEU:HA	1.87	0.41
1:G:29:GLY:HA2	1:G:32:ARG:NH1	2.36	0.41
1:C:30:LEU:HD11	1:E:4:LEU:HA	2.02	0.41
1:E:7:PHE:C	1:E:7:PHE:CD2	2.94	0.41
1:H:4:LEU:O	1:H:8:ARG:HG3	2.21	0.41
1:C:37:GLU:O	1:C:41:VAL:HG13	2.21	0.40
1:F:7:PHE:C	1:F:7:PHE:CD1	2.95	0.40
1:H:3:ARG:HD2	1:H:3:ARG:HA	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:OD2	1:H:39:LYS:NZ[3_656]	2.14	0.06

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	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	B	49/58 (84%)	49 (100%)	0	0	100	100
1	C	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	D	49/58 (84%)	47 (96%)	2 (4%)	0	100	100
1	E	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	F	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	G	47/58 (81%)	47 (100%)	0	0	100	100
1	H	47/58 (81%)	46 (98%)	0	1 (2%)	7	18
All	All	388/464 (84%)	381 (98%)	6 (2%)	1 (0%)	41	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	49	LYS

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	42/49 (86%)	39 (93%)	3 (7%)	14	34
1	B	42/49 (86%)	39 (93%)	3 (7%)	14	34
1	C	42/49 (86%)	38 (90%)	4 (10%)	8	20
1	D	42/49 (86%)	41 (98%)	1 (2%)	49	77
1	E	41/49 (84%)	39 (95%)	2 (5%)	25	52
1	F	42/49 (86%)	40 (95%)	2 (5%)	25	53
1	G	40/49 (82%)	37 (92%)	3 (8%)	13	31
1	H	40/49 (82%)	39 (98%)	1 (2%)	47	76
All	All	331/392 (84%)	312 (94%)	19 (6%)	20	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	49	LYS
1	A	52	GLU
1	B	14	LEU
1	B	49	LYS
1	B	50	SER
1	C	22	GLU
1	C	44	MET
1	C	49	LYS
1	C	50	SER
1	D	38	GLN
1	E	12	LYS
1	E	43	LEU

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Mol	Chain	Res	Type
1	F	46	SER
1	F	51	LEU
1	G	2	SER
1	G	3	ARG
1	G	47	TYR
1	H	47	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	C	15	GLN
1	C	17	GLN
1	G	17	GLN
1	G	38	GLN

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.