



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 09:40 AM EST

PDB ID : 1BSA
Title : CRYSTAL STRUCTURAL ANALYSIS OF MUTATIONS IN THE HYDROPHOBIC CORES OF BARNASE
Authors : Buckle, A.M.; Henrick, K.; Fersht, A.R.
Deposited on : unknown
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

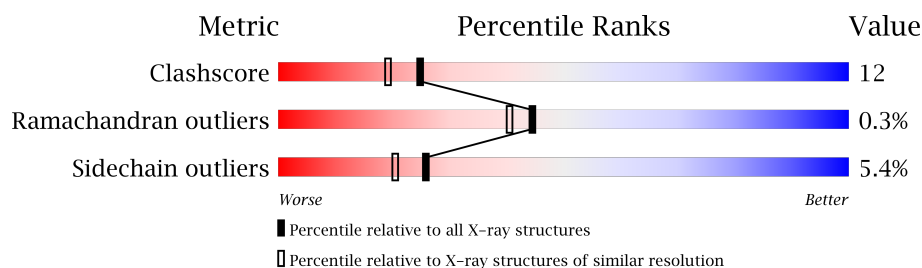
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	110	
1	B	110	
1	C	110	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2784 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 BARNASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	0	0	0
			838	532	145	161			
1	B	107	Total	C	N	O	0	0	0
			839	531	144	164			
1	C	107	Total	C	N	O	0	0	0
			849	538	148	163			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	VAL	ILE	CONFLICT	UNP P00648
B	51	VAL	ILE	CONFLICT	UNP P00648
C	51	VAL	ILE	CONFLICT	UNP P00648

- Molecule 2 is water.

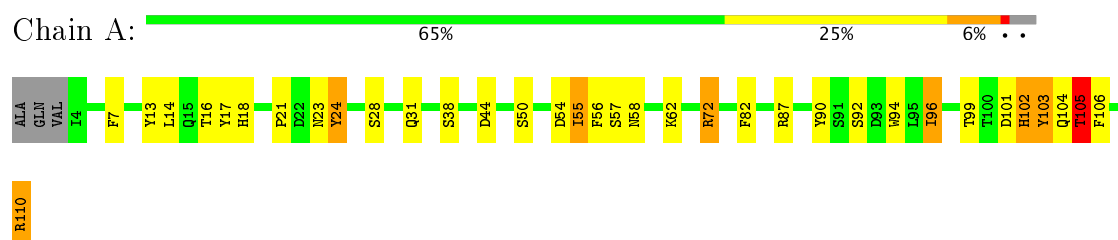
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	0
			77	77		
2	B	84	Total	O	0	0
			84	84		
2	C	97	Total	O	0	0
			97	97		

3 Residue-property plots [i](#)

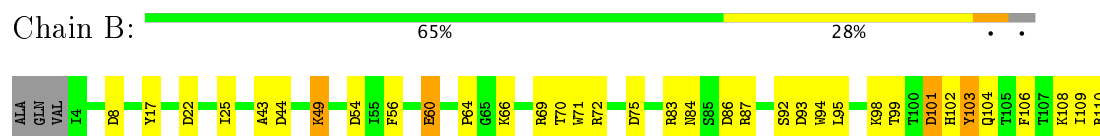
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

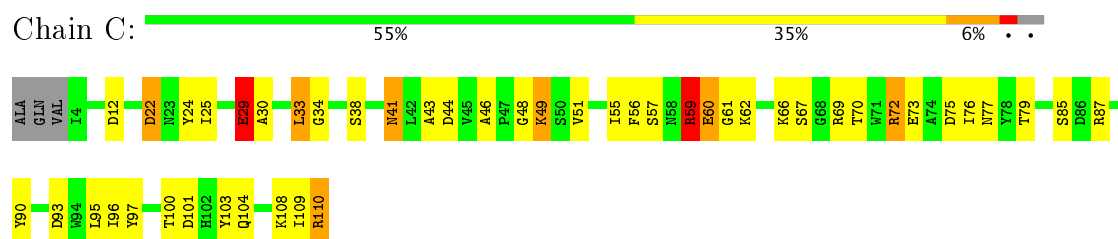
• Molecule 1: BARNASE



• Molecule 1: BARNASE



• Molecule 1: BARNASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	58.63Å 58.63Å 81.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2784	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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	0.96	0/859	1.90	19/1166 (1.6%)
1	B	0.96	0/859	2.16	34/1167 (2.9%)
1	C	1.37	2/870 (0.2%)	2.43	37/1179 (3.1%)
All	All	1.11	2/2588 (0.1%)	2.17	90/3512 (2.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLU	CG-CD	26.33	1.91	1.51
1	C	38	SER	CB-OG	-6.26	1.34	1.42

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	GLU	CA-CB-CG	26.05	170.71	113.40
1	C	110	ARG	NE-CZ-NH2	21.87	131.23	120.30
1	C	87	ARG	NE-CZ-NH2	18.09	129.34	120.30
1	C	29	GLU	CA-CB-CG	13.89	143.96	113.40
1	C	110	ARG	NE-CZ-NH1	-13.25	113.67	120.30
1	C	72	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	B	72	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	B	56	PHE	CB-CG-CD1	-11.54	112.72	120.80
1	B	72	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	C	60	GLU	C-N-CA	11.17	145.76	122.30
1	B	87	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	B	110	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	C	60	GLU	O-C-N	-10.29	105.70	123.20
1	A	24	TYR	CB-CG-CD1	-10.03	114.98	121.00
1	B	8	ASP	CB-CG-OD2	-9.94	109.35	118.30
1	A	54	ASP	CB-CG-OD2	9.76	127.08	118.30
1	C	60	GLU	CB-CA-C	9.53	129.46	110.40
1	B	56	PHE	CB-CG-CD2	9.39	127.37	120.80
1	B	69	ARG	CD-NE-CZ	-9.16	110.78	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	PHE	CB-CG-CD2	-9.04	114.47	120.80
1	B	60	GLU	CG-CD-OE1	8.95	136.19	118.30
1	B	95	LEU	CA-CB-CG	8.91	135.79	115.30
1	B	22	ASP	CB-CG-OD2	-8.66	110.50	118.30
1	C	56	PHE	CB-CG-CD1	-8.58	114.80	120.80
1	B	44	ASP	CB-CG-OD1	-8.53	110.63	118.30
1	B	101	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	C	93	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	83	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	60	GLU	CA-CB-CG	8.25	131.55	113.40
1	C	22	ASP	CB-CG-OD2	8.07	125.56	118.30
1	C	59	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	8	ASP	CB-CG-OD1	7.81	125.33	118.30
1	C	60	GLU	CA-C-O	7.61	136.08	120.10
1	C	61	GLY	CA-C-O	7.60	134.28	120.60
1	A	110	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	90	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	A	110	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	72	ARG	NH1-CZ-NH2	-7.49	111.16	119.40
1	A	102	HIS	C-N-CA	7.38	140.15	121.70
1	C	101	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	60	GLU	CB-CG-CD	6.60	132.01	114.20
1	B	106	PHE	CB-CG-CD1	-6.40	116.32	120.80
1	B	60	GLU	CG-CD-OE2	-6.38	105.54	118.30
1	A	82	PHE	CB-CG-CD1	6.31	125.22	120.80
1	C	22	ASP	CA-CB-CG	-6.26	99.62	113.40
1	C	103	TYR	O-C-N	6.22	132.66	122.70
1	C	87	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
1	A	99	THR	N-CA-CB	6.14	121.97	110.30
1	B	69	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	C	24	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	B	86	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	94	TRP	CA-CB-CG	-6.09	102.13	113.70
1	A	24	TYR	CB-CG-CD2	6.07	124.64	121.00
1	A	44	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	A	87	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	103	TYR	CB-CG-CD2	5.87	124.52	121.00
1	B	75	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	72	ARG	O-C-N	5.78	131.95	122.70
1	C	43	ALA	CB-CA-C	5.71	118.66	110.10
1	B	60	GLU	CB-CG-CD	5.58	129.26	114.20
1	A	105	THR	N-CA-CB	-5.57	99.72	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	LEU	CB-CA-C	-5.55	99.65	110.20
1	A	38	SER	CA-CB-OG	-5.46	96.47	111.20
1	A	55	ILE	CB-CA-C	-5.42	100.75	111.60
1	C	101	ASP	OD1-CG-OD2	-5.39	113.05	123.30
1	B	22	ASP	OD1-CG-OD2	5.35	133.46	123.30
1	C	73	GLU	O-C-N	5.33	131.22	122.70
1	B	93	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	7	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	C	12	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	24	TYR	CB-CG-CD2	5.25	124.15	121.00
1	B	17	TYR	CA-CB-CG	-5.22	103.47	113.40
1	C	59	ARG	CA-C-O	-5.21	109.15	120.10
1	A	105	THR	CA-CB-CG2	5.21	119.69	112.40
1	C	59	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	72	ARG	N-CA-CB	5.17	119.91	110.60
1	B	106	PHE	CB-CG-CD2	5.17	124.42	120.80
1	B	71	TRP	CH2-CZ2-CE2	5.16	122.56	117.40
1	B	101	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	48	GLY	C-N-CA	5.10	134.45	121.70
1	C	72	ARG	CD-NE-CZ	5.10	130.74	123.60
1	C	90	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	B	86	ASP	OD1-CG-OD2	5.09	132.97	123.30
1	C	41	ASN	N-CA-C	5.06	124.66	111.00
1	C	75	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	13	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
1	C	95	LEU	N-CA-C	-5.02	97.45	111.00
1	B	43	ALA	CB-CA-C	5.01	117.62	110.10
1	B	54	ASP	O-C-N	5.01	130.72	122.70
1	C	104	GLN	C-N-CA	5.00	134.20	121.70

There are no chirality outliers.

There are no planarity outliers.

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	838	0	794	21	0
1	B	839	0	785	9	0
1	C	849	0	811	32	0
2	A	77	0	0	0	0
2	B	84	0	0	1	0
2	C	97	0	0	3	0
All	All	2784	0	2390	60	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 (60) 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:C:60:GLU:CG	1:C:60:GLU:CD	1.91	1.38
1:C:60:GLU:CD	1:C:62:LYS:NZ	2.13	1.02
1:C:25:ILE:HD12	1:C:30:ALA:HB2	1.38	1.01
1:C:60:GLU:CD	1:C:62:LYS:HZ1	1.83	0.79
1:C:25:ILE:HB	1:C:29:GLU:HG2	1.64	0.78
1:C:60:GLU:CD	1:C:62:LYS:HZ2	1.86	0.77
1:A:55:ILE:HD11	1:A:72:ARG:CZ	2.16	0.74
1:A:55:ILE:CD1	1:A:72:ARG:CZ	2.68	0.72
1:C:25:ILE:CD1	1:C:30:ALA:HB2	2.19	0.71
1:B:25:ILE:HD13	1:B:49:LYS:HG3	1.74	0.70
1:A:55:ILE:HD11	1:A:72:ARG:NH2	2.09	0.67
1:C:55:ILE:CD1	1:C:70:THR:CG2	2.74	0.66
1:A:57:SER:O	1:A:58:ASN:HB3	2.03	0.59
1:B:104:GLN:CB	2:B:143:HOH:O	2.52	0.58
1:A:101:ASP:OD2	1:A:105:THR:HB	2.05	0.56
1:C:79:THR:HG23	2:C:206:HOH:O	2.04	0.55
1:A:55:ILE:CD1	1:A:72:ARG:NH1	2.69	0.55
1:C:60:GLU:CD	1:C:62:LYS:CE	2.74	0.55
1:A:62:LYS:NZ	1:A:103:TYR:O	2.38	0.54
1:A:57:SER:O	1:A:58:ASN:CB	2.55	0.54
1:A:96:ILE:HG13	1:A:110:ARG:HB2	1.91	0.53
1:A:21:PRO:HB2	1:A:23:ASN:OD1	2.09	0.52
1:A:16:THR:HG22	1:A:17:TYR:N	2.24	0.52
1:C:66:LYS:HG2	1:C:67:SER:N	2.25	0.52
1:C:96:ILE:HB	1:C:110:ARG:HB2	1.92	0.51
1:A:14:LEU:O	1:A:18:HIS:HA	2.10	0.51
1:A:28:SER:HA	1:A:31:GLN:HE21	1.75	0.50
1:C:46:ALA:O	1:C:49:LYS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HD11	1:A:72:ARG:NH1	2.27	0.49
1:B:98:LYS:HG2	1:B:109:ILE:CG2	2.43	0.49
1:C:66:LYS:HE3	1:C:69:ARG:HB2	1.95	0.49
1:B:64:PRO:HG3	1:C:34:GLY:HA2	1.94	0.48
1:C:57:SER:OG	1:C:59:ARG:HG3	2.15	0.47
1:C:55:ILE:HD11	1:C:70:THR:HG21	1.96	0.47
1:C:57:SER:OG	1:C:59:ARG:CG	2.63	0.47
1:C:66:LYS:NZ	1:C:67:SER:O	2.47	0.45
1:B:98:LYS:HG2	1:B:109:ILE:HG21	1.98	0.45
1:B:101:ASP:O	1:B:102:HIS:HB2	2.16	0.45
1:A:24:TYR:HA	1:A:50:SER:O	2.16	0.45
1:A:101:ASP:O	1:A:104:GLN:HG3	2.17	0.44
1:A:21:PRO:HD2	1:A:24:TYR:CD2	2.52	0.44
1:C:55:ILE:HD11	1:C:70:THR:CG2	2.46	0.44
1:A:55:ILE:HD13	1:A:72:ARG:NH1	2.31	0.44
1:C:76:ILE:O	1:C:77:ASN:HB2	2.18	0.43
1:C:22:ASP:N	2:C:179:HOH:O	2.10	0.43
1:C:33:LEU:HD13	1:C:46:ALA:HB2	2.01	0.43
1:B:84:ASN:C	1:B:84:ASN:OD1	2.58	0.42
1:B:108:LYS:HZ2	1:C:33:LEU:HD22	1.85	0.42
1:C:109:ILE:O	1:C:110:ARG:HD3	2.19	0.42
1:A:55:ILE:HG22	1:A:56:PHE:N	2.34	0.42
1:C:85:SER:OG	1:C:100:THR:O	2.37	0.42
1:B:99:THR:OG1	1:B:101:ASP:OD1	2.37	0.42
1:C:41:ASN:O	1:C:44:ASP:HB2	2.20	0.42
1:A:103:TYR:HB3	1:A:106:PHE:HZ	1.84	0.41
1:C:60:GLU:CD	1:C:62:LYS:HE3	2.41	0.41
1:C:55:ILE:HD12	1:C:70:THR:HG23	2.02	0.41
1:C:55:ILE:CD1	1:C:70:THR:HG23	2.50	0.40
1:C:97:TYR:CZ	1:C:108:LYS:HB2	2.56	0.40
1:C:72:ARG:NE	2:C:189:HOH:O	2.13	0.40
1:A:14:LEU:HD22	1:A:94:TRP:HZ3	1.87	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	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
1	B	105/110 (96%)	100 (95%)	4 (4%)	1 (1%)	18	10
1	C	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
All	All	315/330 (96%)	296 (94%)	18 (6%)	1 (0%)	44	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	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	86/92 (94%)	81 (94%)	5 (6%)	23	18
1	B	86/92 (94%)	81 (94%)	5 (6%)	23	18
1	C	88/92 (96%)	84 (96%)	4 (4%)	32	27
All	All	260/276 (94%)	246 (95%)	14 (5%)	26	20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	96	ILE
1	A	102	HIS
1	A	103	TYR
1	A	105	THR
1	B	49	LYS
1	B	60	GLU
1	B	70	THR

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Mol	Chain	Res	Type
1	B	92	SER
1	B	103	TYR
1	C	29	GLU
1	C	49	LYS
1	C	51	VAL
1	C	59	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	C	102	HIS

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.