



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:49 pm GMT

PDB ID : 1B8X  
Title : GLUTATHIONE S-TRANSFERASE FUSED WITH THE NUCLEAR MATRIX TARGETING SIGNAL OF THE TRANSCRIPTION FACTOR AML-1  
Authors : Tang, L.; Guo, B.; Van Wijnen, A.J.; Lian, J.B.; Stein, J.L.; Stein, G.S.; Zhou, G.W.  
Deposited on : 1999-02-03  
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](mailto: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.

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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) : recalc28949

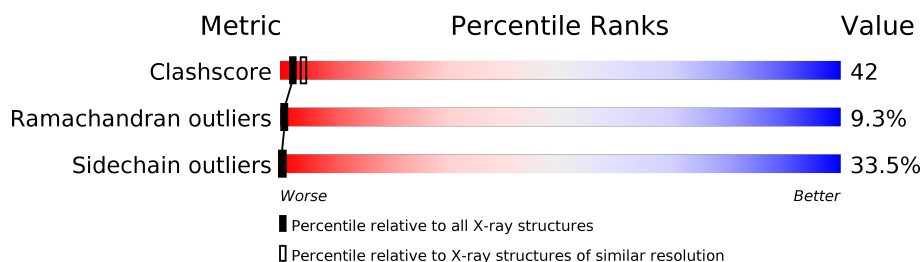
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

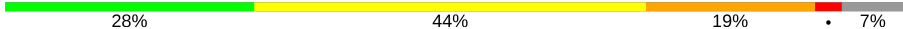
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	280	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2083 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 PROTEIN (AML-1B).

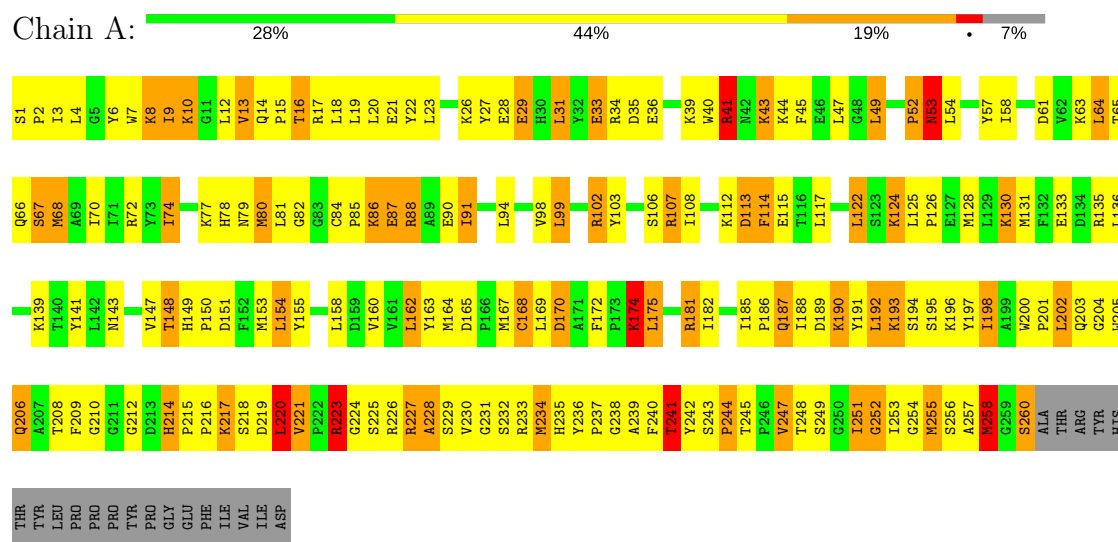
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2083	1343	347	378	15	0	0	0

### 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 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: PROTEIN (AML-1B)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40 Å 93.40 Å 57.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.5 (6.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	11.00	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.209 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 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	0.41	1/2139 (0.0%)	0.65	0/2889

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	SER	C-O	-8.36	1.07	1.23

There are no bond angle outliers.

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	2083	0	2073	176	0
All	All	2083	0	2073	176	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 42.

All (176) 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:241:THR:O	1:A:241:THR:HG23	1.59	1.01
1:A:158:LEU:HD11	1:A:175:LEU:HD22	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HH12	1:A:203:GLN:HE22	1.10	0.98
1:A:232:SER:H	1:A:243:SER:HB2	1.38	0.89
1:A:36:GLU:HB2	1:A:39:LYS:HB2	1.55	0.89
1:A:217:LYS:HE3	1:A:220:LEU:HB2	1.57	0.87
1:A:148:THR:HB	1:A:150:PRO:HD2	1.57	0.86
1:A:251:ILE:HG23	1:A:252:GLY:N	1.90	0.86
1:A:43:LYS:HE3	1:A:47:LEU:HD21	1.59	0.84
1:A:257:ALA:O	1:A:258:MET:HB2	1.79	0.83
1:A:40:TRP:O	1:A:41:ARG:HG2	1.81	0.81
1:A:9:ILE:HG22	1:A:201:PRO:HD2	1.60	0.80
1:A:98:VAL:HG11	1:A:153:MET:HB3	1.65	0.79
1:A:232:SER:HB3	1:A:236:TYR:HE2	1.49	0.77
1:A:7:TRP:HB2	1:A:9:ILE:HD13	1.65	0.77
1:A:241:THR:O	1:A:241:THR:CG2	2.32	0.76
1:A:113:ASP:O	1:A:117:LEU:HG	1.86	0.76
1:A:22:TYR:HB2	1:A:188:ILE:HD11	1.69	0.74
1:A:122:LEU:O	1:A:126:PRO:HD3	1.89	0.73
1:A:102:ARG:HH12	1:A:203:GLN:NE2	1.86	0.73
1:A:202:LEU:HB2	1:A:210:GLY:HA3	1.69	0.72
1:A:2:PRO:HA	1:A:58:ILE:O	1.90	0.72
1:A:14:GLN:HB3	1:A:15:PRO:HD3	1.72	0.71
1:A:64:LEU:HD11	1:A:70:ILE:HG13	1.74	0.70
1:A:86:LYS:H	1:A:86:LYS:HE3	1.56	0.69
1:A:220:LEU:O	1:A:221:VAL:HG13	1.93	0.68
1:A:200:TRP:CG	1:A:201:PRO:HA	2.29	0.67
1:A:232:SER:HB3	1:A:236:TYR:CE2	2.30	0.67
1:A:52:PRO:O	1:A:53:ASN:HB2	1.96	0.65
1:A:99:LEU:O	1:A:103:TYR:HB2	1.96	0.65
1:A:189:ASP:O	1:A:193:LYS:HE3	1.96	0.64
1:A:115:GLU:H	1:A:115:GLU:CD	1.99	0.64
1:A:214:HIS:HB2	1:A:216:PRO:HD3	1.79	0.64
1:A:21:GLU:HG2	1:A:191:TYR:CB	2.28	0.64
1:A:191:TYR:O	1:A:197:TYR:HB2	1.98	0.64
1:A:251:ILE:CG2	1:A:252:GLY:N	2.60	0.63
1:A:86:LYS:N	1:A:86:LYS:HE3	2.13	0.63
1:A:21:GLU:HG2	1:A:191:TYR:HB2	1.79	0.63
1:A:201:PRO:HB2	1:A:210:GLY:O	1.99	0.63
1:A:223:ARG:HD2	1:A:226:ARG:HD2	1.81	0.62
1:A:165:ASP:OD1	1:A:167:MET:HB2	1.99	0.62
1:A:223:ARG:NE	1:A:223:ARG:O	2.32	0.61
1:A:14:GLN:O	1:A:17:ARG:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:HE3	1:A:220:LEU:CB	2.30	0.61
1:A:81:LEU:O	1:A:91:ILE:HG13	2.00	0.61
1:A:214:HIS:O	1:A:216:PRO:HD2	2.01	0.61
1:A:185:ILE:O	1:A:189:ASP:N	2.34	0.60
1:A:36:GLU:HB2	1:A:39:LYS:CB	2.29	0.60
1:A:85:PRO:HD2	1:A:86:LYS:NZ	2.16	0.60
1:A:202:LEU:HB2	1:A:210:GLY:CA	2.31	0.59
1:A:135:ARG:HG3	1:A:135:ARG:O	2.02	0.59
1:A:130:LYS:NZ	1:A:131:MET:HG3	2.18	0.58
1:A:40:TRP:CH2	1:A:44:LYS:HG3	2.39	0.58
1:A:200:TRP:CD2	1:A:215:PRO:HB3	2.39	0.58
1:A:150:PRO:HB3	1:A:153:MET:HE3	1.85	0.57
1:A:149:HIS:ND1	1:A:150:PRO:HD3	2.18	0.57
1:A:64:LEU:HD12	1:A:65:THR:N	2.19	0.57
1:A:223:ARG:CD	1:A:226:ARG:HD2	2.34	0.57
1:A:231:GLY:HA2	1:A:243:SER:O	2.04	0.57
1:A:236:TYR:O	1:A:238:GLY:N	2.37	0.57
1:A:74:ILE:O	1:A:78:HIS:HD2	1.88	0.57
1:A:91:ILE:HD12	1:A:148:THR:HG21	1.87	0.56
1:A:148:THR:O	1:A:151:ASP:HB2	2.06	0.56
1:A:8:LYS:HE2	1:A:31:LEU:CG	2.36	0.55
1:A:68:MET:O	1:A:72:ARG:HG3	2.07	0.55
1:A:27:TYR:HE2	1:A:29:GLU:HG2	1.72	0.54
1:A:90:GLU:O	1:A:94:LEU:HG	2.08	0.54
1:A:10:LYS:HE3	1:A:198:ILE:O	2.08	0.54
1:A:122:LEU:O	1:A:126:PRO:CD	2.54	0.54
1:A:150:PRO:HA	1:A:153:MET:HB2	1.89	0.54
1:A:214:HIS:C	1:A:216:PRO:HD2	2.28	0.54
1:A:247:VAL:HG13	1:A:248:THR:HG23	1.89	0.54
1:A:8:LYS:HD3	1:A:198:ILE:CD1	2.37	0.54
1:A:43:LYS:CE	1:A:47:LEU:HD21	2.35	0.54
1:A:44:LYS:O	1:A:47:LEU:HD12	2.08	0.53
1:A:251:ILE:HG23	1:A:252:GLY:H	1.71	0.53
1:A:198:ILE:HG22	1:A:198:ILE:O	2.09	0.53
1:A:34:ARG:HG2	1:A:205:TRP:CD2	2.44	0.53
1:A:230:VAL:HG22	1:A:230:VAL:O	2.08	0.53
1:A:21:GLU:CG	1:A:191:TYR:HB2	2.39	0.53
1:A:40:TRP:CZ2	1:A:44:LYS:HG3	2.44	0.52
1:A:19:LEU:HG	1:A:23:LEU:HD11	1.92	0.52
1:A:163:TYR:O	1:A:220:LEU:HD11	2.10	0.52
1:A:19:LEU:HD11	1:A:80:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LYS:HE2	1:A:31:LEU:HB3	1.92	0.51
1:A:64:LEU:HD12	1:A:65:THR:O	2.10	0.51
1:A:82:GLY:HA3	1:A:88:ARG:HG3	1.93	0.51
1:A:87:GLU:O	1:A:91:ILE:HG12	2.11	0.51
1:A:103:TYR:O	1:A:107:ARG:HG3	2.11	0.50
1:A:53:ASN:O	1:A:54:LEU:HD23	2.10	0.50
1:A:19:LEU:HG	1:A:23:LEU:CD1	2.40	0.50
1:A:257:ALA:O	1:A:258:MET:CB	2.56	0.50
1:A:223:ARG:C	1:A:223:ARG:HE	2.15	0.50
1:A:27:TYR:CE2	1:A:29:GLU:HG2	2.47	0.50
1:A:103:TYR:HA	1:A:106:SER:OG	2.11	0.50
1:A:40:TRP:O	1:A:41:ARG:CG	2.56	0.50
1:A:68:MET:SD	1:A:99:LEU:HD11	2.52	0.49
1:A:200:TRP:CD1	1:A:201:PRO:HA	2.48	0.49
1:A:16:THR:O	1:A:20:LEU:HD12	2.12	0.49
1:A:8:LYS:HE2	1:A:31:LEU:CB	2.42	0.49
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.69	0.49
1:A:223:ARG:CZ	1:A:226:ARG:HD2	2.43	0.48
1:A:158:LEU:HD21	1:A:175:LEU:HD13	1.96	0.48
1:A:217:LYS:NZ	1:A:220:LEU:HB3	2.28	0.48
1:A:8:LYS:HE2	1:A:31:LEU:HG	1.95	0.48
1:A:154:LEU:HD22	1:A:158:LEU:HG	1.95	0.48
1:A:52:PRO:O	1:A:53:ASN:CB	2.62	0.48
1:A:6:TYR:CD2	1:A:13:VAL:HG12	2.48	0.48
1:A:141:TYR:CE2	1:A:147:VAL:HG23	2.48	0.48
1:A:223:ARG:NE	1:A:223:ARG:C	2.66	0.48
1:A:223:ARG:NE	1:A:226:ARG:HD2	2.28	0.48
1:A:191:TYR:HA	1:A:194:SER:OG	2.14	0.47
1:A:114:PHE:HB3	1:A:208:THR:HG21	1.96	0.47
1:A:236:TYR:CD1	1:A:244:PRO:HG2	2.49	0.47
1:A:8:LYS:HD3	1:A:198:ILE:HD11	1.96	0.47
1:A:223:ARG:C	1:A:225:SER:H	2.18	0.47
1:A:21:GLU:HG3	1:A:187:GLN:O	2.15	0.47
1:A:4:LEU:O	1:A:29:GLU:HA	2.15	0.47
1:A:49:LEU:O	1:A:52:PRO:HD3	2.14	0.47
1:A:19:LEU:HD11	1:A:80:MET:CE	2.45	0.46
1:A:2:PRO:HB2	1:A:57:TYR:CE1	2.50	0.46
1:A:234:MET:O	1:A:235:HIS:HB2	2.16	0.46
1:A:187:GLN:HE21	1:A:187:GLN:HB2	1.53	0.46
1:A:102:ARG:NH1	1:A:203:GLN:HE22	1.94	0.46
1:A:220:LEU:C	1:A:221:VAL:HG22	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:NH1	1:A:226:ARG:HD3	2.31	0.45
1:A:182:ILE:HG22	1:A:188:ILE:HG21	1.99	0.45
1:A:186:PRO:HA	1:A:189:ASP:HB3	1.98	0.45
1:A:200:TRP:CE3	1:A:215:PRO:HB3	2.52	0.45
1:A:23:LEU:HD21	1:A:80:MET:SD	2.57	0.45
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.99	0.45
1:A:34:ARG:HD2	1:A:205:TRP:CG	2.52	0.45
1:A:78:HIS:O	1:A:79:ASN:HB2	2.17	0.45
1:A:202:LEU:HD23	1:A:209:PHE:CE2	2.52	0.44
1:A:214:HIS:C	1:A:216:PRO:CD	2.85	0.44
1:A:103:TYR:HB3	1:A:107:ARG:NH1	2.32	0.44
1:A:223:ARG:O	1:A:225:SER:N	2.51	0.44
1:A:33:GLU:OE1	1:A:34:ARG:HG3	2.17	0.44
1:A:18:LEU:HD21	1:A:155:TYR:CD2	2.53	0.44
1:A:255:MET:HB3	1:A:256:SER:H	1.51	0.44
1:A:3:ILE:O	1:A:3:ILE:HG22	2.18	0.44
1:A:170:ASP:C	1:A:172:PHE:H	2.20	0.44
1:A:9:ILE:HG22	1:A:201:PRO:CD	2.39	0.44
1:A:130:LYS:HZ1	1:A:131:MET:HG3	1.81	0.43
1:A:149:HIS:N	1:A:150:PRO:HD2	2.33	0.43
1:A:162:LEU:HD11	1:A:169:LEU:HB2	2.00	0.43
1:A:188:ILE:O	1:A:192:LEU:HD22	2.18	0.43
1:A:124:LYS:O	1:A:128:MET:HG3	2.18	0.43
1:A:202:LEU:CB	1:A:210:GLY:HA3	2.45	0.43
1:A:163:TYR:CD2	1:A:202:LEU:HD21	2.54	0.43
1:A:9:ILE:CG2	1:A:201:PRO:HD2	2.40	0.42
1:A:22:TYR:HA	1:A:187:GLN:NE2	2.34	0.42
1:A:136:LEU:HD13	1:A:174:LYS:O	2.20	0.42
1:A:200:TRP:CZ3	1:A:202:LEU:HD13	2.55	0.42
1:A:160:VAL:O	1:A:163:TYR:HB2	2.20	0.42
1:A:191:TYR:CD2	1:A:192:LEU:HD13	2.54	0.42
1:A:227:ARG:O	1:A:228:ALA:O	2.38	0.42
1:A:190:LYS:HD3	1:A:190:LYS:HA	1.74	0.42
1:A:223:ARG:CZ	1:A:226:ARG:HB2	2.50	0.41
1:A:247:VAL:O	1:A:248:THR:HG23	2.19	0.41
1:A:22:TYR:HA	1:A:187:GLN:HE21	1.85	0.41
1:A:141:TYR:CE1	1:A:181:ARG:HD2	2.55	0.41
1:A:242:TYR:O	1:A:243:SER:C	2.59	0.41
1:A:8:LYS:HD3	1:A:198:ILE:HD13	2.01	0.41
1:A:44:LYS:HD3	1:A:45:PHE:CE2	2.55	0.41
1:A:34:ARG:HE	1:A:34:ARG:HB3	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:N	1:A:150:PRO:CD	2.84	0.41
1:A:204:GLY:C	1:A:206:GLN:N	2.74	0.41
1:A:141:TYR:CD1	1:A:181:ARG:HD2	2.56	0.41
1:A:4:LEU:HD11	1:A:13:VAL:CG2	2.51	0.41
1:A:72:ARG:NH1	1:A:81:LEU:HD21	2.35	0.41
1:A:91:ILE:H	1:A:91:ILE:HG12	1.53	0.41
1:A:165:ASP:C	1:A:167:MET:H	2.24	0.40
1:A:205:TRP:HA	1:A:212:GLY:H	1.85	0.40
1:A:133:GLU:OE2	1:A:174:LYS:HB2	2.21	0.40
1:A:204:GLY:O	1:A:206:GLN:N	2.54	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	258/280 (92%)	184 (71%)	50 (19%)	24 (9%)	<b>1</b> <b>1</b>

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	LYS
1	A	218	SER
1	A	228	ALA
1	A	249	SER
1	A	253	ILE
1	A	254	GLY
1	A	41	ARG
1	A	53	ASN
1	A	67	SER
1	A	219	ASP
1	A	239	ALA

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Mol	Chain	Res	Type
1	A	252	GLY
1	A	107	ARG
1	A	224	GLY
1	A	237	PRO
1	A	240	PHE
1	A	241	THR
1	A	244	PRO
1	A	258	MET
1	A	52	PRO
1	A	66	GLN
1	A	220	LEU
1	A	223	ARG
1	A	168	CYS

### 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	224/244 (92%)	149 (66%)	75 (34%)	<b>0</b> <b>0</b>

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	8	LYS
1	A	9	ILE
1	A	10	LYS
1	A	12	LEU
1	A	13	VAL
1	A	16	THR
1	A	26	LYS
1	A	28	GLU
1	A	29	GLU
1	A	31	LEU
1	A	33	GLU
1	A	35	ASP

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Mol	Chain	Res	Type
1	A	41	ARG
1	A	43	LYS
1	A	49	LEU
1	A	53	ASN
1	A	61	ASP
1	A	63	LYS
1	A	64	LEU
1	A	67	SER
1	A	68	MET
1	A	74	ILE
1	A	77	LYS
1	A	80	MET
1	A	84	CYS
1	A	86	LYS
1	A	87	GLU
1	A	88	ARG
1	A	91	ILE
1	A	99	LEU
1	A	102	ARG
1	A	108	ILE
1	A	112	LYS
1	A	113	ASP
1	A	114	PHE
1	A	122	LEU
1	A	124	LYS
1	A	130	LYS
1	A	139	LYS
1	A	143	ASN
1	A	148	THR
1	A	154	LEU
1	A	162	LEU
1	A	164	MET
1	A	168	CYS
1	A	170	ASP
1	A	174	LYS
1	A	175	LEU
1	A	181	ARG
1	A	187	GLN
1	A	190	LYS
1	A	192	LEU
1	A	193	LYS
1	A	195	SER

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Mol	Chain	Res	Type
1	A	196	LYS
1	A	198	ILE
1	A	202	LEU
1	A	206	GLN
1	A	214	HIS
1	A	217	LYS
1	A	220	LEU
1	A	221	VAL
1	A	223	ARG
1	A	227	ARG
1	A	229	SER
1	A	233	ARG
1	A	234	MET
1	A	241	THR
1	A	245	THR
1	A	247	VAL
1	A	251	ILE
1	A	255	MET
1	A	258	MET
1	A	260	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	143	ASN
1	A	187	GLN
1	A	203	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 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

### 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.