



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:33 PM UTC

PDB ID : 1B8X / pdb_00001b8x
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

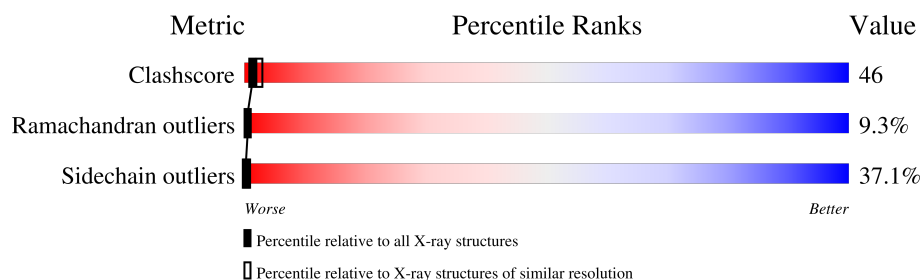
1 Overall quality at a glance

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 $\leq 5\%$.

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

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, α , β , γ	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 ²)	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	0.50	1/2139 (0.0%)	1.07	17/2889 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	SER	C-O	-8.04	1.07	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	SER	CA-C-N	-7.50	115.49	121.86
1	A	249	SER	C-N-CA	-7.50	115.49	121.86
1	A	175	LEU	N-CA-C	-7.42	104.36	113.41
1	A	94	LEU	N-CA-C	-6.98	103.11	111.69
1	A	37	GLY	N-CA-C	-6.96	106.02	114.66
1	A	39	LYS	N-CA-C	-6.72	103.65	110.97
1	A	42	ASN	N-CA-C	-6.51	104.92	112.92
1	A	144	GLY	N-CA-C	6.33	120.67	111.24
1	A	192	LEU	N-CA-C	-6.24	105.53	113.01
1	A	249	SER	N-CA-C	-6.08	97.86	110.80
1	A	114	PHE	N-CA-C	-6.05	104.77	111.36
1	A	88	ARG	N-CA-C	-5.96	105.28	112.54
1	A	130	LYS	N-CA-C	-5.87	106.25	113.41
1	A	152	PHE	N-CA-C	-5.62	106.42	113.28
1	A	177	CYS	N-CA-C	-5.52	105.18	111.14
1	A	16	THR	N-CA-C	-5.36	106.24	112.89
1	A	215	PRO	N-CA-C	5.29	117.15	110.70

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	2083	0	2073	193	0
All	All	2083	0	2073	193	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 46.

All (193) 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:HG23	1:A:241:THR:O	1.59	1.01
1:A:158:LEU:HD11	1:A:175:LEU:HD22	1.38	1.00
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:7:TRP:HB2	1:A:9:ILE:HD13	1.65	0.77
1:A:232:SER:HB3	1:A:236:TYR:HE2	1.49	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:115:GLU:H	1:A:115:GLU:CD	1.99	0.70
1:A:64:LEU:HD11	1:A:70:ILE:HG13	1.74	0.70
1:A:86:LYS:HE3	1:A:86:LYS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE3	1:A:86:LYS:N	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:150:PRO:HA	1:A:153:MET:HE3	1.80	0.62
1:A:165:ASP:OD1	1:A:167:MET:HB2	1.99	0.62
1:A:223:ARG:O	1:A:223:ARG:NE	2.32	0.61
1:A:14:GLN:O	1:A:17:ARG:HB2	2.01	0.61
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:150:PRO:CA	1:A:153:MET:HE3	2.31	0.60
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:O	1:A:135:ARG:HG3	2.02	0.59
1:A:214:HIS:C	1:A:216:PRO:HD2	2.28	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:64:LEU:HD12	1:A:65:THR:N	2.19	0.57
1:A:149:HIS:ND1	1:A:150:PRO:HD3	2.18	0.57
1:A:255:MET:HE2	1:A:256:SER:H	1.70	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:74:ILE:O	1:A:78:HIS:HD2	1.88	0.57
1:A:236:TYR:O	1:A:238:GLY:N	2.37	0.57
1:A:149:HIS:CD2	1:A:153:MET:HE2	2.40	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:MET:HE2	1:A:256:SER:N	2.22	0.55
1:A:150:PRO:HB3	1:A:153:MET:HE3	1.87	0.55
1:A:223:ARG:HE	1:A:223:ARG:C	2.15	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: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:O	1:A:198:ILE:HG22	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:223:ARG:NE	1:A:223:ARG:C	2.66	0.53
1:A:40:TRP:CZ2	1:A:44:LYS:HG3	2.44	0.52
1:A:130:LYS:HZ1	1:A:131:MET:HG3	1.75	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:223:ARG:C	1:A:225:SER:H	2.18	0.52
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:53:ASN:O	1:A:54:LEU:HD23	2.10	0.50
1:A:103:TYR:O	1:A:107:ARG:HG3	2.11	0.50
1:A:19:LEU:HG	1:A:23:LEU:CD1	2.40	0.50
1:A:220:LEU:C	1:A:221:VAL:HG22	2.36	0.50
1:A:257:ALA:O	1:A:258:MET:CB	2.56	0.50
1:A:27:TYR:CE2	1:A:29:GLU:HG2	2.47	0.50
1:A:170:ASP:C	1:A:172:PHE:H	2.20	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:16:THR:O	1:A:20:LEU:HD12	2.12	0.49
1:A:200:TRP:CD1	1:A:201:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:HIS:C	1:A:216:PRO:CD	2.85	0.49
1:A:8:LYS:HE2	1:A:31:LEU:CB	2.42	0.49
1:A:124:LYS:HE2	1:A:124:LYS:HB3	1.69	0.49
1:A:223:ARG:CZ	1:A:226:ARG:HD2	2.43	0.48
1:A:8:LYS:HE2	1:A:31:LEU:HG	1.95	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:150:PRO:CB	1:A:153:MET:HE3	2.43	0.48
1:A:52:PRO:O	1:A:53:ASN:CB	2.62	0.48
1:A:154:LEU:HD22	1:A:158:LEU:HG	1.95	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:226:ARG:HD2	2.28	0.48
1:A:114:PHE:HB3	1:A:208:THR:HG21	1.96	0.47
1:A:191:TYR:HA	1:A:194:SER:OG	2.14	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: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:204:GLY:C	1:A:206:GLN:N	2.74	0.46
1:A:223:ARG:NH1	1:A:226:ARG:HD3	2.31	0.45
1:A:242:TYR:O	1:A:243:SER:C	2.59	0.45
1:A:165:ASP:C	1:A:167:MET:H	2.24	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:34:ARG:HD2	1:A:205:TRP:CG	2.52	0.45
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.99	0.45
1:A:202:LEU:HD23	1:A:209:PHE:CE2	2.52	0.44
1:A:33:GLU:OE1	1:A:34:ARG:HG3	2.17	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:3:ILE:O	1:A:3:ILE:HG22	2.18	0.44
1:A:18:LEU:HD21	1:A:155:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:MET:HB3	1:A:256:SER:H	1.51	0.44
1:A:85:PRO:HD2	1:A:86:LYS:HZ2	1.81	0.44
1:A:78:HIS:O	1:A:79:ASN:HB2	2.17	0.44
1:A:9:ILE:HG22	1:A:201:PRO:CD	2.39	0.44
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:204:GLY:C	1:A:206:GLN:H	2.25	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:170:ASP:C	1:A:172:PHE:N	2.77	0.42
1:A:34:ARG:O	1:A:35:ASP:C	2.63	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:HA	1:A:190:LYS:HD3	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:19:LEU:HD11	1:A:80:MET:HE1	2.02	0.41
1:A:95:GLU:HB2	1:A:153:MET:HE1	2.02	0.41
1:A:8:LYS:HD3	1:A:198:ILE:HD13	2.01	0.41
1:A:141:TYR:CE1	1:A:181:ARG:HD2	2.55	0.41
1:A:44:LYS:HD3	1:A:45:PHE:CE2	2.55	0.41
1:A:223:ARG:C	1:A:225:SER:N	2.77	0.41
1:A:235:HIS:C	1:A:237:PRO:HD3	2.45	0.41
1:A:34:ARG:HE	1:A:34:ARG:HB3	1.63	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:HG12	1:A:91:ILE:H	1.53	0.41
1:A:141:TYR:CD1	1:A:181:ARG:HD2	2.56	0.41
1:A:148:THR:C	1:A:150:PRO:HD2	2.46	0.41
1:A:149:HIS:N	1:A:150:PRO:CD	2.84	0.41
1:A:223:ARG:CD	1:A:223:ARG:C	2.92	0.41
1:A:149:HIS:C	1:A:151:ASP:H	2.29	0.40
1:A:205:TRP:HA	1:A:212:GLY:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:O	1:A:44:LYS:C	2.64	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%)	0 0

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
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

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Mol	Chain	Res	Type
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%)	141 (63%)	83 (37%)	0 0

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	3	ILE
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
1	A	36	GLU
1	A	41	ARG
1	A	43	LYS
1	A	49	LEU
1	A	53	ASN
1	A	61	ASP

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Mol	Chain	Res	Type
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	98	VAL
1	A	99	LEU
1	A	102	ARG
1	A	105	VAL
1	A	108	ILE
1	A	112	LYS
1	A	113	ASP
1	A	115	GLU
1	A	119	VAL
1	A	122	LEU
1	A	124	LYS
1	A	130	LYS
1	A	131	MET
1	A	138	HIS
1	A	139	LYS
1	A	143	ASN
1	A	147	VAL
1	A	148	THR
1	A	154	LEU
1	A	162	LEU
1	A	164	MET
1	A	168	CYS
1	A	175	LEU
1	A	176	VAL
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	208	THR
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	78	HIS
1	A	143	ASN
1	A	187	GLN
1	A	203	GLN
1	A	214	HIS

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 [i](#)

There are no oligosaccharides 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.