



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:41 PM UTC

PDB ID : 1BHJ / pdb_00001bhj
Title : CRYSTAL STRUCTURE OF APO-GLYCINE N-METHYLTRANSFERASE (GNMT)
Authors : Pattanayek, R.; Newcomer, M.E.; Wagner, C.
Deposited on : 1998-06-09
Resolution : 2.50 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

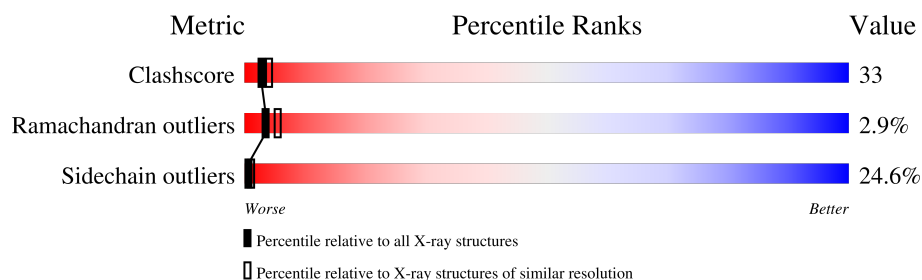
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	292	43% 39% 17%
1	B	292	41% 43% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4675 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 GLYCINE N-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2285	1450	399	425	11			
1	B	292	Total	C	N	O	S	0	0	0
			2285	1450	399	425	11			

- Molecule 2 is water.

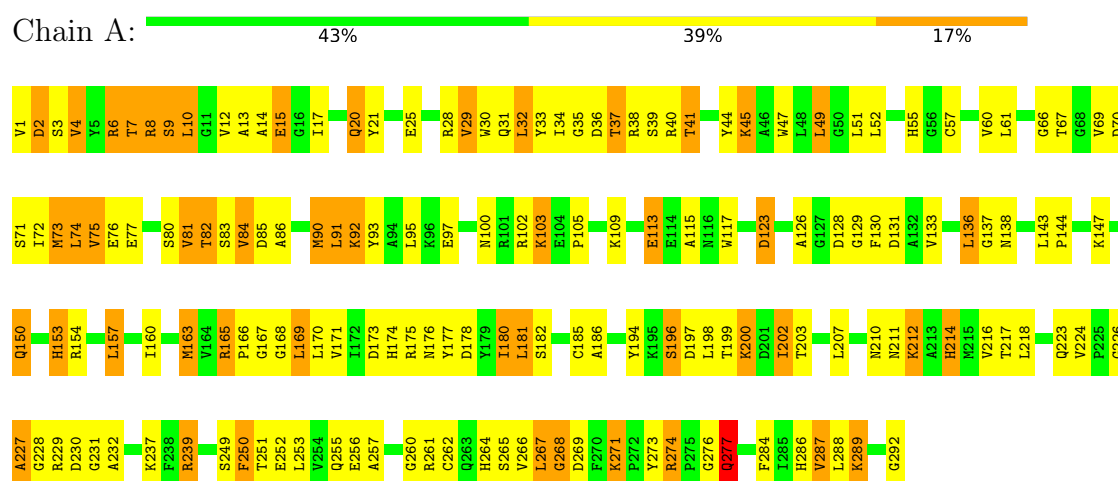
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	50	Total	O	0	0
			50	50		

3 Residue-property plots

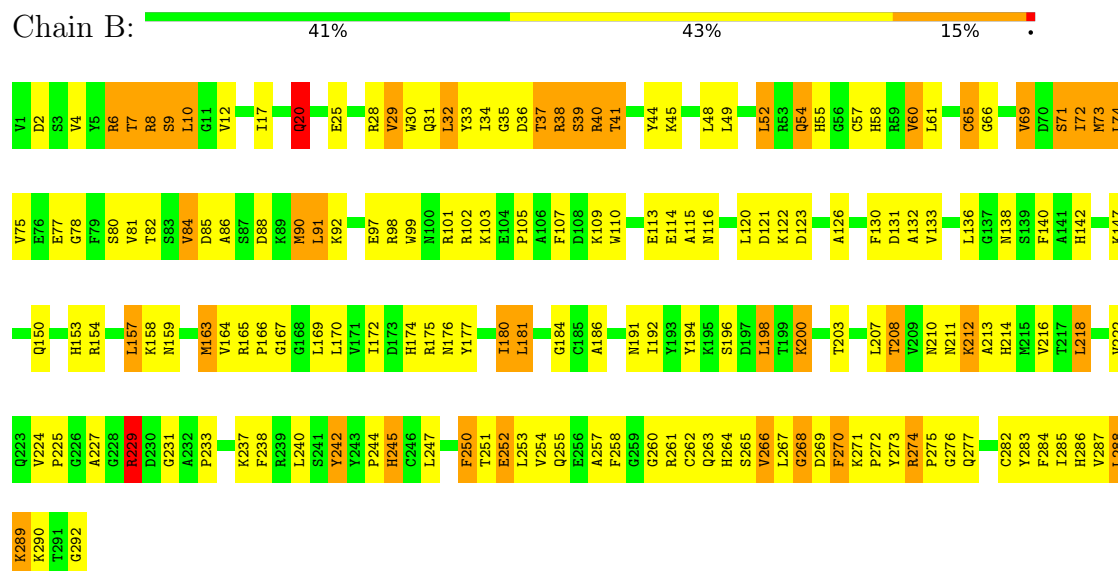
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

• Molecule 1: GLYCINE N-METHYLTRANSFERASE



• Molecule 1: GLYCINE N-METHYLTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 174.21Å 44.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	78.7 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4675	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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	0.50	0/2341	1.02	13/3174 (0.4%)
1	B	0.50	0/2341	1.03	12/3174 (0.4%)
All	All	0.50	0/4682	1.02	25/6348 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	VAL	N-CA-C	8.37	120.62	108.58
1	A	37	THR	N-CA-C	-7.88	104.56	114.56
1	A	81	VAL	N-CA-C	7.46	120.20	108.87
1	A	269	ASP	N-CA-C	-7.12	103.45	111.07
1	B	38	ARG	N-CA-C	7.05	120.35	108.23
1	A	74	LEU	N-CA-C	-6.89	103.85	111.36
1	A	167	GLY	N-CA-C	-6.51	106.70	115.36
1	A	33	TYR	N-CA-C	-6.14	104.86	112.72
1	B	167	GLY	N-CA-C	-6.00	107.56	114.69
1	B	231	GLY	N-CA-C	-5.96	106.50	114.25
1	A	153	HIS	N-CA-C	-5.69	104.98	111.07
1	B	17	ILE	CA-C-N	5.46	125.38	119.76
1	B	17	ILE	C-N-CA	5.46	125.38	119.76
1	B	78	GLY	N-CA-C	5.45	122.85	115.32
1	A	202	ILE	N-CA-C	5.34	115.97	108.17
1	B	20	GLN	N-CA-C	5.32	122.14	110.80
1	A	39	SER	N-CA-C	-5.26	99.59	110.80
1	B	74	LEU	N-CA-C	-5.25	105.63	111.36
1	B	88	ASP	N-CA-C	-5.22	106.86	113.18
1	A	75	VAL	N-CA-C	-5.19	105.26	110.30
1	B	60	VAL	N-CA-C	5.12	116.33	108.71
1	A	178	ASP	N-CA-C	-5.08	105.87	111.71
1	B	266	VAL	N-CA-C	5.05	115.24	108.17
1	A	231	GLY	N-CA-C	-5.05	109.01	115.42
1	A	273	TYR	N-CA-C	5.01	117.57	109.40

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	2285	0	2243	145	0
1	B	2285	0	2243	155	0
2	A	55	0	0	15	0
2	B	50	0	0	3	0
All	All	4675	0	4486	296	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 33.

All (296) 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:38:ARG:HG2	1:A:69:VAL:HG11	1.31	1.09
1:B:37:THR:HG22	1:B:38:ARG:HG3	1.38	1.06
1:A:57:CYS:HB2	2:A:293:HOH:O	1.59	1.00
1:B:57:CYS:HB2	2:B:293:HOH:O	1.61	0.98
1:B:41:THR:HG22	1:B:44:TYR:H	1.27	0.97
1:B:57:CYS:HB3	1:B:131:ASP:HB3	1.48	0.95
1:A:166:PRO:HB3	1:A:292:GLY:HA2	1.48	0.94
1:A:41:THR:HG22	1:A:44:TYR:H	1.36	0.90
1:A:70:ASP:HB2	2:A:313:HOH:O	1.71	0.90
1:B:71:SER:O	1:B:75:VAL:HG23	1.75	0.87
1:B:6:ARG:NH1	1:B:10:LEU:HD13	1.89	0.87
1:A:133:VAL:HG11	2:A:319:HOH:O	1.76	0.85
1:A:38:ARG:HH12	1:A:67:THR:CB	1.89	0.85
1:B:25:GLU:HA	1:B:28:ARG:HD2	1.58	0.85
1:B:126:ALA:HB2	1:B:163:MET:HE3	1.56	0.85
1:B:166:PRO:HB3	1:B:292:GLY:HA2	1.58	0.85
1:A:66:GLY:HA2	1:A:90:MET:HG2	1.57	0.85
1:B:37:THR:CG2	1:B:69:VAL:HG11	2.06	0.83
1:B:273:TYR:HA	1:B:277:GLN:NE2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.45	0.81
1:B:10:LEU:HD12	1:B:20:GLN:HE22	1.45	0.81
1:B:35:GLY:C	1:B:37:THR:H	1.89	0.81
1:B:45:LYS:HG3	1:B:73:MET:HE1	1.63	0.81
1:A:71:SER:O	1:A:75:VAL:HG23	1.81	0.80
1:A:200:LYS:NZ	1:A:200:LYS:HB2	1.98	0.79
1:A:169:LEU:HD12	1:A:289:LYS:HG2	1.64	0.79
1:A:251:THR:O	1:A:255:GLN:HG3	1.83	0.79
1:A:136:LEU:HD11	1:A:171:VAL:HG12	1.65	0.78
1:B:72:ILE:HD11	1:B:97:GLU:HG2	1.66	0.78
1:B:37:THR:HG23	1:B:69:VAL:HG11	1.66	0.76
1:A:138:ASN:ND2	1:A:175:ARG:HG3	1.99	0.76
1:A:200:LYS:HB2	1:A:200:LYS:HZ3	1.48	0.76
1:A:224:VAL:HG23	1:A:227:ALA:HB3	1.67	0.76
1:B:84:VAL:HG11	1:B:115:ALA:HB3	1.69	0.75
1:B:224:VAL:HG23	1:B:227:ALA:HB3	1.67	0.75
1:B:84:VAL:CG1	1:B:115:ALA:HB3	2.20	0.72
1:A:174:HIS:HD2	1:A:175:ARG:O	1.72	0.72
1:B:41:THR:CG2	1:B:44:TYR:H	2.01	0.72
1:A:113:GLU:HA	1:A:113:GLU:OE1	1.89	0.72
1:B:177:TYR:HA	1:B:180:ILE:HG23	1.72	0.72
1:B:41:THR:HG22	1:B:44:TYR:N	2.05	0.71
1:B:273:TYR:HA	1:B:277:GLN:HE21	1.55	0.70
1:A:14:ALA:HB3	1:A:17:ILE:HD11	1.73	0.70
1:B:85:ASP:HB3	1:B:91:LEU:HD13	1.73	0.70
1:B:113:GLU:OE1	1:B:113:GLU:HA	1.91	0.70
1:A:37:THR:O	1:A:194:TYR:HB3	1.92	0.69
1:B:57:CYS:CB	1:B:131:ASP:HB3	2.20	0.69
1:A:150:GLN:HB3	1:A:153:HIS:CD2	2.28	0.69
1:B:150:GLN:HE21	1:B:153:HIS:HD2	1.38	0.69
1:A:264:HIS:HD2	1:A:265:SER:N	1.89	0.69
1:B:10:LEU:HD12	1:B:20:GLN:NE2	2.07	0.69
1:A:35:GLY:HA2	1:A:38:ARG:NE	2.08	0.68
1:B:126:ALA:HB2	1:B:163:MET:CE	2.24	0.68
1:A:105:PRO:O	1:A:109:LYS:HG2	1.93	0.68
1:A:126:ALA:HB2	1:A:163:MET:HE3	1.76	0.68
1:B:57:CYS:HB3	1:B:131:ASP:CB	2.24	0.68
1:A:264:HIS:CD2	1:A:265:SER:N	2.62	0.67
1:A:6:ARG:HD2	1:A:8:ARG:O	1.95	0.67
1:B:7:THR:HG22	1:B:8:ARG:N	2.11	0.66
1:A:38:ARG:NH1	1:A:67:THR:OG1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:HD2	1:A:265:SER:H	1.43	0.66
1:B:150:GLN:HE21	1:B:153:HIS:CD2	2.13	0.66
1:B:35:GLY:C	1:B:37:THR:N	2.52	0.66
1:B:72:ILE:CD1	1:B:97:GLU:HG2	2.25	0.66
1:A:117:TRP:CD1	1:A:160:ILE:HD11	2.32	0.65
1:B:105:PRO:O	1:B:109:LYS:HG2	1.97	0.65
1:A:29:VAL:HA	1:A:32:LEU:HD23	1.79	0.64
1:A:113:GLU:HG3	2:A:315:HOH:O	1.97	0.64
1:B:177:TYR:O	1:B:181:LEU:HB2	1.96	0.64
1:B:6:ARG:NH1	1:B:6:ARG:HG2	2.13	0.64
1:A:72:ILE:O	1:A:76:GLU:HG3	1.97	0.63
1:B:170:LEU:HB3	1:B:288:LEU:HB2	1.79	0.63
1:A:8:ARG:HH11	1:A:13:ALA:HA	1.63	0.63
1:A:226:GLY:C	1:A:228:GLY:H	2.05	0.63
1:A:91:LEU:HD21	1:A:113:GLU:O	1.99	0.63
1:A:150:GLN:HE21	1:A:153:HIS:HD2	1.47	0.62
1:B:54:GLN:HG2	1:B:55:HIS:CE1	2.34	0.62
1:B:29:VAL:HA	1:B:32:LEU:HD23	1.80	0.62
1:B:174:HIS:HD2	1:B:175:ARG:O	1.83	0.62
1:A:36:ASP:HB2	1:A:198:LEU:HD22	1.81	0.62
1:B:174:HIS:ND1	1:B:250:PHE:HD2	1.98	0.60
1:A:264:HIS:CE1	1:A:286:HIS:HD1	2.19	0.60
1:A:38:ARG:CG	1:A:69:VAL:HG11	2.20	0.60
1:B:45:LYS:CG	1:B:73:MET:HE1	2.31	0.60
1:A:25:GLU:HA	1:A:28:ARG:HD2	1.83	0.59
1:B:6:ARG:HD2	1:B:8:ARG:O	2.01	0.59
1:B:158:LYS:HE2	1:B:159:ASN:ND2	2.18	0.58
1:A:287:VAL:HG22	1:A:287:VAL:O	2.03	0.58
1:A:165:ARG:O	1:A:168:GLY:N	2.36	0.58
1:A:84:VAL:HG11	1:A:115:ALA:HB3	1.85	0.58
1:A:117:TRP:CG	1:A:160:ILE:HD11	2.37	0.58
1:A:45:LYS:HE3	2:A:310:HOH:O	2.02	0.58
1:A:73:MET:O	1:A:77:GLU:HG2	2.04	0.58
1:B:225:PRO:HA	1:B:233:PRO:HB3	1.84	0.58
1:A:35:GLY:HA2	1:A:38:ARG:CZ	2.34	0.57
1:A:84:VAL:CG1	1:A:115:ALA:HB3	2.34	0.57
1:B:101:ARG:O	1:B:107:PHE:HB2	2.05	0.57
1:B:65:CYS:HB3	1:B:85:ASP:HB2	1.87	0.57
1:B:200:LYS:CG	1:B:222:VAL:HG22	2.35	0.56
1:B:264:HIS:CD2	1:B:265:SER:N	2.73	0.56
1:A:85:ASP:OD1	1:A:86:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HD13	1:B:186:ALA:HB2	1.87	0.56
1:A:2:ASP:O	1:A:3:SER:HB2	2.06	0.56
1:B:247:LEU:HD22	1:B:284:PHE:CZ	2.40	0.56
1:A:268:GLY:N	1:A:271:LYS:O	2.36	0.56
1:B:30:TRP:O	1:B:34:ILE:HG23	2.06	0.56
1:A:61:LEU:HD12	1:A:82:THR:O	2.06	0.55
1:A:66:GLY:CA	1:A:90:MET:HG2	2.31	0.55
1:A:177:TYR:O	1:A:181:LEU:HB2	2.07	0.55
1:A:57:CYS:HB3	1:A:131:ASP:HB2	1.88	0.55
1:A:37:THR:HA	1:A:196:SER:HA	1.90	0.54
1:A:47:TRP:HZ2	2:A:337:HOH:O	1.90	0.54
1:A:174:HIS:ND1	1:A:250:PHE:HD2	2.06	0.54
1:A:174:HIS:CD2	1:A:175:ARG:O	2.59	0.54
1:A:176:ASN:ND2	1:A:284:PHE:HE2	2.05	0.54
1:A:262:CYS:SG	2:A:294:HOH:O	2.45	0.54
1:B:32:LEU:HD21	1:B:224:VAL:HG12	1.90	0.54
1:B:210:ASN:HB2	1:B:212:LYS:NZ	2.22	0.54
1:A:45:LYS:CG	1:A:73:MET:HE1	2.37	0.54
1:B:274:ARG:O	1:B:277:GLN:HB2	2.08	0.54
1:A:38:ARG:H	1:A:38:ARG:HD3	1.73	0.54
1:B:66:GLY:HA2	1:B:90:MET:HG2	1.89	0.54
1:A:15:GLU:HG2	1:B:142:HIS:CE1	2.43	0.53
1:B:252:GLU:HG3	1:B:253:LEU:N	2.23	0.53
1:A:32:LEU:O	1:A:36:ASP:HB2	2.07	0.53
1:B:37:THR:CG2	1:B:38:ARG:HG3	2.27	0.53
1:B:224:VAL:HG23	1:B:224:VAL:O	2.09	0.53
1:A:36:ASP:CB	1:A:198:LEU:HD22	2.38	0.53
1:A:267:LEU:HD11	2:A:337:HOH:O	2.09	0.53
1:B:41:THR:HG22	1:B:44:TYR:CB	2.38	0.53
1:B:48:LEU:HG	1:B:52:LEU:HD22	1.90	0.53
1:B:255:GLN:HE21	1:B:264:HIS:CB	2.22	0.53
1:B:264:HIS:CE1	1:B:286:HIS:ND1	2.77	0.52
1:B:126:ALA:CB	1:B:163:MET:HE3	2.34	0.52
1:B:275:PRO:C	1:B:277:GLN:H	2.16	0.52
1:B:58:HIS:HB3	2:B:339:HOH:O	2.09	0.52
1:A:38:ARG:HH12	1:A:67:THR:CG2	2.22	0.52
1:A:84:VAL:HG13	1:A:85:ASP:N	2.24	0.52
1:A:226:GLY:O	1:A:228:GLY:N	2.42	0.52
1:A:14:ALA:HB3	1:A:17:ILE:CD1	2.40	0.52
1:A:84:VAL:CG1	1:A:85:ASP:N	2.73	0.52
1:A:25:GLU:HG3	2:A:316:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HE21	1:A:153:HIS:CD2	2.27	0.51
1:B:274:ARG:CZ	1:B:274:ARG:HB3	2.39	0.51
1:B:57:CYS:CB	2:B:293:HOH:O	2.36	0.51
1:B:61:LEU:CD2	1:B:163:MET:HG2	2.41	0.51
1:B:140:PHE:CE1	1:B:157:LEU:HD13	2.45	0.51
1:A:274:ARG:HH12	1:A:277:GLN:HE21	1.59	0.51
1:B:40:ARG:NH1	1:B:194:TYR:OH	2.43	0.51
1:B:267:LEU:HD12	1:B:285:ILE:HB	1.91	0.51
1:A:28:ARG:HB2	2:A:316:HOH:O	2.10	0.51
1:B:85:ASP:OD1	1:B:86:ALA:N	2.43	0.51
1:B:150:GLN:O	1:B:154:ARG:HG3	2.10	0.51
1:B:176:ASN:C	1:B:176:ASN:HD22	2.18	0.51
1:A:217:THR:HG21	1:A:239:ARG:HE	1.75	0.51
1:B:6:ARG:CZ	1:B:10:LEU:HD13	2.41	0.51
1:B:37:THR:CG2	1:B:69:VAL:CG1	2.86	0.51
1:A:97:GLU:O	1:A:100:ASN:HB2	2.11	0.51
1:B:255:GLN:HE21	1:B:264:HIS:HB2	1.76	0.51
1:A:210:ASN:O	1:A:212:LYS:HG3	2.12	0.50
1:B:37:THR:HG22	1:B:38:ARG:N	2.27	0.50
1:A:45:LYS:HG2	1:A:73:MET:HE1	1.92	0.50
1:A:163:MET:HB3	2:A:319:HOH:O	2.11	0.50
1:A:199:THR:HG21	1:A:223:GLN:OE1	2.11	0.50
1:B:208:THR:HG23	1:B:213:ALA:HA	1.93	0.50
1:A:131:ASP:HA	1:A:165:ARG:HE	1.76	0.50
1:A:173:ASP:C	1:A:173:ASP:OD1	2.55	0.50
1:B:274:ARG:NH1	1:B:277:GLN:HG3	2.26	0.50
1:A:197:ASP:HB3	2:A:341:HOH:O	2.11	0.49
1:B:54:GLN:O	1:B:54:GLN:HG3	2.12	0.49
1:B:260:GLY:O	1:B:262:CYS:N	2.46	0.49
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.54	0.49
1:B:263:GLN:HB3	1:B:289:LYS:HB3	1.94	0.49
1:A:41:THR:HG22	1:A:44:TYR:N	2.17	0.49
1:A:30:TRP:O	1:A:34:ILE:HG12	2.12	0.48
1:B:60:VAL:HA	1:B:132:ALA:O	2.13	0.48
1:A:226:GLY:C	1:A:228:GLY:N	2.71	0.48
1:B:98:ARG:O	1:B:99:TRP:C	2.56	0.48
1:A:91:LEU:O	1:A:92:LYS:C	2.57	0.48
1:A:57:CYS:HB3	1:A:131:ASP:CB	2.43	0.48
1:B:242:TYR:N	1:B:242:TYR:CD1	2.82	0.48
1:A:115:ALA:HA	1:A:123:ASP:OD2	2.14	0.47
1:B:266:VAL:HG13	1:B:266:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HB3	1:A:257:ALA:HB2	1.95	0.47
1:A:138:ASN:OD1	1:A:174:HIS:HA	2.14	0.47
1:A:133:VAL:O	1:A:170:LEU:HD12	2.15	0.47
1:B:41:THR:HG21	1:B:192:ILE:O	2.14	0.47
1:B:28:ARG:O	1:B:31:GLN:HB2	2.15	0.47
1:B:170:LEU:CD2	1:B:258:PHE:HZ	2.27	0.47
1:B:254:VAL:O	1:B:257:ALA:HB3	2.15	0.47
1:A:180:ILE:HD13	1:A:186:ALA:HB2	1.96	0.47
1:B:7:THR:HG22	1:B:8:ARG:HB2	1.97	0.47
1:B:218:LEU:HD22	1:B:242:TYR:CE1	2.50	0.47
1:A:8:ARG:NH1	1:A:13:ALA:HA	2.30	0.47
1:A:21:TYR:CE1	1:B:10:LEU:HD23	2.49	0.46
1:B:138:ASN:ND2	1:B:175:ARG:HG3	2.31	0.46
1:A:239:ARG:H	1:B:9:SER:HB2	1.79	0.46
1:B:267:LEU:O	1:B:268:GLY:O	2.33	0.46
1:A:126:ALA:HB1	1:A:129:GLY:HA2	1.96	0.46
1:B:32:LEU:HD11	1:B:198:LEU:HD21	1.96	0.46
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.83	0.46
1:A:61:LEU:HB2	1:A:130:PHE:CD2	2.51	0.46
1:A:136:LEU:HD11	1:A:171:VAL:CG1	2.40	0.46
1:A:180:ILE:HD11	1:A:216:VAL:HG11	1.96	0.46
1:B:169:LEU:HD12	1:B:289:LYS:HG2	1.96	0.46
1:A:73:MET:HE3	1:A:73:MET:HB2	1.74	0.46
1:A:224:VAL:HG23	1:A:224:VAL:O	2.16	0.46
1:B:61:LEU:HB3	1:B:133:VAL:HG22	1.98	0.45
1:B:177:TYR:HD1	1:B:180:ILE:HG12	1.81	0.45
1:A:287:VAL:HG11	2:A:337:HOH:O	2.15	0.45
1:A:38:ARG:HH12	1:A:67:THR:HG21	1.80	0.45
1:A:57:CYS:SG	1:A:131:ASP:HB3	2.57	0.45
1:B:77:GLU:OE1	1:B:77:GLU:HA	2.15	0.45
1:B:191:ASN:HA	1:B:283:TYR:CE1	2.51	0.45
1:B:210:ASN:HB2	1:B:212:LYS:HZ1	1.82	0.45
1:B:268:GLY:N	1:B:271:LYS:O	2.40	0.45
1:B:84:VAL:HG13	1:B:115:ALA:HB3	1.97	0.45
1:A:13:ALA:HB1	2:A:295:HOH:O	2.17	0.45
1:B:120:LEU:HA	1:B:123:ASP:HB2	1.98	0.45
1:B:212:LYS:HB2	1:B:212:LYS:HE2	1.43	0.45
1:A:82:THR:CG2	1:A:130:PHE:HE2	2.30	0.45
1:B:40:ARG:HB2	1:B:194:TYR:CE1	2.52	0.45
1:A:9:SER:O	1:A:20:GLN:NE2	2.50	0.45
1:A:32:LEU:HD12	1:A:198:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:CD1	1:A:97:GLU:HG2	2.47	0.44
1:A:7:THR:HG22	1:A:8:ARG:N	2.32	0.44
1:A:3:SER:O	1:A:4:VAL:HG13	2.18	0.44
1:A:276:GLY:O	1:A:277:GLN:C	2.60	0.44
1:A:30:TRP:CD1	1:B:12:VAL:HB	2.52	0.44
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.77	0.44
1:A:266:VAL:O	1:A:266:VAL:HG13	2.17	0.44
1:B:164:VAL:O	1:B:290:LYS:HD2	2.17	0.44
1:B:170:LEU:HD23	1:B:258:PHE:CZ	2.53	0.44
1:A:143:LEU:HD12	1:A:144:PRO:HD2	2.00	0.43
1:A:180:ILE:HB	1:A:185:CYS:O	2.18	0.43
1:A:253:LEU:O	1:A:256:GLU:HG2	2.17	0.43
1:B:177:TYR:HB2	1:B:245:HIS:O	2.18	0.43
1:B:174:HIS:CD2	1:B:175:ARG:O	2.68	0.43
1:A:136:LEU:N	1:A:136:LEU:HD13	2.33	0.43
1:A:260:GLY:O	1:A:262:CYS:N	2.51	0.43
1:B:6:ARG:HH12	1:B:10:LEU:HD13	1.78	0.43
1:B:174:HIS:ND1	1:B:250:PHE:CD2	2.84	0.43
1:A:230:ASP:C	1:A:232:ALA:H	2.26	0.43
1:B:247:LEU:HD11	1:B:266:VAL:HG21	2.00	0.43
1:B:6:ARG:NH1	1:B:6:ARG:CG	2.80	0.43
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.84	0.43
1:A:60:VAL:HG12	1:A:61:LEU:N	2.33	0.43
1:B:8:ARG:HD2	1:B:12:VAL:HG23	2.00	0.43
1:B:72:ILE:HG13	1:B:110:TRP:CH2	2.54	0.43
1:B:172:ILE:O	1:B:172:ILE:HG23	2.19	0.43
1:B:33:TYR:C	1:B:35:GLY:H	2.25	0.43
1:A:55:HIS:ND1	1:A:55:HIS:N	2.67	0.43
1:A:91:LEU:C	1:A:93:TYR:N	2.76	0.43
1:A:214:HIS:CD2	2:A:321:HOH:O	2.72	0.43
1:A:29:VAL:HA	1:A:32:LEU:CD2	2.47	0.42
1:A:45:LYS:HZ3	1:A:45:LYS:HG3	1.69	0.42
1:B:73:MET:HE3	1:B:73:MET:HB2	1.73	0.42
1:B:116:ASN:O	1:B:120:LEU:N	2.52	0.42
1:A:153:HIS:O	1:A:157:LEU:HD22	2.19	0.42
1:B:40:ARG:HG2	1:B:41:THR:N	2.33	0.42
1:B:216:VAL:HG23	1:B:244:PRO:HD3	2.01	0.42
1:A:157:LEU:HB3	1:A:257:ALA:CB	2.49	0.42
1:B:130:PHE:O	1:B:165:ARG:HB3	2.19	0.42
1:B:275:PRO:C	1:B:277:GLN:N	2.77	0.42
1:B:114:GLU:O	1:B:115:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:O	1:B:184:GLY:N	2.50	0.42
1:B:238:PHE:HE2	1:B:240:LEU:HD11	1.84	0.42
1:B:276:GLY:O	1:B:277:GLN:C	2.62	0.42
1:B:91:LEU:HD12	1:B:91:LEU:HA	1.90	0.42
1:B:200:LYS:HG2	1:B:222:VAL:HG22	2.01	0.42
1:B:200:LYS:NZ	1:B:200:LYS:HB2	2.34	0.42
1:A:45:LYS:HG2	1:A:49:LEU:CD2	2.50	0.42
1:B:191:ASN:HA	1:B:283:TYR:HE1	1.84	0.42
1:A:44:TYR:O	1:A:45:LYS:C	2.63	0.41
1:B:36:ASP:OD2	1:B:196:SER:HB3	2.20	0.41
1:B:150:GLN:NE2	1:B:153:HIS:HD2	2.14	0.41
1:A:169:LEU:CD1	1:A:289:LYS:HG2	2.42	0.41
1:B:268:GLY:CA	1:B:273:TYR:HB2	2.50	0.41
1:B:271:LYS:HB3	1:B:272:PRO:HD2	2.03	0.41
1:A:60:VAL:HG11	1:A:74:LEU:CD1	2.50	0.41
1:B:52:LEU:HD12	1:B:52:LEU:HA	1.87	0.41
1:B:176:ASN:O	1:B:180:ILE:CG2	2.69	0.41
1:B:229:ARG:HA	1:B:229:ARG:HD3	1.71	0.41
1:A:137:GLY:O	1:A:138:ASN:HB3	2.20	0.41
1:B:140:PHE:CZ	1:B:157:LEU:HD13	2.55	0.41
1:B:176:ASN:O	1:B:180:ILE:HG23	2.20	0.41
1:A:202:ILE:HG21	1:A:218:LEU:HG	2.03	0.41
1:B:170:LEU:HD23	1:B:258:PHE:HZ	1.86	0.41
1:A:72:ILE:O	1:A:72:ILE:HG22	2.20	0.41
1:B:37:THR:O	1:B:194:TYR:CD1	2.73	0.41
1:A:6:ARG:NH1	1:A:10:LEU:HD13	2.35	0.40
1:A:154:ARG:HG2	1:A:256:GLU:OE2	2.20	0.40
1:B:33:TYR:C	1:B:35:GLY:N	2.77	0.40
1:B:224:VAL:CG2	1:B:227:ALA:HB3	2.45	0.40
1:A:85:ASP:HB3	1:A:91:LEU:HD13	2.03	0.40
1:B:32:LEU:CD1	1:B:198:LEU:HD21	2.52	0.40

There are no symmetry-related clashes.

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	290/292 (99%)	248 (86%)	34 (12%)	8 (3%)	4	6
1	B	290/292 (99%)	256 (88%)	25 (9%)	9 (3%)	3	5
All	All	580/584 (99%)	504 (87%)	59 (10%)	17 (3%)	3	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ARG
1	B	20	GLN
1	B	39	SER
1	A	4	VAL
1	A	20	GLN
1	A	227	ALA
1	A	277	GLN
1	B	4	VAL
1	B	229	ARG
1	B	54	GLN
1	B	268	GLY
1	B	40	ARG
1	A	40	ARG
1	A	261	ARG
1	A	268	GLY
1	B	65	CYS
1	B	270	PHE

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	242/242 (100%)	181 (75%)	61 (25%)	0	1
1	B	242/242 (100%)	184 (76%)	58 (24%)	1	1
All	All	484/484 (100%)	365 (75%)	119 (25%)	1	1

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	ASP
1	A	6	ARG
1	A	7	THR
1	A	8	ARG
1	A	9	SER
1	A	10	LEU
1	A	12	VAL
1	A	15	GLU
1	A	29	VAL
1	A	31	GLN
1	A	32	LEU
1	A	41	THR
1	A	45	LYS
1	A	49	LEU
1	A	51	LEU
1	A	52	LEU
1	A	73	MET
1	A	80	SER
1	A	81	VAL
1	A	82	THR
1	A	83	SER
1	A	84	VAL
1	A	90	MET
1	A	91	LEU
1	A	92	LYS
1	A	95	LEU
1	A	102	ARG
1	A	103	LYS
1	A	113	GLU
1	A	123	ASP
1	A	128	ASP
1	A	136	LEU
1	A	147	LYS
1	A	150	GLN
1	A	157	LEU
1	A	163	MET
1	A	165	ARG
1	A	169	LEU
1	A	180	ILE
1	A	181	LEU
1	A	182	SER

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Mol	Chain	Res	Type
1	A	196	SER
1	A	200	LYS
1	A	203	THR
1	A	207	LEU
1	A	211	ASN
1	A	212	LYS
1	A	214	HIS
1	A	237	LYS
1	A	239	ARG
1	A	249	SER
1	A	250	PHE
1	A	252	GLU
1	A	267	LEU
1	A	271	LYS
1	A	274	ARG
1	A	277	GLN
1	A	287	VAL
1	A	288	LEU
1	A	289	LYS
1	B	2	ASP
1	B	6	ARG
1	B	7	THR
1	B	8	ARG
1	B	9	SER
1	B	10	LEU
1	B	29	VAL
1	B	32	LEU
1	B	37	THR
1	B	39	SER
1	B	41	THR
1	B	49	LEU
1	B	52	LEU
1	B	69	VAL
1	B	71	SER
1	B	72	ILE
1	B	73	MET
1	B	74	LEU
1	B	80	SER
1	B	82	THR
1	B	84	VAL
1	B	90	MET
1	B	91	LEU

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Mol	Chain	Res	Type
1	B	92	LYS
1	B	102	ARG
1	B	103	LYS
1	B	121	ASP
1	B	122	LYS
1	B	136	LEU
1	B	147	LYS
1	B	157	LEU
1	B	163	MET
1	B	180	ILE
1	B	181	LEU
1	B	198	LEU
1	B	200	LYS
1	B	203	THR
1	B	207	LEU
1	B	208	THR
1	B	211	ASN
1	B	212	LYS
1	B	214	HIS
1	B	218	LEU
1	B	229	ARG
1	B	237	LYS
1	B	242	TYR
1	B	245	HIS
1	B	250	PHE
1	B	251	THR
1	B	252	GLU
1	B	261	ARG
1	B	269	ASP
1	B	270	PHE
1	B	274	ARG
1	B	282	CYS
1	B	287	VAL
1	B	288	LEU
1	B	289	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	153	HIS
1	A	159	ASN

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Mol	Chain	Res	Type
1	A	174	HIS
1	A	176	ASN
1	A	211	ASN
1	A	214	HIS
1	A	255	GLN
1	A	264	HIS
1	B	138	ASN
1	B	150	GLN
1	B	153	HIS
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN
1	B	211	ASN
1	B	255	GLN
1	B	264	HIS
1	B	277	GLN

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 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 ⓘ

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.