



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 09:41 pm GMT

PDB ID : 1D2C
Title : METHYLTRANSFERASE
Authors : Huang, Y.; Takusagawa, F.
Deposited on : 1999-09-23
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 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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

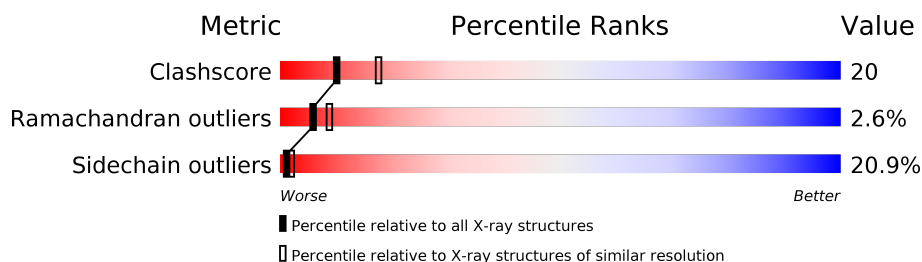
1 Overall quality at a glance

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	122078	4826 (2.50-2.50)
Ramachandran outliers	120005	4734 (2.50-2.50)
Sidechain outliers	119972	4736 (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 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	292	
1	B	292	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4886 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 (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.

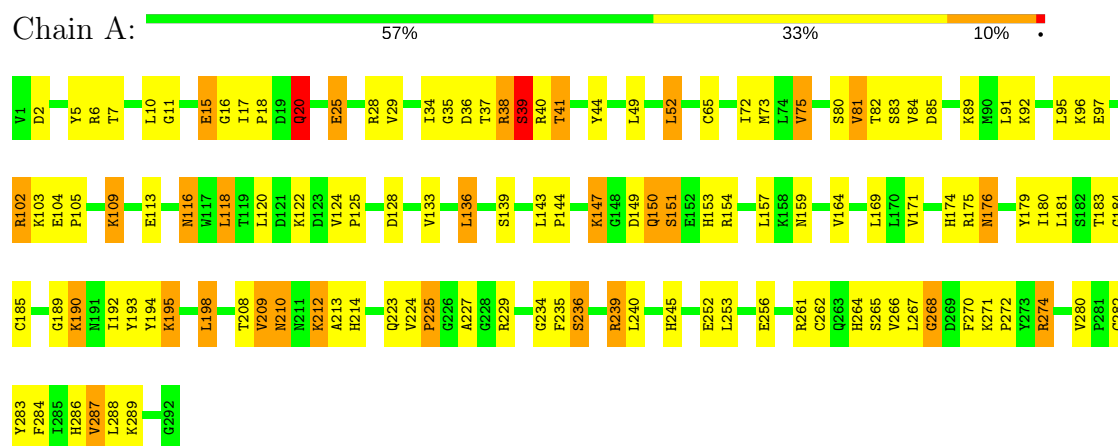
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	193	Total	O	0	0
			193	193		
2	B	123	Total	O	0	0
			123	123		

3 Residue-property plots [i](#)

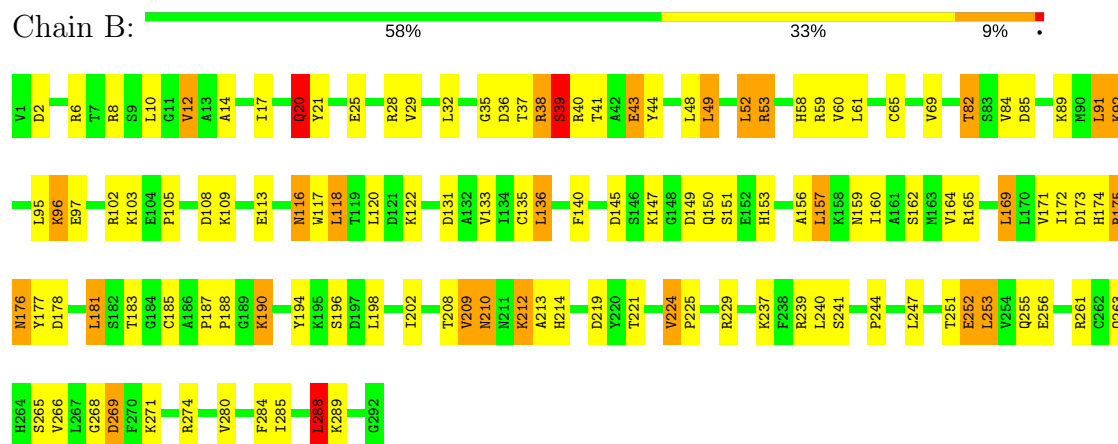
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: PROTEIN (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	86.30Å 175.90Å 45.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.2 (10.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4886	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.38	0/2341	0.64	0/3174
1	B	0.37	0/2341	0.64	1/3174 (0.0%)
All	All	0.38	0/4682	0.64	1/6348 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	LEU	CA-CB-CG	5.59	128.15	115.30

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	2285	0	2243	96	0
1	B	2285	0	2243	96	0
2	A	193	0	0	1	0
2	B	123	0	0	1	0
All	All	4886	0	4486	184	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 20.

All (184) 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:HB3	1:A:38:ARG:HH11	1.15	1.11
1:B:188:PRO:HB3	1:B:202:ILE:HG13	1.55	0.89
1:A:29:VAL:HG21	1:A:236:SER:HB2	1.56	0.87
1:B:209:VAL:HG12	1:B:210:ASN:H	1.41	0.84
1:A:38:ARG:HB3	1:A:38:ARG:NH1	1.94	0.82
1:B:38:ARG:HG2	1:B:38:ARG:HH11	1.45	0.81
1:A:29:VAL:CG2	1:A:236:SER:HB2	2.13	0.78
1:B:175:ARG:HH11	1:B:175:ARG:HG3	1.49	0.77
1:B:269:ASP:O	1:B:285:ILE:HD12	1.89	0.73
1:A:39:SER:HB2	1:A:195:LYS:HG3	1.70	0.72
1:A:40:ARG:HA	1:A:194:TYR:CD1	2.24	0.72
1:A:272:PRO:HG2	1:A:274:ARG:HH22	1.55	0.71
1:A:175:ARG:HG2	1:A:175:ARG:HH11	1.54	0.71
1:A:11:GLY:H	1:A:20:GLN:HE22	1.39	0.71
1:A:37:THR:O	1:A:37:THR:HG23	1.90	0.70
1:A:116:ASN:HD22	1:A:118:LEU:H	1.40	0.69
1:A:272:PRO:C	1:A:274:ARG:HH12	1.97	0.68
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.59	0.67
1:A:5:TYR:HD2	1:B:239:ARG:HH12	1.42	0.67
1:B:174:HIS:HD2	1:B:175:ARG:O	1.77	0.67
1:A:209:VAL:HG23	1:A:214:HIS:CB	2.25	0.67
1:B:43:GLU:OE2	1:B:43:GLU:HA	1.94	0.67
1:B:37:THR:O	1:B:37:THR:HG22	1.94	0.66
1:A:174:HIS:HD2	1:A:175:ARG:O	1.79	0.66
1:A:183:THR:HG22	1:A:185:CYS:HB2	1.76	0.66
1:A:147:LYS:HB3	1:A:149:ASP:OD1	1.96	0.66
1:A:209:VAL:HG12	1:A:210:ASN:H	1.62	0.65
1:B:159:ASN:O	1:B:162:SER:HB2	1.97	0.64
1:B:188:PRO:HB3	1:B:202:ILE:CG1	2.28	0.64
1:A:72:ILE:HD11	1:A:97:GLU:HG2	1.79	0.63
1:B:209:VAL:O	1:B:210:ASN:C	2.38	0.62
1:B:38:ARG:CG	1:B:38:ARG:HH11	2.12	0.62
1:A:65:CYS:HB3	1:A:85:ASP:HB2	1.80	0.61
1:A:212:LYS:HE3	1:A:214:HIS:HB2	1.82	0.60
1:B:136:LEU:HD11	1:B:171:VAL:HG12	1.82	0.60
1:B:247:LEU:HD22	1:B:284:PHE:CE2	2.36	0.60
1:A:25:GLU:OE2	1:A:236:SER:HB3	2.01	0.59
1:A:116:ASN:ND2	1:A:118:LEU:H	2.00	0.59
1:A:136:LEU:HD11	1:A:171:VAL:HG12	1.84	0.59
1:A:209:VAL:O	1:A:210:ASN:C	2.42	0.58
1:B:169:LEU:CD1	1:B:289:LYS:HG3	2.33	0.58
1:B:49:LEU:O	1:B:53:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HG22	1:A:44:TYR:H	1.68	0.58
1:B:40:ARG:HA	1:B:194:TYR:CD2	2.39	0.58
1:B:48:LEU:O	1:B:52:LEU:HD22	2.04	0.58
1:A:11:GLY:H	1:A:20:GLN:NE2	2.00	0.58
1:A:150:GLN:OE1	1:A:153:HIS:HD2	1.87	0.57
1:B:41:THR:HG22	1:B:44:TYR:H	1.68	0.57
1:B:209:VAL:HG12	1:B:210:ASN:N	2.17	0.57
1:A:15:GLU:O	1:B:85:ASP:OD2	2.21	0.56
1:B:156:ALA:O	1:B:160:ILE:HG13	2.05	0.56
1:B:187:PRO:HB2	1:B:190:LYS:HG3	1.87	0.56
1:B:209:VAL:HG23	1:B:214:HIS:CB	2.35	0.56
1:A:154:ARG:HD3	1:A:256:GLU:OE1	2.06	0.56
1:A:264:HIS:CE1	1:A:286:HIS:ND1	2.74	0.56
1:B:150:GLN:OE1	1:B:153:HIS:HD2	1.89	0.56
1:A:264:HIS:HE1	1:A:286:HIS:ND1	2.04	0.55
1:B:209:VAL:HG23	1:B:214:HIS:HB2	1.87	0.55
1:A:38:ARG:HH11	1:A:38:ARG:CB	2.04	0.55
1:B:176:ASN:HD21	1:B:178:ASP:HB2	1.71	0.55
1:B:169:LEU:HD12	1:B:289:LYS:HG3	1.88	0.55
1:B:208:THR:C	1:B:209:VAL:O	2.45	0.55
1:A:65:CYS:SG	1:A:83:SER:HB3	2.47	0.55
1:A:175:ARG:HG2	1:A:175:ARG:NH1	2.21	0.54
1:B:209:VAL:HB	1:B:212:LYS:HE3	1.88	0.54
1:A:35:GLY:O	1:A:38:ARG:CD	2.56	0.54
1:A:143:LEU:O	1:A:153:HIS:HE1	1.90	0.54
1:B:208:THR:HG22	1:B:209:VAL:O	2.08	0.54
1:B:175:ARG:CG	1:B:175:ARG:HH11	2.20	0.53
1:A:280:VAL:HG23	1:A:280:VAL:O	2.08	0.53
1:A:120:LEU:HB3	1:A:159:ASN:HB3	1.90	0.53
1:A:143:LEU:HD12	1:A:144:PRO:HD2	1.90	0.53
1:A:16:GLY:HA3	1:B:117:TRP:CH2	2.43	0.53
1:B:212:LYS:NZ	1:B:214:HIS:ND1	2.58	0.52
1:B:263:GLN:O	1:B:288:LEU:HA	2.10	0.52
1:A:209:VAL:HG23	1:A:214:HIS:HB3	1.90	0.51
1:A:192:ILE:HG13	1:A:193:TYR:N	2.26	0.51
1:B:40:ARG:HG3	1:B:44:TYR:HD2	1.74	0.51
1:A:7:THR:HG23	1:B:241:SER:HB2	1.93	0.51
1:B:176:ASN:ND2	1:B:284:PHE:HE1	2.10	0.50
1:B:40:ARG:HG3	1:B:44:TYR:CD2	2.46	0.50
1:B:221:THR:OG1	1:B:237:LYS:HE3	2.12	0.50
1:A:262:CYS:SG	1:A:288:LEU:HD12	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:HB3	1:A:91:LEU:HD13	1.94	0.50
1:A:208:THR:C	1:A:209:VAL:O	2.45	0.49
1:B:38:ARG:O	1:B:40:ARG:N	2.44	0.49
1:A:274:ARG:NH1	1:A:274:ARG:HG3	2.25	0.49
1:B:145:ASP:OD2	1:B:149:ASP:O	2.29	0.49
1:A:116:ASN:C	1:A:116:ASN:HD22	2.15	0.49
1:B:43:GLU:OE2	1:B:43:GLU:CA	2.61	0.49
1:A:40:ARG:HD2	1:A:73:MET:SD	2.53	0.49
1:B:29:VAL:O	1:B:32:LEU:HB2	2.12	0.49
1:A:39:SER:CB	1:A:195:LYS:HZ2	2.26	0.48
1:B:92:LYS:HE3	1:B:96:LYS:NZ	2.28	0.48
1:B:116:ASN:HD22	1:B:117:TRP:N	2.11	0.48
1:B:269:ASP:O	1:B:285:ILE:CD1	2.61	0.48
1:B:35:GLY:O	1:B:38:ARG:NH2	2.47	0.48
1:B:61:LEU:HD12	1:B:82:THR:O	2.14	0.47
1:A:240:LEU:HD13	1:B:12:VAL:HG21	1.95	0.47
1:B:40:ARG:HB3	1:B:40:ARG:NH1	2.29	0.47
1:B:14:ALA:HB3	1:B:17:ILE:HD11	1.95	0.47
1:A:176:ASN:ND2	1:A:284:PHE:HE1	2.12	0.47
1:A:245:HIS:HD2	2:A:331:HOH:O	1.97	0.47
1:A:75:VAL:HG23	1:A:81:VAL:HG13	1.96	0.47
1:A:183:THR:CG2	1:A:185:CYS:HB2	2.44	0.47
1:B:280:VAL:HG22	1:B:280:VAL:O	2.15	0.47
1:B:116:ASN:O	1:B:120:LEU:N	2.48	0.47
1:B:188:PRO:C	1:B:190:LYS:H	2.19	0.47
1:B:84:VAL:HA	1:B:113:GLU:O	2.15	0.46
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.46
1:A:38:ARG:NH1	1:A:38:ARG:CB	2.71	0.46
1:A:149:ASP:O	1:A:151:SER:N	2.40	0.46
1:A:190:LYS:HE3	1:A:282:CYS:SG	2.55	0.46
1:B:117:TRP:HB3	1:B:156:ALA:HB1	1.98	0.46
1:B:183:THR:HG22	1:B:185:CYS:HB2	1.98	0.46
1:B:92:LYS:HE3	1:B:96:LYS:HZ1	1.81	0.46
1:A:239:ARG:HG3	1:B:8:ARG:HA	1.97	0.45
1:A:227:ALA:HB3	1:A:234:GLY:HA3	1.99	0.45
1:B:65:CYS:HB3	1:B:85:ASP:HB2	1.99	0.45
1:A:209:VAL:HB	1:A:212:LYS:HE2	1.98	0.45
1:B:252:GLU:HG3	1:B:253:LEU:N	2.29	0.45
1:A:11:GLY:O	1:B:89:LYS:NZ	2.49	0.45
1:A:96:LYS:HE3	2:B:317:HOH:O	2.16	0.45
1:B:256:GLU:O	1:B:256:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HG12	1:A:283:TYR:CD1	2.52	0.44
1:A:287:VAL:C	1:A:288:LEU:HD22	2.38	0.44
1:B:116:ASN:HD22	1:B:118:LEU:H	1.65	0.44
1:B:38:ARG:NH1	1:B:38:ARG:CG	2.75	0.44
1:B:175:ARG:CG	1:B:175:ARG:NH1	2.79	0.44
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.88	0.44
1:B:133:VAL:CG2	1:B:164:VAL:HG22	2.47	0.44
1:A:102:ARG:NH1	1:B:108:ASP:OD1	2.51	0.44
1:A:38:ARG:O	1:A:40:ARG:N	2.51	0.44
1:A:272:PRO:HG2	1:A:274:ARG:NH2	2.27	0.43
1:B:212:LYS:O	1:B:213:ALA:C	2.57	0.43
1:B:177:TYR:O	1:B:181:LEU:HB2	2.18	0.43
1:A:133:VAL:HG21	1:A:164:VAL:HG22	2.00	0.43
1:A:272:PRO:O	1:A:274:ARG:NH1	2.49	0.43
1:A:84:VAL:HG12	1:A:113:GLU:HB3	2.01	0.43
1:A:223:GLN:HB2	1:A:235:PHE:CE2	2.54	0.43
1:B:280:VAL:CG2	1:B:280:VAL:O	2.66	0.43
1:B:38:ARG:HG2	1:B:39:SER:N	2.33	0.43
1:A:39:SER:HB2	1:A:195:LYS:CG	2.43	0.43
1:A:52:LEU:HD12	1:A:52:LEU:HA	1.85	0.43
1:A:223:GLN:O	1:A:225:PRO:HD3	2.19	0.43
1:B:105:PRO:O	1:B:109:LYS:HG2	2.18	0.43
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.85	0.43
1:B:176:ASN:ND2	1:B:178:ASP:HB2	2.33	0.43
1:B:181:LEU:HD21	1:B:244:PRO:HB2	2.01	0.42
1:A:36:ASP:CB	1:A:198:LEU:HD22	2.49	0.42
1:A:267:LEU:O	1:A:268:GLY:O	2.37	0.42
1:B:187:PRO:HB2	1:B:190:LYS:CD	2.49	0.42
1:B:36:ASP:CG	1:B:198:LEU:HB2	2.40	0.42
1:A:17:ILE:HA	1:A:18:PRO:HD3	1.94	0.42
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.93	0.42
1:A:34:ILE:O	1:A:37:THR:HG22	2.20	0.42
1:A:280:VAL:CG2	1:A:280:VAL:O	2.67	0.42
1:A:72:ILE:CD1	1:A:97:GLU:HG2	2.47	0.42
1:A:198:LEU:HA	1:A:198:LEU:HD12	1.87	0.42
1:B:187:PRO:HB2	1:B:190:LYS:CG	2.50	0.42
1:A:25:GLU:O	1:A:29:VAL:HG23	2.20	0.42
1:B:251:THR:O	1:B:255:GLN:HG3	2.20	0.42
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.91	0.41
1:B:224:VAL:HG22	1:B:224:VAL:O	2.18	0.41
1:A:192:ILE:HD12	1:A:270:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD12	1:B:91:LEU:HA	1.76	0.41
1:B:117:TRP:CH2	1:B:140:PHE:HA	2.55	0.41
1:B:149:ASP:OD2	1:B:149:ASP:N	2.54	0.41
1:B:173:ASP:C	1:B:173:ASP:OD2	2.59	0.41
1:B:188:PRO:HB3	1:B:202:ILE:CD1	2.50	0.41
1:B:288:LEU:CD2	1:B:288:LEU:N	2.84	0.41
1:A:180:ILE:O	1:A:184:GLY:N	2.49	0.41
1:A:29:VAL:HG21	1:A:236:SER:CB	2.40	0.41
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.93	0.41
1:B:20:GLN:HB3	1:B:21:TYR:CD1	2.56	0.41
1:A:40:ARG:NE	1:A:73:MET:SD	2.94	0.41
1:A:29:VAL:HG22	1:A:236:SER:HB2	1.98	0.41
1:A:105:PRO:O	1:A:109:LYS:HD2	2.21	0.40
1:A:212:LYS:O	1:A:213:ALA:C	2.57	0.40
1:B:135:CYS:HB3	1:B:172:ILE:HG13	2.03	0.40
1:B:219:ASP:HB3	1:B:237:LYS:HE2	2.03	0.40
1:A:104:GLU:HA	1:A:105:PRO:HD2	1.90	0.40
1:A:179:TYR:CD1	1:A:179:TYR:C	2.94	0.40
1:B:58:HIS:N	1:B:131:ASP:OD1	2.53	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	290/292 (99%)	262 (90%)	19 (7%)	9 (3%)	4	6
1	B	290/292 (99%)	261 (90%)	23 (8%)	6 (2%)	8	12
All	All	580/584 (99%)	523 (90%)	42 (7%)	15 (3%)	6	9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	B	39	SER
1	A	209	VAL
1	B	209	VAL
1	B	268	GLY
1	A	39	SER
1	A	150	GLN
1	A	210	ASN
1	A	268	GLY
1	B	20	GLN
1	A	15	GLU
1	B	210	ASN
1	B	225	PRO
1	A	189	GLY
1	A	225	PRO

5.3.2 Protein sidechains [i](#)

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%)	192 (79%)	50 (21%)	1	2
1	B	242/242 (100%)	191 (79%)	51 (21%)	1	2
All	All	484/484 (100%)	383 (79%)	101 (21%)	1	2

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	6	ARG
1	A	10	LEU
1	A	20	GLN
1	A	25	GLU
1	A	28	ARG
1	A	38	ARG
1	A	39	SER
1	A	41	THR

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	52	LEU
1	A	75	VAL
1	A	80	SER
1	A	81	VAL
1	A	82	THR
1	A	89	LYS
1	A	92	LYS
1	A	95	LEU
1	A	102	ARG
1	A	103	LYS
1	A	109	LYS
1	A	116	ASN
1	A	118	LEU
1	A	122	LYS
1	A	128	ASP
1	A	136	LEU
1	A	139	SER
1	A	147	LYS
1	A	151	SER
1	A	157	LEU
1	A	169	LEU
1	A	176	ASN
1	A	181	LEU
1	A	190	LYS
1	A	195	LYS
1	A	198	LEU
1	A	212	LYS
1	A	224	VAL
1	A	229	ARG
1	A	236	SER
1	A	239	ARG
1	A	252	GLU
1	A	253	LEU
1	A	261	ARG
1	A	265	SER
1	A	266	VAL
1	A	271	LYS
1	A	274	ARG
1	A	287	VAL
1	A	289	LYS
1	B	2	ASP

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Mol	Chain	Res	Type
1	B	6	ARG
1	B	10	LEU
1	B	12	VAL
1	B	20	GLN
1	B	25	GLU
1	B	28	ARG
1	B	38	ARG
1	B	39	SER
1	B	43	GLU
1	B	49	LEU
1	B	52	LEU
1	B	53	ARG
1	B	59	ARG
1	B	60	VAL
1	B	69	VAL
1	B	82	THR
1	B	91	LEU
1	B	92	LYS
1	B	95	LEU
1	B	96	LYS
1	B	97	GLU
1	B	102	ARG
1	B	103	LYS
1	B	116	ASN
1	B	118	LEU
1	B	122	LYS
1	B	136	LEU
1	B	147	LYS
1	B	151	SER
1	B	157	LEU
1	B	165	ARG
1	B	169	LEU
1	B	175	ARG
1	B	176	ASN
1	B	181	LEU
1	B	190	LYS
1	B	196	SER
1	B	212	LYS
1	B	224	VAL
1	B	229	ARG
1	B	240	LEU
1	B	252	GLU

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Mol	Chain	Res	Type
1	B	253	LEU
1	B	261	ARG
1	B	265	SER
1	B	266	VAL
1	B	269	ASP
1	B	271	LYS
1	B	274	ARG
1	B	288	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	116	ASN
1	A	153	HIS
1	A	159	ASN
1	A	174	HIS
1	A	176	ASN
1	A	211	ASN
1	A	245	HIS
1	A	255	GLN
1	A	264	HIS
1	B	100	ASN
1	B	116	ASN
1	B	153	HIS
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN

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.