



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:26 am BST

PDB ID : 1R74  
Title : Crystal Structure of Human Glycine N-Methyltransferase  
Authors : Pakhomova, S.; Luka, Z.; Wagner, C.; Newcomer, M.E.  
Deposited on : 2003-10-17  
Resolution : 2.55 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

<https://www.wwpdb.org/validation/2017/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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

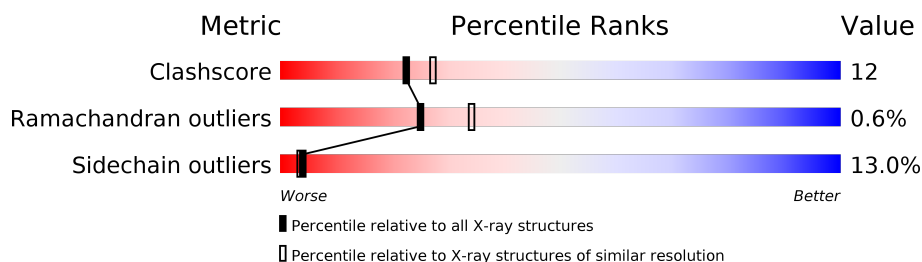
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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 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	294	
1	B	294	

## 2 Entry composition [i](#)

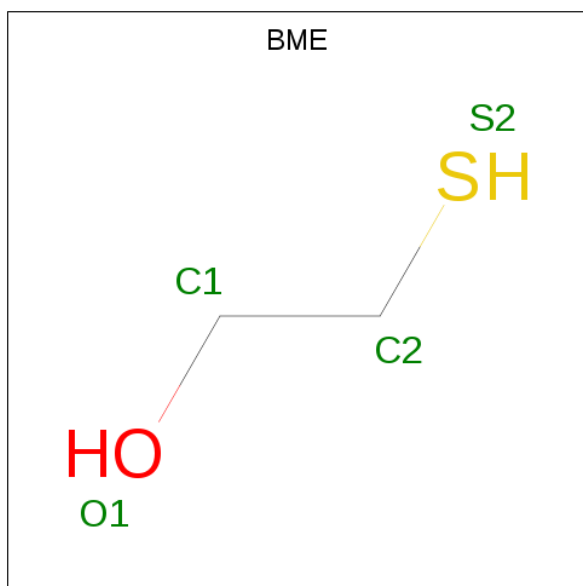
There are 4 unique types of molecules in this entry. The entry contains 4342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

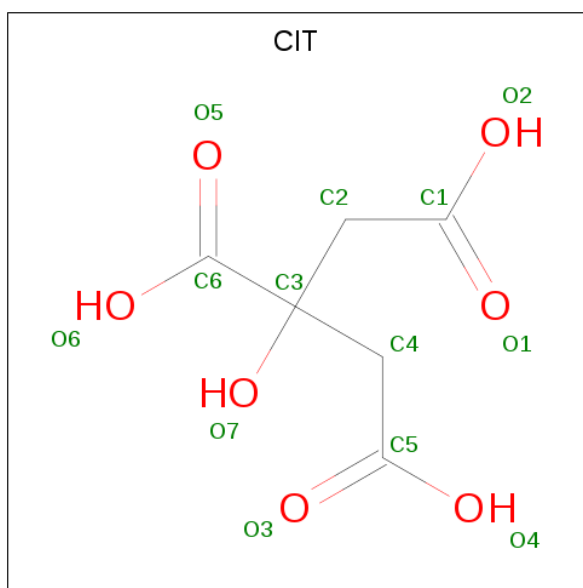
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2076	1323	356	384	13			
1	B	279	Total	C	N	O	S	0	0	0
			2164	1376	374	401	13			

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

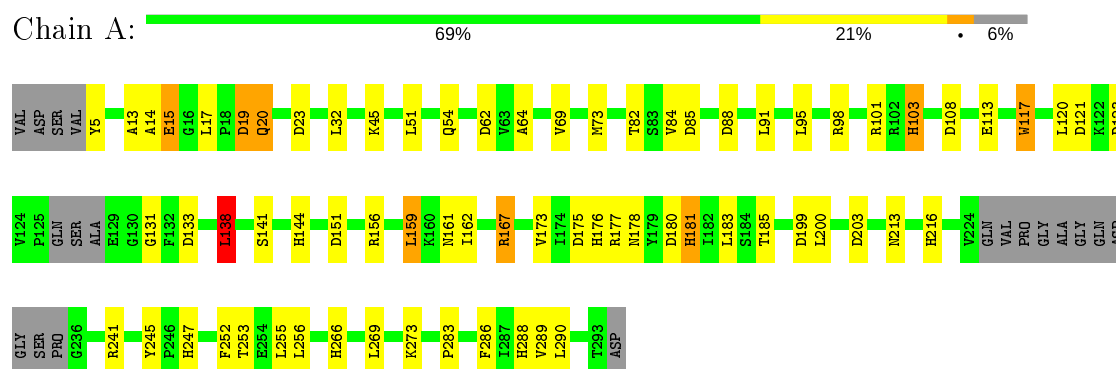
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	59	Total	O	0	0
			59	59		

### 3 Residue-property plots [i](#)

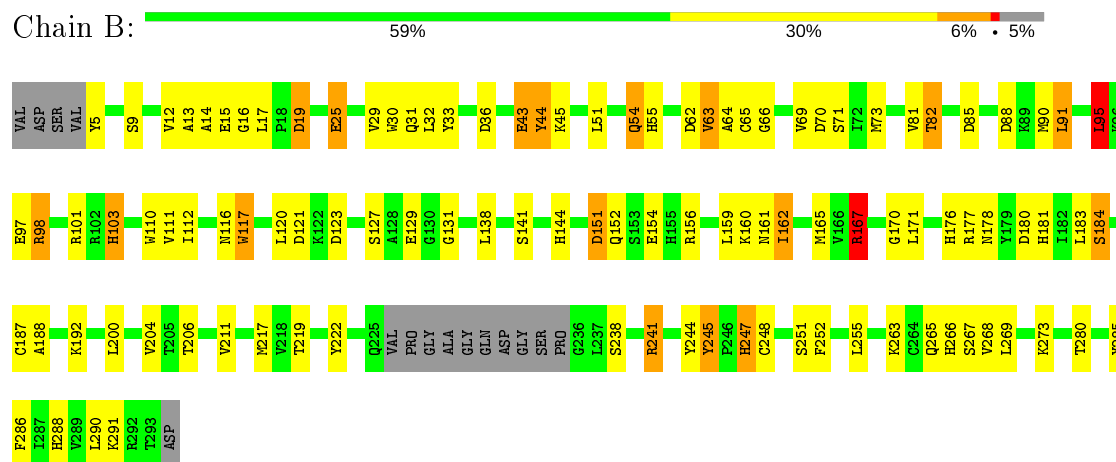
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	75.84Å 83.23Å 114.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.55	Depositor
% Data completeness (in resolution range)	98.4 (12.00-2.55)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.222 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, BME

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	0.87	1/2126 (0.0%)	1.07	15/2896 (0.5%)
1	B	1.49	18/2215 (0.8%)	1.24	14/3007 (0.5%)
All	All	1.22	19/4341 (0.4%)	1.16	29/5903 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	GLN	CG-CD	8.13	1.69	1.51
1	B	63	VAL	CB-CG1	-8.03	1.35	1.52
1	B	184	SER	CB-OG	-7.57	1.32	1.42
1	B	44	TYR	CD1-CE1	7.15	1.50	1.39
1	B	248	CYS	CB-SG	7.01	1.94	1.82
1	B	43	GLU	CG-CD	6.78	1.62	1.51
1	B	69	VAL	CB-CG2	6.73	1.67	1.52
1	B	244	TYR	CD1-CE1	-6.36	1.29	1.39
1	B	160	LYS	CA-CB	6.27	1.67	1.53
1	B	245	TYR	CE2-CZ	6.07	1.46	1.38
1	B	43	GLU	CD-OE1	5.82	1.32	1.25
1	B	154	GLU	CD-OE1	5.58	1.31	1.25
1	B	217	MET	SD-CE	-5.35	1.48	1.77
1	B	71	SER	CB-OG	5.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	VAL	CB-CG2	-5.19	1.42	1.52
1	A	15	GLU	CD-OE1	5.16	1.31	1.25
1	B	188	ALA	CA-CB	-5.13	1.41	1.52
1	B	244	TYR	CD2-CE2	-5.05	1.31	1.39
1	B	285	TYR	CD1-CE1	-5.02	1.31	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CB-CG-OD2	8.24	125.72	118.30
1	B	123	ASP	CB-CG-OD2	7.14	124.72	118.30
1	B	85	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	180	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	133	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	167	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	151	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	88	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	151	ASP	CB-CG-OD2	6.33	123.99	118.30
1	B	62	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	98	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	19	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	123	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	180	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	199	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	88	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	98	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	138	LEU	CB-CG-CD1	5.77	120.81	111.00
1	B	167	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	19	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	98	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	175	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	62	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	203	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	187	CYS	CA-CB-SG	-5.32	104.42	114.00
1	B	95	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	108	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	23	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	162	ILE	CG1-CB-CG2	-5.09	100.21	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	181	HIS	Sidechain
1	B	247	HIS	Sidechain

## 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	2076	0	1938	42	1
1	B	2164	0	2092	64	0
2	A	4	0	5	0	0
2	B	12	0	15	2	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
4	A	1	0	0	0	0
4	B	59	0	0	3	0
All	All	4342	0	4060	97	1

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 (97) 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:B:29:VAL:HG21	1:B:238:SER:HB3	1.37	1.01
1:B:245:TYR:HD2	1:B:247:HIS:CD2	1.80	1.00
1:A:245:TYR:HD2	1:A:247:HIS:HD1	0.99	0.98
1:A:245:TYR:HD2	1:A:247:HIS:ND1	1.67	0.92
1:B:247:HIS:HD1	1:B:252:PHE:HD1	1.16	0.92
1:B:245:TYR:HD2	1:B:247:HIS:HD2	1.16	0.90
1:B:245:TYR:CD2	1:B:247:HIS:CD2	2.60	0.90
1:B:29:VAL:HG21	1:B:238:SER:CB	2.04	0.88
1:A:245:TYR:CD2	1:A:247:HIS:ND1	2.40	0.88
1:A:181:HIS:CE1	1:A:185:THR:HG23	2.11	0.84
1:B:55:HIS:CD2	1:B:171:LEU:HD21	2.13	0.84
1:A:15:GLU:HB3	1:B:64:ALA:HB1	1.61	0.82
1:A:247:HIS:HD2	1:A:252:PHE:CD1	2.04	0.76
1:B:245:TYR:CD2	1:B:247:HIS:HD2	1.99	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:HIS:HD2	1:B:171:LEU:HD21	1.57	0.69
1:A:120:LEU:HB3	1:A:161:ASN:HB3	1.76	0.68
1:B:176:HIS:CE1	1:B:286:PHE:HB2	2.29	0.67
1:A:247:HIS:CD2	1:A:252:PHE:CD1	2.82	0.67
1:A:247:HIS:HD2	1:A:252:PHE:CE1	2.13	0.66
1:A:181:HIS:CE1	1:A:185:THR:CG2	2.79	0.66
1:A:13:ALA:HB2	1:A:19:ASP:OD1	1.96	0.65
1:A:245:TYR:CD2	1:A:247:HIS:CE1	2.86	0.63
1:A:252:PHE:HD2	1:A:288:HIS:CE1	2.19	0.61
1:A:14:ALA:HB1	1:B:144:HIS:HD2	1.64	0.61
1:B:141:SER:HA	1:B:144:HIS:ND1	2.15	0.60
1:B:120:LEU:HB3	1:B:161:ASN:HB3	1.84	0.60
1:B:266:HIS:CE1	1:B:288:HIS:HD2	2.19	0.59
1:B:181:HIS:HD2	4:B:2321:HOH:O	1.85	0.59
1:A:144:HIS:ND1	1:B:14:ALA:HB1	2.18	0.58
1:B:204:VAL:O	2:B:2187:BME:H11	2.02	0.58
1:A:256:LEU:HD12	1:A:288:HIS:ND1	2.19	0.57
1:A:14:ALA:HB1	1:B:144:HIS:CD2	2.38	0.57
1:A:131:GLY:HA3	1:A:167:ARG:HB3	1.87	0.57
1:A:14:ALA:CA	1:B:90:MET:HE1	2.35	0.56
1:A:247:HIS:CD2	1:A:252:PHE:CE1	2.94	0.56
1:A:14:ALA:N	1:B:90:MET:HE1	2.22	0.54
1:B:266:HIS:HE2	1:B:288:HIS:CD2	2.26	0.54
1:B:290:LEU:HD12	1:B:290:LEU:N	2.23	0.54
1:A:181:HIS:NE2	1:A:185:THR:CG2	2.72	0.53
1:A:176:HIS:CE1	1:A:286:PHE:HB2	2.44	0.52
1:A:64:ALA:HB1	1:B:15:GLU:HB3	1.90	0.52
1:A:247:HIS:CD2	1:A:252:PHE:HD1	2.28	0.51
1:B:65:CYS:O	1:B:66:GLY:C	2.45	0.51
1:B:206:THR:OG1	2:B:2187:BME:H12	2.10	0.51
1:B:141:SER:HA	1:B:144:HIS:CE1	2.47	0.50
1:A:181:HIS:NE2	1:A:185:THR:HG21	2.28	0.49
1:B:247:HIS:ND1	1:B:252:PHE:CD1	2.67	0.49
1:B:63:VAL:O	1:B:64:ALA:HB3	2.13	0.49
1:B:266:HIS:NE2	1:B:288:HIS:HD2	2.11	0.48
1:B:266:HIS:NE2	1:B:288:HIS:CD2	2.82	0.48
1:A:19:ASP:O	1:A:20:GLN:C	2.53	0.48
1:A:252:PHE:HD2	1:A:288:HIS:NE2	2.12	0.47
1:B:245:TYR:CD2	1:B:247:HIS:NE2	2.80	0.47
1:A:101:ARG:C	1:A:103:HIS:N	2.68	0.46
1:B:170:GLY:O	1:B:291:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:O	1:A:216:HIS:CD2	2.68	0.46
1:B:101:ARG:C	1:B:103:HIS:N	2.67	0.46
1:B:81:VAL:HG22	1:B:110:TRP:CD1	2.51	0.46
1:A:117:TRP:CZ3	1:B:16:GLY:HA3	2.51	0.46
1:B:247:HIS:ND1	1:B:252:PHE:HD1	1.99	0.45
1:B:101:ARG:C	1:B:103:HIS:H	2.20	0.45
1:B:13:ALA:HB2	1:B:19:ASP:OD1	2.17	0.45
1:A:159:LEU:HA	1:A:162:ILE:HD12	1.98	0.45
1:A:141:SER:HA	1:A:144:HIS:CD2	2.51	0.45
1:B:266:HIS:ND1	1:B:267:SER:N	2.64	0.45
1:A:45:LYS:HG3	1:A:73:MET:SD	2.57	0.44
1:B:192:LYS:HB2	4:B:2304:HOH:O	2.17	0.44
1:B:97:GLU:O	1:B:98:ARG:C	2.54	0.44
1:B:252:PHE:HD2	1:B:288:HIS:CE1	2.36	0.44
1:B:9:SER:O	1:B:12:VAL:HG22	2.18	0.44
1:A:138:LEU:HD11	1:A:173:VAL:HG12	2.00	0.43
1:B:162:ILE:O	1:B:165:MET:HB2	2.18	0.43
1:B:30:TRP:O	1:B:33:TYR:HB3	2.17	0.43
1:B:116:ASN:OD1	1:B:117:TRP:N	2.51	0.43
1:B:151:ASP:O	1:B:152:GLN:HB2	2.19	0.43
1:A:290:LEU:N	1:A:290:LEU:HD12	2.34	0.42
1:B:204:VAL:HG22	1:B:222:TYR:CD2	2.53	0.42
1:B:266:HIS:HE1	1:B:268:VAL:HG22	1.83	0.42
1:B:95:LEU:HD13	1:B:112:ILE:HG21	2.00	0.42
1:A:101:ARG:C	1:A:103:HIS:H	2.21	0.42
1:B:181:HIS:CD2	4:B:2321:HOH:O	2.67	0.42
1:A:253:THR:HG23	1:A:266:HIS:CE1	2.55	0.41
1:B:131:GLY:HA3	1:B:167:ARG:HB3	2.02	0.41
1:B:45:LYS:HG3	1:B:73:MET:SD	2.60	0.41
1:B:204:VAL:HG22	1:B:222:TYR:CE2	2.56	0.41
1:B:247:HIS:ND1	1:B:252:PHE:CE1	2.87	0.41
1:B:25:GLU:O	1:B:29:VAL:HG23	2.20	0.41
1:A:84:VAL:HA	1:A:113:GLU:O	2.20	0.41
1:B:266:HIS:HE1	1:B:268:VAL:CG2	2.34	0.41
1:A:14:ALA:C	1:B:90:MET:HE1	2.42	0.41
1:B:178:ASN:OD1	1:B:178:ASN:C	2.60	0.40
1:A:178:ASN:ND2	1:A:283:PRO:O	2.46	0.40
1:B:219:THR:CG2	1:B:241:ARG:HD3	2.51	0.40
1:B:44:TYR:HH	1:B:70:ASP:CG	2.24	0.40
1:B:266:HIS:C	1:B:266:HIS:ND1	2.74	0.40
1:A:253:THR:HG23	1:A:266:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:THR:HB	1:B:111:VAL:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:O	1:A:213:ASN:ND2[2_745]	2.10	0.10

## 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	269/294 (92%)	256 (95%)	13 (5%)	0	100	100
1	B	275/294 (94%)	257 (94%)	15 (6%)	3 (1%)	14	19
All	All	544/588 (92%)	513 (94%)	28 (5%)	3 (1%)	25	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	SER
1	B	129	GLU
1	B	91	LEU

### 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	206/245 (84%)	181 (88%)	25 (12%)	5	4
1	B	226/245 (92%)	195 (86%)	31 (14%)	3	3
All	All	432/490 (88%)	376 (87%)	56 (13%)	4	3

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	17	LEU
1	A	20	GLN
1	A	32	LEU
1	A	51	LEU
1	A	54	GLN
1	A	69	VAL
1	A	82	THR
1	A	91	LEU
1	A	95	LEU
1	A	103	HIS
1	A	117	TRP
1	A	121	ASP
1	A	138	LEU
1	A	156	ARG
1	A	159	LEU
1	A	167	ARG
1	A	177	ARG
1	A	183	LEU
1	A	200	LEU
1	A	241	ARG
1	A	255	LEU
1	A	269	LEU
1	A	273	LYS
1	A	289	VAL
1	B	5	TYR
1	B	17	LEU
1	B	25	GLU
1	B	31	GLN
1	B	32	LEU
1	B	36	ASP
1	B	43	GLU
1	B	51	LEU
1	B	54	GLN
1	B	82	THR

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Mol	Chain	Res	Type
1	B	91	LEU
1	B	95	LEU
1	B	103	HIS
1	B	117	TRP
1	B	121	ASP
1	B	138	LEU
1	B	156	ARG
1	B	159	LEU
1	B	167	ARG
1	B	177	ARG
1	B	183	LEU
1	B	184	SER
1	B	200	LEU
1	B	241	ARG
1	B	251	SER
1	B	255	LEU
1	B	263	LYS
1	B	265	GLN
1	B	269	LEU
1	B	273	LYS
1	B	280	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	54	GLN
1	A	176	HIS
1	A	216	HIS
1	B	20	GLN
1	B	152	GLN
1	B	265	GLN
1	B	288	HIS

### 5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BME	B	2187	1	3,3,3	0.31	0	1,2,2	1.50	0
3	CIT	B	2001	-	3,12,12	4.86	2 (66%)	3,17,17	2.45	1 (33%)
3	CIT	A	1001	-	3,12,12	1.55	1 (33%)	3,17,17	1.71	1 (33%)
2	BME	B	2284	1	3,3,3	0.55	0	1,2,2	0.18	0
2	BME	B	2264	1	3,3,3	0.43	0	1,2,2	0.70	0
2	BME	A	1187	1	3,3,3	0.27	0	1,2,2	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	B	2187	1	-	1/1/1/1	-
3	CIT	B	2001	-	-	3/6/16/16	-
3	CIT	A	1001	-	-	0/6/16/16	-
2	BME	B	2284	1	-	0/1/1/1	-
2	BME	B	2264	1	-	0/1/1/1	-
2	BME	A	1187	1	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	CIT	O7-C3	7.76	1.55	1.43
3	B	2001	CIT	C2-C3	3.17	1.59	1.54
3	A	1001	CIT	O7-C3	2.29	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	CIT	C3-C2-C1	4.22	121.74	114.98
3	A	1001	CIT	C4-C3-C2	2.65	116.41	109.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2187	BME	O1-C1-C2-S2
3	B	2001	CIT	O7-C3-C4-C5
3	B	2001	CIT	C6-C3-C4-C5
3	B	2001	CIT	C2-C3-C4-C5
2	A	1187	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2187	BME	2	0

## 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.