



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:16 am BST

PDB ID : 1R8X
Title : Crystal Structure of Mouse Glycine N-Methyltransferase (Tetragonal Form)
Authors : Pakhomova, S.; Luka, Z.; Wagner, C.; Newcomer, M.E.
Deposited on : 2003-10-28
Resolution : 2.95 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
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

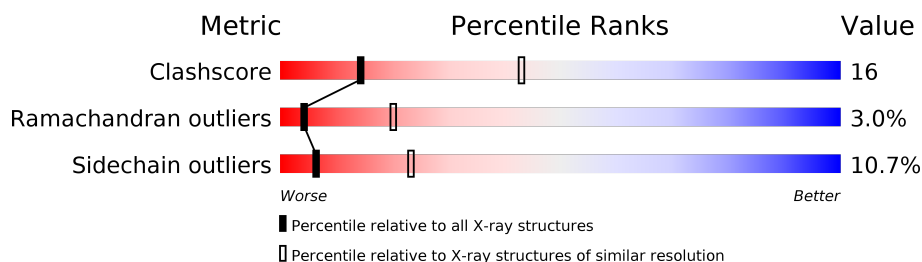
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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 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	
1	B	292	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	A	1247	-	X	-	-
3	TRS	B	2263	-	X	-	-

2 Entry composition [i](#)

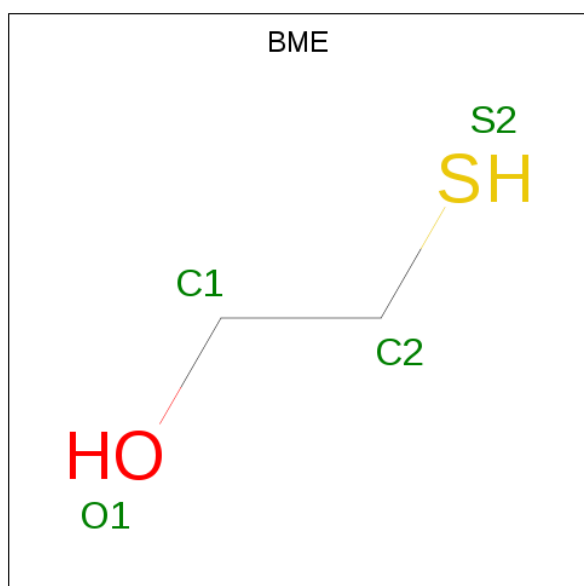
There are 4 unique types of molecules in this entry. The entry contains 4409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

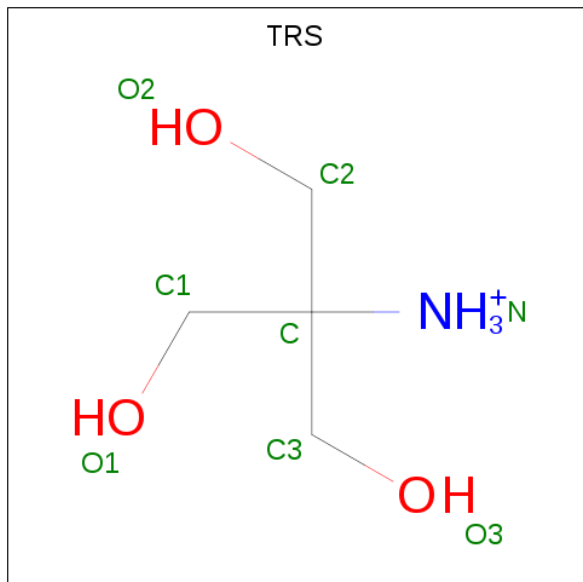
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2152	1363	369	407	13			
1	B	284	Total	C	N	O	S	0	0	0
			2204	1403	381	407	13			

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	12	Total	O	0	0
			12	12		

3 Residue-property plots [i](#)

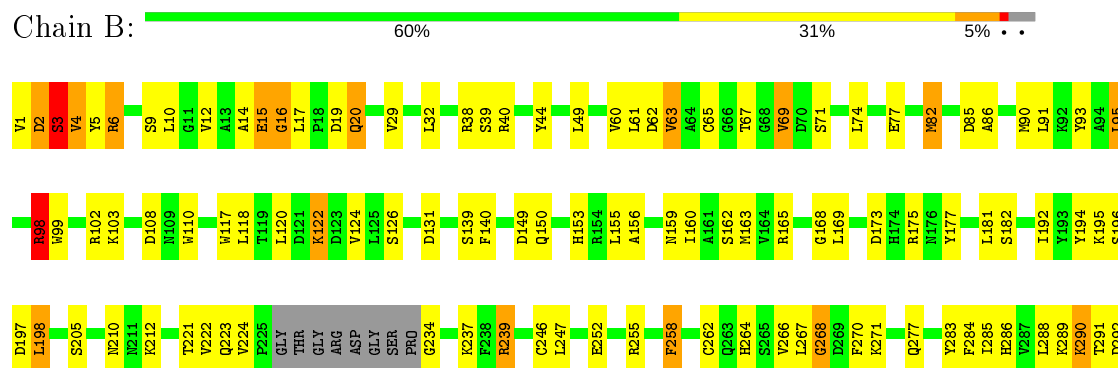
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.70 Å 70.70 Å 266.03 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.50 – 2.95	Depositor
% Data completeness (in resolution range)	99.8 (10.50-2.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4409	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 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	1.03	4/2203 (0.2%)	1.10	9/3001 (0.3%)
1	B	1.19	4/2257 (0.2%)	1.18	9/3065 (0.3%)
All	All	1.12	8/4460 (0.2%)	1.14	18/6066 (0.3%)

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	2
1	B	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	VAL	CB-CG1	-6.32	1.39	1.52
1	A	5	TYR	CG-CD1	6.18	1.47	1.39
1	A	6	ARG	CB-CG	-6.02	1.36	1.52
1	B	252	GLU	CD-OE1	5.79	1.32	1.25
1	B	177	TYR	CD2-CE2	-5.74	1.30	1.39
1	A	209	VAL	CB-CG2	-5.70	1.40	1.52
1	A	54	GLN	CA-CB	5.25	1.65	1.53
1	B	3	SER	CA-CB	5.06	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASP	CB-CG-OD2	8.05	125.55	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	15	GLU	C-N-CA	-7.33	106.92	122.30
1	A	62	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	173	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	62	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	246	CYS	CA-CB-SG	6.70	126.06	114.00
1	A	6	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	108	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	98	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	239	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	B	98	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	178	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	2	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	15	GLU	C-N-CA	-5.32	111.13	122.30
1	A	269	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	290	LYS	N-CA-C	5.22	125.10	111.00
1	B	239	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Peptide
1	A	16	GLY	Peptide
1	B	16	GLY	Peptide
1	B	262	CYS	Peptide

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	2152	0	2005	71	0
1	B	2204	0	2125	74	0
2	A	8	0	10	2	0
2	B	8	0	10	1	0
3	A	8	0	12	0	0
3	B	8	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	2	0
4	B	12	0	0	1	0
All	All	4409	0	4174	133	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 16.

All (133) 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:3:SER:O	1:B:4:VAL:HG23	1.62	0.98
1:A:49:LEU:HD11	1:A:77:GLU:HG3	1.47	0.94
1:A:63:VAL:CG1	1:A:117:TRP:HE1	1.87	0.87
1:B:82:MET:CE	1:B:124:VAL:HG13	2.06	0.85
1:B:63:VAL:CG1	1:B:117:TRP:HE1	1.95	0.80
1:B:49:LEU:HD11	1:B:77:GLU:HG3	1.67	0.77
1:B:3:SER:O	1:B:4:VAL:CG2	2.31	0.76
1:A:99:TRP:CH2	1:B:98:ARG:HD3	2.21	0.76
1:A:61:LEU:CD2	1:A:163:MET:HE3	2.17	0.75
1:B:82:MET:HE1	1:B:124:VAL:HG13	1.68	0.75
1:A:20:GLN:HB2	4:A:1254:HOH:O	1.87	0.74
1:A:82:MET:CE	1:A:124:VAL:HG13	2.19	0.73
1:A:82:MET:HE1	1:A:124:VAL:HG13	1.70	0.73
1:A:144:PRO:HB2	2:A:1146:BME:H21	1.72	0.70
1:A:264:HIS:HE1	1:A:286:HIS:HD2	1.39	0.70
1:A:239:ARG:HD3	1:B:6:ARG:O	1.92	0.70
1:A:117:TRP:CZ3	1:B:16:GLY:HA3	2.27	0.69
1:B:264:HIS:HE1	1:B:286:HIS:HD2	1.41	0.68
1:B:4:VAL:O	1:B:4:VAL:HG12	1.93	0.68
1:A:63:VAL:HG11	1:A:117:TRP:HE1	1.59	0.65
1:A:4:VAL:O	1:A:4:VAL:HG12	1.96	0.65
1:B:223:GLN:HA	1:B:234:GLY:O	1.97	0.65
1:B:192:ILE:HG12	1:B:283:TYR:CD1	2.32	0.64
1:A:264:HIS:CE1	1:A:286:HIS:HD2	2.16	0.64
1:B:63:VAL:HG12	1:B:117:TRP:HE1	1.63	0.64
1:B:150:GLN:HG2	1:B:153:HIS:ND1	2.13	0.63
1:B:85:ASP:OD2	1:B:86:ALA:N	2.31	0.63
1:A:124:VAL:HG11	1:A:163:MET:CE	2.28	0.63
1:B:156:ALA:O	1:B:160:ILE:HG13	1.99	0.63
1:B:69:VAL:HG23	3:B:2263:TRS:H21	1.80	0.63
1:A:124:VAL:HG11	1:A:163:MET:HE1	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLN:HA	1:B:20:GLN:NE2	2.16	0.61
1:B:264:HIS:CE1	1:B:286:HIS:HD2	2.18	0.61
1:A:117:TRP:CD1	1:A:160:ILE:HD11	2.35	0.61
1:B:169:LEU:HA	1:B:288:LEU:O	2.01	0.60
1:B:124:VAL:HG11	1:B:163:MET:HE1	1.83	0.60
1:B:1:VAL:O	1:B:3:SER:N	2.31	0.60
1:A:174:HIS:HE1	1:A:286:HIS:HE1	1.50	0.59
1:A:267:LEU:HB2	1:A:285:ILE:HB	1.83	0.59
1:B:82:MET:HE2	1:B:124:VAL:HG13	1.83	0.59
1:B:61:LEU:HD13	1:B:82:MET:HG2	1.84	0.59
1:A:264:HIS:HE1	1:A:286:HIS:CD2	2.21	0.58
1:A:61:LEU:HD21	1:A:163:MET:HE3	1.85	0.58
1:A:16:GLY:HA3	1:B:117:TRP:CZ3	2.38	0.58
1:A:49:LEU:CD1	1:A:77:GLU:HG3	2.28	0.58
1:A:220:TYR:CE1	1:A:240:LEU:HD12	2.39	0.57
1:A:223:GLN:HA	1:A:234:GLY:O	2.04	0.57
1:A:150:GLN:HG2	1:A:153:HIS:ND1	2.18	0.57
1:B:124:VAL:HG11	1:B:163:MET:CE	2.34	0.57
1:A:117:TRP:CH2	1:B:16:GLY:HA3	2.41	0.56
1:B:264:HIS:HE1	1:B:286:HIS:CD2	2.23	0.56
1:A:40:ARG:HG3	1:A:194:TYR:CE2	2.40	0.56
1:B:124:VAL:CG1	1:B:163:MET:HE1	2.35	0.56
1:B:63:VAL:HG11	1:B:117:TRP:HE1	1.69	0.56
1:B:20:GLN:HA	1:B:20:GLN:HE21	1.70	0.55
1:A:6:ARG:O	1:B:239:ARG:HD3	2.07	0.55
1:A:85:ASP:OD2	1:B:15:GLU:O	2.25	0.55
1:B:2:ASP:O	1:B:3:SER:O	2.26	0.53
1:B:255:ARG:HD3	2:B:2262:BME:H21	1.89	0.53
1:B:291:THR:O	1:B:292:ASP:CB	2.57	0.53
1:A:174:HIS:CE1	1:A:286:HIS:HE1	2.27	0.53
1:B:118:LEU:HD22	1:B:155:LEU:HD23	1.90	0.52
1:B:63:VAL:CG1	1:B:117:TRP:NE1	2.70	0.52
1:B:14:ALA:HB3	1:B:17:LEU:HD12	1.92	0.52
1:A:124:VAL:CG1	1:A:163:MET:HE1	2.41	0.51
1:A:98:ARG:HD3	1:B:99:TRP:CH2	2.45	0.51
1:B:258:PHE:CD1	1:B:258:PHE:N	2.79	0.51
1:B:247:LEU:HD13	1:B:284:PHE:CG	2.45	0.50
1:B:19:ASP:OD1	4:B:2272:HOH:O	2.19	0.50
1:A:192:ILE:HD12	1:A:270:PHE:CZ	2.47	0.49
1:A:64:ALA:HB2	1:A:117:TRP:CZ2	2.47	0.49
1:A:247:LEU:HD13	1:A:284:PHE:CG	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD22	1:A:163:MET:HE3	1.94	0.49
1:B:131:ASP:OD1	1:B:165:ARG:NH1	2.43	0.48
1:A:114:GLU:HG3	4:A:1248:HOH:O	2.13	0.48
1:A:82:MET:HE2	1:A:124:VAL:HG13	1.96	0.48
1:B:120:LEU:HB3	1:B:159:ASN:HB3	1.95	0.48
1:B:95:LEU:HD12	1:B:98:ARG:NH1	2.28	0.48
1:A:142:HIS:O	1:B:17:LEU:HD21	2.14	0.48
1:B:181:LEU:HA	1:B:181:LEU:HD23	1.63	0.47
1:B:69:VAL:HG23	3:B:2263:TRS:C2	2.44	0.47
1:A:118:LEU:HD22	1:A:155:LEU:HD23	1.97	0.47
1:A:191:ASN:OD1	1:A:191:ASN:C	2.53	0.47
1:A:156:ALA:O	1:A:160:ILE:HG13	2.14	0.46
1:A:144:PRO:CB	2:A:1146:BME:H21	2.44	0.46
1:B:61:LEU:CD2	1:B:163:MET:HE3	2.44	0.46
1:A:120:LEU:HB3	1:A:159:ASN:HB3	1.97	0.46
1:B:67:THR:HG22	1:B:93:TYR:HB2	1.98	0.46
1:B:98:ARG:HG3	1:B:110:TRP:CE3	2.51	0.46
1:A:6:ARG:NH2	1:A:10:LEU:HD21	2.31	0.46
1:B:6:ARG:NH2	1:B:10:LEU:HD21	2.31	0.46
1:B:49:LEU:CD1	1:B:77:GLU:HG3	2.42	0.46
1:A:15:GLU:OE2	3:B:2263:TRS:H12	2.16	0.45
1:B:20:GLN:CA	1:B:20:GLN:HE21	2.29	0.45
1:B:222:VAL:HG12	1:B:223:GLN:N	2.31	0.45
1:B:268:GLY:N	1:B:271:LYS:O	2.45	0.45
1:A:15:GLU:HG3	1:B:90:MET:SD	2.56	0.45
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.53	0.45
1:B:40:ARG:HA	1:B:194:TYR:CD2	2.52	0.45
1:A:165:ARG:O	1:A:168:GLY:N	2.49	0.45
1:A:16:GLY:HA3	1:B:117:TRP:CH2	2.51	0.45
1:B:44:TYR:HB2	1:B:270:PHE:CZ	2.51	0.45
1:A:72:ILE:HD13	1:A:97:GLU:HG2	1.98	0.44
1:A:258:PHE:N	1:A:258:PHE:CD1	2.85	0.44
1:B:139:SER:O	1:B:140:PHE:C	2.54	0.44
1:A:169:LEU:HA	1:A:288:LEU:O	2.18	0.44
1:B:122:LYS:HG2	1:B:122:LYS:H	1.64	0.43
1:B:267:LEU:HB2	1:B:285:ILE:HB	1.99	0.43
1:A:84:VAL:HA	1:A:113:GLU:O	2.18	0.43
1:A:269:ASP:O	1:A:270:PHE:HB2	2.19	0.43
1:B:290:LYS:HB3	1:B:291:THR:H	1.41	0.43
1:B:221:THR:HG23	1:B:237:LYS:HD3	2.01	0.43
1:A:188:PRO:HB3	1:A:202:ILE:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:O	1:A:49:LEU:HB2	2.20	0.42
1:B:198:LEU:HD12	1:B:198:LEU:HA	1.64	0.42
1:A:63:VAL:CG1	1:A:117:TRP:NE1	2.68	0.42
1:A:8:ARG:NH1	1:A:13:ALA:HA	2.34	0.42
1:A:175:ARG:HD2	1:A:175:ARG:HH11	1.74	0.42
1:B:168:GLY:O	1:B:289:LYS:HA	2.19	0.42
1:A:20:GLN:HA	1:A:20:GLN:NE2	2.35	0.42
1:A:201:ASP:HB3	1:A:221:THR:HG23	2.01	0.42
1:A:20:GLN:HE21	1:A:20:GLN:HA	1.85	0.41
1:A:99:TRP:CH2	1:B:98:ARG:CD	2.99	0.41
1:A:98:ARG:HG3	1:A:110:TRP:CE3	2.55	0.41
1:A:224:VAL:HG13	1:A:234:GLY:HA3	2.02	0.41
1:B:9:SER:O	1:B:12:VAL:HG22	2.21	0.41
1:A:159:ASN:O	1:A:160:ILE:C	2.58	0.41
1:A:44:TYR:O	1:A:45:LYS:C	2.57	0.41
1:A:85:ASP:OD2	1:A:86:ALA:N	2.54	0.40
1:B:82:MET:HE2	1:B:124:VAL:CG1	2.50	0.40
1:A:138:ASN:O	1:A:138:ASN:CG	2.60	0.40
1:A:124:VAL:O	1:A:126:SER:N	2.55	0.40
1:B:32:LEU:HA	1:B:32:LEU:HD23	1.86	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	279/292 (96%)	243 (87%)	28 (10%)	8 (3%)	4	21
1	B	280/292 (96%)	247 (88%)	24 (9%)	9 (3%)	4	19
All	All	559/584 (96%)	490 (88%)	52 (9%)	17 (3%)	4	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	20	GLN
1	B	2	ASP
1	B	3	SER
1	B	4	VAL
1	B	20	GLN
1	A	268	GLY
1	B	5	TYR
1	B	268	GLY
1	A	199	THR
1	B	162	SER
1	A	77	GLU
1	A	106	SER
1	A	260	GLY
1	B	210	ASN
1	B	224	VAL
1	A	124	VAL

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	218/246 (89%)	197 (90%)	21 (10%)	8	28
1	B	230/246 (94%)	203 (88%)	27 (12%)	5	20
All	All	448/492 (91%)	400 (89%)	48 (11%)	6	23

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	38	ARG
1	A	39	SER
1	A	45	LYS
1	A	49	LEU
1	A	60	VAL
1	A	65	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	67	THR
1	A	69	VAL
1	A	91	LEU
1	A	95	LEU
1	A	102	ARG
1	A	126	SER
1	A	196	SER
1	A	208	THR
1	A	212	LYS
1	A	237	LYS
1	A	239	ARG
1	A	258	PHE
1	A	266	VAL
1	A	277	GLN
1	B	6	ARG
1	B	29	VAL
1	B	38	ARG
1	B	39	SER
1	B	60	VAL
1	B	65	CYS
1	B	69	VAL
1	B	71	SER
1	B	82	MET
1	B	91	LEU
1	B	95	LEU
1	B	98	ARG
1	B	102	ARG
1	B	103	LYS
1	B	122	LYS
1	B	126	SER
1	B	175	ARG
1	B	182	SER
1	B	195	LYS
1	B	196	SER
1	B	197	ASP
1	B	198	LEU
1	B	205	SER
1	B	212	LYS
1	B	258	PHE
1	B	266	VAL
1	B	277	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	31	GLN
1	A	109	ASN
1	A	174	HIS
1	A	264	HIS
1	A	286	HIS
1	B	20	GLN
1	B	31	GLN
1	B	109	ASN
1	B	150	GLN
1	B	174	HIS
1	B	245	HIS
1	B	264	HIS
1	B	286	HIS

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 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	A	1246	1	3,3,3	1.11	0	1,2,2	1.33	0
3	TRS	B	2263	-	7,7,7	1.10	0	9,9,9	2.50	5 (55%)
2	BME	A	1146	1	3,3,3	0.80	0	1,2,2	0.10	0
3	TRS	A	1247	-	7,7,7	0.43	0	9,9,9	1.37	1 (11%)
2	BME	B	2262	1	3,3,3	0.39	0	1,2,2	0.18	0
2	BME	B	2146	1	3,3,3	0.99	0	1,2,2	1.33	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	A	1246	1	-	1/1/1/1	-
3	TRS	B	2263	-	-	8/9/9/9	-
2	BME	A	1146	1	-	0/1/1/1	-
3	TRS	A	1247	-	-	9/9/9/9	-
2	BME	B	2262	1	-	1/1/1/1	-
2	BME	B	2146	1	-	1/1/1/1	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2263	TRS	O3-C3-C	4.91	126.57	111.00
3	B	2263	TRS	C3-C-C1	3.05	120.27	110.81
3	B	2263	TRS	C3-C-N	-2.46	100.62	107.98
3	B	2263	TRS	O2-C2-C	2.40	118.61	111.00
3	A	1247	TRS	O3-C3-C	2.30	118.27	111.00
3	B	2263	TRS	C1-C-N	-2.18	101.47	107.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1246	BME	O1-C1-C2-S2
3	B	2263	TRS	C3-C-C1-O1
3	B	2263	TRS	C1-C-C2-O2
3	B	2263	TRS	C3-C-C2-O2
3	B	2263	TRS	N-C-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1247	TRS	C2-C-C1-O1
3	A	1247	TRS	C3-C-C1-O1
3	A	1247	TRS	N-C-C1-O1
3	A	1247	TRS	C3-C-C2-O2
3	A	1247	TRS	N-C-C2-O2
2	B	2262	BME	O1-C1-C2-S2
2	B	2146	BME	O1-C1-C2-S2
3	B	2263	TRS	C2-C-C1-O1
3	A	1247	TRS	C1-C-C3-O3
3	A	1247	TRS	C2-C-C3-O3
3	B	2263	TRS	N-C-C1-O1
3	B	2263	TRS	N-C-C3-O3
3	A	1247	TRS	C1-C-C2-O2
3	A	1247	TRS	N-C-C3-O3
3	B	2263	TRS	C2-C-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2263	TRS	3	0
2	A	1146	BME	2	0
2	B	2262	BME	1	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.