



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:04 pm GMT

PDB ID : 2AZT
Title : Crystal structure of H176N mutant of human Glycine N-Methyltransferase
Authors : Luka, Z.; Pakhomova, S.; Luka, Y.; Newcomer, M.E.; Wagner, C.
Deposited on : 2005-09-12
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

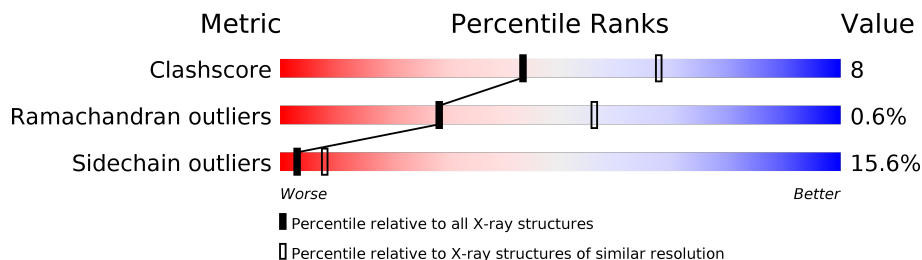
1 Overall quality at a glance

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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (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 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	295	
1	B	295	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4355 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	276	Total	C	N	O	S	0	0	0
			2109	1343	364	389	13			
1	B	277	Total	C	N	O	S	0	0	0
			2159	1372	375	399	13			

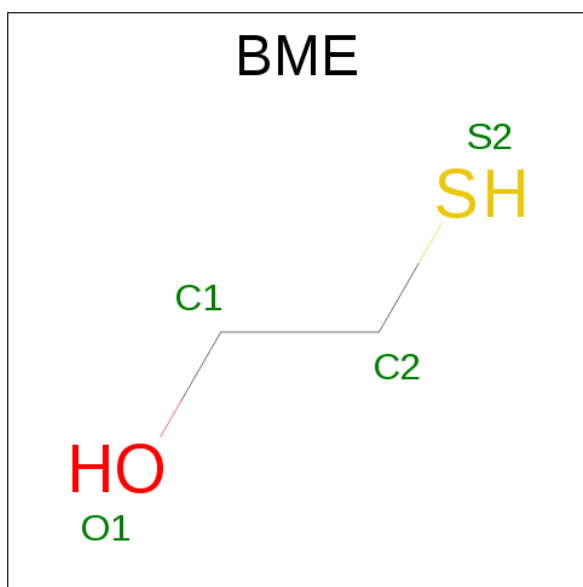
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASN	HIS	ENGINEERED	UNP Q14749
B	176	ASN	HIS	ENGINEERED	UNP Q14749

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

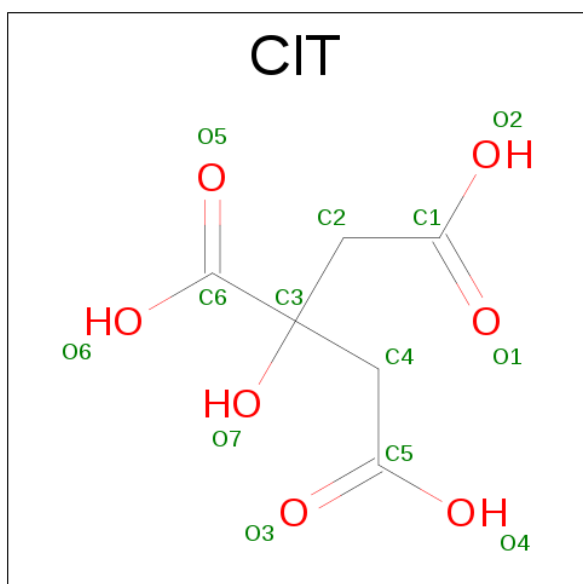
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 5 is water.

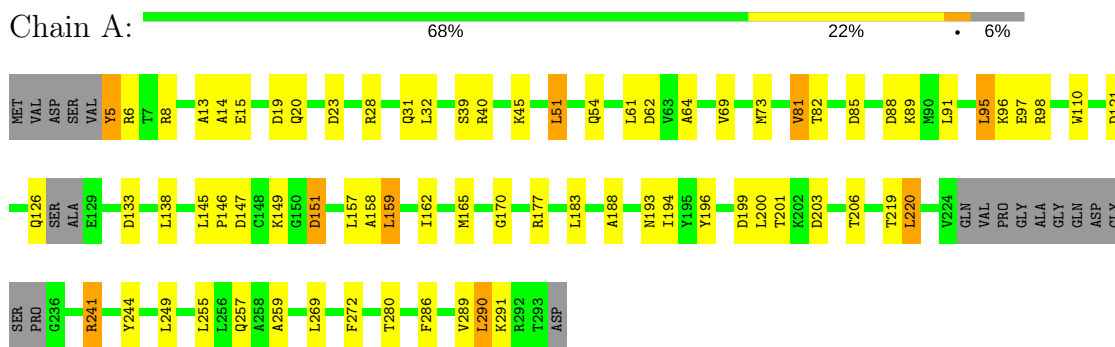
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	35	Total	O	0	0
			35	35		

3 Residue-property plots [i](#)

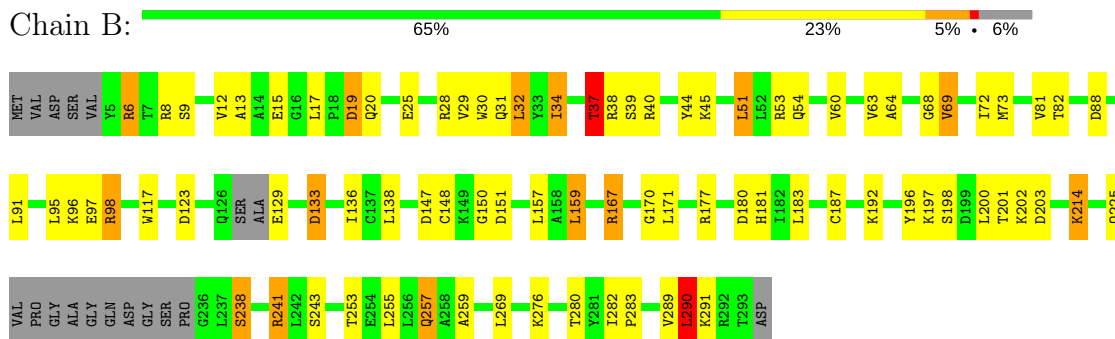
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 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	76.12Å 83.28Å 115.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.9 (13.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.236 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: CL, BME, CIT

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	0.69	0/2158	0.98	11/2933 (0.4%)
1	B	1.11	2/2208 (0.1%)	1.14	13/2994 (0.4%)
All	All	0.93	2/4366 (0.0%)	1.06	24/5927 (0.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	HIS	C-O	5.54	1.33	1.23
1	B	60	VAL	CB-CG2	-5.18	1.42	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	CYS	CA-CB-SG	-8.29	99.09	114.00
1	B	180	ASP	CB-CG-OD2	8.21	125.69	118.30
1	B	51	LEU	CA-CB-CG	7.95	133.59	115.30
1	A	290	LEU	CA-CB-CG	7.93	133.53	115.30
1	B	19	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	290	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	121	ASP	CB-CG-OD2	6.78	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	85	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	133	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	51	LEU	CA-CB-CG	6.39	130.00	115.30
1	B	88	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	133	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	177	ARG	CG-CD-NE	6.00	124.41	111.80
1	B	53	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	203	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	177	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	98	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	23	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	203	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	98	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	199	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	88	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	214	LYS	CD-CE-NZ	-5.06	100.06	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	TYR	Peptide
1	B	129	GLU	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	2109	0	2006	30	0
1	B	2159	0	2098	41	0
2	B	1	0	0	0	0
3	A	8	0	10	1	0
3	B	12	0	15	1	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	35	0	0	4	0
All	All	4355	0	4139	65	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 8.

All (65) 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	1.53	0.90
1:B:29:VAL:HG21	1:B:238:SER:CB	2.07	0.84
1:A:15:GLU:HB3	1:B:64:ALA:HB1	1.67	0.76
1:B:133:ASP:HA	1:B:167:ARG:HE	1.49	0.74
1:B:37:THR:OG1	1:B:69:VAL:HG21	1.92	0.69
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.60	0.66
1:A:45:LYS:HG3	1:A:73:MET:SD	2.38	0.64
1:A:241:ARG:HG2	1:B:8:ARG:HA	1.80	0.63
1:A:13:ALA:HB2	1:A:19:ASP:OD1	1.98	0.63
1:A:8:ARG:HA	1:B:241:ARG:HG2	1.81	0.62
1:B:197:LYS:HE2	1:B:198:SER:O	1.99	0.62
1:A:188:ALA:HB3	1:A:220:LEU:HD11	1.80	0.61
1:A:206:THR:OG1	3:A:1188:BME:H12	2.00	0.61
1:B:63:VAL:HG11	1:B:117:TRP:HE1	1.67	0.60
1:B:32:LEU:HD22	5:B:3021:HOH:O	2.02	0.59
1:B:68:GLY:O	1:B:72:ILE:HG13	2.04	0.58
1:B:170:GLY:O	1:B:291:LYS:HA	2.04	0.57
1:A:158:ALA:O	1:A:162:ILE:HD12	2.03	0.57
1:A:147:ASP:OD1	1:A:151:ASP:O	2.22	0.57
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.71	0.56
1:A:40:ARG:HG3	1:A:196:TYR:CE2	2.43	0.54
1:B:40:ARG:HG3	1:B:196:TYR:CE2	2.43	0.53
1:A:220:LEU:HD23	1:A:244:TYR:CE1	2.42	0.53
1:B:13:ALA:HB2	1:B:19:ASP:OD1	2.09	0.52
1:B:192:LYS:HG3	3:B:2285:BME:S2	2.50	0.52
1:B:192:LYS:HB2	5:B:3012:HOH:O	2.10	0.50
1:B:133:ASP:HA	1:B:167:ARG:NE	2.24	0.50
1:A:13:ALA:N	1:B:30:TRP:CZ2	2.78	0.50
1:B:40:ARG:HG2	1:B:44:TYR:HD2	1.78	0.49
1:B:136:ILE:O	1:B:136:ILE:HG13	2.14	0.48
1:B:30:TRP:CE2	1:B:34:ILE:HG12	2.49	0.48
1:A:6:ARG:NH1	1:A:6:ARG:HG3	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:OD1	1:B:151:ASP:O	2.32	0.47
1:B:9:SER:O	1:B:12:VAL:HG22	2.15	0.47
1:A:159:LEU:HB3	1:A:259:ALA:HB2	1.97	0.46
1:A:61:LEU:CD2	1:A:165:MET:HG3	2.45	0.46
1:A:193:ASN:HB3	1:A:196:TYR:O	2.15	0.46
1:A:64:ALA:HB1	1:B:15:GLU:HB3	1.97	0.46
1:B:6:ARG:CG	1:B:6:ARG:HH11	2.29	0.46
1:A:170:GLY:O	1:A:291:LYS:HA	2.17	0.45
1:B:171:LEU:HA	1:B:290:LEU:O	2.16	0.45
1:A:194:ILE:HD12	1:A:272:PHE:CZ	2.52	0.44
1:A:81:VAL:HG22	1:A:110:TRP:CD1	2.53	0.43
1:A:62:ASP:OD1	1:A:62:ASP:C	2.56	0.43
1:A:97:GLU:O	1:A:98:ARG:C	2.57	0.43
1:B:45:LYS:HG3	1:B:73:MET:SD	2.59	0.43
1:A:219:THR:CG2	1:A:241:ARG:HD3	2.49	0.43
1:B:150:GLY:C	1:B:151:ASP:O	2.56	0.43
1:B:282:ILE:HA	1:B:283:PRO:HD3	1.87	0.43
1:B:29:VAL:HG21	1:B:238:SER:HB2	1.95	0.42
1:B:68:GLY:HA2	5:B:3004:HOH:O	2.19	0.42
1:B:159:LEU:HB3	1:B:259:ALA:HB2	2.01	0.42
1:A:241:ARG:HE	1:A:241:ARG:HB2	1.64	0.41
1:A:89:LYS:HB2	1:B:19:ASP:OD1	2.20	0.41
1:B:253:THR:O	1:B:257:GLN:HG2	2.20	0.41
1:B:276:LYS:HE2	5:B:3033:HOH:O	2.19	0.41
1:B:40:ARG:HG3	1:B:196:TYR:CZ	2.55	0.41
1:A:14:ALA:O	1:A:15:GLU:C	2.56	0.41
1:A:145:LEU:HA	1:A:146:PRO:HD3	1.98	0.41
1:B:34:ILE:HA	1:B:34:ILE:HD12	1.89	0.41
1:B:6:ARG:NH1	1:B:6:ARG:CG	2.84	0.41
1:A:249:LEU:HD13	1:A:286:PHE:CG	2.55	0.41
1:A:95:LEU:HD12	1:A:98:ARG:NH2	2.37	0.40
1:B:257:GLN:H	1:B:257:GLN:HG2	1.75	0.40
1:B:97:GLU:O	1:B:98:ARG:C	2.60	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	270/295 (92%)	251 (93%)	18 (7%)	1 (0%)	38	66
1	B	271/295 (92%)	248 (92%)	21 (8%)	2 (1%)	25	53
All	All	541/590 (92%)	499 (92%)	39 (7%)	3 (1%)	28	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	THR
1	A	151	ASP
1	B	38	ARG

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	214/246 (87%)	184 (86%)	30 (14%)	4	10
1	B	227/246 (92%)	188 (83%)	39 (17%)	2	6
All	All	441/492 (90%)	372 (84%)	69 (16%)	3	8

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	20	GLN
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	31	GLN
1	A	32	LEU
1	A	39	SER
1	A	51	LEU
1	A	54	GLN
1	A	69	VAL
1	A	81	VAL
1	A	82	THR
1	A	91	LEU
1	A	95	LEU
1	A	96	LYS
1	A	126	GLN
1	A	138	LEU
1	A	149	LYS
1	A	157	LEU
1	A	159	LEU
1	A	183	LEU
1	A	200	LEU
1	A	201	THR
1	A	220	LEU
1	A	241	ARG
1	A	255	LEU
1	A	257	GLN
1	A	269	LEU
1	A	280	THR
1	A	289	VAL
1	A	290	LEU
1	B	6	ARG
1	B	17	LEU
1	B	20	GLN
1	B	25	GLU
1	B	28	ARG
1	B	31	GLN
1	B	32	LEU
1	B	34	ILE
1	B	37	THR
1	B	39	SER
1	B	51	LEU
1	B	54	GLN
1	B	69	VAL
1	B	81	VAL
1	B	82	THR

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Mol	Chain	Res	Type
1	B	91	LEU
1	B	95	LEU
1	B	96	LYS
1	B	138	LEU
1	B	148	CYS
1	B	157	LEU
1	B	159	LEU
1	B	167	ARG
1	B	177	ARG
1	B	183	LEU
1	B	200	LEU
1	B	201	THR
1	B	202	LYS
1	B	214	LYS
1	B	225	GLN
1	B	238	SER
1	B	241	ARG
1	B	243	SER
1	B	255	LEU
1	B	257	GLN
1	B	269	LEU
1	B	280	THR
1	B	289	VAL
1	B	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	161	ASN
1	A	247	HIS
1	B	152	GLN
1	B	161	ASN
1	B	225	GLN
1	B	265	GLN

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](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
4	CIT	A	1000	-	3,12,12	1.93	1 (33%)	3,17,17	2.53	2 (66%)
3	BME	A	1188	1	3,3,3	0.39	0	2,2,2	0.35	0
3	BME	A	1285	1	3,3,3	0.65	0	2,2,2	0.30	0
4	CIT	B	2000	-	3,12,12	2.23	1 (33%)	3,17,17	3.49	2 (66%)
3	BME	B	2188	1	3,3,3	0.34	0	2,2,2	0.33	0
3	BME	B	2249	1	3,3,3	0.45	0	2,2,2	0.08	0
3	BME	B	2285	1	3,3,3	0.44	0	2,2,2	1.35	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
4	CIT	A	1000	-	-	0/6/16/16	0/0/0/0
3	BME	A	1188	1	-	0/1/1/1	0/0/0/0
3	BME	A	1285	1	-	0/1/1/1	0/0/0/0
4	CIT	B	2000	-	-	0/6/16/16	0/0/0/0
3	BME	B	2188	1	-	0/1/1/1	0/0/0/0
3	BME	B	2249	1	-	0/1/1/1	0/0/0/0
3	BME	B	2285	1	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	CIT	O7-C3	3.32	1.48	1.43
4	B	2000	CIT	O7-C3	3.60	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2000	CIT	C3-C4-C5	-5.43	106.47	114.95
4	A	1000	CIT	C3-C2-C1	-3.80	109.01	114.95
4	B	2000	CIT	C3-C2-C1	-2.47	111.10	114.95
4	A	1000	CIT	C3-C4-C5	-2.17	111.57	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1188	BME	1	0
3	B	2285	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.