



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:56 pm BST

PDB ID : 3THS  
Title : Crystal structure of rat native liver Glycine N-methyltransferase complexed with 5-methyltetrahydrofolate pentaglutamate  
Authors : Luka, Z.; Pakhomova, S.; Loukachevitch, L.V.; Newcomer, M.E.; Wagner, C.  
Deposited on : 2011-08-19  
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](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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

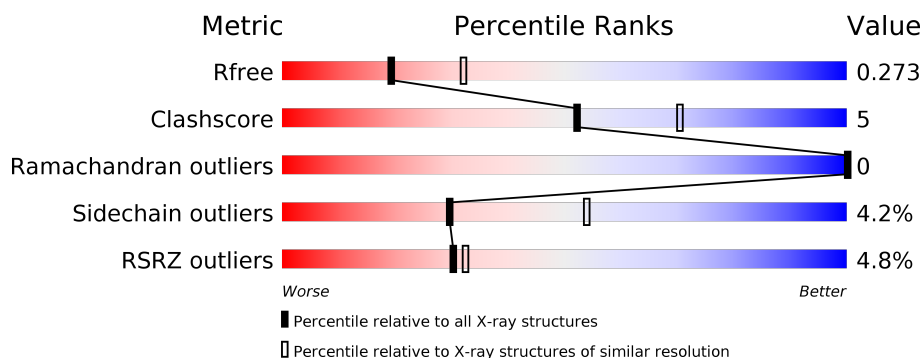
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 86%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>11%</span> <span>86%</span> <span>11%</span> </div> </div>
1	B	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 13%, green 83%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>13%</span> <span>83%</span> <span>13%</span> </div> </div>
1	C	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, orange 1%, yellow 14%, green 83%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>11%</span> <span>83%</span> <span>14%</span> </div> </div>
1	D	293	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 9%, green 88%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>88%</span> <span>9%</span> </div> </div>
2	E	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, grey 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>50%</span> <span>50%</span> </div> </div>
2	F	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 17%, yellow 33%, grey 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>17%</span> <span>33%</span> <span>50%</span> </div> </div>

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
2	GGL	F	2	-	-	X	-
2	GGL	F	3	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9091 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	284	Total	C	N	O	S	0	0	0
			2225	1415	385	414	11			
1	B	286	Total	C	N	O	S	0	0	0
			2243	1428	388	416	11			
1	C	285	Total	C	N	O	S	0	0	0
			2224	1412	386	415	11			
1	D	284	Total	C	N	O	S	0	0	0
			2226	1416	386	413	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ACE	-	ACETYLATION	UNP P13255
B	300	ACE	-	ACETYLATION	UNP P13255
C	300	ACE	-	ACETYLATION	UNP P13255
D	300	ACE	-	ACETYLATION	UNP P13255

- Molecule 2 is a protein called 5-methyltetrahydrofolate pentaglutamate.

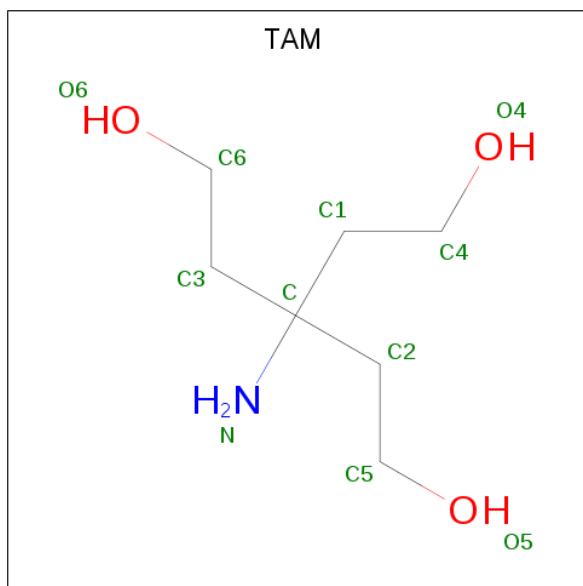
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	1
			33	20	8	5			
2	F	3	Total	C	N	O	0	0	1
			33	20	8	5			

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	1
			8	4	2	2		

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			11	7	1	3		

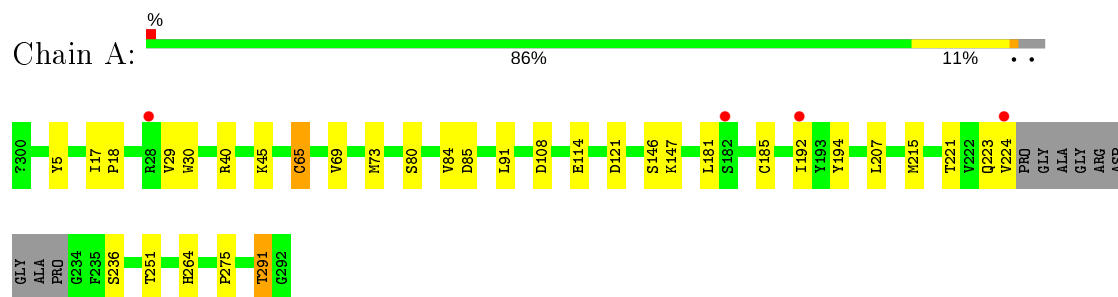
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	30	Total 30	O 30	0	0
5	C	13	Total 13	O 13	0	0
5	D	14	Total 14	O 14	0	0

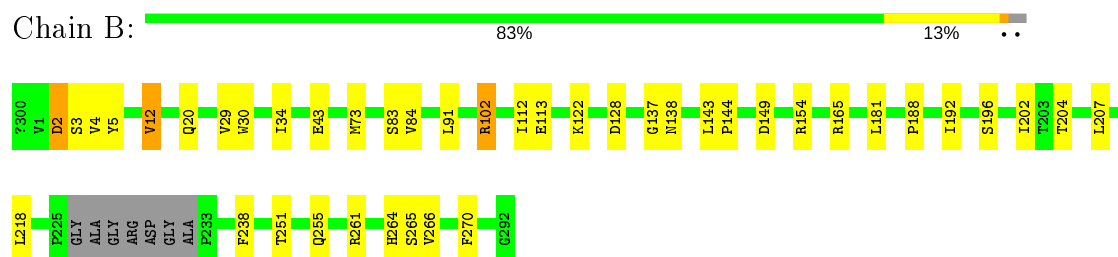
### 3 Residue-property plots [i](#)

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.

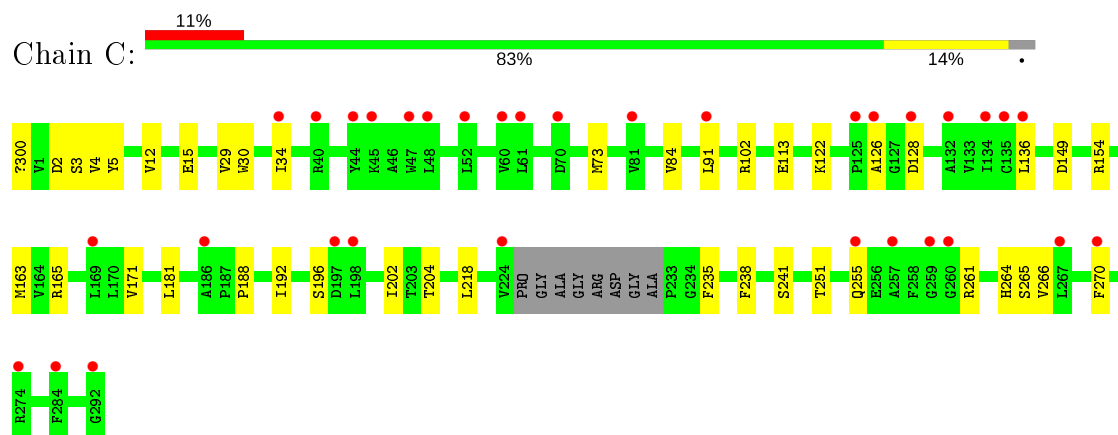
- Molecule 1: Glycine N-methyltransferase



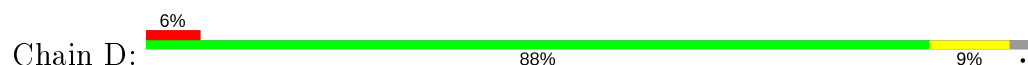
- Molecule 1: Glycine N-methyltransferase

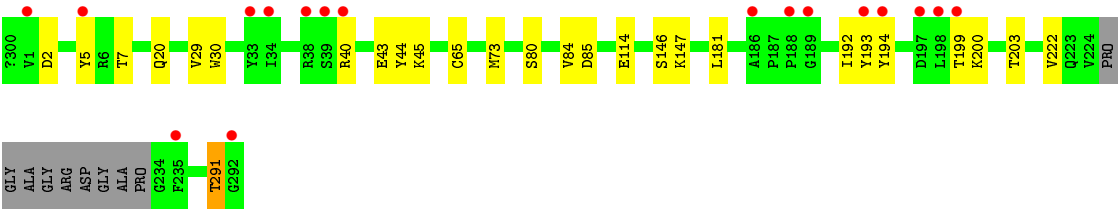


- Molecule 1: Glycine N-methyltransferase

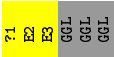


- Molecule 1: Glycine N-methyltransferase

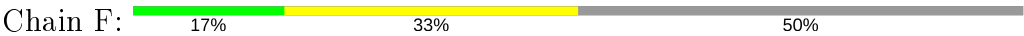




- Molecule 2: 5-methyltetrahydrofolate pentaglutamate



- Molecule 2: 5-methyltetrahydrofolate pentaglutamate





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.04 Å   61.05 Å   146.35 Å 90.00°   128.92°   90.00°	Depositor
Resolution (Å)	48.22 – 2.50 48.22 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.22-2.50) 99.3 (48.22-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.48 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.280 0.227 , 0.273	Depositor DCC
$R_{free}$ test set	2256 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GGL, TAM, 03O, ACE, 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	0.83	3/2276 (0.1%)	0.78	1/3086 (0.0%)
1	B	0.89	1/2296 (0.0%)	0.81	1/3113 (0.0%)
1	C	0.66	0/2275	0.72	2/3085 (0.1%)
1	D	0.82	2/2277 (0.1%)	0.78	0/3087
All	All	0.81	6/9124 (0.1%)	0.77	4/12371 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	CYS	CB-SG	-6.47	1.71	1.82
1	B	43	GLU	CG-CD	6.14	1.61	1.51
1	A	114	GLU	CB-CG	5.99	1.63	1.52
1	D	43	GLU	CG-CD	5.59	1.60	1.51
1	A	114	GLU	CG-CD	5.47	1.60	1.51
1	D	114	GLU	CB-CG	5.42	1.62	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	C	15	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	2	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	121	ASP	CB-CG-OD1	5.05	122.84	118.30

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	2225	0	2176	25	1
1	B	2243	0	2201	25	0
1	C	2224	0	2170	22	1
1	D	2226	0	2180	28	0
2	E	33	0	22	12	0
2	F	33	0	22	13	0
3	B	8	0	10	0	0
4	B	11	0	17	0	0
5	A	31	0	0	0	0
5	B	30	0	0	0	0
5	C	13	0	0	1	0
5	D	14	0	0	1	0
All	All	9091	0	8798	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 5.

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:D:200:LYS:NZ	1:D:222:VAL:HG12	1.20	1.45
1:D:200:LYS:NZ	1:D:222:VAL:CG1	2.02	1.21
1:D:200:LYS:HZ3	1:D:222:VAL:CG1	1.61	1.07
1:A:29:VAL:HG21	1:A:236:SER:HB2	1.51	0.93
1:A:5:TYR:CZ	2:E:2:GGL:HB2	2.08	0.87
1:A:29:VAL:HG21	1:A:236:SER:CB	2.04	0.86
1:D:200:LYS:HZ3	1:D:222:VAL:HG12	1.22	0.85
1:D:200:LYS:HZ3	1:D:222:VAL:HG11	1.43	0.82
2:E:1:03O:C11	2:E:1:03O:O4	2.31	0.77
1:D:200:LYS:HZ2	1:D:222:VAL:HG12	0.86	0.75
2:E:1:03O:H112	2:E:1:03O:O4	1.90	0.72
1:C:300:ACE:H3	1:C:3:SER:OG	1.91	0.71
1:D:5:TYR:CZ	2:F:2:GGL:HB2	2.26	0.68
1:A:185:CYS:SG	5:C:301:HOH:O	2.50	0.68
1:D:5:TYR:CE2	2:F:2:GGL:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LYS:HZ2	1:D:222:VAL:CG1	1.82	0.67
1:B:207:LEU:HD22	2:E:1:03O:H71	1.77	0.67
1:C:149:ASP:O	1:C:154:ARG:NH2	2.27	0.67
1:A:45:LYS:HG3	1:A:73:MET:SD	2.35	0.66
1:A:5:TYR:CE1	2:E:2:GGL:C	2.78	0.66
1:A:5:TYR:CE2	2:E:2:GGL:HB2	2.31	0.65
1:C:29:VAL:HG12	1:C:238:PHE:CD1	2.34	0.63
2:F:1:03O:H112	2:F:1:03O:O4	1.98	0.62
1:C:4:VAL:O	1:C:4:VAL:HG23	1.99	0.61
1:D:40:ARG:HA	1:D:194:TYR:CD1	2.35	0.61
1:A:29:VAL:HG21	1:A:236:SER:HB3	1.82	0.61
1:B:149:ASP:O	1:B:154:ARG:NH2	2.34	0.60
1:D:45:LYS:HG3	1:D:73:MET:SD	2.43	0.59
1:B:5:TYR:HB2	2:F:1:03O:H91	1.85	0.58
2:F:1:03O:C11	2:F:1:03O:O4	2.54	0.55
1:D:65:CYS:HB3	1:D:85:ASP:HB2	1.90	0.53
1:D:291:THR:HG23	1:D:291:THR:O	2.08	0.53
1:C:192:ILE:HD12	1:C:270:PHE:CZ	2.43	0.53
1:C:4:VAL:O	1:C:4:VAL:CG2	2.57	0.52
1:B:264:HIS:CE1	1:B:266:VAL:HG12	2.45	0.52
1:C:264:HIS:CE1	1:C:266:VAL:HG12	2.45	0.52
1:C:84:VAL:HA	1:C:113:GLU:O	2.11	0.51
1:D:29:VAL:CG1	1:D:222:VAL:HG11	2.40	0.51
1:C:251:THR:HG23	1:C:264:HIS:CE1	2.45	0.51
1:A:291:THR:CG2	1:A:291:THR:O	2.58	0.51
1:C:29:VAL:HG12	1:C:238:PHE:HD1	1.75	0.50
1:B:251:THR:HG23	1:B:264:HIS:CE1	2.47	0.50
1:B:143:LEU:HD12	1:B:144:PRO:HD2	1.94	0.49
1:A:207:LEU:HD21	2:F:2:GGL:HA	1.94	0.49
1:B:30:TRP:CZ2	1:B:34:ILE:HG21	2.48	0.49
1:A:30:TRP:CG	1:B:12:VAL:HG22	2.48	0.49
1:D:5:TYR:CD1	2:F:2:GGL:C	2.96	0.48
1:A:291:THR:HG23	1:A:291:THR:O	2.13	0.48
1:B:29:VAL:HG12	1:B:238:PHE:HD1	1.78	0.48
1:C:126:ALA:HB2	1:C:163:MET:CE	2.43	0.48
1:A:207:LEU:CD2	2:F:2:GGL:HA	2.43	0.48
1:A:251:THR:HG23	1:A:264:HIS:CE1	2.49	0.48
1:B:5:TYR:CD1	2:F:1:03O:H16	2.49	0.48
1:D:5:TYR:CE1	2:F:2:GGL:C	2.95	0.48
1:B:204:THR:HG23	1:B:218:LEU:CD2	2.44	0.48
1:C:5:TYR:HB2	2:E:1:03O:C11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:THR:O	1:D:291:THR:CG2	2.62	0.48
1:A:65:CYS:HB3	1:A:85:ASP:HB2	1.96	0.47
1:A:29:VAL:CG2	1:A:236:SER:HB2	2.33	0.47
1:B:188:PRO:HB3	1:B:202:ILE:HD12	1.96	0.47
1:D:44:TYR:CD1	1:D:193:TYR:HD2	2.33	0.47
1:B:4:VAL:HG23	1:B:4:VAL:O	2.14	0.47
1:B:84:VAL:HA	1:B:113:GLU:O	2.15	0.47
1:C:12:VAL:HG22	1:D:30:TRP:CG	2.49	0.46
1:D:29:VAL:HG11	1:D:222:VAL:HG13	1.97	0.46
1:B:2:ASP:OD2	1:D:20:GLN:HG2	2.16	0.46
1:D:29:VAL:CG1	1:D:222:VAL:CG1	2.94	0.46
1:B:83:SER:O	1:B:112:ILE:HA	2.16	0.46
1:A:108:ASP:OD1	1:B:102:ARG:NH1	2.48	0.46
1:A:5:TYR:CB	2:E:1:03O:C17	2.95	0.45
1:B:137:GLY:O	1:B:138:ASN:HB3	2.16	0.45
1:A:215:MET:HE1	2:F:2:GGL:OXT	2.17	0.45
1:B:192:ILE:HD12	1:B:270:PHE:CZ	2.51	0.45
1:B:29:VAL:HG12	1:B:238:PHE:CD1	2.52	0.45
1:C:5:TYR:HB2	2:E:1:03O:H111	1.98	0.45
1:C:136:LEU:HD21	1:C:171:VAL:HG12	2.00	0.44
1:B:20:GLN:HG2	1:D:2:ASP:OD2	2.16	0.44
1:B:207:LEU:CD2	2:E:1:03O:H71	2.45	0.43
1:A:223:GLN:O	1:A:224:VAL:HG23	2.19	0.43
1:C:235:PHE:CG	1:C:235:PHE:O	2.71	0.43
1:C:126:ALA:HB2	1:C:163:MET:HE2	2.00	0.43
1:D:199:THR:O	1:D:200:LYS:HD3	2.18	0.43
1:A:5:TYR:HB3	2:E:1:03O:C17	2.50	0.42
1:D:5:TYR:CE1	2:F:2:GGL:HB2	2.54	0.42
1:A:40:ARG:HA	1:A:194:TYR:CD1	2.55	0.42
1:C:30:TRP:CZ2	1:C:34:ILE:HG21	2.55	0.41
1:C:29:VAL:HG12	1:C:238:PHE:CE1	2.54	0.41
1:C:204:THR:HG23	1:C:218:LEU:CD2	2.50	0.41
1:A:5:TYR:OH	2:E:3:GGL:N	2.53	0.41
1:B:20:GLN:HA	1:D:2:ASP:OD1	2.21	0.41
1:C:241:SER:HB2	1:D:7:THR:HG23	2.01	0.41
1:A:17:ILE:HA	1:A:18:PRO:HD3	1.96	0.41
1:B:3:SER:HB2	2:F:1:03O:O4	2.21	0.41
1:A:29:VAL:CG2	1:A:236:SER:CB	2.89	0.41
1:B:4:VAL:O	1:B:4:VAL:CG2	2.69	0.41
1:D:203:THR:HG22	5:D:297:HOH:O	2.20	0.40
1:C:188:PRO:HB3	1:C:202:ILE:HD12	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:275:PRO:O	1:C:154:ARG:NH1[2_556]	2.17	0.03

## 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	280/293 (96%)	272 (97%)	8 (3%)	0	100	100
1	B	282/293 (96%)	273 (97%)	9 (3%)	0	100	100
1	C	281/293 (96%)	269 (96%)	12 (4%)	0	100	100
1	D	280/293 (96%)	273 (98%)	7 (2%)	0	100	100
All	All	1123/1172 (96%)	1087 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	236/242 (98%)	226 (96%)	10 (4%)	30	54
1	B	239/242 (99%)	227 (95%)	12 (5%)	24	46
1	C	235/242 (97%)	224 (95%)	11 (5%)	26	49
1	D	236/242 (98%)	229 (97%)	7 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	946/968 (98%)	906 (96%)	40 (4%)	30	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	80	SER
1	A	84	VAL
1	A	91	LEU
1	A	146	SER
1	A	147	LYS
1	A	181	LEU
1	A	192	ILE
1	A	221	THR
1	A	291	THR
1	B	12	VAL
1	B	73	MET
1	B	91	LEU
1	B	102	ARG
1	B	122	LYS
1	B	128	ASP
1	B	165	ARG
1	B	181	LEU
1	B	196	SER
1	B	255	GLN
1	B	261	ARG
1	B	265	SER
1	C	73	MET
1	C	91	LEU
1	C	102	ARG
1	C	122	LYS
1	C	128	ASP
1	C	165	ARG
1	C	181	LEU
1	C	196	SER
1	C	255	GLN
1	C	261	ARG
1	C	265	SER
1	D	80	SER
1	D	84	VAL
1	D	146	SER
1	D	147	LYS

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Mol	Chain	Res	Type
1	D	181	LEU
1	D	192	ILE
1	D	291	THR

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	255	GLN
1	B	255	GLN
1	C	150	GLN
1	C	211	ASN
1	C	255	GLN
1	D	138	ASN
1	D	263	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Of 4 non-standard protein/DNA/RNA residues modelled in this entry, 2 are modelled with single atom - leaving 2 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	$\# Z  > 2$
2	GGL	E	2	2	4,8,9	0.59	0	2,9,11	0.65	0
2	GGL	F	2	2	4,8,9	0.61	0	2,9,11	0.92	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	GGL	E	2	2	-	3/3/8/9	-
2	GGL	F	2	2	-	3/3/8/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GGL	N-CA-CB-CG
2	E	2	GGL	C-CA-CB-CG
2	E	2	GGL	CA-CB-CG-CD
2	F	2	GGL	N-CA-CB-CG
2	F	2	GGL	C-CA-CB-CG
2	F	2	GGL	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GGL	3	0
2	F	2	GGL	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	BME	B	400[B]	1	3,3,3	0.28	0	1,2,2	1.06	0
3	BME	B	400[A]	1	3,3,3	0.96	0	1,2,2	1.66	0
4	TAM	B	293	-	7,10,10	1.78	1 (14%)	9,12,12	1.87	4 (44%)

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
3	BME	B	400[B]	1	-	0/1/1/1	-
3	BME	B	400[A]	1	-	1/1/1/1	-
4	TAM	B	293	-	-	7/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	293	TAM	C1-C4	4.07	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	293	TAM	O4-C4-C1	2.91	119.17	111.39
4	B	293	TAM	C3-C-N	-2.70	100.40	108.09
4	B	293	TAM	O5-C5-C2	2.50	118.08	111.39
4	B	293	TAM	C3-C-C2	2.28	114.53	110.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400[A]	BME	O1-C1-C2-S2
4	B	293	TAM	C2-C-C1-C4
4	B	293	TAM	N-C-C1-C4
4	B	293	TAM	C1-C-C2-C5
4	B	293	TAM	C-C3-C6-O6
4	B	293	TAM	C3-C-C1-C4
4	B	293	TAM	C3-C-C2-C5
4	B	293	TAM	N-C-C2-C5

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	2:GGL	C	3:GGL	N	5.60
1	E	2:GGL	C	3:GGL	N	4.73

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	283/293 (96%)	0.08	4 (1%) 75 77	30, 39, 57, 68	1 (0%)
1	B	285/293 (97%)	-0.07	0 100 100	28, 37, 48, 57	0
1	C	284/293 (96%)	0.69	33 (11%) 4 4	28, 37, 48, 57	1 (0%)
1	D	283/293 (96%)	0.32	17 (6%) 21 22	30, 39, 57, 68	0
2	E	0/6	-	-	-	-
2	F	0/6	-	-	-	-
All	All	1135/1184 (95%)	0.26	54 (4%) 30 32	28, 38, 53, 68	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	292	GLY	7.4
1	D	189	GLY	7.0
1	C	270	PHE	6.2
1	D	188	PRO	5.9
1	C	292	GLY	5.5
1	D	39	SER	5.4
1	D	38	ARG	4.9
1	D	199	THR	4.8
1	C	61	LEU	4.7
1	D	40	ARG	4.6
1	C	48	LEU	4.5
1	C	255	GLN	4.3
1	C	134	ILE	4.1
1	D	235	PHE	4.1
1	C	126	ALA	4.0
1	C	186	ALA	4.0
1	C	135	CYS	3.9
1	D	198	LEU	3.9
1	C	132	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	125	PRO	3.6
1	C	197	ASP	3.6
1	C	259	GLY	3.4
1	C	136	LEU	3.3
1	A	192	ILE	3.2
1	C	52	LEU	3.2
1	C	198	LEU	3.1
1	C	60	VAL	3.0
1	D	194	TYR	3.0
1	C	169	LEU	2.9
1	C	284	PHE	2.8
1	C	34	ILE	2.7
1	C	44	TYR	2.7
1	C	70	ASP	2.7
1	C	128	ASP	2.6
1	C	260	GLY	2.6
1	A	182	SER	2.6
1	D	1	VAL	2.4
1	A	224	VAL	2.4
1	D	186	ALA	2.4
1	D	197	ASP	2.3
1	C	40	ARG	2.3
1	C	81	VAL	2.3
1	D	34	ILE	2.3
1	D	5	TYR	2.3
1	A	28	ARG	2.2
1	C	274	ARG	2.2
1	C	45	LYS	2.2
1	C	257	ALA	2.2
1	C	47	TRP	2.2
1	C	224	VAL	2.2
1	D	33	TYR	2.1
1	D	193	TYR	2.1
1	C	91	LEU	2.1
1	C	267	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GGL	F	3	1/10	0.36	0.59	98,98,98,98	0
2	GGL	E	2	9/10	0.72	0.36	95,96,98,98	0
2	GGL	E	3	1/10	0.74	0.22	99,99,99,99	0
2	GGL	F	2	9/10	0.83	0.47	96,97,99,99	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TAM	B	293	11/11	0.68	0.25	62,67,68,72	0
3	BME	B	400[A]	4/4	0.75	0.28	43,45,45,50	4
3	BME	B	400[B]	4/4	0.75	0.28	33,40,45,52	4

### 6.5 Other polymers [i](#)

There are no such residues in this entry.