



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 04:45 PM EDT

PDB ID : 4L8W  
Title : Crystal structure of gamma glutamyl hydrolase (H218N) from zebrafish complex with MTX polyglutamate  
Authors : Chuankhayan, P.; Kao, T.-T.; Chen, C.-J.; Fu, T.-F.  
Deposited on : 2013-06-18  
Resolution : 2.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
buster-report	:	1.1.7 (2018)
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)	:	2.37.1

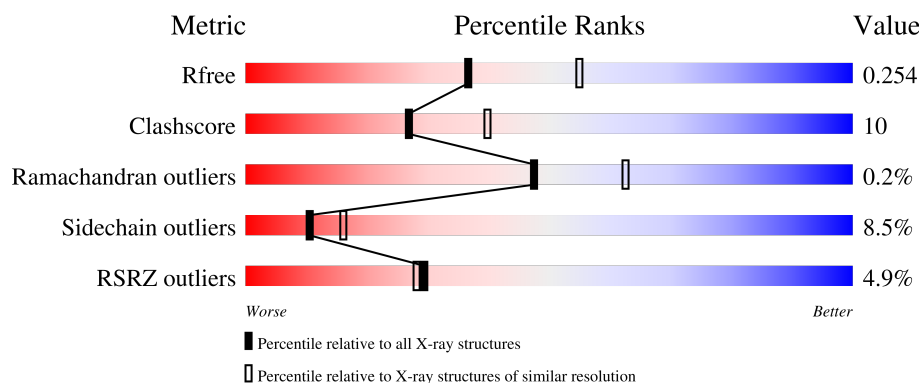
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


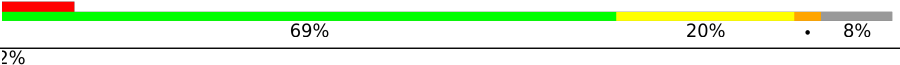
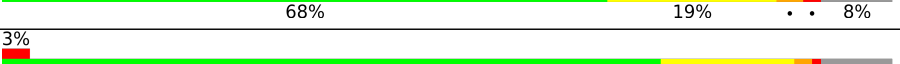
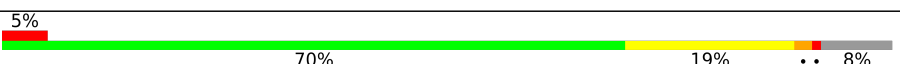

The reported resolution of this entry is 2.39 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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	B	312	 4% 72% 17% 8%
1	D	312	 8% 69% 20% 8%
1	E	312	 2% 68% 19% 8%
1	G	312	 3% 74% 15% 8%
1	I	312	 5% 70% 19% 8%

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Mol	Chain	Length	Quality of chain
1	K	312	<div><div></div><div>5%</div><div>69%</div><div>20%</div><div>• • 8%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14329 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.

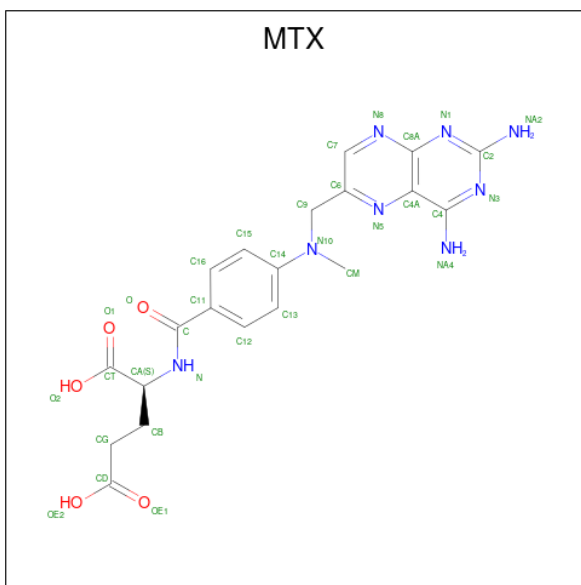
- Molecule 1 is a protein called Gamma-glutamyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	I	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	B	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	E	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	G	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	K	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			

There are 6 discrepancies between the modelled and reference sequences:

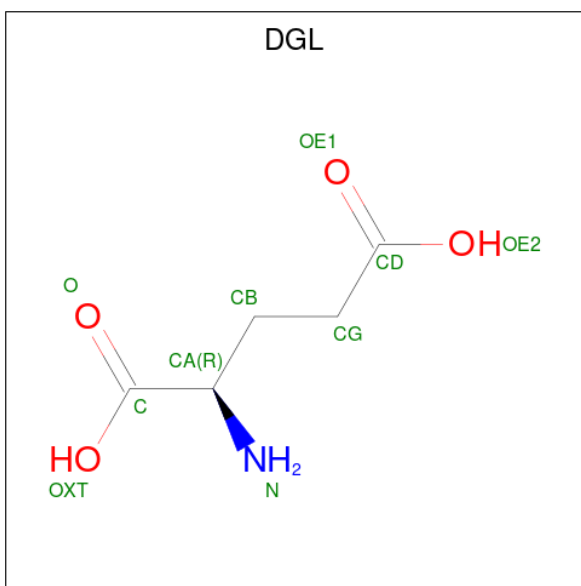
Chain	Residue	Modelled	Actual	Comment	Reference
D	218	ASN	HIS	engineered mutation	UNP Q6NY42
I	218	ASN	HIS	engineered mutation	UNP Q6NY42
B	218	ASN	HIS	engineered mutation	UNP Q6NY42
E	218	ASN	HIS	engineered mutation	UNP Q6NY42
G	218	ASN	HIS	engineered mutation	UNP Q6NY42
K	218	ASN	HIS	engineered mutation	UNP Q6NY42

- Molecule 2 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total 32	C 20	N 8	O 4	0	0
2	G	1	Total 32	C 20	N 8	O 4	0	0

- Molecule 3 is D-GLUTAMIC ACID (three-letter code: DGL) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total 9	C 5	N 1	O 3	0	0
3	I	1	Total 10	C 5	N 1	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			9	5	1	3		
3	G	1	Total	C	N	O	0	0
			10	5	1	4		

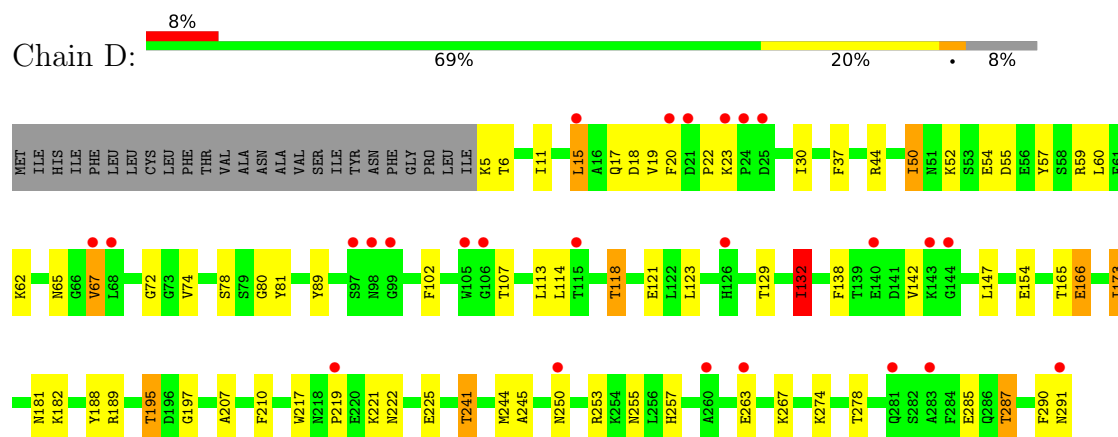
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	42	Total	O	0	0
			42	42		
4	I	58	Total	O	0	0
			58	58		
4	B	84	Total	O	0	0
			84	84		
4	E	75	Total	O	0	0
			75	75		
4	G	95	Total	O	0	0
			95	95		
4	K	31	Total	O	0	0
			31	31		

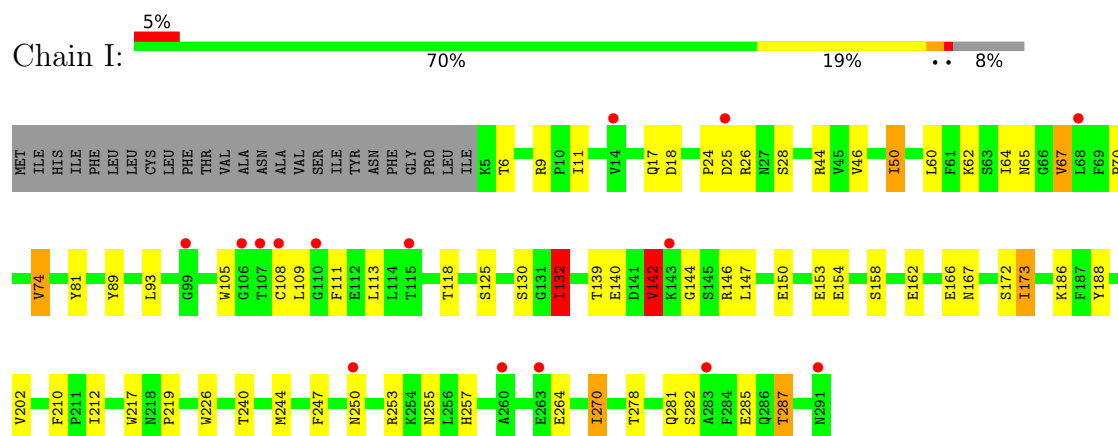
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

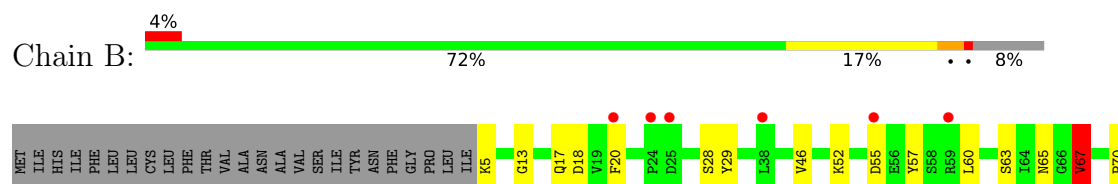
#### • Molecule 1: Gamma-glutamyl hydrolase

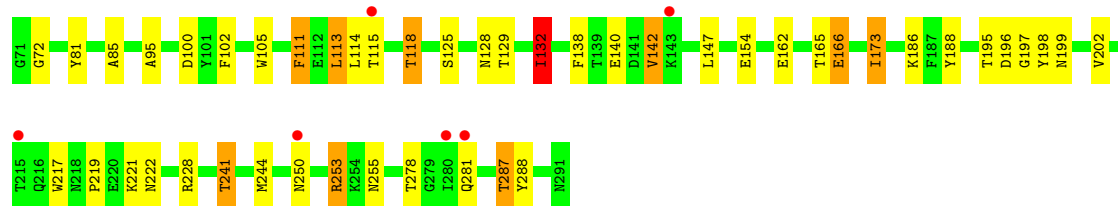


#### • Molecule 1: Gamma-glutamyl hydrolase

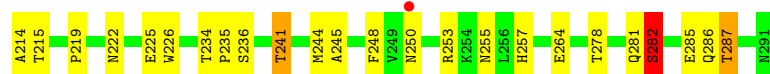
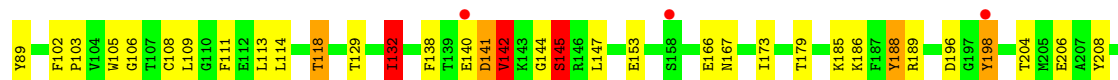


#### • Molecule 1: Gamma-glutamyl hydrolase

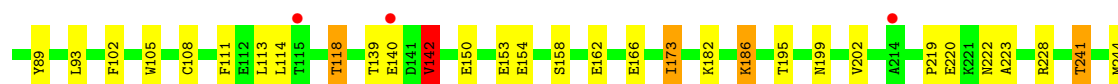
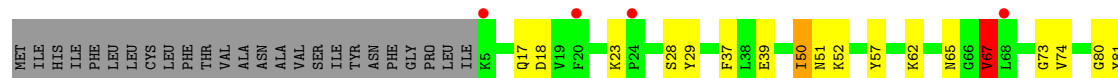
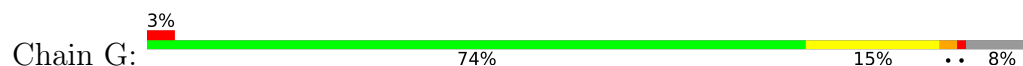




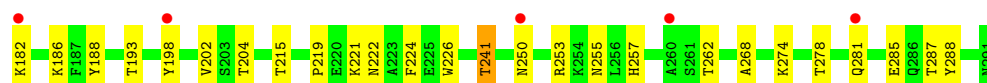
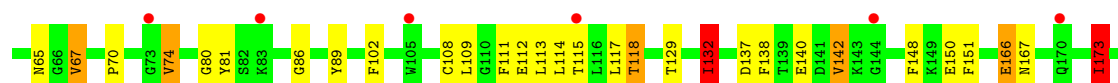
• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.59Å 60.41Å 157.06Å 90.00° 100.98° 90.00°	Depositor
Resolution (Å)	29.63 – 2.39 29.63 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.63-2.39) 98.5 (29.63-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.193 , 0.258 0.193 , 0.254	Depositor DCC
$R_{free}$ test set	4102 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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 i

### 5.1 Standard geometry i

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

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	B	1.09	9/2371 (0.4%)	0.93	5/3217 (0.2%)
1	D	0.99	3/2371 (0.1%)	0.87	3/3217 (0.1%)
1	E	1.06	5/2371 (0.2%)	0.91	6/3217 (0.2%)
1	G	1.09	7/2371 (0.3%)	0.88	3/3217 (0.1%)
1	I	1.02	2/2371 (0.1%)	0.89	4/3217 (0.1%)
1	K	0.95	4/2371 (0.2%)	0.84	2/3217 (0.1%)
All	All	1.03	30/14226 (0.2%)	0.89	23/19302 (0.1%)

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	I	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	108	CYS	CB-SG	-7.78	1.69	1.82
1	B	188	TYR	CD1-CE1	-7.41	1.28	1.39
1	B	154	GLU	CG-CD	7.02	1.62	1.51
1	G	154	GLU	CG-CD	6.25	1.61	1.51
1	K	140	GLU	CG-CD	6.24	1.61	1.51
1	E	188	TYR	CD2-CE2	-6.21	1.30	1.39
1	G	140	GLU	CG-CD	6.16	1.61	1.51
1	D	188	TYR	CD2-CE2	-6.03	1.30	1.39
1	B	154	GLU	CB-CG	5.99	1.63	1.52
1	G	220	GLU	CG-CD	5.92	1.60	1.51
1	G	223	ALA	CA-CB	5.82	1.64	1.52
1	B	140	GLU	CG-CD	5.79	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	188	TYR	CD2-CE2	-5.77	1.30	1.39
1	B	142	VAL	CB-CG1	-5.73	1.40	1.52
1	E	140	GLU	CG-CD	5.73	1.60	1.51
1	E	188	TYR	CD1-CE1	-5.72	1.30	1.39
1	K	140	GLU	CB-CG	5.65	1.62	1.52
1	B	188	TYR	CD2-CE2	-5.64	1.30	1.39
1	K	188	TYR	CD1-CE1	-5.54	1.31	1.39
1	G	150	GLU	CG-CD	5.49	1.60	1.51
1	B	198	TYR	CD1-CE1	-5.43	1.31	1.39
1	D	154	GLU	CG-CD	5.35	1.59	1.51
1	G	39	GLU	CG-CD	5.34	1.59	1.51
1	I	153	GLU	CG-CD	5.33	1.59	1.51
1	B	198	TYR	CD2-CE2	-5.19	1.31	1.39
1	E	198	TYR	CB-CG	5.05	1.59	1.51
1	I	188	TYR	CE2-CZ	-5.04	1.31	1.38
1	E	56	GLU	CG-CD	5.04	1.59	1.51
1	B	197	GLY	C-N	-5.02	1.22	1.34
1	D	154	GLU	CB-CG	5.00	1.61	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ILE	CB-CA-C	-7.24	97.11	111.60
1	E	50	ILE	C-N-CA	-6.60	105.20	121.70
1	G	67	VAL	CB-CA-C	-6.34	99.35	111.40
1	B	132	ILE	CB-CA-C	-6.23	99.14	111.60
1	I	67	VAL	CB-CA-C	-6.09	99.82	111.40
1	G	142	VAL	CB-CA-C	-6.08	99.85	111.40
1	B	67	VAL	CB-CA-C	-6.06	99.89	111.40
1	E	132	ILE	CB-CA-C	-5.94	99.72	111.60
1	E	142	VAL	CB-CA-C	-5.92	100.16	111.40
1	G	228	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	E	9	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	I	132	ILE	CB-CA-C	-5.69	100.22	111.60
1	B	253	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	189	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	15	LEU	CA-CB-CG	-5.48	102.69	115.30
1	K	132	ILE	CB-CA-C	-5.46	100.67	111.60
1	E	196	ASP	CB-CG-OD1	5.42	123.18	118.30
1	E	67	VAL	CB-CA-C	-5.33	101.27	111.40
1	B	142	VAL	CB-CA-C	-5.33	101.28	111.40
1	I	142	VAL	CB-CA-C	-5.29	101.35	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	K	173	ILE	CB-CA-C	-5.23	101.15	111.60
1	I	67	VAL	CG1-CB-CG2	5.03	118.95	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	144	GLY	Peptide

## 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	B	2307	0	2227	42	0
1	D	2307	0	2228	53	0
1	E	2307	0	2228	55	0
1	G	2307	0	2228	39	0
1	I	2307	0	2228	42	0
1	K	2307	0	2228	56	0
2	G	32	0	20	3	0
2	I	32	0	20	1	0
3	G	19	0	10	0	0
3	I	19	0	10	0	0
4	B	84	0	0	0	0
4	D	42	0	0	2	0
4	E	75	0	0	0	0
4	G	95	0	0	0	0
4	I	58	0	0	1	0
4	K	31	0	0	0	0
All	All	14329	0	13427	280	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 10.

All (280) 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:129:THR:HA	1:D:132:ILE:HD11	1.35	1.04
1:D:65:ASN:HD22	1:D:255:ASN:HD22	1.05	1.03
1:I:250:ASN:ND2	1:I:253:ARG:HH11	1.61	0.97
1:K:250:ASN:ND2	1:K:253:ARG:HH11	1.63	0.96
1:G:50:ILE:HD11	1:G:81:TYR:HA	1.46	0.96
1:I:65:ASN:HD22	1:I:255:ASN:HD22	1.02	0.94
1:K:65:ASN:HD22	1:K:255:ASN:HD22	1.06	0.94
1:D:222:ASN:HB2	1:D:241:THR:CG2	1.97	0.93
1:I:173:ILE:CD1	1:I:202:VAL:HB	2.02	0.90
1:I:105:TRP:HH2	1:I:244:MET:HE3	1.39	0.86
1:E:278:THR:HG21	1:E:287:THR:HG23	1.59	0.84
1:G:65:ASN:HD22	1:G:255:ASN:HD22	1.21	0.84
1:E:219:PRO:O	1:E:241:THR:HB	1.78	0.83
1:I:250:ASN:ND2	1:I:253:ARG:NH1	2.28	0.82
1:B:222:ASN:HB2	1:B:241:THR:CG2	2.10	0.81
1:G:219:PRO:O	1:G:241:THR:HB	1.81	0.80
1:I:65:ASN:HD22	1:I:255:ASN:ND2	1.79	0.79
1:K:173:ILE:HD13	1:K:202:VAL:HB	1.65	0.79
1:E:65:ASN:HD22	1:E:255:ASN:HD22	1.33	0.76
1:K:129:THR:HA	1:K:132:ILE:HD11	1.67	0.76
1:G:50:ILE:HG23	1:G:51:ASN:CG	2.07	0.75
1:B:65:ASN:HD22	1:B:255:ASN:HD22	1.35	0.74
1:K:204:THR:HG23	1:K:215:THR:HG22	1.67	0.74
1:I:173:ILE:HD13	1:I:202:VAL:HB	1.68	0.74
1:K:114:LEU:O	1:K:118:THR:HG23	1.89	0.72
1:G:50:ILE:HD11	1:G:81:TYR:CA	2.19	0.72
1:D:222:ASN:HB2	1:D:241:THR:HG22	1.70	0.72
1:D:222:ASN:HB2	1:D:241:THR:HG21	1.71	0.72
1:B:173:ILE:HD12	1:B:202:VAL:HB	1.73	0.71
1:K:222:ASN:HB2	1:K:241:THR:CG2	2.21	0.70
1:E:222:ASN:HB2	1:E:241:THR:CG2	2.21	0.70
1:K:50:ILE:HD11	1:K:81:TYR:H	1.54	0.70
1:K:222:ASN:HB2	1:K:241:THR:HG21	1.73	0.70
1:G:50:ILE:HG23	1:G:51:ASN:ND2	2.07	0.70
1:B:250:ASN:ND2	1:B:253:ARG:HH11	1.90	0.70
1:D:114:LEU:O	1:D:118:THR:HG23	1.93	0.69
1:K:250:ASN:HD22	1:K:253:ARG:HD2	1.57	0.69
1:K:250:ASN:ND2	1:K:253:ARG:NH1	2.39	0.69
1:K:278:THR:HG21	1:K:287:THR:CG2	2.23	0.69
1:G:50:ILE:CG2	1:G:51:ASN:ND2	2.56	0.68
1:E:278:THR:CG2	1:E:287:THR:HG23	2.24	0.68
1:E:114:LEU:O	1:E:118:THR:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ILE:HG13	1:G:80:GLY:HA3	1.76	0.67
1:K:67:VAL:HG22	1:K:102:PHE:HE2	1.57	0.67
1:K:255:ASN:HD21	1:K:257:HIS:CG	2.12	0.67
1:D:129:THR:CA	1:D:132:ILE:HD11	2.20	0.67
1:B:278:THR:HG21	1:B:287:THR:HG23	1.74	0.67
1:I:173:ILE:HD11	1:I:202:VAL:HB	1.77	0.67
1:D:166:GLU:HG2	1:D:221:LYS:HD2	1.76	0.67
1:K:138:PHE:CD2	1:K:142:VAL:HG11	2.30	0.66
1:B:105:TRP:HH2	1:B:244:MET:HE1	1.61	0.66
1:D:278:THR:HG21	1:D:287:THR:HG23	1.78	0.66
1:I:105:TRP:CH2	1:I:244:MET:HE3	2.26	0.65
1:B:67:VAL:HG22	1:B:102:PHE:HE2	1.61	0.65
1:D:17:GLN:OE1	1:D:72:GLY:HA3	1.97	0.65
1:I:9:ARG:NH1	4:I:432:HOH:O	2.21	0.65
1:E:129:THR:HA	1:E:132:ILE:HD11	1.80	0.64
1:D:20:PHE:O	1:D:22:PRO:HD3	1.98	0.63
1:K:173:ILE:CD1	1:K:202:VAL:HB	2.27	0.63
1:G:50:ILE:HG13	1:G:80:GLY:C	2.18	0.63
1:K:111:PHE:CE2	1:K:173:ILE:HD11	2.33	0.63
1:D:65:ASN:HD22	1:D:255:ASN:ND2	1.86	0.63
1:K:111:PHE:CZ	1:K:173:ILE:HD11	2.34	0.63
1:E:222:ASN:HB2	1:E:241:THR:HG21	1.80	0.62
1:K:67:VAL:HG22	1:K:102:PHE:CE2	2.34	0.62
1:E:204:THR:HG23	1:E:215:THR:HG22	1.82	0.62
1:G:139:THR:O	1:G:142:VAL:HG22	1.99	0.62
1:K:137:ASP:HB2	1:K:193:THR:O	1.99	0.62
1:G:105:TRP:HH2	1:G:244:MET:HE3	1.64	0.62
1:D:195:THR:HG23	1:D:197:GLY:H	1.65	0.61
1:B:222:ASN:HB2	1:B:241:THR:HG21	1.81	0.61
1:B:111:PHE:CZ	1:B:173:ILE:HD11	2.37	0.60
1:G:89:TYR:CE2	1:G:93:LEU:HD11	2.37	0.60
1:D:219:PRO:O	1:D:241:THR:HB	2.02	0.60
1:G:50:ILE:HG13	1:G:80:GLY:CA	2.31	0.60
1:I:132:ILE:HD12	1:I:167:ASN:HB2	1.82	0.59
1:B:70:PRO:HD2	1:B:81:TYR:HE1	1.67	0.59
1:D:89:TYR:OH	1:D:118:THR:HB	2.04	0.58
1:G:65:ASN:HD22	1:G:255:ASN:ND2	1.99	0.58
1:D:114:LEU:O	1:D:118:THR:CG2	2.52	0.58
1:K:65:ASN:HD22	1:K:255:ASN:ND2	1.89	0.58
1:K:18:ASP:HB2	1:K:74:VAL:HG21	1.86	0.57
1:I:11:ILE:CG2	1:I:46:VAL:HG23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:VAL:HG22	1:E:102:PHE:HE2	1.69	0.57
1:B:52:LYS:HB2	1:B:57:TYR:CZ	2.40	0.57
1:K:278:THR:CG2	1:K:287:THR:HG22	2.35	0.56
1:D:250:ASN:ND2	1:D:253:ARG:HH11	2.03	0.56
1:I:62:LYS:O	1:I:257:HIS:HB3	2.05	0.56
1:E:281:GLN:O	1:E:282:SER:O	2.24	0.56
1:E:118:THR:HG21	1:E:188:TYR:OH	2.06	0.56
1:E:281:GLN:HA	1:E:281:GLN:NE2	2.21	0.56
1:K:278:THR:HG21	1:K:287:THR:HG22	1.87	0.56
1:D:67:VAL:HG22	1:D:102:PHE:HE2	1.70	0.55
1:D:62:LYS:O	1:D:257:HIS:HB3	2.06	0.55
1:E:198:TYR:CD1	1:E:198:TYR:O	2.60	0.55
1:K:26:ARG:O	1:K:26:ARG:HG2	2.06	0.55
1:E:250:ASN:ND2	1:E:253:ARG:HH11	2.05	0.55
1:E:141:ASP:OD1	1:E:141:ASP:N	2.40	0.55
1:E:281:GLN:NE2	1:E:281:GLN:CA	2.69	0.55
1:G:255:ASN:ND2	1:G:257:HIS:H	2.05	0.55
1:E:142:VAL:O	1:E:145:SER:HB3	2.07	0.55
1:D:207:ALA:HB3	1:D:210:PHE:O	2.07	0.54
1:B:219:PRO:O	1:B:241:THR:HB	2.06	0.54
1:D:50:ILE:HD11	1:D:81:TYR:HA	1.88	0.54
1:B:114:LEU:O	1:B:118:THR:HG23	2.07	0.54
1:B:278:THR:CG2	1:B:287:THR:HG23	2.39	0.53
1:I:74:VAL:HG12	1:I:109:LEU:HD21	1.89	0.53
1:G:105:TRP:CH2	1:G:244:MET:HE3	2.42	0.53
1:D:278:THR:CG2	1:D:287:THR:HG23	2.39	0.53
1:D:132:ILE:HD12	1:B:128:ASN:CG	2.29	0.53
1:B:196:ASP:OD1	1:B:199:ASN:N	2.41	0.53
1:K:108:CYS:O	1:K:111:PHE:HB3	2.08	0.53
1:K:112:GLU:O	1:K:115:THR:OG1	2.23	0.53
1:K:129:THR:CA	1:K:132:ILE:HD11	2.38	0.52
1:E:255:ASN:ND2	1:E:257:HIS:H	2.08	0.52
1:I:111:PHE:HZ	1:I:173:ILE:HD11	1.75	0.52
1:B:105:TRP:CH2	1:B:244:MET:HE1	2.44	0.52
1:E:70:PRO:HD2	1:E:81:TYR:HE1	1.74	0.52
1:I:24:PRO:O	1:I:25:ASP:HB2	2.08	0.52
1:E:226:TRP:HB2	1:E:285:GLU:OE1	2.09	0.52
1:G:255:ASN:HD21	1:G:257:HIS:CG	2.28	0.52
1:K:250:ASN:ND2	1:K:253:ARG:HD2	2.25	0.52
1:G:222:ASN:HB2	1:G:241:THR:CG2	2.39	0.52
1:B:85:ALA:HB3	1:B:113:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TRP:HH2	1:B:244:MET:CE	2.21	0.52
1:D:52:LYS:HB2	1:D:57:TYR:CE2	2.45	0.51
1:G:73:GLY:O	2:G:301:MTX:H7	2.09	0.51
1:D:166:GLU:CG	1:D:221:LYS:HD2	2.41	0.51
1:D:19:VAL:HG12	1:D:20:PHE:N	2.26	0.51
1:I:173:ILE:HD12	1:I:173:ILE:O	2.09	0.51
1:B:111:PHE:HZ	1:B:173:ILE:HD11	1.74	0.51
1:K:219:PRO:O	1:K:241:THR:HB	2.10	0.50
1:D:52:LYS:HB2	1:D:57:TYR:CZ	2.47	0.50
1:E:138:PHE:HB3	1:E:142:VAL:HG21	1.92	0.50
1:E:103:PRO:HB2	1:E:248:PHE:HE1	1.76	0.50
1:K:278:THR:HG21	1:K:287:THR:HG21	1.92	0.50
1:E:281:GLN:HA	1:E:281:GLN:HE21	1.76	0.50
1:B:29:TYR:HA	1:B:288:TYR:O	2.11	0.50
1:B:105:TRP:CH2	1:B:244:MET:CE	2.95	0.50
1:K:89:TYR:OH	1:K:118:THR:HB	2.12	0.49
1:E:278:THR:OG1	1:E:287:THR:CG2	2.60	0.49
1:G:111:PHE:CE2	1:G:173:ILE:HD11	2.48	0.49
1:K:13:GLY:HA2	1:K:46:VAL:O	2.12	0.49
1:G:222:ASN:HB2	1:G:241:THR:HG21	1.95	0.49
2:G:301:MTX:H7	2:G:301:MTX:HM2	1.93	0.49
1:I:250:ASN:HD22	1:I:253:ARG:HH11	1.55	0.49
1:E:278:THR:OG1	1:E:287:THR:HG22	2.12	0.49
1:K:148:PHE:HA	1:K:151:PHE:CD1	2.48	0.49
1:K:166:GLU:CG	1:K:221:LYS:HD2	2.42	0.49
1:D:250:ASN:ND2	1:D:253:ARG:NH1	2.60	0.49
1:G:17:GLN:O	1:G:28:SER:HA	2.12	0.49
1:B:65:ASN:HD22	1:B:255:ASN:ND2	2.06	0.49
1:G:67:VAL:HG22	1:G:102:PHE:HE2	1.78	0.49
1:E:89:TYR:OH	1:E:118:THR:HB	2.13	0.48
1:D:37:PHE:CE2	1:D:245:ALA:HB2	2.49	0.48
1:D:132:ILE:HD12	1:B:128:ASN:ND2	2.29	0.48
1:K:52:LYS:HB2	1:K:57:TYR:CZ	2.49	0.48
1:K:17:GLN:O	1:K:28:SER:HA	2.14	0.48
1:B:129:THR:HA	1:B:132:ILE:HD11	1.96	0.48
1:E:145:SER:HA	1:E:206:GLU:OE2	2.13	0.48
1:G:114:LEU:O	1:G:118:THR:HG23	2.13	0.48
1:D:132:ILE:HG23	1:B:128:ASN:HB2	1.94	0.48
1:D:138:PHE:CD2	1:D:142:VAL:HG11	2.49	0.47
1:K:198:TYR:O	1:K:198:TYR:CD1	2.67	0.47
1:K:46:VAL:HG22	1:K:268:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:THR:HB	1:B:217:TRP:CE3	2.49	0.47
1:G:278:THR:HG21	1:G:287:THR:HG23	1.96	0.47
1:K:50:ILE:HD11	1:K:81:TYR:N	2.27	0.47
1:K:198:TYR:O	1:K:198:TYR:HD1	1.98	0.47
1:B:95:ALA:O	1:B:100:ASP:HB3	2.15	0.47
1:E:17:GLN:OE1	1:E:72:GLY:HA3	2.15	0.47
1:E:234:THR:O	1:E:235:PRO:C	2.51	0.47
1:E:179:THR:HG23	1:E:185:LYS:HE2	1.95	0.46
1:I:285:GLU:OE2	1:I:285:GLU:HA	2.15	0.46
1:E:50:ILE:HA	1:E:50:ILE:HD12	1.49	0.46
1:E:138:PHE:HB3	1:E:142:VAL:CG2	2.45	0.46
1:D:44:ARG:HD3	1:K:226:TRP:CG	2.50	0.46
1:E:106:GLY:O	1:E:214:ALA:HA	2.15	0.46
1:E:278:THR:HG21	1:E:287:THR:CG2	2.39	0.46
1:E:67:VAL:HG22	1:E:102:PHE:CE2	2.50	0.46
1:E:105:TRP:HH2	1:E:244:MET:HE3	1.80	0.46
1:G:278:THR:OG1	1:G:287:THR:CG2	2.63	0.46
1:D:65:ASN:ND2	1:D:255:ASN:HD22	1.90	0.46
1:E:281:GLN:HB2	1:E:282:SER:H	1.50	0.46
1:I:17:GLN:O	1:I:28:SER:HA	2.15	0.46
1:I:255:ASN:HD21	1:I:257:HIS:CG	2.34	0.46
1:I:89:TYR:CE2	1:I:93:LEU:HD11	2.50	0.46
1:I:146:ARG:NH2	1:I:210:PHE:O	2.49	0.46
1:G:278:THR:OG1	1:G:287:THR:HG23	2.16	0.45
1:B:173:ILE:CD1	1:B:202:VAL:HB	2.45	0.45
1:K:108:CYS:HB3	1:K:109:LEU:H	1.49	0.45
1:D:50:ILE:HA	1:D:50:ILE:HD12	1.53	0.45
1:I:111:PHE:CZ	1:I:173:ILE:HD11	2.51	0.45
1:I:240:THR:O	1:I:244:MET:HG2	2.17	0.45
1:I:226:TRP:CG	1:E:44:ARG:HD3	2.52	0.45
1:B:278:THR:OG1	1:B:287:THR:CG2	2.65	0.45
1:D:197:GLY:HA2	1:B:195:THR:HG23	1.99	0.45
1:I:158:SER:O	1:I:162:GLU:HB2	2.17	0.45
1:D:138:PHE:HD2	1:D:142:VAL:HG11	1.81	0.45
1:I:108:CYS:HG	2:I:301:MTX:CD	2.30	0.45
1:I:70:PRO:HD2	1:I:81:TYR:HE1	1.82	0.45
1:I:50:ILE:HA	1:I:50:ILE:HD12	1.46	0.44
1:B:67:VAL:HG22	1:B:102:PHE:CE2	2.49	0.44
1:G:50:ILE:HA	1:G:50:ILE:HD12	1.67	0.44
1:K:222:ASN:HB2	1:K:241:THR:HG22	1.98	0.44
1:D:173:ILE:H	1:D:173:ILE:HG13	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:TRP:CH2	1:I:244:MET:CE	2.99	0.44
1:K:48:VAL:HG22	1:K:60:LEU:CD1	2.47	0.44
1:I:65:ASN:ND2	1:I:255:ASN:HD22	1.87	0.44
1:B:17:GLN:O	1:B:28:SER:HA	2.17	0.44
1:B:166:GLU:CG	1:B:221:LYS:HD2	2.48	0.44
1:E:189:ARG:HB2	1:E:208:TYR:CE2	2.53	0.44
1:G:158:SER:O	1:G:162:GLU:HB2	2.17	0.44
1:E:264:GLU:OE1	1:G:264:GLU:OE1	2.35	0.44
1:K:132:ILE:HD12	1:K:167:ASN:HB2	1.99	0.44
1:E:103:PRO:HB2	1:E:248:PHE:CE1	2.52	0.44
1:K:86:GLY:HA2	1:K:117:LEU:HD21	2.00	0.44
1:D:11:ILE:HD11	1:D:44:ARG:NH1	2.33	0.44
1:D:19:VAL:HG12	1:D:20:PHE:H	1.83	0.44
1:D:165:THR:HB	1:D:217:TRP:CE3	2.53	0.44
1:D:132:ILE:HD12	1:B:128:ASN:OD1	2.18	0.44
1:D:173:ILE:HA	4:D:310:HOH:O	2.18	0.43
1:D:274:LYS:HD3	1:K:274:LYS:HB3	2.00	0.43
1:G:37:PHE:CE2	1:G:245:ALA:HB2	2.53	0.43
1:K:173:ILE:HD12	1:K:173:ILE:H	1.82	0.43
1:E:225:GLU:OE2	1:E:285:GLU:HG2	2.18	0.43
2:G:301:MTX:HM2	2:G:301:MTX:C7	2.48	0.43
1:I:132:ILE:CD1	1:I:167:ASN:HB2	2.46	0.43
1:K:29:TYR:HA	1:K:288:TYR:O	2.19	0.43
1:B:165:THR:HB	1:B:217:TRP:CD2	2.54	0.43
1:K:226:TRP:HB2	1:K:285:GLU:OE1	2.19	0.43
1:B:17:GLN:OE1	1:B:72:GLY:HA3	2.18	0.43
1:E:37:PHE:CE2	1:E:245:ALA:HB2	2.53	0.43
1:K:111:PHE:HE2	1:K:173:ILE:HD11	1.83	0.43
1:E:23:LYS:HE3	1:E:23:LYS:HA	2.00	0.42
1:D:123:LEU:HD11	1:D:181:ASN:HD22	1.85	0.42
1:B:147:LEU:O	1:B:147:LEU:HD23	2.19	0.42
1:E:132:ILE:HD12	1:E:132:ILE:N	2.34	0.42
1:E:132:ILE:HD12	1:E:167:ASN:HB2	2.00	0.42
1:B:111:PHE:CD2	1:B:111:PHE:C	2.92	0.42
1:G:278:THR:CG2	1:G:287:THR:HG23	2.49	0.42
1:K:36:LYS:HB3	1:K:224:PHE:CE1	2.54	0.42
1:I:270:ILE:HD13	1:I:270:ILE:O	2.19	0.42
1:I:65:ASN:HA	1:I:255:ASN:ND2	2.35	0.42
1:D:30:ILE:HG13	1:D:290:PHE:HE1	1.83	0.42
1:D:278:THR:OG1	1:D:287:THR:CG2	2.67	0.42
1:I:9:ARG:HB3	1:I:44:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PHE:CD2	1:B:142:VAL:HG11	2.54	0.42
1:E:65:ASN:HD22	1:E:255:ASN:ND2	2.08	0.42
1:G:186:LYS:O	1:G:186:LYS:HD3	2.20	0.42
1:D:244:MET:HE3	1:D:244:MET:HB3	1.90	0.42
1:E:198:TYR:O	1:E:198:TYR:CG	2.73	0.42
1:K:60:LEU:O	1:K:61:PHE:C	2.57	0.42
1:D:55:ASP:HB3	1:D:59:ARG:NH2	2.35	0.41
1:B:13:GLY:HA2	1:B:46:VAL:O	2.20	0.41
1:D:5:LYS:HB3	1:D:5:LYS:HE3	1.69	0.41
1:E:255:ASN:HD21	1:E:257:HIS:CG	2.38	0.41
1:E:36:LYS:NZ	1:E:286:GLN:NE2	2.68	0.41
1:G:62:LYS:O	1:G:257:HIS:HB3	2.19	0.41
1:E:108:CYS:O	1:E:111:PHE:HB3	2.19	0.41
1:I:278:THR:OG1	1:I:287:THR:CG2	2.68	0.41
1:E:36:LYS:NZ	1:E:286:GLN:HE21	2.18	0.41
1:K:70:PRO:HD2	1:K:81:TYR:HE1	1.86	0.41
1:D:225:GLU:OE2	1:D:285:GLU:HG2	2.21	0.41
1:I:173:ILE:HD13	1:I:202:VAL:CB	2.43	0.41
1:I:278:THR:OG1	1:I:287:THR:HG23	2.20	0.41
1:E:74:VAL:HG12	1:E:109:LEU:HD21	2.03	0.41
1:G:50:ILE:HD11	1:G:81:TYR:N	2.36	0.41
1:G:195:THR:HA	1:G:199:ASN:O	2.21	0.41
1:D:182:LYS:HB3	4:D:303:HOH:O	2.21	0.41
1:K:50:ILE:HG13	1:K:80:GLY:HA3	2.03	0.41
1:G:52:LYS:HB2	1:G:57:TYR:CZ	2.55	0.40
1:B:115:THR:HG21	1:B:173:ILE:HG12	2.04	0.40
1:G:89:TYR:OH	1:G:118:THR:HB	2.21	0.40
1:G:173:ILE:HD12	1:G:202:VAL:HB	2.04	0.40
1:D:50:ILE:HG13	1:D:80:GLY:HA3	2.02	0.40
1:I:247:PHE:CD2	1:I:247:PHE:C	2.94	0.40
1:E:132:ILE:HD12	1:E:132:ILE:H	1.87	0.40
1:I:217:TRP:O	1:I:219:PRO:HD3	2.22	0.40
1:I:139:THR:O	1:I:142:VAL:HG22	2.21	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	B	285/312 (91%)	271 (95%)	14 (5%)	0	100	100
1	D	285/312 (91%)	270 (95%)	15 (5%)	0	100	100
1	E	285/312 (91%)	271 (95%)	11 (4%)	3 (1%)	14	20
1	G	285/312 (91%)	273 (96%)	12 (4%)	0	100	100
1	I	285/312 (91%)	269 (94%)	16 (6%)	0	100	100
1	K	285/312 (91%)	268 (94%)	17 (6%)	0	100	100
All	All	1710/1872 (91%)	1622 (95%)	85 (5%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	282	SER
1	E	144	GLY
1	E	145	SER

### 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	B	250/272 (92%)	231 (92%)	19 (8%)	13	20
1	D	250/272 (92%)	226 (90%)	24 (10%)	8	12
1	E	250/272 (92%)	229 (92%)	21 (8%)	11	16
1	G	250/272 (92%)	233 (93%)	17 (7%)	16	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	250/272 (92%)	222 (89%)	28 (11%)	6	8
1	K	250/272 (92%)	231 (92%)	19 (8%)	13	20
All	All	1500/1632 (92%)	1372 (92%)	128 (8%)	10	16

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	15	LEU
1	D	18	ASP
1	D	23	LYS
1	D	50	ILE
1	D	54	GLU
1	D	60	LEU
1	D	67	VAL
1	D	74	VAL
1	D	78	SER
1	D	107	THR
1	D	113	LEU
1	D	118	THR
1	D	121	GLU
1	D	132	ILE
1	D	147	LEU
1	D	166	GLU
1	D	173	ILE
1	D	195	THR
1	D	241	THR
1	D	263	GLU
1	D	267	LYS
1	D	287	THR
1	D	291	ASN
1	I	6	THR
1	I	18	ASP
1	I	26	ARG
1	I	50	ILE
1	I	60	LEU
1	I	64	ILE
1	I	67	VAL
1	I	74	VAL
1	I	113	LEU
1	I	118	THR

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Mol	Chain	Res	Type
1	I	125	SER
1	I	130	SER
1	I	132	ILE
1	I	140	GLU
1	I	142	VAL
1	I	147	LEU
1	I	150	GLU
1	I	154	GLU
1	I	166	GLU
1	I	172	SER
1	I	173	ILE
1	I	186	LYS
1	I	212	ILE
1	I	264	GLU
1	I	270	ILE
1	I	281	GLN
1	I	282	SER
1	I	287	THR
1	B	5	LYS
1	B	18	ASP
1	B	20	PHE
1	B	55	ASP
1	B	60	LEU
1	B	63	SER
1	B	67	VAL
1	B	111	PHE
1	B	113	LEU
1	B	118	THR
1	B	125	SER
1	B	132	ILE
1	B	162	GLU
1	B	166	GLU
1	B	173	ILE
1	B	186	LYS
1	B	241	THR
1	B	281	GLN
1	B	287	THR
1	E	18	ASP
1	E	23	LYS
1	E	50	ILE
1	E	58	SER
1	E	67	VAL

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Mol	Chain	Res	Type
1	E	74	VAL
1	E	113	LEU
1	E	118	THR
1	E	132	ILE
1	E	141	ASP
1	E	142	VAL
1	E	145	SER
1	E	147	LEU
1	E	153	GLU
1	E	166	GLU
1	E	173	ILE
1	E	186	LYS
1	E	236	SER
1	E	241	THR
1	E	282	SER
1	E	287	THR
1	G	18	ASP
1	G	23	LYS
1	G	29	TYR
1	G	50	ILE
1	G	67	VAL
1	G	74	VAL
1	G	113	LEU
1	G	118	THR
1	G	142	VAL
1	G	153	GLU
1	G	166	GLU
1	G	173	ILE
1	G	182	LYS
1	G	186	LYS
1	G	241	THR
1	G	282	SER
1	G	287	THR
1	K	5	LYS
1	K	15	LEU
1	K	50	ILE
1	K	58	SER
1	K	60	LEU
1	K	67	VAL
1	K	74	VAL
1	K	113	LEU
1	K	118	THR

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Mol	Chain	Res	Type
1	K	132	ILE
1	K	142	VAL
1	K	150	GLU
1	K	166	GLU
1	K	173	ILE
1	K	182	LYS
1	K	186	LYS
1	K	241	THR
1	K	262	THR
1	K	281	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	216	GLN
1	D	218	ASN
1	D	250	ASN
1	D	255	ASN
1	D	272	ASN
1	D	286	GLN
1	I	128	ASN
1	I	167	ASN
1	I	218	ASN
1	I	250	ASN
1	I	255	ASN
1	I	272	ASN
1	I	281	GLN
1	I	286	GLN
1	B	128	ASN
1	B	216	GLN
1	B	218	ASN
1	B	250	ASN
1	B	255	ASN
1	B	272	ASN
1	B	281	GLN
1	B	286	GLN
1	E	128	ASN
1	E	167	ASN
1	E	170	GLN
1	E	218	ASN
1	E	250	ASN
1	E	255	ASN

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Mol	Chain	Res	Type
1	E	272	ASN
1	E	281	GLN
1	E	286	GLN
1	G	167	ASN
1	G	218	ASN
1	G	250	ASN
1	G	255	ASN
1	G	272	ASN
1	G	286	GLN
1	K	216	GLN
1	K	218	ASN
1	K	250	ASN
1	K	255	ASN
1	K	281	GLN
1	K	286	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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
3	DGL	G	302	3,2	7,8,9	0.87	0	7,9,11	1.15	0
3	DGL	I	303	3	8,9,9	1.92	2 (25%)	10,11,11	1.33	1 (10%)
2	MTX	I	301	3	34,34,35	1.82	4 (11%)	44,47,49	2.11	13 (29%)
2	MTX	G	301	3	34,34,35	1.99	7 (20%)	44,47,49	2.42	13 (29%)
3	DGL	I	302	3,2	7,8,9	0.98	0	7,9,11	1.14	1 (14%)
3	DGL	G	303	3	8,9,9	1.92	2 (25%)	10,11,11	1.25	1 (10%)

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	DGL	G	302	3,2	-	1/7/8/9	-
3	DGL	I	303	3	-	5/9/9/9	-
2	MTX	I	301	3	-	2/23/24/25	0/3/3/3
2	MTX	G	301	3	-	7/23/24/25	0/3/3/3
3	DGL	I	302	3,2	-	3/7/8/9	-
3	DGL	G	303	3	-	7/9/9/9	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	MTX	C7-N8	6.46	1.42	1.31
2	I	301	MTX	C9-C6	-6.28	1.40	1.51
2	G	301	MTX	C9-C6	-5.73	1.41	1.51
2	I	301	MTX	C7-N8	4.81	1.39	1.31
2	I	301	MTX	C11-C	-3.81	1.42	1.50
2	G	301	MTX	C11-C	-3.75	1.42	1.50
3	G	303	DGL	CG-CD	3.27	1.58	1.50
3	I	303	DGL	CG-CD	3.23	1.58	1.50
3	I	303	DGL	CB-CA	2.88	1.59	1.53
3	G	303	DGL	CB-CA	2.83	1.59	1.53
2	G	301	MTX	CM-N10	2.58	1.50	1.46
2	I	301	MTX	CM-N10	2.56	1.50	1.46
2	G	301	MTX	C9-N10	2.50	1.51	1.46
2	G	301	MTX	CA-N	2.11	1.50	1.45
2	G	301	MTX	C6-N5	2.03	1.36	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	MTX	C2-N1-C8A	5.89	122.09	115.36
2	G	301	MTX	N8-C8A-N1	5.22	121.78	115.82
2	G	301	MTX	N1-C2-N3	-5.21	120.28	127.22
2	G	301	MTX	C6-C9-N10	5.04	122.24	113.60
2	I	301	MTX	C2-N1-C8A	4.98	121.04	115.36
2	I	301	MTX	N1-C2-N3	-4.68	120.98	127.22
2	G	301	MTX	CB-CG-CD	-4.42	99.70	112.29
2	I	301	MTX	C6-C7-N8	-4.07	119.14	123.13
2	G	301	MTX	C6-C7-N8	-4.06	119.15	123.13
2	I	301	MTX	N8-C8A-N1	3.93	120.31	115.82
2	I	301	MTX	C6-C9-N10	3.85	120.19	113.60
2	G	301	MTX	C7-N8-C8A	3.78	120.49	116.69
2	G	301	MTX	C7-C6-N5	-3.57	118.52	120.85
2	G	301	MTX	C4-C4A-N5	3.56	123.06	120.33
2	I	301	MTX	CB-CG-CD	-3.43	102.53	112.29
2	I	301	MTX	C15-C14-N10	-3.16	117.07	121.62
2	G	301	MTX	C6-N5-C4A	3.02	122.92	118.04
2	I	301	MTX	C7-N8-C8A	2.72	119.43	116.69
2	I	301	MTX	C8A-C4A-N5	-2.52	119.37	122.41
2	G	301	MTX	O1-CT-CA	-2.49	114.06	122.26
2	G	301	MTX	C8A-C4A-N5	-2.49	119.40	122.41
3	G	303	DGL	CG-CB-CA	2.47	119.60	113.84
3	I	303	DGL	CB-CA-N	2.44	116.57	110.17
2	G	301	MTX	CB-CA-N	2.37	115.66	110.88
3	I	302	DGL	CB-CA-N	-2.33	104.06	110.17
2	I	301	MTX	CA-N-C	-2.32	115.93	121.60
2	I	301	MTX	C4-C4A-N5	2.16	121.99	120.33
2	I	301	MTX	C6-N5-C4A	2.13	121.49	118.04
2	I	301	MTX	C11-C-N	2.01	120.92	117.06

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	302	DGL	C-CA-CB-CG
2	G	301	MTX	N-C-C11-C12
2	G	301	MTX	N-C-C11-C16
2	G	301	MTX	O-C-C11-C12
3	G	303	DGL	OXT-C-CA-CB
2	I	301	MTX	C13-C14-N10-CM
2	I	301	MTX	C15-C14-N10-CM
2	G	301	MTX	O-C-C11-C16
3	G	303	DGL	O-C-CA-CB

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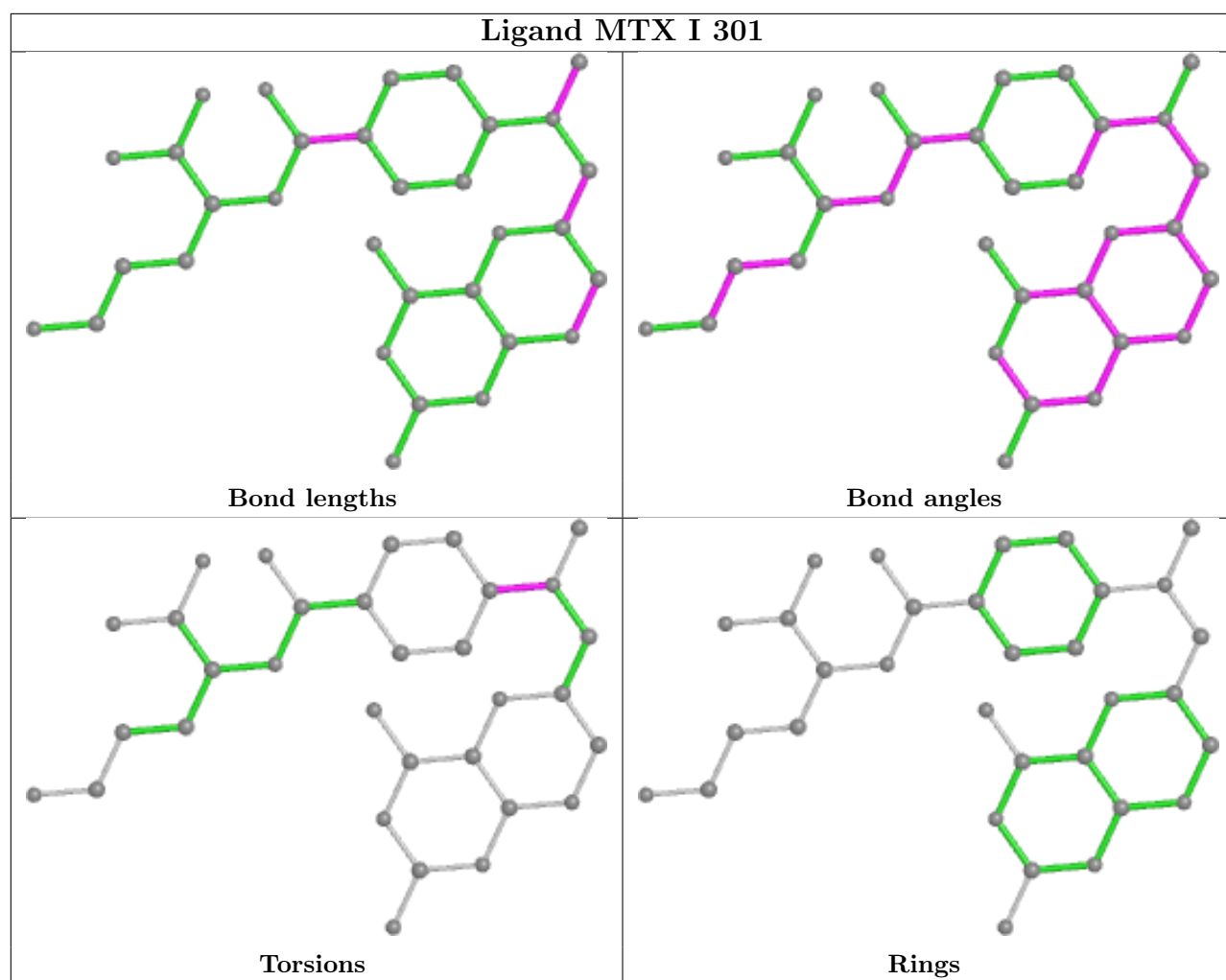
Mol	Chain	Res	Type	Atoms
2	G	301	MTX	C15-C14-N10-CM
3	G	303	DGL	OXT-C-CA-N
2	G	301	MTX	C13-C14-N10-CM
3	I	303	DGL	OXT-C-CA-CB
3	G	303	DGL	CA-CB-CG-CD
3	I	302	DGL	N-CA-CB-CG
3	I	303	DGL	O-C-CA-CB
3	I	303	DGL	CA-CB-CG-CD
2	G	301	MTX	CA-CB-CG-CD
3	G	303	DGL	OE1-CD-CG-CB
3	G	303	DGL	O-C-CA-N
3	I	303	DGL	OE1-CD-CG-CB
3	G	303	DGL	OE2-CD-CG-CB
3	I	303	DGL	OE2-CD-CG-CB
3	G	302	DGL	OXT-C-CA-N
3	I	302	DGL	OXT-C-CA-N

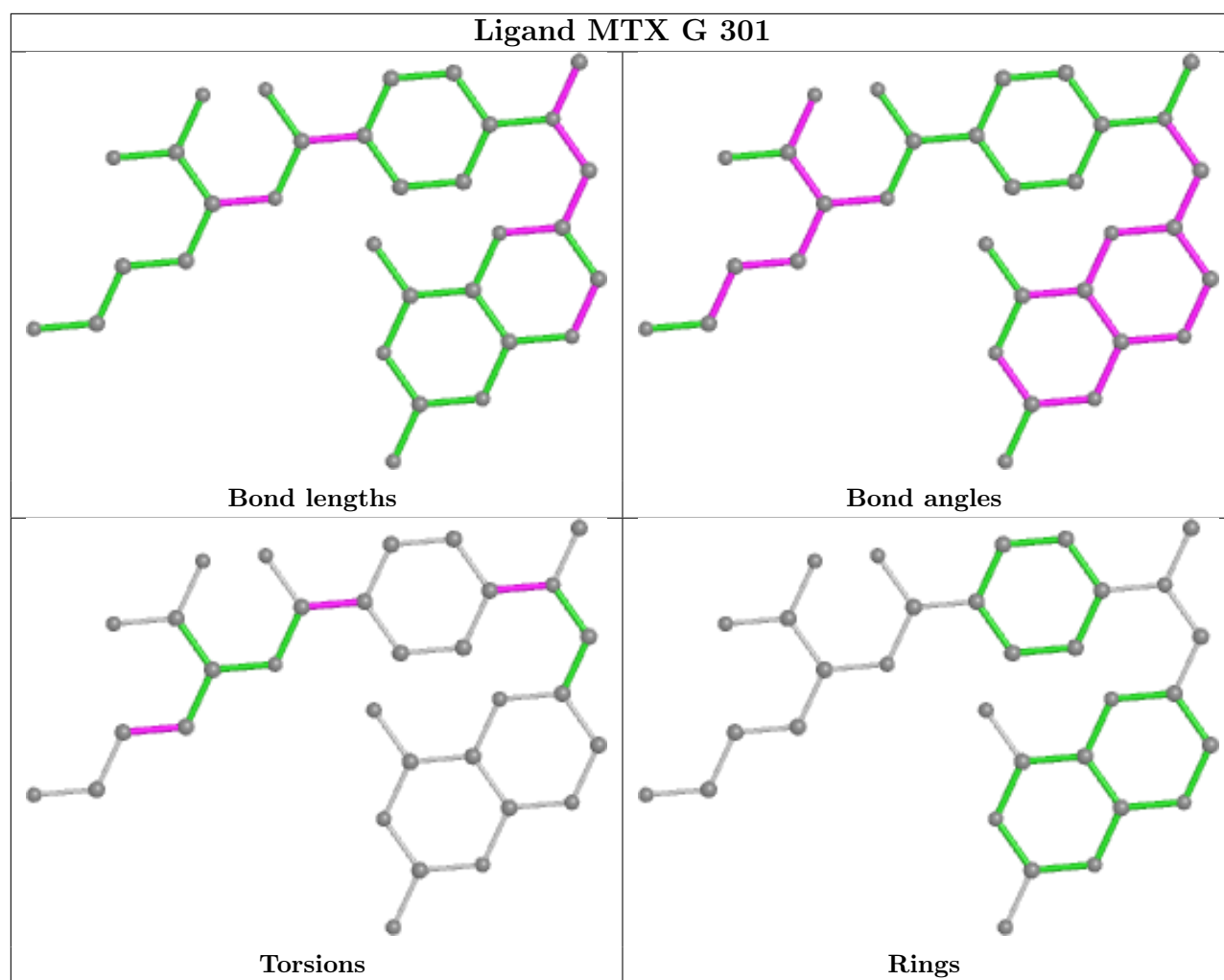
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	301	MTX	1	0
2	G	301	MTX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 ⓘ

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	B	287/312 (91%)	0.09	12 (4%)	36 35	12, 27, 44, 56	5 (1%)
1	D	287/312 (91%)	0.35	25 (8%)	10 9	20, 35, 55, 72	5 (1%)
1	E	287/312 (91%)	0.08	6 (2%)	63 61	14, 28, 45, 57	5 (1%)
1	G	287/312 (91%)	-0.00	10 (3%)	44 43	10, 24, 40, 53	5 (1%)
1	I	287/312 (91%)	0.22	15 (5%)	27 26	18, 31, 49, 56	5 (1%)
1	K	287/312 (91%)	0.41	17 (5%)	22 21	21, 38, 60, 70	5 (1%)
All	All	1722/1872 (91%)	0.19	85 (4%)	29 28	10, 30, 52, 72	30 (1%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	PHE	6.6
1	K	198	TYR	5.1
1	E	20	PHE	4.7
1	D	21	ASP	4.6
1	E	198	TYR	4.3
1	G	20	PHE	4.3
1	D	250	ASN	4.2
1	B	250	ASN	3.8
1	K	250	ASN	3.7
1	I	107	THR	3.5
1	K	20	PHE	3.5
1	E	250	ASN	3.4
1	G	250	ASN	3.3
1	D	24	PRO	3.3
1	D	291	ASN	3.3
1	K	21	ASP	3.3
1	B	115	THR	3.2
1	D	115	THR	3.2
1	G	5	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	250	ASN	3.2
1	D	281	GLN	3.1
1	D	283	ALA	3.1
1	K	144	GLY	3.1
1	K	55	ASP	2.9
1	K	182	LYS	2.9
1	K	59	ARG	2.8
1	D	25	ASP	2.8
1	I	283	ALA	2.8
1	B	281	GLN	2.8
1	I	115	THR	2.8
1	G	115	THR	2.8
1	I	106	GLY	2.7
1	D	23	LYS	2.7
1	D	260	ALA	2.7
1	B	280	ILE	2.7
1	B	55	ASP	2.7
1	E	22	PRO	2.6
1	D	144	GLY	2.6
1	I	110	GLY	2.6
1	B	20	PHE	2.6
1	I	260	ALA	2.6
1	E	140	GLU	2.5
1	K	83	LYS	2.5
1	E	158	SER	2.5
1	I	99	GLY	2.5
1	D	105	TRP	2.5
1	D	106	GLY	2.5
1	D	68	LEU	2.4
1	K	115	THR	2.4
1	K	73	GLY	2.4
1	G	24	PRO	2.4
1	D	67	VAL	2.4
1	G	283	ALA	2.3
1	G	281	GLN	2.3
1	I	291	ASN	2.3
1	K	281	GLN	2.3
1	D	98	ASN	2.3
1	B	59	ARG	2.3
1	I	68	LEU	2.2
1	B	38	LEU	2.2
1	D	99	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	143	LYS	2.2
1	D	143	LYS	2.2
1	D	97	SER	2.2
1	D	126	HIS	2.2
1	I	263	GLU	2.2
1	I	108	CYS	2.1
1	D	219	PRO	2.1
1	I	14	VAL	2.1
1	K	50	ILE	2.1
1	B	24	PRO	2.1
1	K	260	ALA	2.1
1	D	140	GLU	2.1
1	G	68	LEU	2.1
1	D	263	GLU	2.1
1	K	53	SER	2.1
1	I	25	ASP	2.1
1	B	215	THR	2.1
1	K	105	TRP	2.1
1	G	140	GLU	2.0
1	D	15	LEU	2.0
1	B	25	ASP	2.0
1	G	214	ALA	2.0
1	B	143	LYS	2.0
1	K	170	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

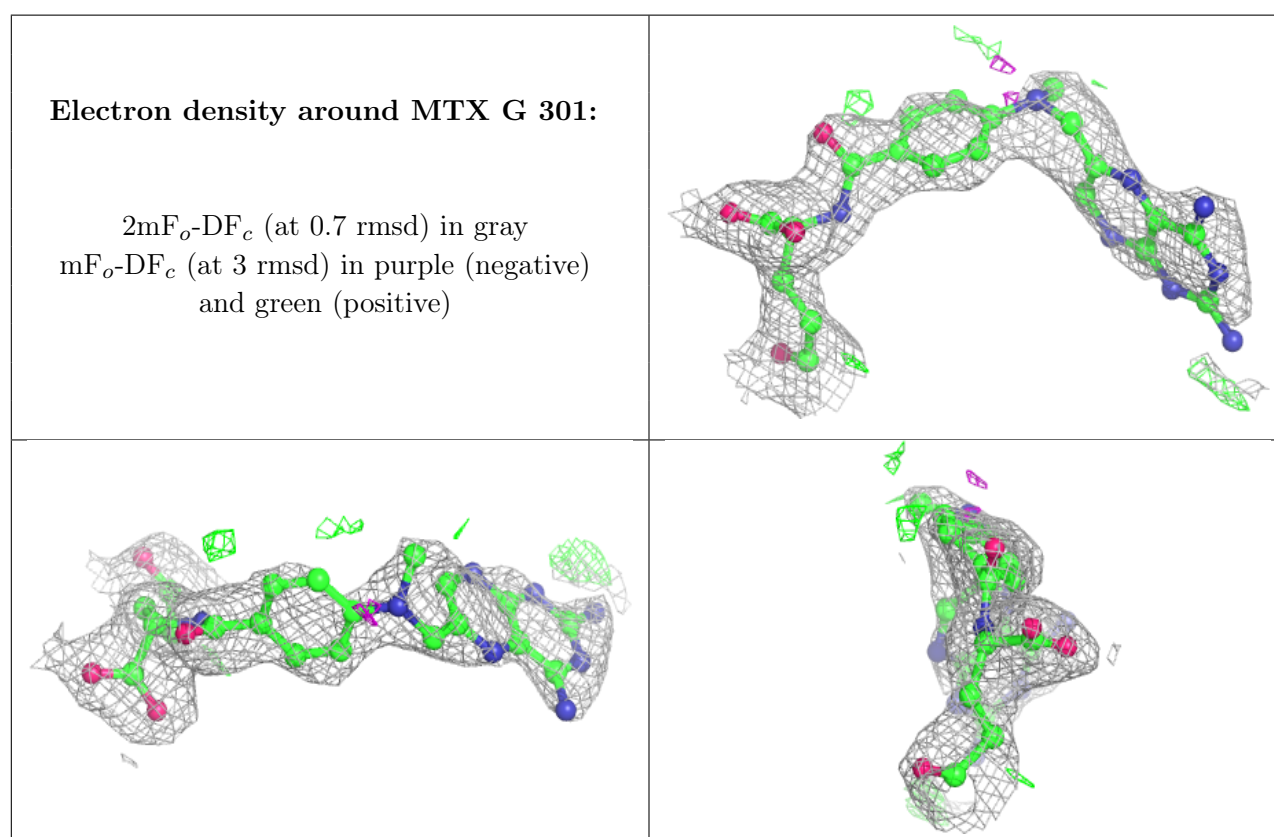
There are no monosaccharides in this entry.

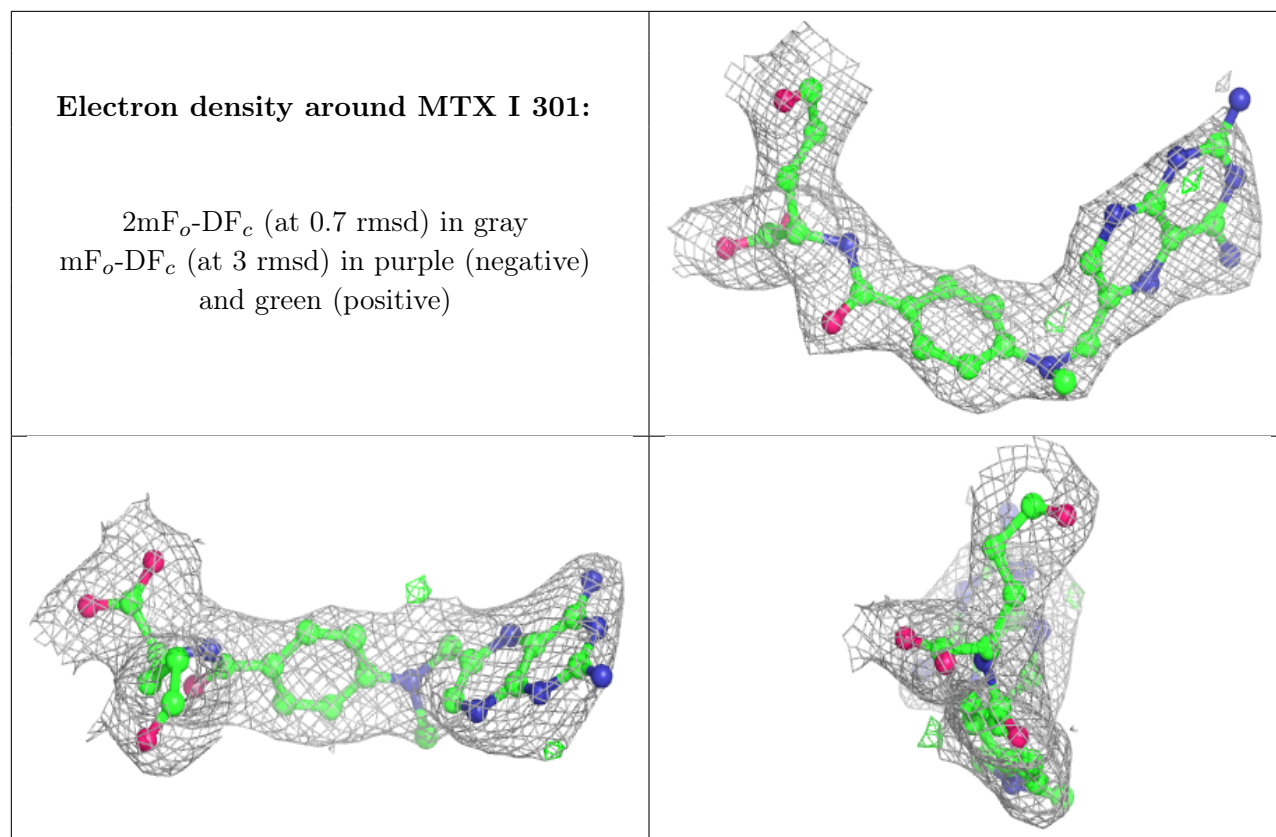
## 6.4 Ligands [i](#)

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
3	DGL	I	303	10/10	0.73	0.30	65,67,69,71	0
3	DGL	G	303	10/10	0.74	0.30	62,65,68,69	0
2	MTX	G	301	32/33	0.75	0.28	44,66,87,87	0
2	MTX	I	301	32/33	0.78	0.20	44,60,79,80	0
3	DGL	I	302	9/10	0.79	0.21	54,59,62,63	0
3	DGL	G	302	9/10	0.83	0.24	52,57,59,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.