



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:11 PM UTC

PDB ID : 4L8W / pdb_00004l8w
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

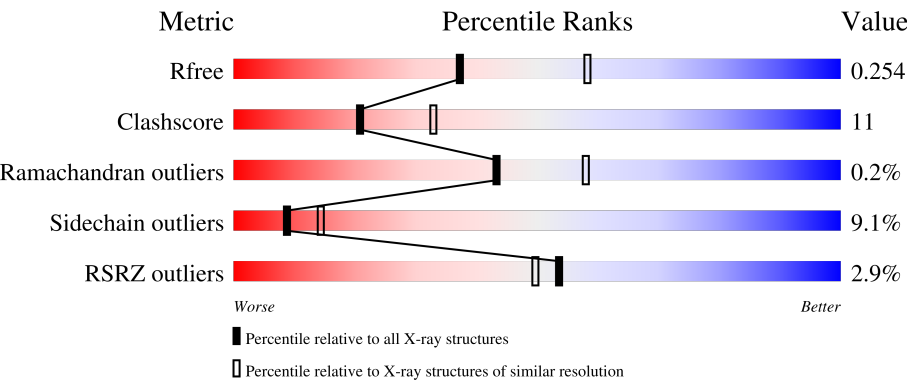
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	2% 70% 19% .. 8%
1	D	312	3% 68% 20% .. 8%
1	E	312	3% 68% 20% .. 8%
1	G	312	3% 72% 17% .. 8%
1	I	312	2% 70% 18% .. 8%

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Mol	Chain	Length	Quality of chain
1	K	312	4% 68% 21% • • 8%

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.

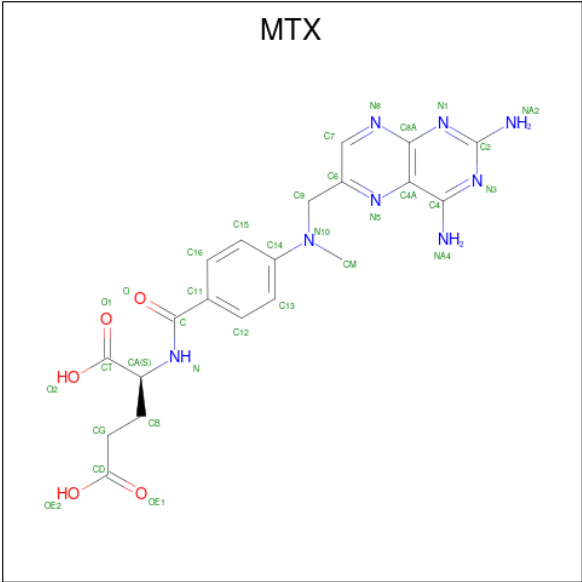
- Molecule 1 is a protein called Gamma-glutamyl hydrolase.

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:

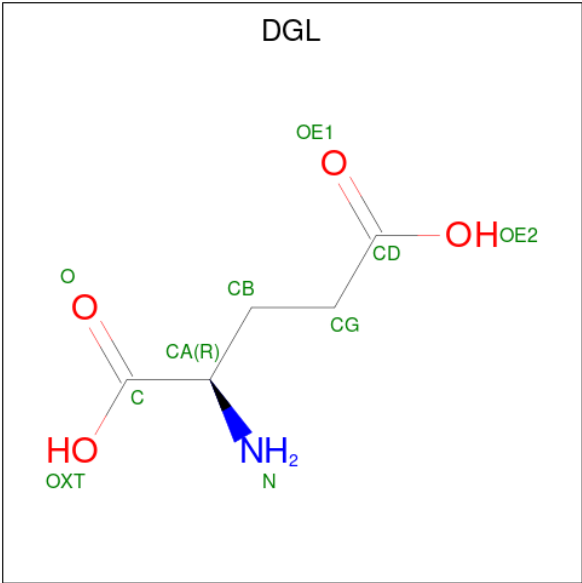
Chain	Residue	Modelled	Actual	Comment	Reference
D	218	ASN	HIS	engineered mutation	UNP Q6NY42
I	218	ASN	HIS	engineered mutation	UNP Q6NY42
B	218	ASN	HIS	engineered mutation	UNP Q6NY42
E	218	ASN	HIS	engineered mutation	UNP Q6NY42
G	218	ASN	HIS	engineered mutation	UNP Q6NY42
K	218	ASN	HIS	engineered mutation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

- Molecule 2 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: C₅H₉NO₄).



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

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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		

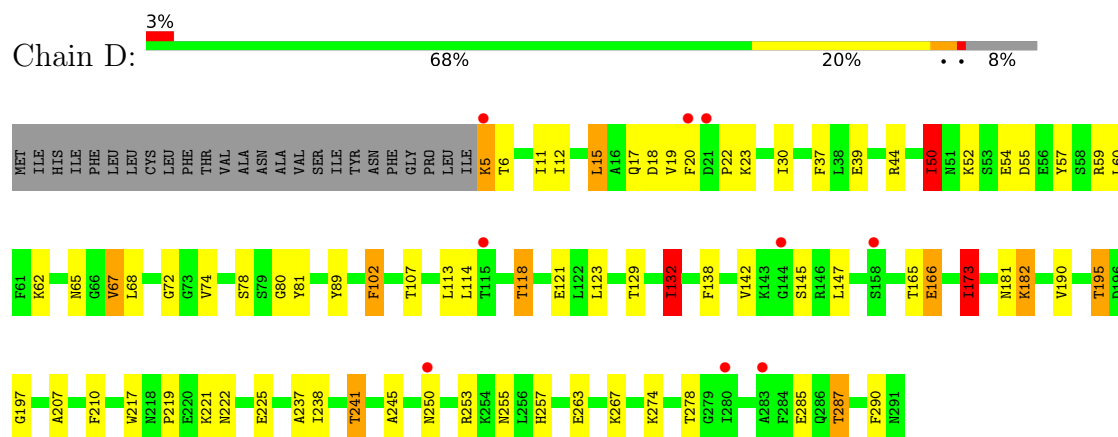
- Molecule 4 is water.

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		

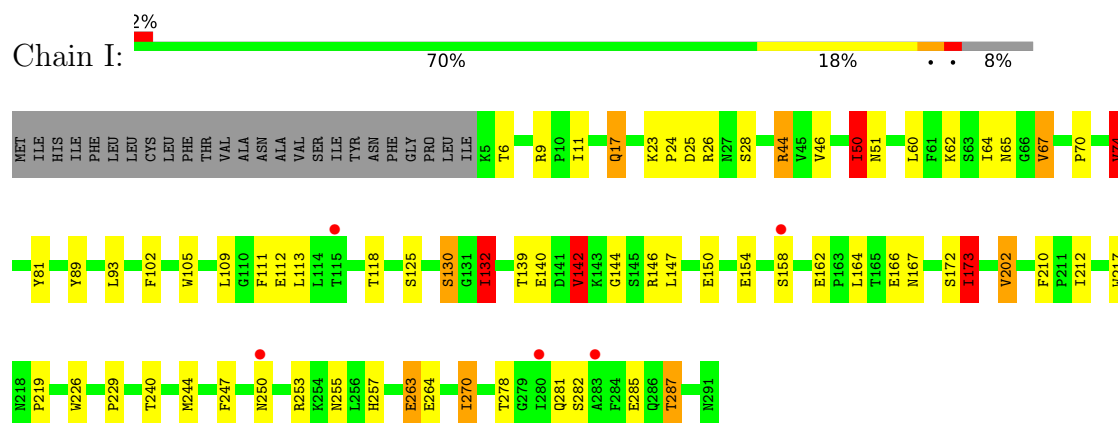
3 Residue-property plots [i](#)

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.

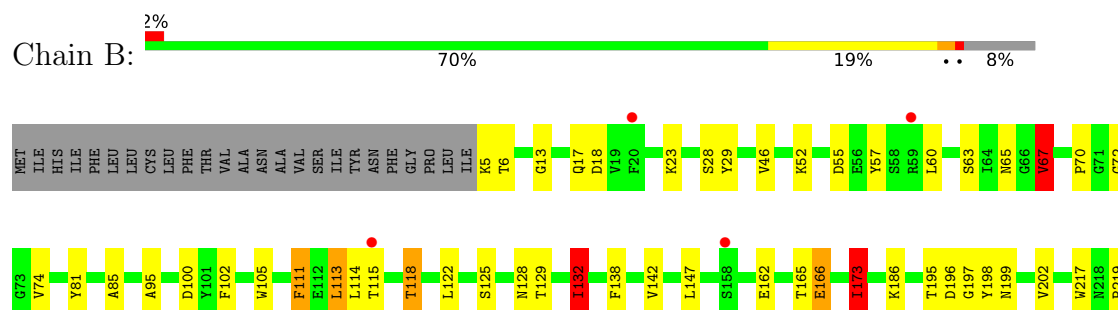
• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase

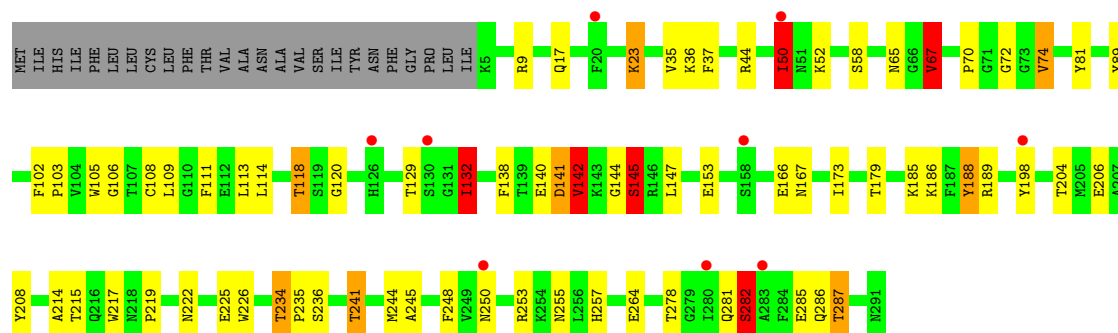


• Molecule 1: Gamma-glutamyl hydrolase

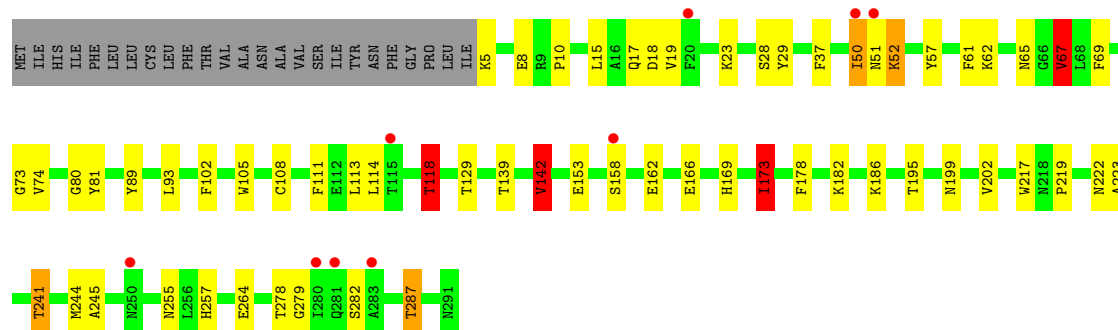




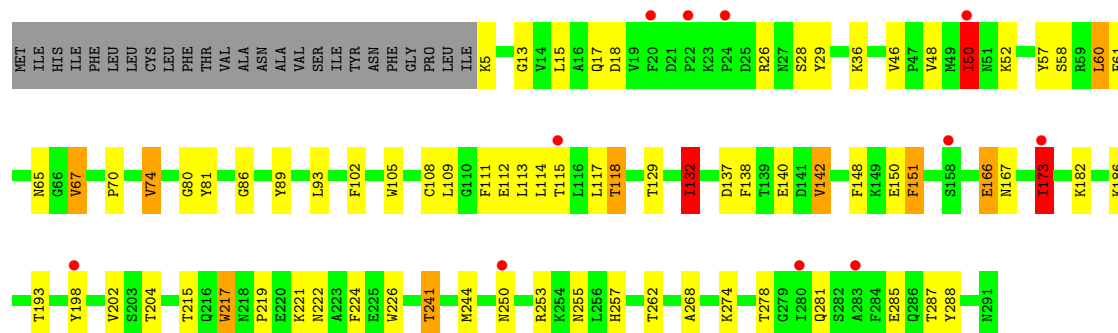
• Molecule 1: Gamma-glutamyl hydrolase



• 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, α , β , γ	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) 98.8 (29.63-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	4157 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DGL, MTX

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	1.20	1/2371 (0.0%)	1.20	8/3217 (0.2%)
1	D	1.10	4/2371 (0.2%)	1.15	8/3217 (0.2%)
1	E	1.16	2/2371 (0.1%)	1.19	10/3217 (0.3%)
1	G	1.21	2/2371 (0.1%)	1.15	8/3217 (0.2%)
1	I	1.14	2/2371 (0.1%)	1.21	17/3217 (0.5%)
1	K	1.06	0/2371	1.13	7/3217 (0.2%)
All	All	1.15	11/14226 (0.1%)	1.17	58/19302 (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	I	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	GLY	C-N	-7.99	1.22	1.33
1	G	223	ALA	CA-CB	6.93	1.64	1.53
1	I	202	VAL	CA-CB	6.02	1.61	1.54
1	G	108	CYS	C-O	-5.62	1.16	1.24
1	D	102	PHE	CA-C	5.43	1.57	1.52
1	D	237	ALA	CA-CB	5.38	1.61	1.53
1	I	229	PRO	C-O	-5.38	1.17	1.24
1	D	190	VAL	CA-CB	5.35	1.60	1.54
1	D	12	ILE	CA-C	-5.20	1.46	1.52
1	E	9	ARG	CA-C	5.19	1.58	1.53
1	E	35	VAL	CA-CB	5.04	1.60	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	50	ILE	CA-C-N	-8.55	105.20	121.54
1	E	50	ILE	C-N-CA	-8.55	105.20	121.54
1	D	132	ILE	CB-CA-C	-7.80	97.11	110.30
1	I	50	ILE	N-CA-C	7.52	118.44	111.45
1	I	23	LYS	CA-C-N	-7.32	112.46	119.85
1	I	23	LYS	C-N-CA	-7.32	112.46	119.85
1	D	50	ILE	N-CA-C	7.21	119.23	111.58
1	I	112	GLU	N-CA-C	-6.76	103.99	111.36
1	I	142	VAL	CB-CA-C	-6.74	101.35	112.26
1	I	102	PHE	CA-C-N	-6.74	113.32	120.66
1	I	102	PHE	C-N-CA	-6.74	113.32	120.66
1	K	50	ILE	N-CA-C	6.66	118.26	111.00
1	B	132	ILE	CB-CA-C	-6.57	99.14	111.30
1	G	67	VAL	CB-CA-C	-6.57	99.35	110.71
1	K	173	ILE	CB-CA-C	-6.50	101.15	110.83
1	B	6	THR	CB-CA-C	-6.40	98.21	110.24
1	E	132	ILE	CB-CA-C	-6.37	99.72	111.18
1	B	67	VAL	CB-CA-C	-6.26	99.89	110.71
1	G	279	GLY	N-CA-C	6.25	121.72	114.16
1	B	173	ILE	CB-CA-C	-6.09	102.55	110.84
1	I	67	VAL	CB-CA-C	-6.08	99.82	110.71
1	E	50	ILE	N-CA-C	6.05	120.88	112.35
1	I	130	SER	N-CA-C	6.02	118.80	111.82
1	D	173	ILE	CB-CA-C	-5.92	102.32	110.96
1	E	67	VAL	CB-CA-C	-5.89	101.27	110.69
1	K	132	ILE	CB-CA-C	-5.84	100.67	111.18
1	I	173	ILE	CB-CA-C	-5.80	103.95	110.96
1	B	240	THR	N-CA-C	-5.78	104.89	111.07
1	I	132	ILE	CB-CA-C	-5.70	100.22	110.48
1	G	173	ILE	CB-CA-C	-5.69	102.36	110.83
1	I	51	ASN	N-CA-C	5.67	119.32	111.55
1	B	282	SER	N-CA-C	5.61	117.15	110.19
1	B	198	TYR	CA-C-N	-5.55	113.48	121.42
1	B	198	TYR	C-N-CA	-5.55	113.48	121.42
1	I	44	ARG	N-CA-C	-5.53	101.56	110.14
1	G	69	PHE	CA-C-N	-5.48	115.09	120.52
1	G	69	PHE	C-N-CA	-5.48	115.09	120.52
1	D	50	ILE	CA-C-N	-5.45	115.48	122.79
1	D	50	ILE	C-N-CA	-5.45	115.48	122.79
1	D	15	LEU	N-CA-C	5.38	117.50	109.59
1	I	74	VAL	N-CA-C	-5.25	100.68	108.45
1	G	142	VAL	CB-CA-C	-5.25	99.85	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	GLY	N-CA-C	-5.25	108.08	115.32
1	D	182	LYS	N-CA-C	-5.20	105.68	112.23
1	I	164	LEU	N-CA-C	5.19	119.70	113.17
1	I	50	ILE	CA-C-N	-5.17	113.42	122.62
1	I	50	ILE	C-N-CA	-5.17	113.42	122.62
1	E	234	THR	CA-C-N	-5.16	113.44	119.32
1	E	234	THR	C-N-CA	-5.16	113.44	119.32
1	G	118	THR	CB-CA-C	5.16	120.14	110.70
1	E	142	VAL	CB-CA-C	-5.11	100.16	111.77
1	G	61	PHE	N-CA-C	-5.09	105.81	111.36
1	K	217	TRP	N-CA-C	5.07	116.47	110.19
1	K	140	GLU	N-CA-C	-5.05	106.38	112.54
1	E	188	TYR	N-CA-C	5.04	117.18	109.07
1	D	145	SER	N-CA-C	5.03	117.97	110.52
1	K	151	PHE	CA-C-N	-5.01	114.79	119.85
1	K	151	PHE	C-N-CA	-5.01	114.79	119.85

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 [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	B	2307	0	2228	45	0
1	D	2307	0	2228	56	0
1	E	2307	0	2228	58	0
1	G	2307	0	2228	45	0
1	I	2307	0	2228	45	0
1	K	2307	0	2228	62	0
2	G	32	0	20	3	0
2	I	32	0	20	0	0
3	G	19	0	10	0	0
3	I	19	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	13428	303	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 11.

All (303) 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: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:50:ILE:HG23	1:G:51:ASN:CG	2.07	0.80
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:B:105:TRP:CH2	1:B:244:MET:HE3	2.17	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: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:B:105:TRP:HH2	1:B:244:MET:HE3	1.51	0.74
1:I:105:TRP:HH2	1:I:244:MET:HE3	1.51	0.74
1:I:173:ILE:HD13	1:I:202:VAL:HB	1.68	0.74
1:I:105:TRP:CH2	1:I:244:MET:HE3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:50:ILE:HG13	1:G:80:GLY:C	2.18	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
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:D:278:THR:HG21	1:D:287:THR:HG23	1.78	0.66
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: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:217:TRP:CD1	1:K:217:TRP:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:217:TRP:H	1:B:217:TRP:CD1	2.17	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:E:105:TRP:HH2	1:E:244:MET:HE3	1.67	0.58
1:D:89:TYR:OH	1:D:118:THR:HB	2.04	0.58
1:K:105:TRP:CH2	1:K:244:MET:HE3	2.39	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:E:105:TRP:CH2	1:E:244:MET:HE3	2.39	0.57
1:K:18:ASP:HB2	1:K:74:VAL:HG21	1.86	0.57
1:D:132:ILE:HD12	1:B:128:ASN:CG	2.29	0.57
1:I:11:ILE:CG2	1:I:46:VAL:HG23	2.34	0.57
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: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:K:105:TRP:HH2	1:K:244:MET:HE3	1.72	0.55
1:E:281:GLN:NE2	1:E:281:GLN:CA	2.69	0.54
1:D:207:ALA:HB3	1:D:210:PHE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:278:THR:CG2	1:D:287:THR:HG23	2.39	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: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
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:D:217:TRP:H	1:D:217:TRP:CD1	2.29	0.50
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:G:105:TRP:CH2	1:G:244:MET:HE3	2.46	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:E:234:THR:O	1:E:235:PRO:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:36:LYS:HZ2	1:E:286:GLN:HE21	1.59	0.49
1:G:105:TRP:HH2	1:G:244:MET:HE3	1.78	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:I:217:TRP:H	1:I:217:TRP:CD1	2.31	0.47
1:G:50:ILE:CG1	1:G:80:GLY:C	2.87	0.47
1:D:138:PHE:CD2	1:D:142:VAL:HG11	2.49	0.47
1:I:105:TRP:HH2	1:I:244:MET:CE	2.21	0.47
1:K:198:TYR:O	1:K:198:TYR:CD1	2.67	0.47
1:B:111:PHE:C	1:B:111:PHE:CD2	2.92	0.47
1:G:129:THR:OG1	1:G:169:HIS:O	2.33	0.47
1:K:46:VAL:HG22	1:K:268:ALA:O	2.15	0.47
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:179:THR:HG23	1:E:185:LYS:HE2	1.95	0.46
1:K:60:LEU:O	1:K:61:PHE:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:TRP:H	1:E:217:TRP:CD1	2.33	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:B:105:TRP:CZ2	1:B:244:MET:HE3	2.51	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:I:247:PHE:CD2	1:I:247:PHE:C	2.94	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:89:TYR:HH	1:D:118:THR:HB	1.82	0.45
1:D:138:PHE:HD2	1:D:142:VAL:HG11	1.81	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
1:D:39:GLU:OE1	1:K:36:LYS:NZ	2.46	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:8:GLU:C	1:G:10:PRO:HD3	2.42	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:G:29:TYR:C	1:G:29:TYR:CD2	2.94	0.44
1:K:132:ILE:HD12	1:K:167:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:105:TRP:CH2	1:B:244:MET:CE	2.95	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:G:217:TRP:H	1:G:217:TRP:CD1	2.35	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:K:111:PHE:C	1:K:111:PHE:CD2	2.97	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:E:111:PHE:C	1:E:111:PHE:CD2	2.96	0.43
1:K:111:PHE:HE2	1:K:173:ILE:HD11	1.83	0.43
1:I:111:PHE:CD2	1:I:111:PHE:C	2.97	0.42
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: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:G:178:PHE:C	1:G:178:PHE:CD2	2.97	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
1:B:138:PHE:CD2	1:B:142:VAL:HG11	2.54	0.42
1:I:263:GLU:CD	1:I:263:GLU:H	2.28	0.42
1:E:65:ASN:HD22	1:E:255:ASN:ND2	2.08	0.42
1:K:102:PHE:C	1:K:102:PHE:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:LYS:O	1:G:186:LYS:HD3	2.20	0.42
1:E:198:TYR:O	1:E:198:TYR:CG	2.73	0.42
1:D:55:ASP:HB3	1:D:59:ARG:NH2	2.35	0.41
1:I:244:MET:HE3	1:I:244:MET:HB3	1.93	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: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:68:LEU:HD23	1:D:68:LEU:C	2.46	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: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
1:B:284:PHE:O	1:B:285:GLU:C	2.63	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%)	11	18
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%)	43	58

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%)	227 (91%)	23 (9%)	8	14
1	D	250/272 (92%)	225 (90%)	25 (10%)	7	11
1	E	250/272 (92%)	228 (91%)	22 (9%)	9	15
1	G	250/272 (92%)	231 (92%)	19 (8%)	12	21
1	I	250/272 (92%)	222 (89%)	28 (11%)	6	9
1	K	250/272 (92%)	230 (92%)	20 (8%)	11	19
All	All	1500/1632 (92%)	1363 (91%)	137 (9%)	9	14

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	5	LYS
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	238	ILE
1	D	241	THR
1	D	263	GLU
1	D	267	LYS
1	D	287	THR
1	I	6	THR
1	I	17	GLN
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
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

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Mol	Chain	Res	Type
1	I	166	GLU
1	I	172	SER
1	I	173	ILE
1	I	212	ILE
1	I	263	GLU
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	23	LYS
1	B	55	ASP
1	B	60	LEU
1	B	63	SER
1	B	67	VAL
1	B	74	VAL
1	B	111	PHE
1	B	113	LEU
1	B	118	THR
1	B	122	LEU
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	263	GLU
1	B	276	GLU
1	B	281	GLN
1	B	287	THR
1	E	23	LYS
1	E	50	ILE
1	E	52	LYS
1	E	58	SER
1	E	67	VAL
1	E	74	VAL
1	E	113	LEU
1	E	118	THR
1	E	132	ILE

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Mol	Chain	Res	Type
1	E	140	GLU
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	5	LYS
1	G	15	LEU
1	G	18	ASP
1	G	19	VAL
1	G	23	LYS
1	G	50	ILE
1	G	52	LYS
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	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	93	LEU
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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	216	GLN
1	D	250	ASN
1	D	255	ASN
1	D	272	ASN
1	D	286	GLN
1	I	126	HIS
1	I	128	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	250	ASN
1	B	255	ASN
1	B	272	ASN
1	B	286	GLN
1	E	27	ASN
1	E	51	ASN
1	E	98	ASN
1	E	128	ASN
1	E	216	GLN
1	E	250	ASN
1	E	255	ASN
1	E	281	GLN
1	E	286	GLN
1	G	126	HIS
1	G	250	ASN

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Mol	Chain	Res	Type
1	G	255	ASN
1	G	286	GLN
1	K	181	ASN
1	K	216	GLN
1	K	250	ASN
1	K	255	ASN
1	K	281	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 oligosaccharides 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
2	MTX	G	301	3	33,34,35	1.99	7 (21%)	45,47,49	2.49	15 (33%)
3	DGL	G	302	3,2	6,8,9	0.91	0	6,9,11	0.73	0
3	DGL	I	303	3	8,9,9	1.94	2 (25%)	8,11,11	1.33	1 (12%)
2	MTX	I	301	3	33,34,35	1.82	5 (15%)	45,47,49	2.16	13 (28%)
3	DGL	I	302	3,2	6,8,9	1.05	1 (16%)	6,9,11	1.09	1 (16%)
3	DGL	G	303	3	8,9,9	1.94	2 (25%)	8,11,11	1.30	1 (12%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	MTX	C7-N8	6.23	1.42	1.31
2	I	301	MTX	C9-C6	-6.12	1.40	1.51
2	G	301	MTX	C9-C6	-5.59	1.41	1.51
2	I	301	MTX	C7-N8	4.63	1.39	1.31
2	I	301	MTX	C11-C	-3.62	1.42	1.50
2	G	301	MTX	C11-C	-3.57	1.42	1.50
3	G	303	DGL	CG-CD	3.29	1.58	1.50
3	I	303	DGL	CG-CD	3.25	1.58	1.50
3	I	303	DGL	CB-CA	2.84	1.59	1.53
3	G	303	DGL	CB-CA	2.80	1.59	1.53
2	G	301	MTX	CM-N10	2.74	1.50	1.46
2	I	301	MTX	CM-N10	2.72	1.50	1.46
2	G	301	MTX	C9-N10	2.47	1.51	1.46
2	G	301	MTX	C6-N5	2.14	1.36	1.32
2	G	301	MTX	CA-N	2.13	1.50	1.45
3	I	302	DGL	O-C	2.03	1.28	1.22
2	I	301	MTX	CA-N	2.01	1.50	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	MTX	C2-N1-C8A	6.12	122.09	115.48
2	G	301	MTX	N8-C8A-N1	5.51	121.78	115.77
2	G	301	MTX	N1-C2-N3	-5.45	120.28	127.21
2	G	301	MTX	C6-C9-N10	5.42	122.24	112.95
2	I	301	MTX	C2-N1-C8A	5.16	121.04	115.48
2	I	301	MTX	N1-C2-N3	-4.90	120.98	127.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	MTX	CB-CG-CD	-4.48	99.70	112.27
2	I	301	MTX	C6-C9-N10	4.23	120.19	112.95
2	I	301	MTX	C6-C7-N8	-4.17	119.14	123.14
2	I	301	MTX	N8-C8A-N1	4.17	120.31	115.77
2	G	301	MTX	C6-C7-N8	-4.16	119.15	123.14
2	G	301	MTX	C7-C6-N5	-3.63	118.52	120.87
2	G	301	MTX	C4-C4A-N5	3.56	123.06	120.33
2	G	301	MTX	C9-N10-C14	-3.51	115.92	120.17
2	I	301	MTX	CB-CG-CD	-3.47	102.53	112.27
2	G	301	MTX	C6-N5-C4A	3.36	122.92	118.17
2	I	301	MTX	C15-C14-N10	-3.24	117.07	121.59
2	I	301	MTX	C8A-C4A-N5	-2.67	119.37	122.35
2	G	301	MTX	C8A-C4A-N5	-2.64	119.40	122.35
2	G	301	MTX	O1-CT-CA	-2.54	114.06	122.26
3	G	303	DGL	CG-CB-CA	2.50	119.60	113.86
3	I	303	DGL	CB-CA-N	2.48	116.57	110.12
2	I	301	MTX	C9-N10-C14	-2.46	117.19	120.17
2	G	301	MTX	CB-CA-N	2.40	115.66	110.91
2	G	301	MTX	C7-N8-C8A	2.36	120.49	117.20
2	I	301	MTX	CA-N-C	-2.35	115.93	121.56
2	I	301	MTX	C6-N5-C4A	2.35	121.49	118.17
3	I	302	DGL	CB-CA-N	-2.32	104.06	110.12
2	I	301	MTX	C4-C4A-N5	2.16	121.99	120.33
2	I	301	MTX	C11-C-N	2.09	120.92	117.04
2	G	301	MTX	CB-CA-CT	-2.02	105.57	110.35

There are no chirality outliers.

All (27) 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
2	G	301	MTX	O-C-C11-C16
2	I	301	MTX	C13-C14-N10-CM
2	I	301	MTX	C15-C14-N10-CM
3	G	303	DGL	OXT-C-CA-CB
3	G	303	DGL	OXT-C-CA-N
2	G	301	MTX	C15-C14-N10-CM
3	G	303	DGL	O-C-CA-CB
2	G	301	MTX	C13-C14-N10-CM

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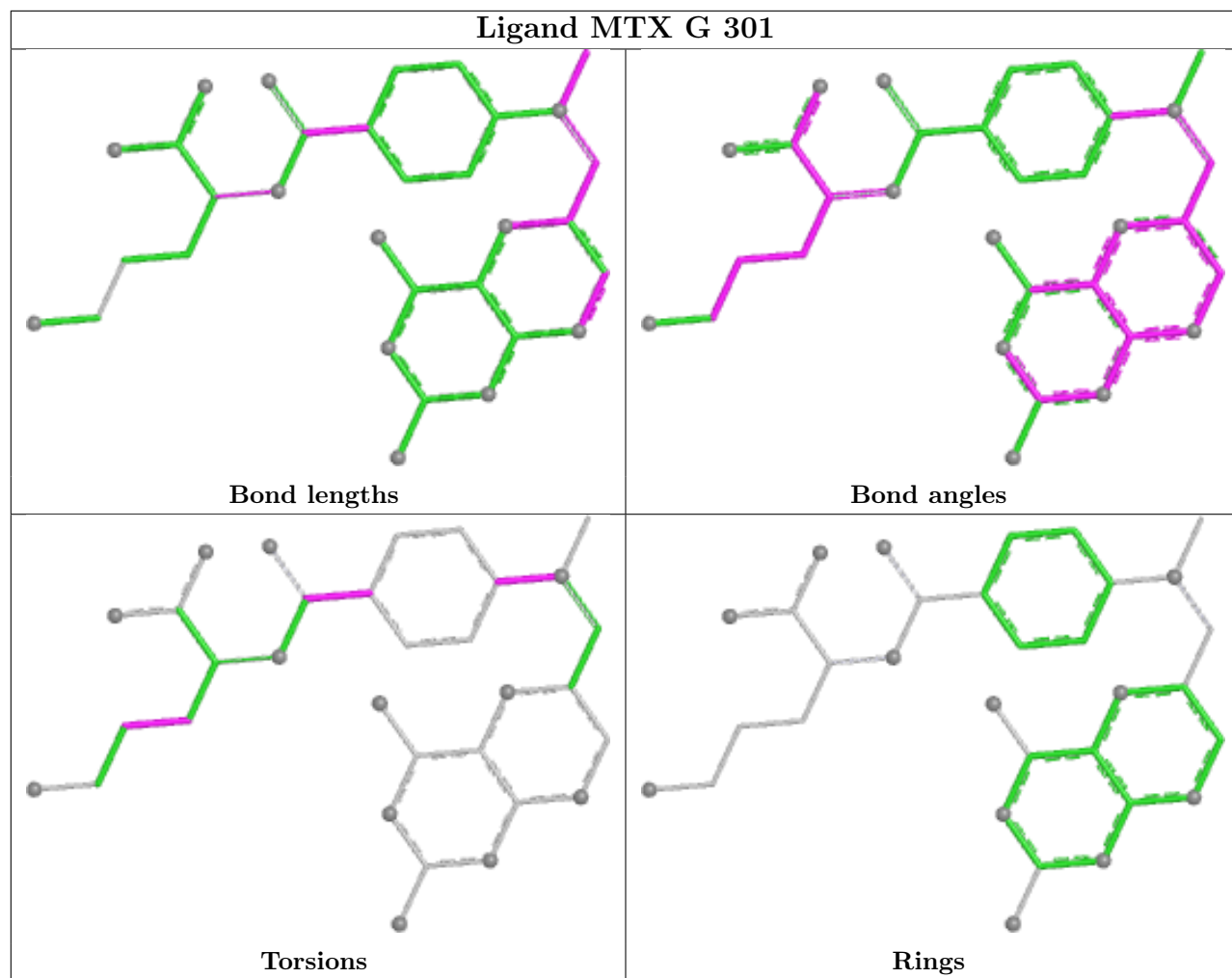
Mol	Chain	Res	Type	Atoms
3	I	303	DGL	O-C-CA-CB
3	I	302	DGL	N-CA-CB-CG
3	G	303	DGL	CA-CB-CG-CD
3	I	303	DGL	OXT-C-CA-CB
3	I	303	DGL	CA-CB-CG-CD
3	G	303	DGL	O-C-CA-N
3	G	303	DGL	OE1-CD-CG-CB
3	G	303	DGL	OE2-CD-CG-CB
3	G	302	DGL	OXT-C-CA-N
3	I	303	DGL	OE1-CD-CG-CB
3	I	302	DGL	OXT-C-CA-N
3	I	303	DGL	OE2-CD-CG-CB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

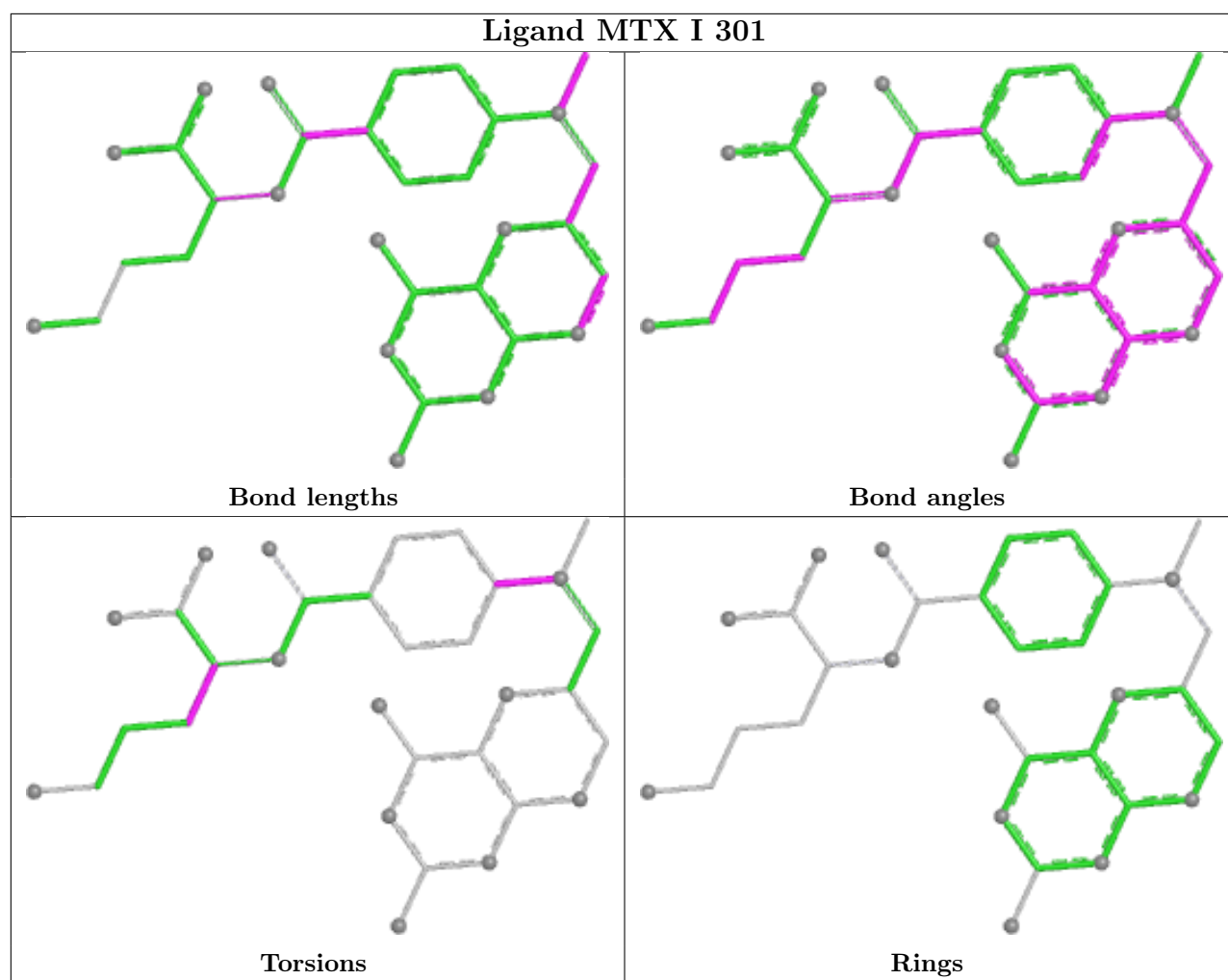
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 95th 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 ²)	Q<0.9
1	B	287/312 (91%)	-0.22	7 (2%) 59 55	6, 27, 44, 56	5 (1%)
1	D	287/312 (91%)	0.13	9 (3%) 51 47	10, 35, 55, 72	5 (1%)
1	E	287/312 (91%)	-0.18	9 (3%) 51 47	7, 28, 45, 57	5 (1%)
1	G	287/312 (91%)	-0.30	9 (3%) 51 47	5, 24, 40, 53	5 (1%)
1	I	287/312 (91%)	-0.07	5 (1%) 69 65	9, 31, 49, 56	5 (1%)
1	K	287/312 (91%)	0.25	11 (3%) 44 40	10, 38, 60, 70	5 (1%)
All	All	1722/1872 (91%)	-0.06	50 (2%) 53 50	5, 30, 52, 72	30 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	SER	6.9
1	E	250	ASN	6.8
1	D	250	ASN	6.8
1	K	158	SER	6.4
1	D	283	ALA	6.3
1	K	250	ASN	6.1
1	B	250	ASN	6.1
1	D	158	SER	6.0
1	I	250	ASN	5.9
1	I	158	SER	5.8
1	I	283	ALA	5.7
1	G	158	SER	5.3
1	B	283	ALA	4.8
1	G	250	ASN	4.7
1	B	158	SER	4.7
1	K	280	ILE	4.3
1	G	283	ALA	4.3
1	K	283	ALA	4.2
1	K	198	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	280	ILE	4.0
1	D	115	THR	3.9
1	E	283	ALA	3.7
1	E	198	TYR	3.5
1	G	280	ILE	3.5
1	B	115	THR	3.4
1	B	280	ILE	3.3
1	G	51	ASN	3.2
1	I	280	ILE	3.2
1	E	280	ILE	3.0
1	D	20	PHE	3.0
1	E	20	PHE	2.9
1	G	50	ILE	2.8
1	K	24	PRO	2.7
1	G	115	THR	2.6
1	B	20	PHE	2.6
1	K	115	THR	2.6
1	D	5	LYS	2.5
1	K	20	PHE	2.5
1	I	115	THR	2.4
1	B	59	ARG	2.3
1	G	20	PHE	2.2
1	K	50	ILE	2.2
1	K	22	PRO	2.2
1	K	173	ILE	2.1
1	D	21	ASP	2.1
1	E	50	ILE	2.1
1	D	144	GLY	2.1
1	E	126	HIS	2.0
1	G	281	GLN	2.0
1	E	130	SER	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](#)

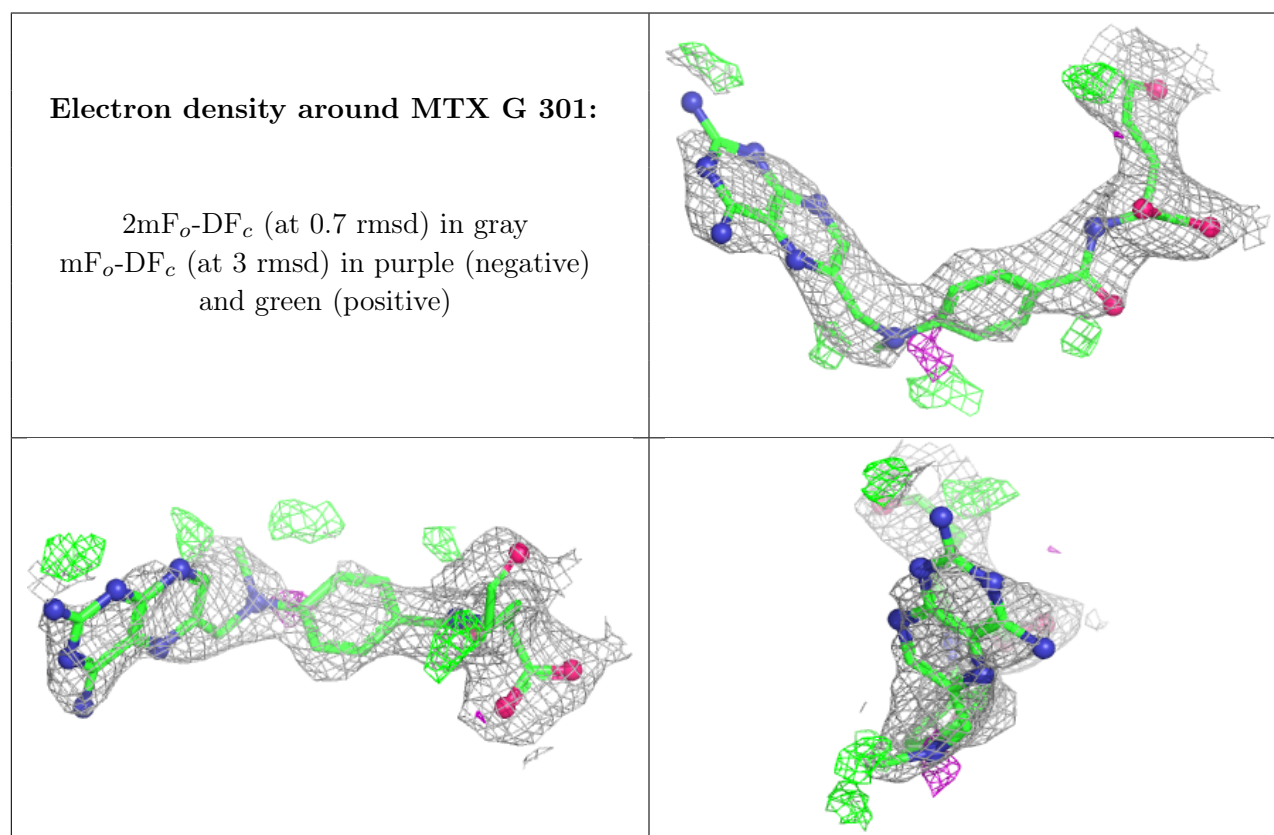
There are no oligosaccharides in this entry.

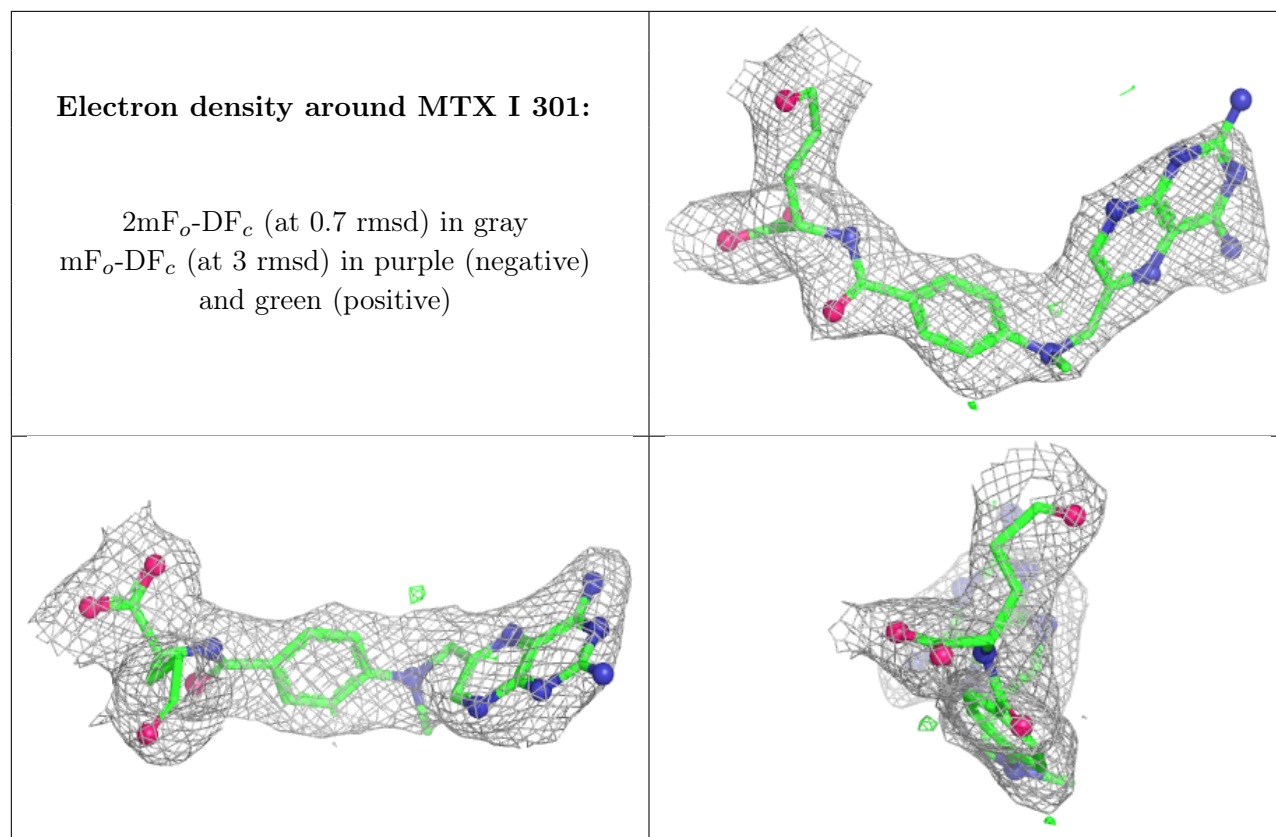
6.4 Ligands ⓘ

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, 95th 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(Å ²)	Q<0.9
3	DGL	G	303	10/10	0.65	0.17	62,65,68,69	0
3	DGL	I	303	10/10	0.68	0.21	65,67,69,71	0
2	MTX	G	301	32/33	0.76	0.16	44,66,87,87	0
3	DGL	I	302	9/10	0.80	0.16	54,59,62,63	0
3	DGL	G	302	9/10	0.82	0.18	52,57,59,63	0
2	MTX	I	301	32/33	0.86	0.13	44,60,79,80	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.