



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:26 PM EDT

PDB ID : 1LVK / pdb_00001lvk
Title : X-RAY CRYSTAL STRUCTURE OF THE MG (DOT) 2'(3')-O-(N-MET
HYLANTHRANILOYL) NUCLEOTIDE BOUND TO DICTYOSTELIUM
DISCOIDEUM MYOSIN MOTOR DOMAIN
Authors : Bauer, C.B.; Kuhlman, P.A.; Bagshaw, C.R.; Rayment, I.
Deposited on : 1997-09-05
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

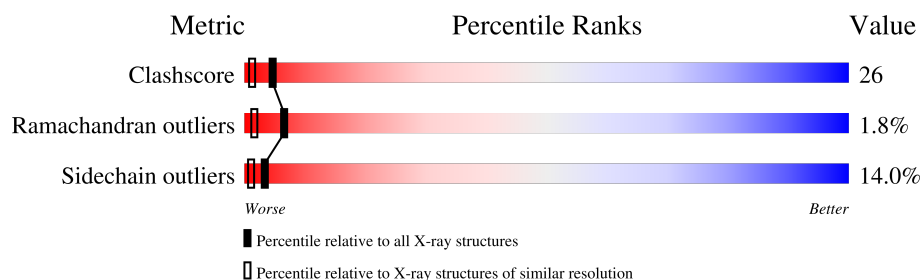
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5954 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	743	5905	3754	1016	1119	16	0	0	0

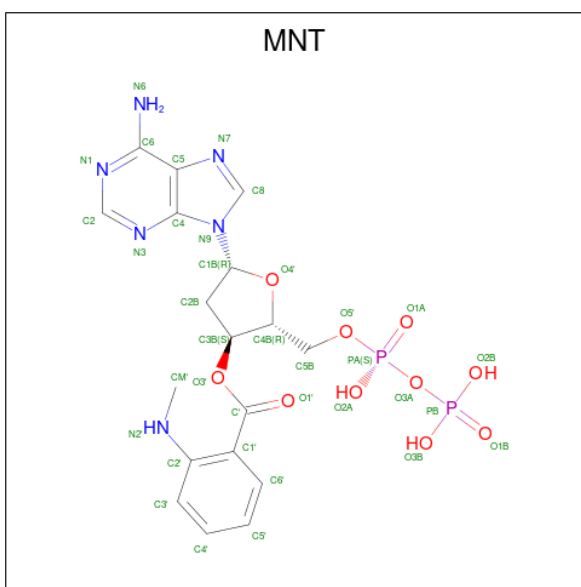
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	VAL	conflict	UNP P08799
A	273	THR	GLU	conflict	UNP P08799
A	274	SER	THR	conflict	UNP P08799
A	312	CYS	TYR	conflict	UNP P08799
A	321	GLU	SER	conflict	UNP P08799
A	322	ASP	GLU	conflict	UNP P08799
A	443	SER	GLN	conflict	UNP P08799
A	489	VAL	LEU	conflict	UNP P08799
A	493	LYS	GLU	conflict	UNP P08799
A	628	LEU	ILE	conflict	UNP P08799
A	707	ASP	LEU	conflict	UNP P08799
A	737	PHE	TYR	conflict	UNP P08799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

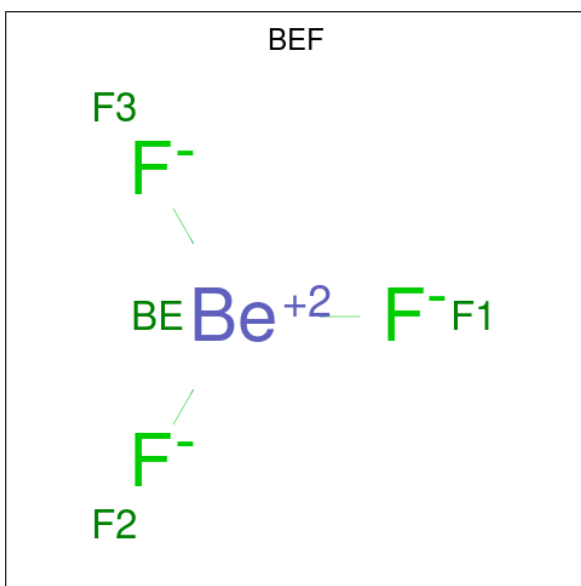
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'(3')-O-N-METHYLANTHRANILOYL-ADENOSINE-5'-DIPHOSPHATE (CCD ID: MNT) (formula: C₁₈H₂₂N₆O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 42	C 23	N 7	O 10	P 2	0	1

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Be 1	F 3	0	0

- Molecule 5 is water.

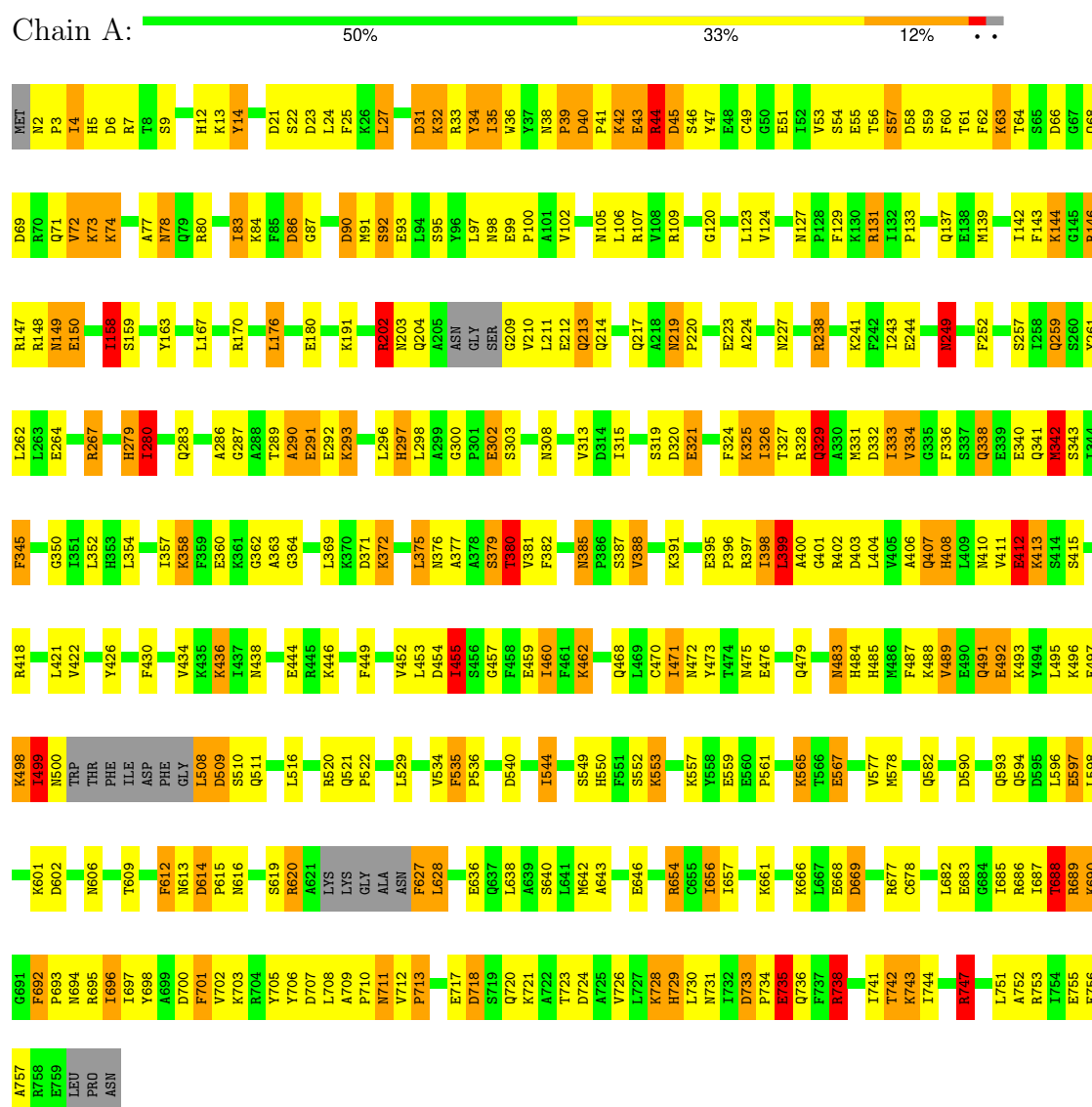
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: MYOSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.90Å 179.90Å 53.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.6 (20.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5954	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MNT, MG, BEF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.38	26/6017 (0.4%)	1.91	134/8122 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	LYS	CE-NZ	-11.90	1.13	1.49
1	A	550	HIS	CE1-NE2	7.93	1.40	1.32
1	A	131	ARG	NE-CZ	7.26	1.41	1.33
1	A	540	ASP	CG-OD1	7.16	1.39	1.25
1	A	109	ARG	NE-CZ	6.28	1.40	1.33
1	A	180	GLU	CD-OE1	6.20	1.37	1.25
1	A	45	ASP	CG-OD1	6.09	1.36	1.25
1	A	668	GLU	CD-OE2	6.01	1.36	1.25
1	A	638	LEU	CA-CB	5.94	1.62	1.53
1	A	340	GLU	CD-OE1	5.85	1.36	1.25
1	A	202	ARG	CZ-NH2	5.72	1.40	1.33
1	A	86	ASP	CA-CB	5.69	1.60	1.53
1	A	326	ILE	CA-CB	-5.63	1.47	1.54
1	A	267	ARG	NE-CZ	5.63	1.39	1.33
1	A	21	ASP	CG-OD1	5.59	1.35	1.25
1	A	360	GLU	CD-OE2	5.56	1.35	1.25
1	A	148	ARG	CZ-NH1	5.49	1.40	1.32
1	A	297	HIS	CD2-NE2	5.36	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLU	CD-OE1	5.29	1.35	1.25
1	A	499	ILE	C-O	-5.23	1.17	1.24
1	A	471	ILE	CA-CB	5.21	1.60	1.54
1	A	567	GLU	CD-OE2	5.17	1.35	1.25
1	A	529	LEU	CA-CB	5.12	1.61	1.53
1	A	279	HIS	CD2-NE2	5.10	1.43	1.37
1	A	43	GLU	CD-OE2	5.10	1.35	1.25
1	A	212	GLU	CD-OE2	5.04	1.34	1.25

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PHE	CA-CB-CG	-14.49	99.31	113.80
1	A	718	ASP	CA-CB-CG	-13.24	99.36	112.60
1	A	729	HIS	CA-CB-CG	-12.74	101.06	113.80
1	A	713	PRO	N-CA-CB	11.58	115.41	103.25
1	A	408	HIS	CA-CB-CG	-11.01	102.79	113.80
1	A	297	HIS	CA-CB-CG	-10.41	103.39	113.80
1	A	711	ASN	CA-CB-CG	10.16	122.76	112.60
1	A	627	PHE	CA-CB-CG	9.55	123.35	113.80
1	A	735	GLU	N-CA-CB	9.35	126.29	110.49
1	A	602	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	238	ARG	NE-CZ-NH1	9.16	130.66	121.50
1	A	41	PRO	N-CA-CB	9.02	113.15	102.60
1	A	489	VAL	CB-CA-C	8.76	123.96	112.14
1	A	654	ARG	NE-CZ-NH2	-8.56	111.50	119.20
1	A	455	ILE	CA-CB-CG2	8.48	124.92	110.50
1	A	491	GLN	CB-CG-CD	-8.32	98.45	112.60
1	A	462	LYS	CB-CA-C	-7.99	97.52	110.79
1	A	692	PHE	CA-C-N	7.94	127.50	119.24
1	A	692	PHE	C-N-CA	7.94	127.50	119.24
1	A	262	LEU	N-CA-CB	-7.90	100.01	111.70
1	A	385	ASN	CB-CA-C	7.86	119.12	110.08
1	A	707	ASP	CA-CB-CG	-7.85	104.75	112.60
1	A	158	ILE	CB-CA-C	7.83	124.29	112.16
1	A	657	ILE	CB-CA-C	7.59	118.00	110.94
1	A	280	ILE	CA-CB-CG2	7.53	123.30	110.50
1	A	259	GLN	CB-CG-CD	7.52	125.39	112.60
1	A	202	ARG	CB-CA-C	7.43	124.17	111.68
1	A	612	PHE	CA-CB-CG	-7.31	106.49	113.80
1	A	731	ASN	CA-CB-CG	7.30	119.90	112.60
1	A	46	SER	N-CA-CB	7.29	122.42	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	CA-CB-CG	-7.27	106.53	113.80
1	A	606	ASN	CB-CA-C	7.15	123.86	110.63
1	A	688	THR	N-CA-CB	-7.13	98.98	109.82
1	A	565	LYS	CB-CA-C	-7.11	98.22	110.09
1	A	44	ARG	N-CA-CB	7.00	122.33	110.49
1	A	219	ASN	CA-C-N	6.90	127.19	119.32
1	A	219	ASN	C-N-CA	6.90	127.19	119.32
1	A	455	ILE	N-CA-CB	-6.90	98.51	111.62
1	A	385	ASN	CA-C-O	6.88	123.76	119.29
1	A	219	ASN	CA-CB-CG	-6.84	105.76	112.60
1	A	42	LYS	N-CA-C	-6.82	104.22	112.54
1	A	472	ASN	CA-CB-CG	-6.77	105.83	112.60
1	A	402	ARG	N-CA-C	-6.74	105.58	113.88
1	A	25	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	412	GLU	CB-CA-C	-6.60	99.84	110.79
1	A	499	ILE	CB-CA-C	6.53	122.00	111.29
1	A	516	LEU	CA-C-O	6.45	127.39	120.55
1	A	438	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	315	ILE	N-CA-CB	6.34	119.87	111.25
1	A	107	ARG	CG-CD-NE	-6.23	98.30	112.00
1	A	620	ARG	N-CA-C	6.20	117.83	111.14
1	A	476	GLU	CB-CA-C	-6.11	100.64	110.79
1	A	669	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	619	SER	CB-CA-C	-6.11	97.31	110.45
1	A	44	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	692	PHE	O-C-N	6.01	126.78	121.37
1	A	485	HIS	CA-CB-CG	-5.93	107.87	113.80
1	A	654	ARG	NH1-CZ-NH2	5.93	127.01	119.30
1	A	90	ASP	CA-CB-CG	5.92	118.53	112.60
1	A	380	THR	N-CA-CB	5.88	118.50	109.91
1	A	485	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	A	74	LYS	N-CA-C	-5.84	104.91	111.28
1	A	511	GLN	N-CA-CB	5.81	118.67	110.12
1	A	213	GLN	N-CA-CB	-5.79	101.61	110.12
1	A	755	GLU	CB-CG-CD	5.77	122.40	112.60
1	A	57	SER	N-CA-CB	-5.76	99.84	110.32
1	A	492	GLU	CB-CA-C	-5.74	101.27	110.79
1	A	449	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	252	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	78	ASN	N-CA-CB	5.64	118.79	110.49
1	A	683	GLU	CB-CG-CD	5.61	122.13	112.60
1	A	72	VAL	CB-CA-C	-5.58	101.14	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	238	ARG	CD-NE-CZ	5.56	132.19	124.40
1	A	550	HIS	ND1-CG-CD2	5.56	111.66	106.10
1	A	320	ASP	CB-CA-C	5.55	120.11	110.68
1	A	144	LYS	CG-CD-CE	5.54	124.05	111.30
1	A	127	ASN	O-C-N	5.52	126.22	121.30
1	A	257	SER	CA-CB-OG	-5.51	100.08	111.10
1	A	549	SER	CA-CB-OG	-5.49	100.12	111.10
1	A	345	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	44	ARG	CG-CD-NE	5.47	124.04	112.00
1	A	627	PHE	N-CA-CB	5.47	119.80	110.50
1	A	34	TYR	N-CA-C	5.46	118.55	110.46
1	A	559	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	148	ARG	NE-CZ-NH2	-5.42	114.33	119.20
1	A	540	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	590	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	238	ARG	CG-CD-NE	-5.37	100.18	112.00
1	A	21	ASP	CB-CA-C	-5.37	102.41	110.90
1	A	561	PRO	CB-CA-C	-5.37	104.36	111.23
1	A	636	GLU	N-CA-CB	-5.35	102.31	110.07
1	A	747	ARG	CA-CB-CG	-5.34	103.41	114.10
1	A	402	ARG	CB-CA-C	5.34	117.68	109.03
1	A	701	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	176	LEU	O-C-N	5.32	129.83	123.13
1	A	468	GLN	N-CA-CB	5.30	118.01	110.16
1	A	150	GLU	CA-CB-CG	5.30	124.69	114.10
1	A	334	VAL	CB-CA-C	5.29	118.47	111.70
1	A	249	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	483	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	457	GLY	N-CA-C	-5.24	102.52	112.27
1	A	280	ILE	N-CA-CB	5.23	119.59	110.65
1	A	743	LYS	CB-CA-C	-5.20	99.14	109.79
1	A	399	LEU	N-CA-C	5.19	116.62	109.15
1	A	693	PRO	N-CA-CB	5.19	108.81	103.15
1	A	452	VAL	CA-C-N	-5.18	115.79	123.05
1	A	452	VAL	C-N-CA	-5.18	115.79	123.05
1	A	459	GLU	CG-CD-OE1	5.13	130.20	118.40
1	A	280	ILE	CB-CG1-CD1	-5.13	103.03	113.80
1	A	733	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	4	ILE	N-CA-CB	5.11	119.38	110.65
1	A	129	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	619	SER	N-CA-C	5.09	116.81	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	MET	N-CA-CB	5.09	117.34	109.91
1	A	606	ASN	N-CA-CB	5.08	118.05	110.22
1	A	41	PRO	CB-CA-C	5.08	117.43	110.52
1	A	678	CYS	N-CA-C	5.07	117.70	111.82
1	A	614	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	597	GLU	CB-CA-C	-5.06	102.39	110.79
1	A	553	LYS	CB-CA-C	-5.05	101.51	111.06
1	A	244	GLU	CA-CB-CG	-5.05	104.00	114.10
1	A	249	ASN	CB-CG-ND2	5.05	123.98	116.40
1	A	475	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	14	TYR	N-CA-C	5.05	119.59	113.38
1	A	202	ARG	N-CA-CB	5.05	117.96	110.49
1	A	131	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	170	ARG	N-CA-CB	5.04	119.56	111.91
1	A	516	LEU	O-C-N	-5.04	116.78	122.12
1	A	244	GLU	N-CA-CB	-5.03	102.12	110.47
1	A	45	ASP	CB-CA-C	5.03	118.41	109.65
1	A	329	GLN	N-CA-CB	-5.02	102.73	110.01
1	A	738	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	A	388	VAL	N-CA-CB	-5.01	103.07	110.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	606	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5905	0	5820	305	0
2	A	1	0	0	0	0
3	A	42	0	16	0	0
4	A	4	0	0	0	0
5	A	2	0	0	0	0
All	All	5954	0	5836	305	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 26.

All (305) 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:A:4:ILE:HD11	1:A:142:ILE:HG23	1.19	1.10
1:A:686:ARG:HA	1:A:689:ARG:HH12	1.09	1.07
1:A:249:ASN:ND2	1:A:249:ASN:H	1.42	1.05
1:A:410:ASN:H	1:A:413:LYS:HZ3	1.03	1.02
1:A:139:MET:HA	1:A:142:ILE:HD12	1.43	0.99
1:A:735:GLU:HA	1:A:738:ARG:HH22	1.27	0.97
1:A:735:GLU:HA	1:A:738:ARG:NH2	1.82	0.94
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.50	0.93
1:A:735:GLU:CA	1:A:738:ARG:HH22	1.84	0.90
1:A:321:GLU:O	1:A:325:LYS:HE3	1.71	0.90
1:A:62:PHE:HE1	1:A:72:VAL:HG23	1.35	0.90
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.02	0.89
1:A:290:ALA:HA	1:A:293:LYS:HD3	1.53	0.89
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.79	0.88
1:A:289:THR:HB	1:A:291:GLU:OE2	1.72	0.88
1:A:686:ARG:HA	1:A:689:ARG:NH1	1.88	0.87
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.09	0.87
1:A:689:ARG:HH11	1:A:689:ARG:HB3	1.40	0.87
1:A:289:THR:HB	1:A:291:GLU:CD	2.00	0.86
1:A:249:ASN:ND2	1:A:249:ASN:N	2.25	0.85
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.41	0.85
1:A:395:GLU:HA	1:A:407:GLN:O	1.76	0.84
1:A:642:MET:O	1:A:646:GLU:HG2	1.77	0.84
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.42	0.84
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.58	0.84
1:A:62:PHE:HE1	1:A:72:VAL:CG2	1.91	0.83
1:A:53:VAL:HG11	1:A:63:LYS:HD2	1.62	0.82
1:A:724:ASP:O	1:A:728:LYS:HB2	1.79	0.82
1:A:454:ASP:O	1:A:455:ILE:HD12	1.80	0.82
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.08	0.81
1:A:695:ARG:C	1:A:696:ILE:HD12	2.06	0.81
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.07	0.81
1:A:735:GLU:CB	1:A:738:ARG:HH22	1.95	0.80
1:A:40:ASP:OD2	1:A:42:LYS:HB2	1.82	0.79
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.65	0.79
1:A:410:ASN:H	1:A:413:LYS:NZ	1.80	0.78
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.65	0.78
1:A:219:ASN:N	1:A:220:PRO:HD2	1.97	0.78
1:A:697:ILE:HB	1:A:700:ASP:OD2	1.84	0.77
1:A:139:MET:HA	1:A:142:ILE:CD1	2.13	0.76
1:A:493:LYS:HE3	1:A:743:LYS:HE3	1.67	0.75
1:A:321:GLU:H	1:A:321:GLU:CD	1.90	0.75
1:A:59:SER:HB2	1:A:72:VAL:O	1.87	0.75
1:A:399:LEU:C	1:A:399:LEU:HD12	2.10	0.74
1:A:436:LYS:NZ	1:A:436:LYS:HB3	2.04	0.73
1:A:329:GLN:O	1:A:333:ILE:HD12	1.87	0.73
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.70	0.73
1:A:453:LEU:CD1	1:A:455:ILE:HD13	2.20	0.72
1:A:62:PHE:CE1	1:A:72:VAL:HG23	2.22	0.72
1:A:210:VAL:O	1:A:214:GLN:HG3	1.90	0.72
1:A:87:GLY:H	1:A:105:ASN:ND2	1.88	0.72
1:A:238:ARG:HD3	1:A:264:GLU:OE1	1.89	0.71
1:A:410:ASN:N	1:A:413:LYS:HZ3	1.84	0.70
1:A:249:ASN:H	1:A:249:ASN:HD22	1.33	0.70
1:A:31:ASP:OD1	1:A:31:ASP:N	2.20	0.70
1:A:147:ARG:HB2	1:A:150:GLU:HG3	1.73	0.69
1:A:64:THR:HG23	1:A:68:GLN:O	1.92	0.69
1:A:376:ASN:O	1:A:380:THR:HG23	1.92	0.69
1:A:302:GLU:H	1:A:302:GLU:CD	2.00	0.69
1:A:139:MET:CA	1:A:142:ILE:HD12	2.21	0.69
1:A:123:LEU:HD22	1:A:158:ILE:HG21	1.74	0.69
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.21	0.68
1:A:397:ARG:HA	1:A:406:ALA:HA	1.74	0.68
1:A:399:LEU:HD12	1:A:400:ALA:N	2.09	0.68
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.25	0.67
1:A:338:GLN:O	1:A:342:MET:SD	2.52	0.67
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.09	0.67
1:A:33:ARG:NH2	1:A:55:GLU:OE2	2.28	0.67
1:A:493:LYS:HE3	1:A:743:LYS:CE	2.23	0.67
1:A:410:ASN:ND2	1:A:413:LYS:HD3	2.11	0.66
1:A:493:LYS:CE	1:A:743:LYS:HE3	2.25	0.66
1:A:24:LEU:N	1:A:24:LEU:HD23	2.11	0.66
1:A:735:GLU:CA	1:A:738:ARG:NH2	2.53	0.66
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.29	0.66
1:A:59:SER:HA	1:A:74:LYS:HG3	1.77	0.66
1:A:567:GLU:HB3	1:A:578:MET:CE	2.27	0.65
1:A:38:ASN:C	1:A:40:ASP:H	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:O	1:A:44:ARG:HG2	1.97	0.64
1:A:72:VAL:HG12	1:A:73:LYS:N	2.12	0.64
1:A:146:ARG:HD2	1:A:150:GLU:OE1	1.97	0.64
1:A:56:THR:O	1:A:74:LYS:NZ	2.22	0.64
1:A:493:LYS:HE3	1:A:743:LYS:NZ	2.12	0.63
1:A:508:LEU:O	1:A:509:ASP:HB2	1.98	0.63
1:A:696:ILE:HD12	1:A:696:ILE:N	2.12	0.63
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.33	0.63
1:A:327:THR:HG22	1:A:331:MET:HE2	1.80	0.63
1:A:362:GLY:O	1:A:364:GLY:N	2.31	0.63
1:A:436:LYS:HB3	1:A:436:LYS:HZ3	1.60	0.63
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.80	0.62
1:A:454:ASP:C	1:A:455:ILE:HD12	2.24	0.62
1:A:124:VAL:HG13	1:A:656:ILE:HD13	1.81	0.62
1:A:224:ALA:O	1:A:280:ILE:HG13	1.99	0.62
1:A:202:ARG:HH11	1:A:202:ARG:CG	2.10	0.62
1:A:325:LYS:N	1:A:325:LYS:HE2	2.14	0.62
1:A:735:GLU:HB3	1:A:738:ARG:HH22	1.62	0.62
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.24	0.61
1:A:372:LYS:O	1:A:376:ASN:ND2	2.34	0.61
1:A:689:ARG:HH11	1:A:689:ARG:CB	2.11	0.61
1:A:733:ASP:O	1:A:736:GLN:HB2	2.01	0.61
1:A:397:ARG:HB3	1:A:404:LEU:HD11	1.81	0.60
1:A:726:VAL:O	1:A:730:LEU:HG	2.01	0.60
1:A:209:GLY:O	1:A:213:GLN:HB2	2.01	0.60
1:A:123:LEU:HD22	1:A:158:ILE:CG2	2.32	0.60
1:A:733:ASP:OD1	1:A:734:PRO:HD2	2.02	0.59
1:A:430:PHE:O	1:A:434:VAL:HG23	2.03	0.59
1:A:59:SER:HB3	1:A:73:LYS:NZ	2.17	0.59
1:A:643:ALA:O	1:A:646:GLU:HB2	2.02	0.59
1:A:552:SER:O	1:A:553:LYS:HB2	2.02	0.58
1:A:567:GLU:HB3	1:A:578:MET:HE1	1.84	0.58
1:A:2:ASN:HB3	1:A:5:HIS:HD2	1.68	0.58
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.33	0.58
1:A:59:SER:CA	1:A:74:LYS:HG3	2.33	0.58
1:A:2:ASN:CB	1:A:5:HIS:HD2	2.17	0.57
1:A:3:PRO:HB3	1:A:9:SER:CB	2.34	0.57
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.69	0.57
1:A:694:ASN:C	1:A:695:ARG:HG3	2.28	0.56
1:A:2:ASN:HB3	1:A:5:HIS:CD2	2.41	0.56
1:A:286:ALA:HB1	1:A:321:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:SD	1:A:342:MET:N	2.78	0.56
1:A:56:THR:HG1	1:A:58:ASP:CG	2.13	0.56
1:A:371:ASP:OD1	1:A:372:LYS:N	2.38	0.56
1:A:544:ILE:O	1:A:544:ILE:HG13	2.05	0.56
1:A:176:LEU:N	1:A:176:LEU:HD12	2.21	0.55
1:A:412:GLU:O	1:A:412:GLU:HG2	2.04	0.55
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.87	0.55
1:A:64:THR:OG1	1:A:68:GLN:N	2.39	0.54
1:A:408:HIS:ND1	1:A:408:HIS:C	2.63	0.54
1:A:87:GLY:H	1:A:105:ASN:HD21	1.52	0.54
1:A:404:LEU:C	1:A:404:LEU:HD13	2.33	0.54
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.42	0.54
1:A:3:PRO:HB3	1:A:9:SER:HB2	1.90	0.54
1:A:147:ARG:HG3	1:A:147:ARG:NH1	2.22	0.53
1:A:241:LYS:H	1:A:455:ILE:HD12	1.72	0.53
1:A:326:ILE:O	1:A:329:GLN:HB3	2.08	0.53
1:A:241:LYS:CD	1:A:243:ILE:HD11	2.38	0.53
1:A:249:ASN:N	1:A:249:ASN:HD22	1.98	0.53
1:A:147:ARG:H	1:A:150:GLU:CD	2.15	0.53
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.90	0.53
1:A:358:LYS:HB2	1:A:358:LYS:NZ	2.24	0.53
1:A:27:LEU:HD13	1:A:27:LEU:N	2.24	0.53
1:A:45:ASP:OD2	1:A:677:ARG:NH1	2.42	0.53
1:A:484:HIS:O	1:A:487:PHE:HB3	2.08	0.53
1:A:2:ASN:ND2	1:A:5:HIS:CD2	2.78	0.52
1:A:124:VAL:CG1	1:A:656:ILE:HD13	2.38	0.52
1:A:415:SER:OG	1:A:418:ARG:NH2	2.39	0.52
1:A:336:PHE:O	1:A:341:GLN:NE2	2.38	0.52
1:A:289:THR:HG23	1:A:292:GLU:OE2	2.09	0.52
1:A:453:LEU:HD12	1:A:455:ILE:HD13	1.92	0.52
1:A:535:PHE:CD1	1:A:535:PHE:N	2.75	0.52
1:A:696:ILE:N	1:A:696:ILE:CD1	2.72	0.51
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.92	0.51
1:A:98:ASN:O	1:A:102:VAL:HG23	2.11	0.51
1:A:289:THR:C	1:A:291:GLU:N	2.68	0.51
1:A:61:THR:OG1	1:A:71:GLN:OE1	2.28	0.51
1:A:39:PRO:O	1:A:40:ASP:HB3	2.10	0.51
1:A:397:ARG:HD2	1:A:404:LEU:CD1	2.41	0.51
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.93	0.51
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.92	0.51
1:A:289:THR:O	1:A:293:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:HD13	1:A:577:VAL:HG22	1.92	0.51
1:A:241:LYS:H	1:A:455:ILE:CD1	2.23	0.51
1:A:341:GLN:O	1:A:345:PHE:CD2	2.64	0.51
1:A:385:ASN:ND2	1:A:388:VAL:CG2	2.74	0.51
1:A:614:ASP:OD1	1:A:615:PRO:HD2	2.11	0.51
1:A:43:GLU:O	1:A:44:ARG:HB3	2.12	0.50
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.44	0.50
1:A:375:LEU:O	1:A:379:SER:OG	2.29	0.50
1:A:62:PHE:CE1	1:A:72:VAL:CG2	2.83	0.49
1:A:297:HIS:ND1	1:A:297:HIS:N	2.60	0.49
1:A:329:GLN:O	1:A:332:ASP:HB2	2.12	0.49
1:A:410:ASN:CG	1:A:413:LYS:HD3	2.37	0.49
1:A:702:VAL:HG13	1:A:712:VAL:HG11	1.94	0.49
1:A:308:ASN:C	1:A:308:ASN:OD1	2.53	0.49
1:A:325:LYS:HE2	1:A:325:LYS:CA	2.42	0.49
1:A:328:ARG:HA	1:A:331:MET:HE3	1.94	0.49
1:A:289:THR:C	1:A:293:LYS:HD2	2.38	0.49
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.93	0.48
1:A:259:GLN:CG	1:A:261:TYR:CZ	2.96	0.48
1:A:319:SER:OG	1:A:321:GLU:HG2	2.13	0.48
1:A:695:ARG:N	1:A:696:ILE:HD12	2.28	0.48
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.41	0.48
1:A:61:THR:OG1	1:A:71:GLN:HG2	2.13	0.48
1:A:296:LEU:O	1:A:297:HIS:HB2	2.13	0.48
1:A:597:GLU:O	1:A:601:LYS:HG3	2.12	0.48
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.49	0.48
1:A:479:GLN:HE21	1:A:483:ASN:ND2	2.12	0.48
1:A:508:LEU:HB3	1:A:509:ASP:H	1.13	0.48
1:A:47:TYR:CE2	1:A:100:PRO:HG3	2.49	0.48
1:A:509:ASP:OD1	1:A:557:LYS:NZ	2.45	0.48
1:A:23:ASP:N	1:A:23:ASP:OD1	2.46	0.47
1:A:56:THR:OG1	1:A:58:ASP:OD1	2.27	0.47
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.55	0.47
1:A:158:ILE:HD13	1:A:159:SER:N	2.29	0.47
1:A:385:ASN:ND2	1:A:388:VAL:HG21	2.29	0.47
1:A:376:ASN:O	1:A:380:THR:CG2	2.61	0.47
1:A:614:ASP:OD1	1:A:616:ASN:HB2	2.15	0.47
1:A:62:PHE:O	1:A:69:ASP:HA	2.15	0.47
1:A:534:VAL:O	1:A:536:PRO:HD3	2.15	0.47
1:A:279:HIS:O	1:A:283:GLN:HG3	2.15	0.46
1:A:377:ALA:O	1:A:381:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:CG1	1:A:73:LYS:N	2.79	0.46
1:A:137:GLN:O	1:A:137:GLN:HG3	2.12	0.46
1:A:213:GLN:O	1:A:217:GLN:HG2	2.16	0.46
1:A:488:LYS:O	1:A:492:GLU:HG3	2.16	0.46
1:A:710:PRO:HD3	1:A:729:HIS:CE1	2.50	0.46
1:A:729:HIS:CD2	1:A:729:HIS:C	2.90	0.46
1:A:293:LYS:HA	1:A:298:LEU:HD12	1.96	0.46
1:A:690:LYS:HB2	1:A:690:LYS:HE2	1.69	0.46
1:A:753:ARG:O	1:A:756:GLU:HB2	2.16	0.46
1:A:302:GLU:CD	1:A:302:GLU:N	2.72	0.46
1:A:3:PRO:O	1:A:12:HIS:HD2	1.99	0.46
1:A:64:THR:N	1:A:68:GLN:O	2.48	0.46
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.51	0.46
1:A:83:ILE:HD11	1:A:86:ASP:OD2	2.16	0.46
1:A:238:ARG:HD2	1:A:267:ARG:NE	2.31	0.45
1:A:399:LEU:HD12	1:A:401:GLY:H	1.80	0.45
1:A:61:THR:HA	1:A:71:GLN:HG2	1.97	0.45
1:A:385:ASN:CG	1:A:388:VAL:HG23	2.42	0.45
1:A:708:LEU:HD13	1:A:757:ALA:HB3	1.97	0.45
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.98	0.45
1:A:40:ASP:OD2	1:A:42:LYS:CB	2.60	0.45
1:A:223:GLU:O	1:A:227:ASN:HB2	2.17	0.45
1:A:92:SER:OG	1:A:120:GLY:N	2.49	0.45
1:A:701:PHE:CE1	1:A:705:TYR:CD2	3.04	0.45
1:A:724:ASP:OD1	1:A:728:LYS:HD2	2.16	0.45
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.47	0.45
1:A:354:LEU:O	1:A:418:ARG:HD3	2.17	0.45
1:A:685:ILE:O	1:A:686:ARG:C	2.59	0.45
1:A:241:LYS:N	1:A:455:ILE:HD11	2.31	0.45
1:A:436:LYS:NZ	1:A:436:LYS:CB	2.76	0.44
1:A:692:PHE:CD2	1:A:747:ARG:HG2	2.52	0.44
1:A:83:ILE:CD1	1:A:86:ASP:OD2	2.65	0.44
1:A:72:VAL:HG12	1:A:73:LYS:H	1.81	0.44
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.53	0.44
1:A:289:THR:HG1	1:A:292:GLU:HG3	1.81	0.44
1:A:698:TYR:CD1	1:A:720:GLN:HA	2.53	0.44
1:A:397:ARG:HG3	1:A:406:ALA:HB2	2.00	0.44
1:A:99:GLU:HB2	1:A:100:PRO:HD3	2.00	0.44
1:A:241:LYS:HE3	1:A:243:ILE:HD11	2.00	0.43
1:A:677:ARG:HG3	1:A:682:LEU:HD12	2.00	0.43
1:A:289:THR:O	1:A:291:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.17	0.43
1:A:470:CYS:O	1:A:473:TYR:HB3	2.19	0.43
1:A:694:ASN:HB3	1:A:696:ILE:HD11	2.00	0.43
1:A:333:ILE:O	1:A:334:VAL:C	2.60	0.43
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.18	0.43
1:A:38:ASN:C	1:A:40:ASP:N	2.69	0.43
1:A:241:LYS:N	1:A:455:ILE:CD1	2.82	0.43
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.54	0.43
1:A:471:ILE:HD12	1:A:471:ILE:HA	1.89	0.43
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.54	0.42
1:A:289:THR:HB	1:A:291:GLU:OE1	2.18	0.42
1:A:385:ASN:HB3	1:A:388:VAL:HG21	2.00	0.42
1:A:219:ASN:N	1:A:220:PRO:CD	2.72	0.42
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.65	0.42
1:A:60:PHE:O	1:A:71:GLN:HA	2.19	0.42
1:A:217:GLN:O	1:A:220:PRO:HG2	2.20	0.42
1:A:158:ILE:HD12	1:A:158:ILE:HG23	1.56	0.42
1:A:241:LYS:HD2	1:A:243:ILE:CD1	2.41	0.42
1:A:149:ASN:ND2	1:A:149:ASN:C	2.78	0.42
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.84	0.42
1:A:692:PHE:O	1:A:695:ARG:NE	2.40	0.42
1:A:35:ILE:HG12	1:A:78:ASN:O	2.20	0.42
1:A:59:SER:HB3	1:A:73:LYS:HZ2	1.81	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.42
1:A:689:ARG:HH11	1:A:689:ARG:CG	2.33	0.42
1:A:385:ASN:CG	1:A:388:VAL:CG2	2.93	0.42
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.55	0.42
1:A:90:ASP:HB3	1:A:93:GLU:HG3	2.02	0.42
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.54	0.41
1:A:289:THR:C	1:A:291:GLU:H	2.27	0.41
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.84	0.41
1:A:521:GLN:HA	1:A:522:PRO:C	2.45	0.41
1:A:747:ARG:HH11	1:A:747:ARG:HD3	1.54	0.41
1:A:4:ILE:O	1:A:4:ILE:HG22	2.18	0.41
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.84	0.41
1:A:399:LEU:HD12	1:A:401:GLY:N	2.35	0.41
1:A:497:GLU:O	1:A:498:LYS:HB3	2.20	0.41
1:A:61:THR:OG1	1:A:71:GLN:CD	2.64	0.41
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.55	0.41
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.74	0.41
1:A:687:ILE:HG22	1:A:688:THR:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:CB	1:A:71:GLN:HG2	2.51	0.41
1:A:296:LEU:C	1:A:297:HIS:ND1	2.79	0.41
1:A:702:VAL:O	1:A:706:TYR:HB3	2.19	0.41
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.23	0.41
1:A:146:ARG:HA	1:A:150:GLU:OE1	2.20	0.41
1:A:397:ARG:HE	1:A:397:ARG:HB2	1.46	0.41
1:A:2:ASN:C	1:A:4:ILE:N	2.78	0.41
1:A:83:ILE:HA	1:A:83:ILE:HD12	1.35	0.41
1:A:87:GLY:N	1:A:105:ASN:HD21	2.18	0.41
1:A:388:VAL:HG23	1:A:388:VAL:H	1.39	0.41
1:A:400:ALA:N	1:A:403:ASP:O	2.49	0.41
1:A:412:GLU:OE2	1:A:413:LYS:HG3	2.20	0.41
1:A:499:ILE:HG22	1:A:500:ASN:N	2.36	0.41
1:A:609:THR:O	1:A:613:ASN:HB2	2.20	0.41
1:A:620:ARG:HB3	1:A:628:LEU:CD2	2.51	0.41
1:A:654:ARG:O	1:A:656:ILE:HD12	2.21	0.41
1:A:354:LEU:HD13	1:A:421:LEU:HD23	2.03	0.40
1:A:396:PRO:HD2	1:A:407:GLN:O	2.20	0.40
1:A:479:GLN:HE21	1:A:483:ASN:HD21	1.68	0.40
1:A:391:LYS:O	1:A:395:GLU:N	2.46	0.40
1:A:91:MET:CE	1:A:106:LEU:HD13	2.51	0.40
1:A:32:LYS:H	1:A:32:LYS:HG2	1.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	735/762 (96%)	692 (94%)	30 (4%)	13 (2%)	6 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	203	ASN
1	A	363	ALA
1	A	44	ARG
1	A	509	ASP
1	A	711	ASN
1	A	204	GLN
1	A	498	LYS
1	A	290	ALA
1	A	499	ILE
1	A	7	ARG
1	A	713	PRO
1	A	39	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	636/666 (96%)	547 (86%)	89 (14%)	3 1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	22	SER
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	44	ARG
1	A	54	SER
1	A	57	SER
1	A	63	LYS
1	A	66	ASP
1	A	73	LYS
1	A	83	ILE
1	A	84	LYS

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Mol	Chain	Res	Type
1	A	92	SER
1	A	131	ARG
1	A	144	LYS
1	A	146	ARG
1	A	149	ASN
1	A	158	ILE
1	A	191	LYS
1	A	202	ARG
1	A	211	LEU
1	A	249	ASN
1	A	280	ILE
1	A	291	GLU
1	A	293	LYS
1	A	302	GLU
1	A	303	SER
1	A	313	VAL
1	A	321	GLU
1	A	325	LYS
1	A	329	GLN
1	A	333	ILE
1	A	338	GLN
1	A	342	MET
1	A	343	SER
1	A	357	ILE
1	A	358	LYS
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	398	ILE
1	A	399	LEU
1	A	407	GLN
1	A	411	VAL
1	A	412	GLU
1	A	413	LYS
1	A	422	VAL
1	A	436	LYS
1	A	444	GLU
1	A	446	LYS
1	A	455	ILE
1	A	460	ILE

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Mol	Chain	Res	Type
1	A	462	LYS
1	A	489	VAL
1	A	491	GLN
1	A	495	LEU
1	A	496	LYS
1	A	499	ILE
1	A	508	LEU
1	A	510	SER
1	A	520	ARG
1	A	544	ILE
1	A	565	LYS
1	A	582	GLN
1	A	627	PHE
1	A	628	LEU
1	A	640	SER
1	A	656	ILE
1	A	661	LYS
1	A	666	LYS
1	A	669	ASP
1	A	688	THR
1	A	689	ARG
1	A	690	LYS
1	A	696	ILE
1	A	703	LYS
1	A	717	GLU
1	A	723	THR
1	A	728	LYS
1	A	735	GLU
1	A	738	ARG
1	A	742	THR
1	A	744	ILE
1	A	747	ARG
1	A	751	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	HIS
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	479	GLN
1	A	480	GLN
1	A	491	GLN
1	A	521	GLN
1	A	582	GLN
1	A	594	GLN
1	A	633	GLN
1	A	649	ASN
1	A	720	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BEF	A	1000	3	0,3,3	-	-	-		
3	MNT	A	999[B]	-	38,39,39	2.41	10 (26%)	56,58,58	2.69	19 (33%)
3	MNT	A	999[A]	-	38,39,39	2.39	11 (28%)	56,58,58	2.84	20 (35%)

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	MNT	A	999[B]	-	-	6/26/38/38	0/4/4/4
3	MNT	A	999[A]	-	-	4/26/38/38	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999[A]	MNT	C2B-C3B	-9.75	1.32	1.52
3	A	999[B]	MNT	C2B-C3B	-9.75	1.32	1.52
3	A	999[A]	MNT	C8-N7	4.25	1.39	1.31
3	A	999[B]	MNT	C8-N7	4.25	1.39	1.31
3	A	999[B]	MNT	C6'-C1'	4.17	1.46	1.39
3	A	999[A]	MNT	C6'-C1'	3.53	1.45	1.39
3	A	999[B]	MNT	C5'-C6'	3.47	1.44	1.38
3	A	999[A]	MNT	PA-O3A	-3.43	1.55	1.59
3	A	999[B]	MNT	PA-O3A	-3.43	1.55	1.59
3	A	999[A]	MNT	C1'-C2'	3.32	1.46	1.41
3	A	999[B]	MNT	C4'-C3'	3.16	1.44	1.38
3	A	999[A]	MNT	C3'-C2'	3.16	1.44	1.39
3	A	999[A]	MNT	C2-N1	3.00	1.39	1.33
3	A	999[B]	MNT	C2-N1	3.00	1.39	1.33
3	A	999[A]	MNT	C5'-C4'	2.76	1.44	1.38
3	A	999[A]	MNT	O3'-C'	2.71	1.40	1.34
3	A	999[B]	MNT	O3'-C'	2.71	1.40	1.34
3	A	999[B]	MNT	C1'-C2'	2.71	1.45	1.41
3	A	999[A]	MNT	C5'-C6'	2.32	1.42	1.38
3	A	999[A]	MNT	C5-C4	2.01	1.42	1.39
3	A	999[B]	MNT	C5-C4	2.01	1.42	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999[A]	MNT	C2'-C1'-C'	-10.59	105.61	122.11
3	A	999[B]	MNT	C3'-C2'-N2'	-9.11	109.98	121.33
3	A	999[B]	MNT	C6'-C1'-C'	-6.45	105.61	118.66
3	A	999[A]	MNT	O3'-C'-O1'	-6.24	113.40	123.55
3	A	999[B]	MNT	O3'-C'-O1'	-6.24	113.40	123.55
3	A	999[A]	MNT	C1'-C2'-N2'	5.97	127.91	121.36
3	A	999[A]	MNT	C3'-C2'-N2'	-5.83	114.07	121.33
3	A	999[A]	MNT	N6-C6-N1	-5.61	105.88	118.38
3	A	999[B]	MNT	N6-C6-N1	-5.61	105.88	118.38
3	A	999[A]	MNT	O3'-C3B-C4B	4.25	119.18	109.37
3	A	999[B]	MNT	O3'-C3B-C4B	4.25	119.18	109.37
3	A	999[A]	MNT	C6'-C1'-C'	4.22	127.18	118.66
3	A	999[A]	MNT	C2B-C3B-C4B	4.17	111.04	102.93
3	A	999[B]	MNT	C2B-C3B-C4B	4.17	111.04	102.93
3	A	999[A]	MNT	O3'-C'-C1'	4.15	118.31	111.71
3	A	999[B]	MNT	O3'-C'-C1'	4.15	118.31	111.71
3	A	999[A]	MNT	O3'-C3B-C2B	4.13	119.17	109.21
3	A	999[B]	MNT	O3'-C3B-C2B	4.13	119.17	109.21
3	A	999[B]	MNT	C1'-C2'-N2'	4.10	125.86	121.36
3	A	999[B]	MNT	C2'-C1'-C'	3.26	127.18	122.11
3	A	999[A]	MNT	C3B-O3'-C'	3.25	124.38	117.33
3	A	999[B]	MNT	C3B-O3'-C'	3.25	124.38	117.33
3	A	999[A]	MNT	N3-C4-N9	-3.23	121.68	127.17
3	A	999[B]	MNT	N3-C4-N9	-3.23	121.68	127.17
3	A	999[B]	MNT	C4'-C5'-C6'	3.12	124.09	120.24
3	A	999[A]	MNT	C4'-C3'-C2'	2.66	124.09	118.69
3	A	999[A]	MNT	C3B-C2B-C1B	2.64	107.92	102.89
3	A	999[B]	MNT	C3B-C2B-C1B	2.64	107.92	102.89
3	A	999[A]	MNT	C5-C4-N9	2.63	108.67	105.81
3	A	999[B]	MNT	C5-C4-N9	2.63	108.67	105.81
3	A	999[A]	MNT	O4'-C1B-N9	-2.54	103.40	107.96
3	A	999[B]	MNT	O4'-C1B-N9	-2.54	103.40	107.96
3	A	999[A]	MNT	C3'-C2'-C1'	-2.32	116.34	119.37
3	A	999[A]	MNT	C2-N3-C4	-2.29	106.24	111.83
3	A	999[B]	MNT	C2-N3-C4	-2.29	106.24	111.83
3	A	999[A]	MNT	C5-C4-N3	2.10	129.60	126.72
3	A	999[B]	MNT	C5-C4-N3	2.10	129.60	126.72
3	A	999[A]	MNT	C5-N7-C8	-2.06	100.22	103.45
3	A	999[B]	MNT	C5-N7-C8	-2.06	100.22	103.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

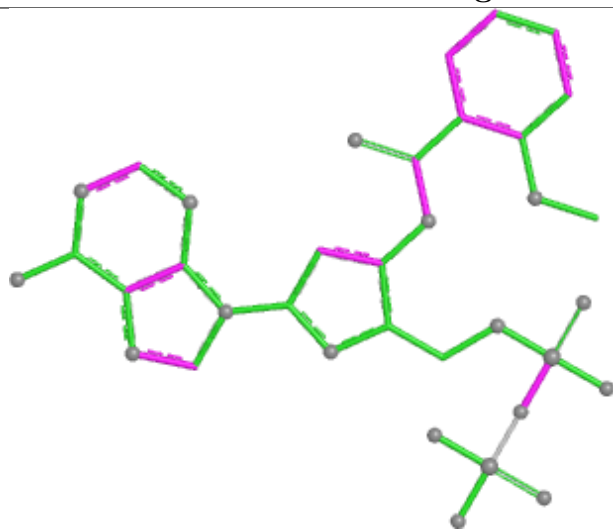
Mol	Chain	Res	Type	Atoms
3	A	999[A]	MNT	PA-O3A-PB-O2B
3	A	999[B]	MNT	PA-O3A-PB-O2B
3	A	999[B]	MNT	C1'-C2'-N2'-CM'
3	A	999[A]	MNT	O4'-C1B-N9-C4
3	A	999[B]	MNT	O4'-C1B-N9-C4
3	A	999[A]	MNT	PA-O3A-PB-O3B
3	A	999[B]	MNT	PA-O3A-PB-O3B
3	A	999[A]	MNT	C1'-C'-O3'-C3B
3	A	999[B]	MNT	C1'-C'-O3'-C3B
3	A	999[B]	MNT	C3'-C2'-N2'-CM'

There are no ring outliers.

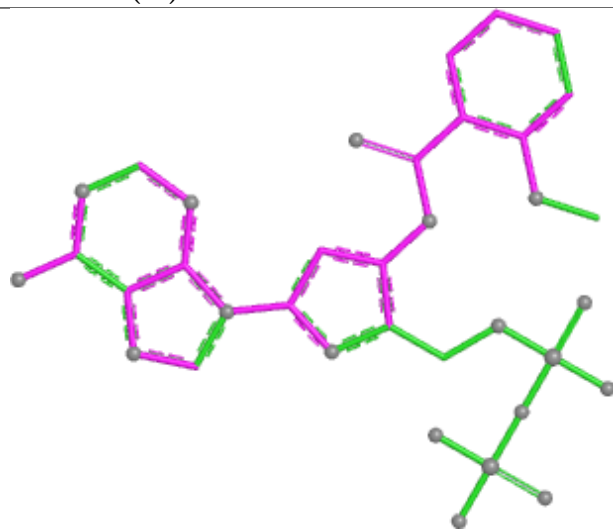
No monomer is involved in short contacts.

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.

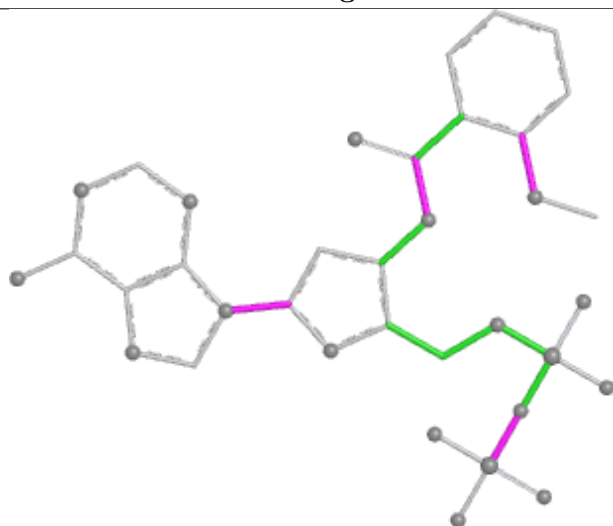
Ligand MNT A 999 (B)



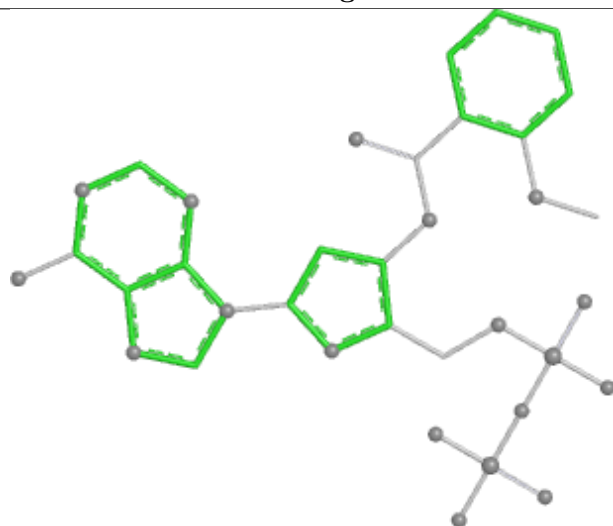
Bond lengths



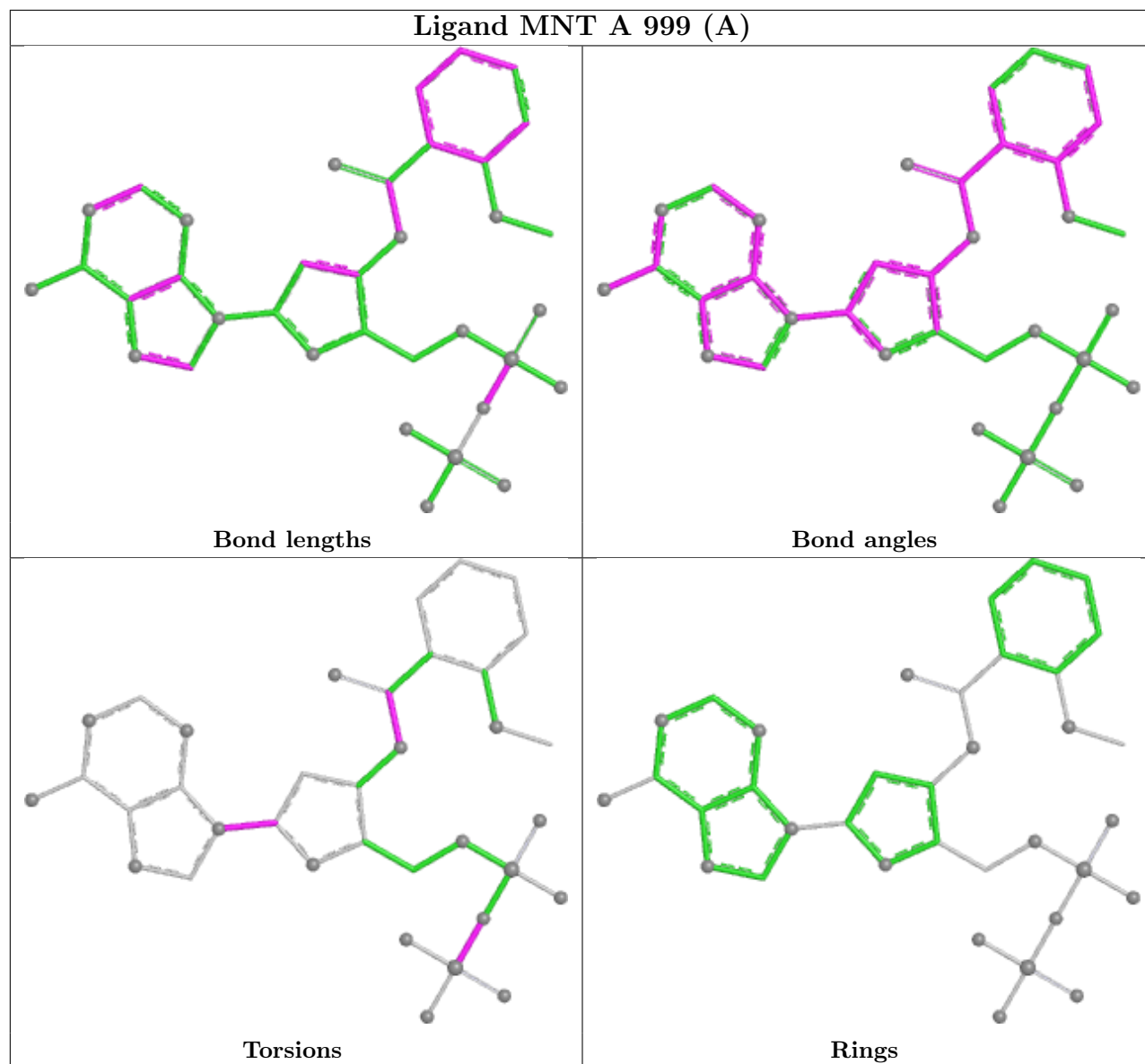
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.