Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 08:35 AM EST

PDB ID	:	1LVK
Title	:	X-RAY CRYSTAL STRUCTURE OF THE MG (DOT) 2'(3')-O-(N-METHYLANTHRANILOYL) 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 (i) 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 (1)) were used in the production of this report:

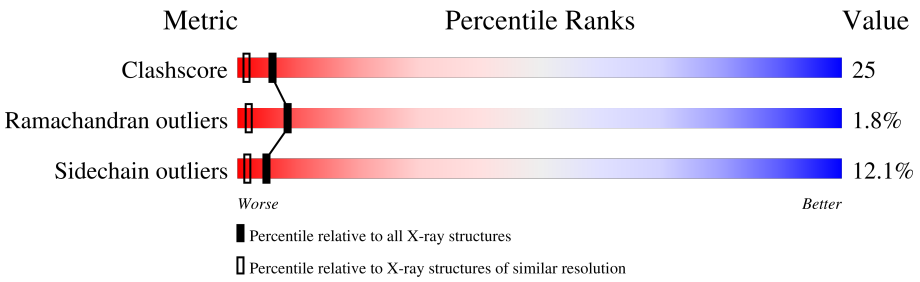
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	50% 33% 11% • •

2 Entry composition (i)

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

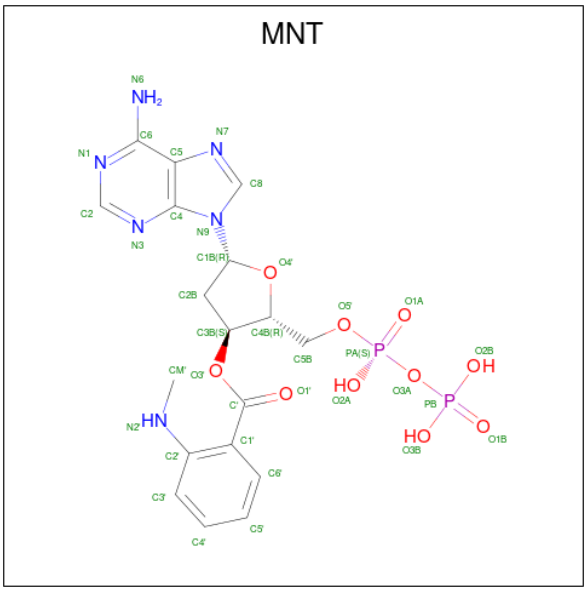
There are 12 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

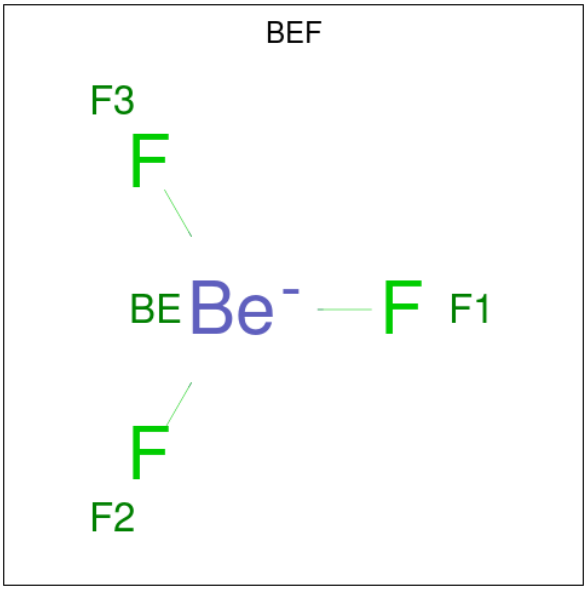
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is 2'(3')-O-N-METHYLANTHRANILOYL-ADENOSINE-5'-DIPHOSPHATE (three-letter code: MNT) (formula: $C_{18}H_{22}N_6O_{10}P_2$).



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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



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

- Molecule 5 is water.

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

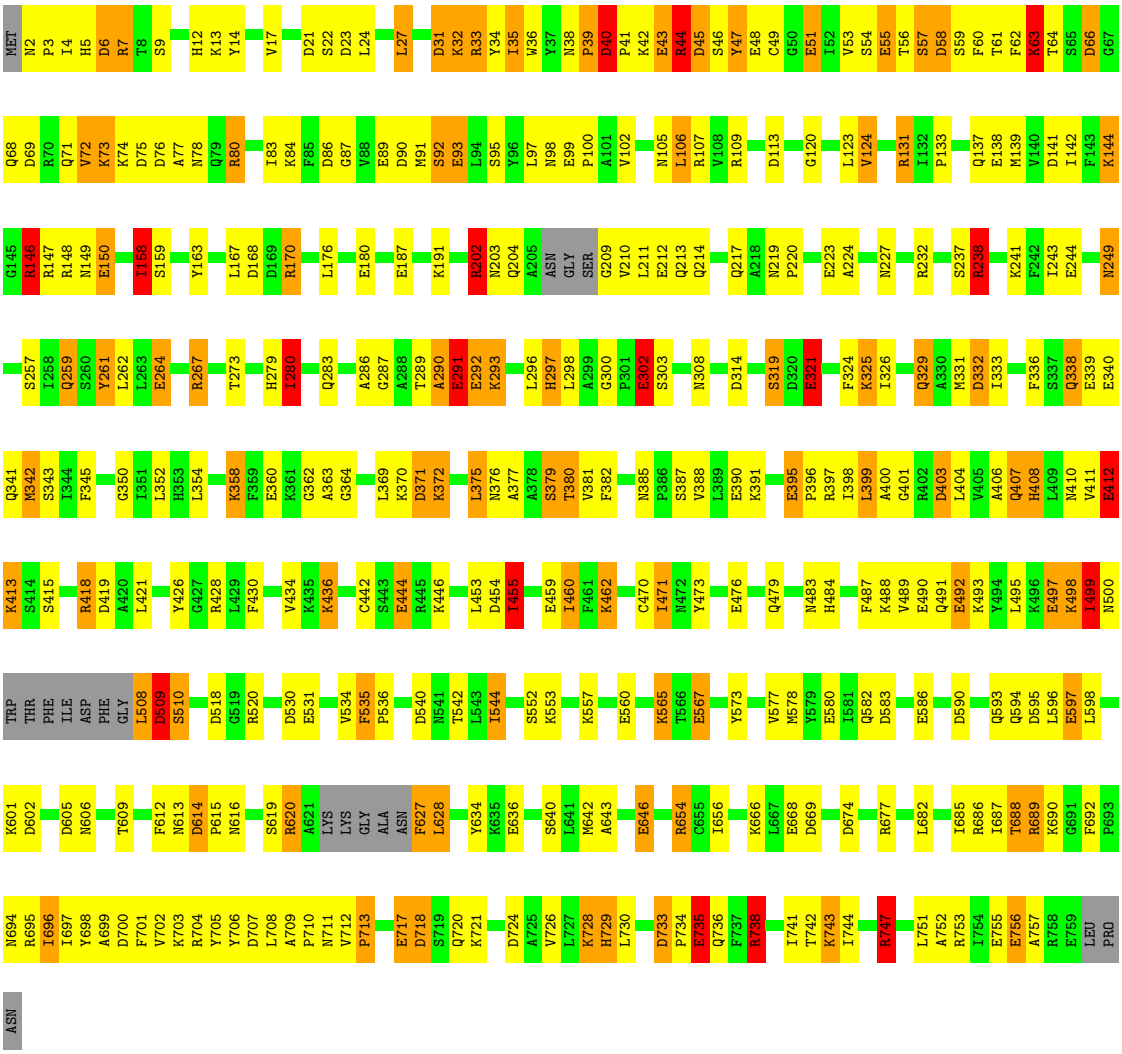
3 Residue-property plots (i)

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. 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

Chain A: 50% 33% 11%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	1.24	48/6017 (0.8%)	1.70	122/8122 (1.5%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	LYS	CE-NZ	-14.16	1.13	1.49
1	A	180	GLU	CD-OE1	10.44	1.37	1.25
1	A	668	GLU	CD-OE2	10.11	1.36	1.25
1	A	340	GLU	CD-OE1	9.84	1.36	1.25
1	A	360	GLU	CD-OE2	9.33	1.35	1.25
1	A	492	GLU	CD-OE1	8.86	1.35	1.25
1	A	567	GLU	CD-OE2	8.66	1.35	1.25
1	A	43	GLU	CD-OE2	8.54	1.35	1.25
1	A	212	GLU	CD-OE2	8.43	1.34	1.25
1	A	138	GLU	CD-OE1	8.30	1.34	1.25
1	A	636	GLU	CD-OE1	8.26	1.34	1.25
1	A	531	GLU	CD-OE1	8.21	1.34	1.25
1	A	264	GLU	CD-OE2	-8.06	1.16	1.25
1	A	339	GLU	CD-OE1	8.01	1.34	1.25
1	A	580	GLU	CD-OE1	7.32	1.33	1.25
1	A	291	GLU	CD-OE2	7.29	1.33	1.25
1	A	412	GLU	CD-OE1	7.13	1.33	1.25
1	A	51	GLU	CD-OE1	7.13	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	GLU	CD-OE2	6.96	1.33	1.25
1	A	510	SER	CB-OG	6.90	1.51	1.42
1	A	717	GLU	CD-OE1	6.87	1.33	1.25
1	A	55	GLU	CD-OE2	6.83	1.33	1.25
1	A	390	GLU	CD-OE1	6.76	1.33	1.25
1	A	490	GLU	CD-OE2	6.66	1.32	1.25
1	A	395	GLU	CD-OE2	6.58	1.32	1.25
1	A	187	GLU	CD-OE1	6.45	1.32	1.25
1	A	48	GLU	CD-OE1	6.41	1.32	1.25
1	A	131	ARG	NE-CZ	6.15	1.41	1.33
1	A	444	GLU	CD-OE1	6.14	1.32	1.25
1	A	244	GLU	CD-OE1	6.06	1.32	1.25
1	A	202	ARG	CZ-NH2	6.03	1.40	1.33
1	A	540	ASP	CG-OD1	5.92	1.39	1.25
1	A	756	GLU	CD-OE1	5.87	1.32	1.25
1	A	560	GLU	CD-OE2	5.87	1.32	1.25
1	A	148	ARG	CZ-NH1	5.68	1.40	1.33
1	A	237	SER	CB-OG	5.55	1.49	1.42
1	A	89	GLU	CD-OE1	5.42	1.31	1.25
1	A	292	GLU	CD-OE2	5.38	1.31	1.25
1	A	109	ARG	NE-CZ	5.31	1.40	1.33
1	A	321	GLU	CD-OE2	5.28	1.31	1.25
1	A	497	GLU	CD-OE1	5.27	1.31	1.25
1	A	476	GLU	CD-OE1	5.23	1.31	1.25
1	A	586	GLU	CD-OE2	5.15	1.31	1.25
1	A	597	GLU	CD-OE2	5.15	1.31	1.25
1	A	302	GLU	CD-OE2	5.13	1.31	1.25
1	A	755	GLU	CD-OE1	5.11	1.31	1.25
1	A	93	GLU	CG-CD	5.11	1.59	1.51
1	A	45	ASP	CG-OD1	5.03	1.36	1.25

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH1	20.73	130.66	120.30
1	A	654	ARG	NE-CZ-NH2	-17.61	111.50	120.30
1	A	738	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	A	238	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	A	148	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	314	ASP	CB-CG-OD1	-10.70	108.67	118.30
1	A	170	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	713	PRO	N-CA-CB	10.09	115.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	261	TYR	CB-CG-CD2	-9.77	115.14	121.00
1	A	718	ASP	CB-CG-OD2	-9.02	110.18	118.30
1	A	7	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	735	GLU	N-CA-CB	8.72	126.29	110.60
1	A	590	ASP	CB-CG-OD1	-8.43	110.71	118.30
1	A	674	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	A	518	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	41	PRO	N-CA-CB	8.21	113.15	103.30
1	A	46	SER	N-CA-CB	7.95	122.42	110.50
1	A	738	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	7	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	518	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	A	21	ASP	CB-CG-OD1	-7.57	111.49	118.30
1	A	261	TYR	CB-CG-CD1	7.49	125.49	121.00
1	A	75	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	530	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	729	HIS	CA-CB-CG	-7.38	101.06	113.60
1	A	40	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	704	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	141	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	583	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	57	SER	N-CA-CB	-7.11	99.84	110.50
1	A	267	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	707	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	455	ILE	CA-CB-CG2	7.01	124.92	110.90
1	A	419	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	66	ASP	CB-CG-OD1	-6.95	112.04	118.30
1	A	530	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	A	654	ARG	NH1-CZ-NH2	6.92	127.01	119.40
1	A	202	ARG	CB-CA-C	6.89	124.17	110.40
1	A	131	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	76	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	58	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	605	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	619	SER	CB-CA-C	-6.73	97.31	110.10
1	A	606	ASN	CB-CA-C	6.73	123.86	110.40
1	A	168	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	44	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	141	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	489	VAL	CB-CA-C	6.61	123.96	111.40
1	A	747	ARG	NE-CZ-NH1	-6.59	117.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ARG	N-CA-CB	6.51	122.33	110.60
1	A	168	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	113	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	33	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	462	LYS	CB-CA-C	-6.44	97.52	110.40
1	A	107	ARG	CG-CD-NE	-6.43	98.30	111.80
1	A	718	ASP	CA-CB-CG	-6.38	99.36	113.40
1	A	408	HIS	CA-CB-CG	-6.36	102.79	113.60
1	A	158	ILE	CB-CA-C	6.34	124.29	111.60
1	A	232	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	267	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	6	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	704	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	273	THR	CA-CB-CG2	-6.24	103.66	112.40
1	A	232	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	471	ILE	CG1-CB-CG2	-6.23	97.69	111.40
1	A	280	ILE	CA-CB-CG2	6.20	123.30	110.90
1	A	80	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	419	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	238	ARG	CD-NE-CZ	6.13	132.19	123.60
1	A	590	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	565	LYS	CB-CA-C	-6.09	98.22	110.40
1	A	535	PHE	CA-CB-CG	-6.08	99.31	113.90
1	A	297	HIS	CA-CB-CG	-6.01	103.39	113.60
1	A	614	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	674	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	620	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	688	THR	N-CA-CB	-5.96	98.98	110.30
1	A	17	VAL	CA-CB-CG1	-5.95	101.97	110.90
1	A	459	GLU	CG-CD-OE1	5.95	130.20	118.30
1	A	403	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	106	LEU	CB-CG-CD2	-5.90	100.98	111.00
1	A	508	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	A	44	ARG	CG-CD-NE	5.83	124.04	111.80
1	A	595	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	146	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	743	LYS	CB-CA-C	-5.63	99.14	110.40
1	A	699	ALA	CB-CA-C	5.63	118.54	110.10
1	A	6	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	332	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	238	ARG	CG-CD-NE	-5.53	100.18	111.80
1	A	418	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	371	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	72	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	180	GLU	CB-CA-C	-5.39	99.61	110.40
1	A	371	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	319	SER	N-CA-CB	5.39	118.58	110.50
1	A	403	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	455	ILE	N-CA-CB	-5.34	98.51	110.80
1	A	542	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	442	CYS	CA-CB-SG	-5.33	104.41	114.00
1	A	733	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	634	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
1	A	33	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	259	GLN	CB-CG-CD	5.30	125.39	111.60
1	A	412	GLU	CB-CA-C	-5.28	99.84	110.40
1	A	634	TYR	CG-CD2-CE2	5.26	125.51	121.30
1	A	614	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	602	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	499	ILE	CB-CA-C	5.20	122.00	111.60
1	A	573	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
1	A	262	LEU	N-CA-CB	-5.20	100.01	110.40
1	A	47	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	150	GLU	CA-CB-CG	5.13	124.69	113.40
1	A	63	LYS	CD-CE-NZ	5.13	123.49	111.70
1	A	44	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	605	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	627	PHE	N-CA-CB	5.11	119.80	110.60
1	A	124	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	459	GLU	CG-CD-OE2	-5.06	108.18	118.30
1	A	491	GLN	CB-CG-CD	-5.06	98.45	111.60
1	A	302	GLU	CG-CD-OE2	-5.00	108.29	118.30

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	298	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	298	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 25.

All (298) 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: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:410:ASN:H	1:A:413:LYS:HZ3	0.95	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: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:689:ARG:HH11	1:A:689:ARG:HB3	1.40	0.87
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:741:ILE:HG22	1:A:742:THR:HG23	1.58	0.84
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HB	1:A:291:GLU:CD	2.00	0.81
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.08	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:60:PHE:CE2	1:A:74:LYS:HG2	2.18	0.78
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:695:ARG:C	1:A:696:ILE:HD12	2.06	0.76
1:A:410:ASN:H	1:A:413:LYS:NZ	1.80	0.76
1:A:493:LYS:HE3	1:A:743:LYS:HE3	1.67	0.75
1:A:59:SER:HB2	1:A:72:VAL:O	1.87	0.75
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:321:GLU:H	1:A:321:GLU:CD	1.90	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:399:LEU:C	1:A:399:LEU:HD12	2.10	0.71
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:GLU:H	1:A:302:GLU:CD	2.00	0.64
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: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: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:567:GLU:HB3	1:A:578:MET:HE1	1.83	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:38:ASN:C	1:A:40:ASP:H	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:C	1:A:455:ILE:HD12	2.24	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: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
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.24	0.56
1:A:342:MET:SD	1:A:342:MET:N	2.78	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:410:ASN:N	1:A:413:LYS:HZ3	1.81	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:87:GLY:H	1:A:105:ASN:HD21	1.52	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: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:694:ASN:C	1:A:695:ARG:HG3	2.28	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:331:MET:HE3	1:A:345:PHE:HZ	1.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HG1	1:A:58:ASP:CG	2.13	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
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:408:HIS:ND1	1:A:408:HIS:C	2.63	0.50
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:137:GLN:HG3	1:A:137:GLN:O	2.12	0.50
1:A:147:ARG:H	1:A:150:GLU:CD	2.15	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:404:LEU:C	1:A:404:LEU:HD13	2.33	0.49
1:A:702:VAL:HG13	1:A:712:VAL:HG11	1.94	0.49
1:A:325:LYS:HE2	1:A:325:LYS:CA	2.42	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:23:ASP:N	1:A:23:ASP:OD1	2.46	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:56:THR:OG1	1:A:58:ASP:OD1	2.27	0.47
1:A:331:MET:CE	1:A:345:PHE:HZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:THR:C	1:A:291:GLU:N	2.68	0.46
1:A:377:ALA:O	1:A:381:VAL:HG22	2.16	0.46
1:A:72:VAL:CG1	1:A:73:LYS:N	2.79	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:509:ASP:OD1	1:A:557:LYS:NZ	2.45	0.46
1:A:710:PRO:HD3	1:A:729:HIS:CE1	2.50	0.46
1:A:308:ASN:C	1:A:308:ASN:OD1	2.53	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: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: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:578:MET:HE2	1:A:578:MET:HB3	1.64	0.45
1:A:410:ASN:CG	1:A:413:LYS:HD3	2.37	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:289:THR:C	1:A:293:LYS:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:331:MET:CE	1:A:345:PHE:CZ	3.01	0.43
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
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:300:GLY:HA3	1:A:302:GLU:OE2	2.18	0.43
1:A:4:ILE:O	1:A:4:ILE:HG22	2.18	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: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: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:38:ASN:C	1:A:40:ASP:N	2.69	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:331:MET:HE3	1:A:345:PHE:CZ	2.54	0.42
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.54	0.41
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.84	0.41
1:A:747:ARG:HH11	1:A:747:ARG:HD3	1.54	0.41
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.84	0.41
1:A:729:HIS:CD2	1:A:729:HIS:C	2.90	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:163:TYR:CE2	1:A:167:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:61:THR:CB	1:A:71:GLN:HG2	2.51	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: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:59:SER:HB3	1:A:73:LYS:HZ2	1.82	0.41
1:A:385:ASN:CG	1:A:388:VAL:HG23	2.42	0.41
1:A:388:VAL:H	1:A:388:VAL:HG23	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:59:SER:HB3	1:A:73:LYS:HZ3	1.84	0.40
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
1:A:685:ILE:O	1:A:686:ARG:C	2.59	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%)	8 2

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	636/666 (96%)	559 (88%)	77 (12%)	5 1

All (77) 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

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Mol	Chain	Res	Type
1	A	57	SER
1	A	63	LYS
1	A	66	ASP
1	A	73	LYS
1	A	84	LYS
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	170	ARG
1	A	191	LYS
1	A	202	ARG
1	A	211	LEU
1	A	238	ARG
1	A	249	ASN
1	A	257	SER
1	A	280	ILE
1	A	291	GLU
1	A	293	LYS
1	A	302	GLU
1	A	303	SER
1	A	321	GLU
1	A	325	LYS
1	A	329	GLN
1	A	338	GLN
1	A	342	MET
1	A	343	SER
1	A	358	LYS
1	A	370	LYS
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	399	LEU
1	A	407	GLN
1	A	411	VAL
1	A	412	GLU
1	A	413	LYS
1	A	436	LYS

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Mol	Chain	Res	Type
1	A	444	GLU
1	A	446	LYS
1	A	455	ILE
1	A	460	ILE
1	A	462	LYS
1	A	495	LEU
1	A	509	ASP
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	666	LYS
1	A	669	ASP
1	A	689	ARG
1	A	696	ILE
1	A	703	LYS
1	A	717	GLU
1	A	728	LYS
1	A	735	GLU
1	A	738	ARG
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 (15) 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	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	483	ASN

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	582	GLN
1	A	594	GLN
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 monosaccharides 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	3,2	0,3,3	-	-	-		
3	MNT	A	999[B]	-	35,39,39	2.21	8 (22%)	43,58,58	3.01	16 (37%)
3	MNT	A	999[A]	-	35,39,39	2.20	8 (22%)	43,58,58	3.19	17 (39%)

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]	-	-	5/22/38/38	0/4/4/4
3	MNT	A	999[A]	-	-	3/22/38/38	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999[A]	MNT	C2B-C3B	-9.29	1.32	1.52
3	A	999[B]	MNT	C2B-C3B	-9.29	1.32	1.52
3	A	999[B]	MNT	C6'-C1'	4.00	1.46	1.39
3	A	999[A]	MNT	C6'-C1'	3.39	1.45	1.39
3	A	999[A]	MNT	C1'-C2'	3.30	1.46	1.41
3	A	999[A]	MNT	C3'-C2'	3.05	1.44	1.39
3	A	999[A]	MNT	C8-N7	2.89	1.39	1.34
3	A	999[B]	MNT	C8-N7	2.89	1.39	1.34
3	A	999[A]	MNT	C2-N1	2.87	1.39	1.33
3	A	999[B]	MNT	C2-N1	2.87	1.39	1.33
3	A	999[B]	MNT	C5'-C6'	2.81	1.44	1.38
3	A	999[A]	MNT	O3'-C'	2.73	1.40	1.34
3	A	999[B]	MNT	O3'-C'	2.73	1.40	1.34
3	A	999[B]	MNT	C1'-C2'	2.69	1.45	1.41
3	A	999[B]	MNT	C4'-C3'	2.56	1.44	1.38
3	A	999[A]	MNT	C5'-C4'	2.38	1.44	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999[A]	MNT	C2'-C1'-C'	-10.56	105.61	122.20
3	A	999[B]	MNT	C3'-C2'-N2'	-8.98	109.98	121.23
3	A	999[B]	MNT	C6'-C1'-C'	-6.36	105.61	118.66
3	A	999[A]	MNT	O3'-C'-O1'	-6.21	113.40	123.53
3	A	999[B]	MNT	O3'-C'-O1'	-6.21	113.40	123.53
3	A	999[A]	MNT	N6-C6-N1	-6.12	105.88	118.57
3	A	999[B]	MNT	N6-C6-N1	-6.12	105.88	118.57
3	A	999[A]	MNT	C1'-C2'-N2'	5.73	127.91	121.25
3	A	999[A]	MNT	C3'-C2'-N2'	-5.71	114.07	121.23
3	A	999[A]	MNT	C5-C6-N6	4.93	127.84	120.35
3	A	999[B]	MNT	C5-C6-N6	4.93	127.84	120.35
3	A	999[A]	MNT	O3'-C'-C1'	4.25	118.31	111.69
3	A	999[B]	MNT	O3'-C'-C1'	4.25	118.31	111.69
3	A	999[A]	MNT	O3'-C3B-C4B	4.22	119.18	109.42
3	A	999[B]	MNT	O3'-C3B-C4B	4.22	119.18	109.42
3	A	999[A]	MNT	O3'-C3B-C2B	4.19	119.17	109.18
3	A	999[B]	MNT	O3'-C3B-C2B	4.19	119.17	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999[A]	MNT	C6'-C1'-C'	4.16	127.18	118.66
3	A	999[A]	MNT	C2B-C3B-C4B	4.13	111.04	102.98
3	A	999[B]	MNT	C2B-C3B-C4B	4.13	111.04	102.98
3	A	999[A]	MNT	C3B-O3'-C'	4.03	124.38	117.38
3	A	999[B]	MNT	C3B-O3'-C'	4.03	124.38	117.38
3	A	999[B]	MNT	C1'-C2'-N2'	3.97	125.86	121.25
3	A	999[B]	MNT	C2'-C1'-C'	3.17	127.18	122.20
3	A	999[A]	MNT	C4'-C3'-C2'	2.63	124.09	118.62
3	A	999[A]	MNT	C3B-C2B-C1B	2.60	107.92	102.93
3	A	999[B]	MNT	C3B-C2B-C1B	2.60	107.92	102.93
3	A	999[B]	MNT	C4'-C5'-C6'	2.56	124.09	120.19
3	A	999[A]	MNT	C5-C6-N1	-2.53	114.61	120.35
3	A	999[B]	MNT	C5-C6-N1	-2.53	114.61	120.35
3	A	999[A]	MNT	C3'-C2'-C1'	-2.32	116.34	119.38
3	A	999[A]	MNT	C5B-C4B-C3B	2.04	119.19	114.53
3	A	999[B]	MNT	C5B-C4B-C3B	2.04	119.19	114.53

There are no chirality outliers.

All (8) 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	C1'-C'-O3'-C3B
3	A	999[B]	MNT	C1'-C'-O3'-C3B
3	A	999[A]	MNT	PA-O3A-PB-O3B
3	A	999[B]	MNT	PA-O3A-PB-O3B
3	A	999[B]	MNT	C3'-C2'-N2'-CM'

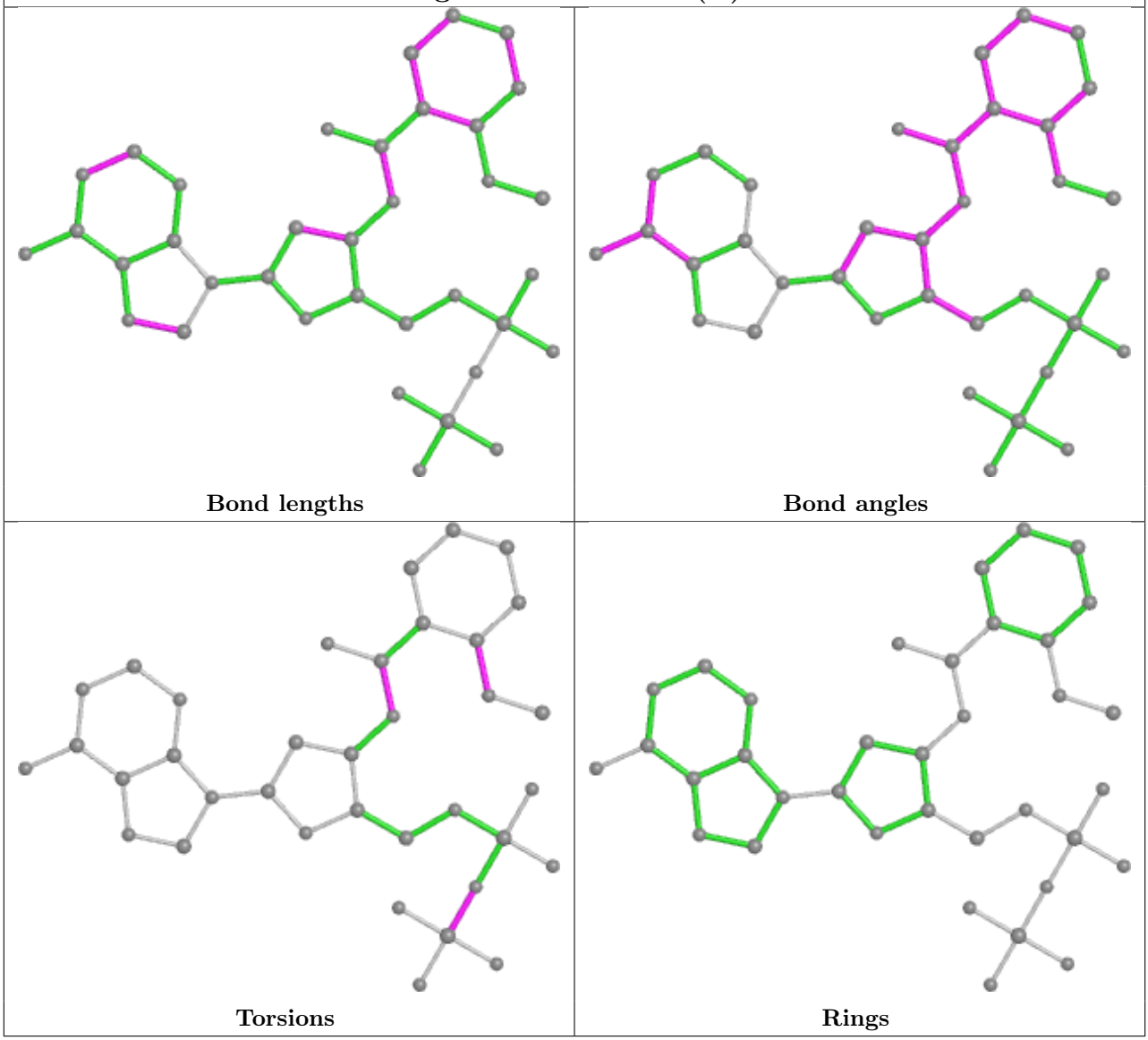
There are no ring outliers.

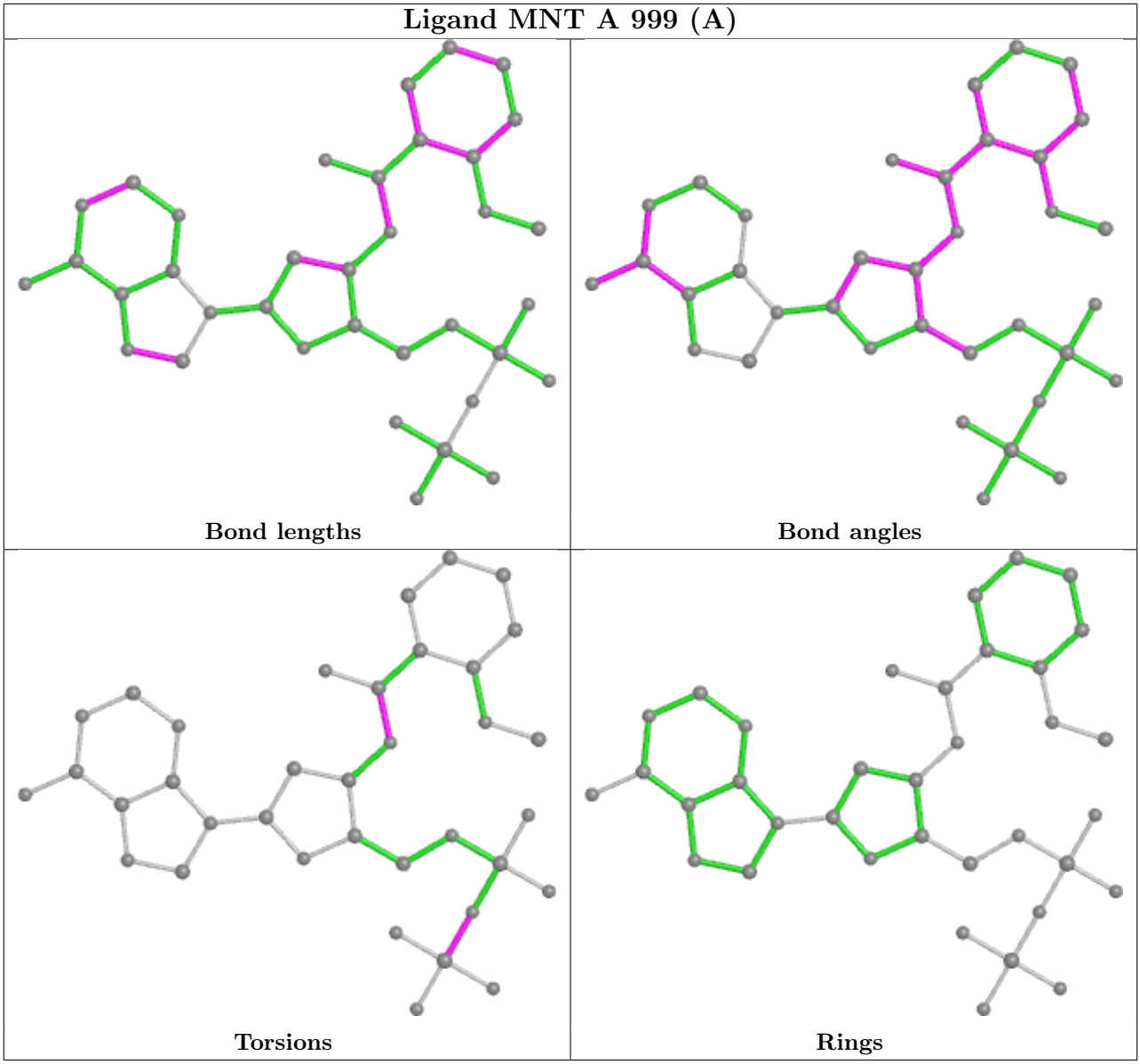
No monomer is involved in short contacts.

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 then 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)





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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.