



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:05 AM UTC

PDB ID : 1FPC / pdb_00001fpc
Title : ACTIVE SITE MIMETIC INHIBITION OF THROMBIN
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-10-16
Resolution : 2.30 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)
Xtrriage (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) : 2.49

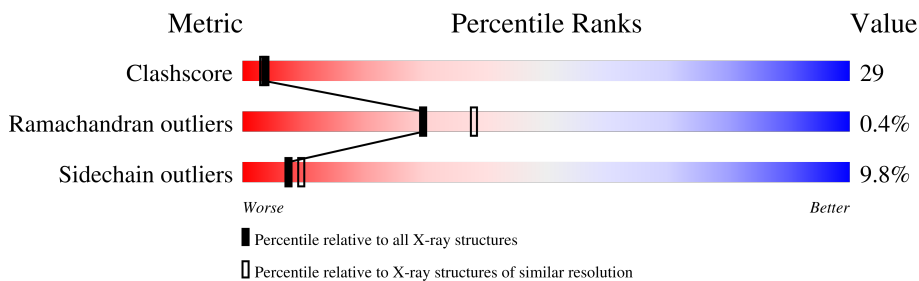
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	L	36	
2	H	259	
3	I	12	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2527 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 thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	26	212	135	32	44	1	0	0	0

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	248	1993	1270	353	356	14	0	0	0

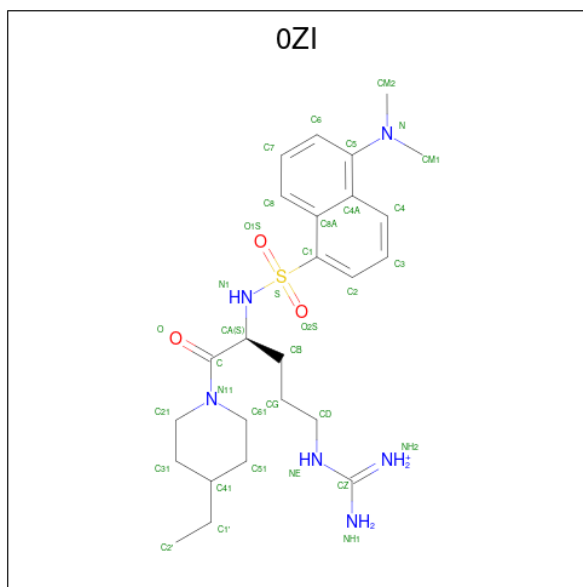
- Molecule 3 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	10	86	54	10	21	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	53	ASN	ASP	conflict	UNP P28504

- Molecule 4 is amino{[(4S)-4-({[5-(dimethylamino)naphthalen-1-yl]sulfonyl}amino)-5-(4-ethylpiperidin-1-yl)-5-oxopentyl]amino}methaniminium (CCD ID: 0ZI) (formula: C₂₅H₃₉N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	S	0	0
			35	25	6	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	19	Total	O	0	0
			19	19		
5	H	180	Total	O	0	0
			180	180		
5	I	2	Total	O	0	0
			2	2		

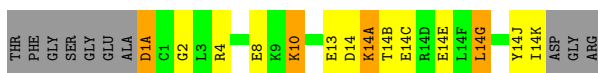
3 Residue-property plots [i](#)

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.

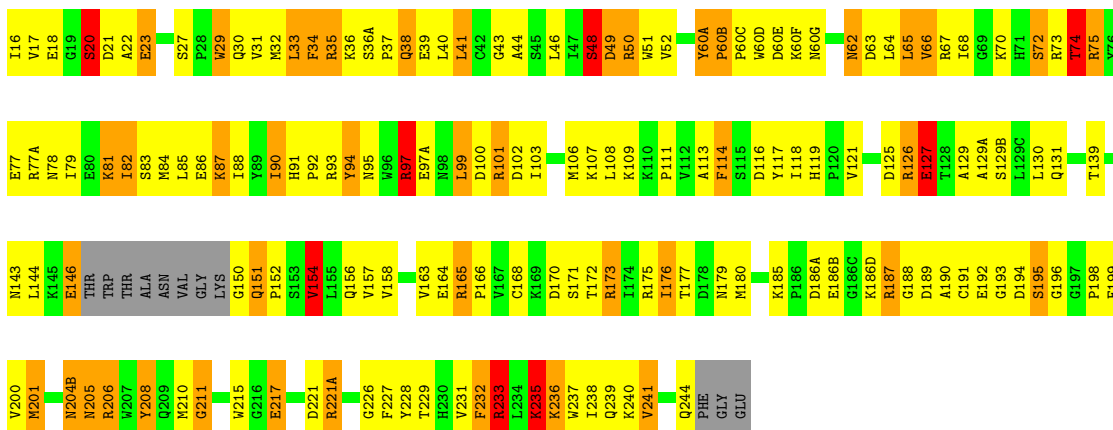
- Molecule 1: thrombin

Chain L: 



- Molecule 2: thrombin

Chain H: 



- Molecule 3: Hirudin

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 72.60Å 73.80Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.147 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2527	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: 0ZI, TYS

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	L	1.28	0/214	2.26	12/285 (4.2%)
2	H	1.45	10/2044 (0.5%)	2.59	151/2765 (5.5%)
3	I	0.92	0/70	2.28	4/91 (4.4%)
All	All	1.42	10/2328 (0.4%)	2.55	167/3141 (5.3%)

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
2	H	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	78	ASN	N-CA	8.10	1.55	1.46
2	H	77(A)	ARG	C-O	6.35	1.31	1.24
2	H	206	ARG	NE-CZ	-5.66	1.26	1.33
2	H	206	ARG	CD-NE	-5.65	1.38	1.46
2	H	172	THR	N-CA	5.27	1.52	1.46
2	H	29	TRP	N-CA	5.23	1.52	1.46
2	H	73	ARG	NE-CZ	5.16	1.38	1.33
2	H	208	TYR	C-O	5.13	1.30	1.24
2	H	215	TRP	NE1-CE2	-5.09	1.31	1.37
2	H	68	ILE	CA-CB	5.03	1.60	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	CD-NE-CZ	39.62	179.86	124.40
2	H	77(A)	ARG	CA-C-O	-17.04	101.08	121.02
2	H	48	SER	CA-C-O	-11.51	108.96	121.05
2	H	221(A)	ARG	NE-CZ-NH1	-11.36	110.14	121.50
2	H	189	ASP	CA-CB-CG	11.20	123.80	112.60
2	H	79	ILE	CB-CA-C	11.16	121.19	111.71
2	H	211	GLY	CA-C-N	10.41	136.09	123.19
2	H	211	GLY	C-N-CA	10.41	136.09	123.19
3	I	58	GLU	CB-CG-CD	10.18	129.90	112.60
2	H	164	GLU	CB-CG-CD	9.55	128.83	112.60
2	H	62	ASN	OD1-CG-ND2	9.48	132.08	122.60
2	H	77(A)	ARG	CA-C-N	-9.18	107.82	122.79
2	H	77(A)	ARG	C-N-CA	-9.18	107.82	122.79
2	H	78	ASN	CA-CB-CG	8.92	121.52	112.60
2	H	205	ASN	OD1-CG-ND2	-8.89	113.71	122.60
2	H	118	ILE	O-C-N	8.59	130.70	122.97
2	H	221(A)	ARG	CD-NE-CZ	-8.51	112.49	124.40
2	H	74	THR	N-CA-CB	-8.41	97.71	110.33
2	H	60(D)	TRP	CA-C-O	-8.28	109.47	120.15
2	H	127	GLU	CB-CG-CD	8.28	126.68	112.60
2	H	186(D)	LYS	CA-C-O	-8.25	111.81	120.89
2	H	60(G)	ASN	CA-CB-CG	8.20	120.80	112.60
2	H	114	PHE	CA-CB-CG	-8.18	105.62	113.80
2	H	231	VAL	O-C-N	8.13	129.88	121.91
1	L	14(E)	GLU	CB-CG-CD	8.12	126.41	112.60
2	H	231	VAL	CA-C-O	-8.01	112.68	121.17
2	H	74	THR	N-CA-C	7.98	123.36	112.90
2	H	170	ASP	CA-CB-CG	-7.96	104.64	112.60
2	H	23	GLU	CB-CG-CD	7.91	126.05	112.60
2	H	77(A)	ARG	N-CA-CB	7.84	123.05	109.72
2	H	176	ILE	CA-CB-CG2	7.70	123.59	110.50
3	I	56	PHE	CA-CB-CG	-7.62	106.18	113.80
2	H	119	HIS	CB-CA-C	7.59	120.45	109.45
2	H	103	ILE	O-C-N	7.54	129.53	122.97
2	H	129(B)	SER	CA-C-O	-7.41	110.26	119.38
2	H	190	ALA	N-CA-C	-7.37	101.02	110.53
2	H	67	ARG	NE-CZ-NH2	7.37	125.83	119.20
2	H	125	ASP	CA-CB-CG	-7.36	105.24	112.60
2	H	64	LEU	N-CA-C	7.29	121.36	109.85
2	H	35	ARG	NE-CZ-NH2	-7.17	112.75	119.20
2	H	192	GLU	CA-CB-CG	7.15	128.40	114.10
2	H	97	ARG	CD-NE-CZ	-7.14	114.41	124.40
2	H	158	VAL	CA-C-O	-7.07	114.64	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	83	SER	O-C-N	7.05	131.91	123.24
2	H	63	ASP	CA-CB-CG	7.00	119.60	112.60
2	H	129(A)	ALA	CA-C-O	-6.99	113.38	121.07
2	H	129(A)	ALA	N-CA-CB	6.89	120.29	109.82
2	H	171	SER	CA-C-O	-6.89	110.98	119.18
2	H	179	ASN	CA-C-O	-6.87	108.64	119.23
2	H	187	ARG	N-CA-C	6.87	117.11	108.45
2	H	172	THR	CA-C-O	-6.82	114.13	121.36
2	H	116	ASP	CA-C-O	-6.77	112.45	120.10
2	H	154	VAL	N-CA-CB	-6.75	99.43	111.93
2	H	116	ASP	O-C-N	6.62	129.97	122.22
2	H	64	LEU	CA-C-N	6.60	133.18	122.29
2	H	64	LEU	C-N-CA	6.60	133.18	122.29
2	H	238	ILE	CA-C-N	6.57	129.41	120.54
2	H	238	ILE	C-N-CA	6.57	129.41	120.54
2	H	232	PHE	CA-CB-CG	-6.57	107.23	113.80
2	H	43	GLY	N-CA-C	-6.53	102.26	112.58
1	L	1(A)	ASP	CA-CB-CG	-6.49	106.11	112.60
2	H	77	GLU	CB-CG-CD	6.49	123.64	112.60
1	L	2	GLY	CA-C-O	-6.48	111.74	119.00
2	H	204(B)	ASN	CB-CA-C	6.47	120.88	109.75
2	H	175	ARG	NE-CZ-NH1	-6.44	115.06	121.50
2	H	170	ASP	O-C-N	6.44	131.34	122.46
2	H	187	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	L	10	LYS	CB-CG-CD	6.32	125.85	111.30
2	H	117	TYR	O-C-N	6.28	129.84	122.24
2	H	176	ILE	N-CA-CB	-6.27	103.46	110.99
2	H	101	ARG	NE-CZ-NH2	-6.27	113.56	119.20
2	H	22	ALA	N-CA-CB	-6.24	101.43	110.36
2	H	151	GLN	OE1-CD-NE2	6.24	128.84	122.60
2	H	168	CYS	CA-C-O	6.24	127.93	121.07
1	L	14(G)	LEU	CB-CA-C	6.22	121.12	110.79
2	H	20	SER	O-C-N	6.21	130.19	122.92
2	H	200	VAL	N-CA-C	6.19	118.38	108.85
2	H	163	VAL	O-C-N	6.18	129.44	123.14
2	H	204(B)	ASN	N-CA-CB	-6.18	102.06	110.95
1	L	14(B)	THR	CA-C-O	-6.10	112.69	119.34
2	H	198	PRO	CA-C-O	-6.09	114.51	122.19
2	H	127	GLU	CA-CB-CG	6.05	126.20	114.10
2	H	126	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	H	75	ARG	CB-CG-CD	6.02	125.14	111.30
2	H	27	SER	CB-CA-C	6.01	120.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	ARG	CA-C-O	6.00	127.30	121.00
2	H	114	PHE	O-C-N	6.00	129.63	122.79
1	L	14(A)	LYS	CA-CB-CG	5.99	126.08	114.10
2	H	38	GLN	N-CA-C	-5.99	100.98	109.96
2	H	186(D)	LYS	N-CA-C	-5.99	99.30	108.76
1	L	14(A)	LYS	N-CA-CB	5.95	120.44	110.32
2	H	63	ASP	N-CA-C	-5.89	105.59	112.89
2	H	173	ARG	CD-NE-CZ	5.88	132.63	124.40
2	H	75	ARG	CA-C-O	5.83	128.35	121.36
2	H	233	ARG	NE-CZ-NH2	-5.81	113.97	119.20
2	H	95	ASN	CA-CB-CG	5.80	118.40	112.60
2	H	232	PHE	CA-C-N	5.73	128.53	120.28
2	H	232	PHE	C-N-CA	5.73	128.53	120.28
2	H	172	THR	O-C-N	5.71	129.60	122.92
2	H	73	ARG	CA-C-N	5.71	132.02	121.52
2	H	73	ARG	C-N-CA	5.71	132.02	121.52
2	H	38	GLN	OE1-CD-NE2	5.67	128.27	122.60
2	H	193	GLY	O-C-N	5.66	129.42	122.46
2	H	51	TRP	CA-C-O	5.64	126.58	120.32
1	L	13	GLU	CA-CB-CG	5.62	125.34	114.10
2	H	196	GLY	CA-C-O	-5.61	113.10	119.04
2	H	35	ARG	NH1-CZ-NH2	5.57	126.54	119.30
2	H	27	SER	N-CA-CB	-5.53	103.60	110.79
2	H	199	PHE	N-CA-C	-5.52	99.52	108.52
2	H	116	ASP	CA-CB-CG	5.52	118.12	112.60
1	L	4	ARG	CD-NE-CZ	5.52	132.13	124.40
2	H	113	ALA	O-C-N	5.52	129.51	123.22
2	H	52	VAL	CB-CA-C	5.51	118.79	110.63
2	H	20	SER	CA-C-N	-5.51	113.55	121.42
2	H	20	SER	C-N-CA	-5.51	113.55	121.42
2	H	34	PHE	CA-CB-CG	5.51	119.31	113.80
3	I	57	GLU	CA-C-N	5.51	128.53	120.71
3	I	57	GLU	C-N-CA	5.51	128.53	120.71
2	H	75	ARG	CA-CB-CG	-5.45	103.20	114.10
2	H	77(A)	ARG	NE-CZ-NH1	-5.45	116.05	121.50
2	H	44	ALA	CA-C-O	-5.43	112.74	120.51
2	H	66	VAL	CB-CA-C	5.42	118.47	110.77
2	H	173	ARG	N-CA-CB	5.42	118.61	110.65
2	H	192	GLU	CB-CG-CD	5.41	121.80	112.60
2	H	221(A)	ARG	NH1-CZ-NH2	5.40	126.32	119.30
2	H	93	ARG	CA-CB-CG	-5.34	103.43	114.10
2	H	226	GLY	N-CA-C	-5.33	105.26	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	208	TYR	N-CA-C	5.32	117.58	108.90
2	H	217	GLU	O-C-N	5.32	129.12	122.63
2	H	244	GLN	CB-CG-CD	5.31	121.63	112.60
2	H	146	GLU	N-CA-CB	5.29	119.49	110.50
2	H	179	ASN	CA-CB-CG	-5.28	107.32	112.60
2	H	33	LEU	CA-C-N	-5.27	115.56	122.99
2	H	33	LEU	C-N-CA	-5.27	115.56	122.99
2	H	173	ARG	N-CA-C	-5.26	106.88	113.72
2	H	66	VAL	N-CA-CB	-5.26	104.80	111.64
2	H	78	ASN	OD1-CG-ND2	-5.26	117.34	122.60
2	H	131	GLN	N-CA-CB	-5.22	102.04	110.71
2	H	38	GLN	CA-C-O	-5.21	114.81	120.81
2	H	72	SER	CA-C-N	5.21	127.53	120.65
2	H	72	SER	C-N-CA	5.21	127.53	120.65
2	H	102	ASP	N-CA-CB	-5.19	103.09	110.46
2	H	38	GLN	O-C-N	5.19	129.31	122.93
2	H	176	ILE	CA-CB-CG1	-5.19	101.58	110.40
2	H	189	ASP	O-C-N	5.19	128.48	123.29
2	H	49	ASP	CA-CB-CG	-5.18	107.42	112.60
2	H	126	ARG	CA-C-O	5.17	126.22	120.63
2	H	151	GLN	O-C-N	5.16	127.06	121.23
2	H	116	ASP	CA-C-N	-5.10	114.58	122.49
2	H	116	ASP	C-N-CA	-5.10	114.58	122.49
2	H	30	GLN	OE1-CD-NE2	5.10	127.70	122.60
2	H	164	GLU	CB-CA-C	-5.08	101.52	109.70
2	H	46	LEU	O-C-N	5.08	128.97	123.13
2	H	66	VAL	CA-C-N	5.08	130.32	123.11
2	H	66	VAL	C-N-CA	5.08	130.32	123.11
2	H	75	ARG	N-CA-C	5.07	118.39	110.32
2	H	60(A)	TYR	N-CA-CB	-5.07	104.79	111.23
2	H	46	LEU	CA-C-N	-5.04	115.81	122.16
2	H	46	LEU	C-N-CA	-5.04	115.81	122.16
2	H	60(B)	PRO	N-CA-C	5.04	116.85	110.70
1	L	8	GLU	O-C-N	5.04	127.26	122.07
1	L	13	GLU	CA-C-O	-5.03	115.34	121.28
2	H	199	PHE	CA-CB-CG	5.03	118.83	113.80
2	H	235	LYS	O-C-N	5.03	127.45	122.12
2	H	73	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	H	187	ARG	NE-CZ-NH1	5.01	126.51	121.50
2	H	118	ILE	CB-CA-C	-5.01	104.70	110.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	ARG	Sidechain
2	H	233	ARG	Mainchain
2	H	94	TYR	Sidechain

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	L	212	0	211	11	0
2	H	1993	0	1952	121	0
3	I	86	0	64	4	0
4	H	35	0	38	6	0
5	H	180	0	0	15	0
5	I	2	0	0	0	0
5	L	19	0	0	2	0
All	All	2527	0	2265	132	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 29.

All (132) 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:L:1(A):ASP:HB3	5:L:506:HOH:O	1.51	1.09
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.55	1.04
2:H:236:LYS:HE2	2:H:239:GLN:HE22	1.28	0.97
2:H:18:GLU:HG3	2:H:187:ARG:HG3	1.44	0.96
1:L:14(J):TYR:O	1:L:14(K):ILE:HB	1.67	0.93
2:H:81:LYS:HB3	2:H:81:LYS:NZ	1.86	0.91
2:H:38:GLN:HB2	5:H:491:HOH:O	1.69	0.91
2:H:236:LYS:HE2	2:H:239:GLN:NE2	1.87	0.90
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.73	0.89
2:H:81:LYS:HB3	2:H:81:LYS:HZ3	1.38	0.89
2:H:35:ARG:O	2:H:38:GLN:HA	1.75	0.87
2:H:205:ASN:HB3	5:H:499:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:NH1	2:H:107:LYS:HD3	1.92	0.84
2:H:208:TYR:HB2	5:H:461:HOH:O	1.78	0.83
2:H:70:LYS:HE3	2:H:72:SER:O	1.79	0.82
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.13	0.81
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.82	0.79
2:H:143:ASN:HA	2:H:150:GLY:O	1.86	0.74
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.52	0.74
2:H:85:LEU:HD13	2:H:106:MET:HE3	1.69	0.74
2:H:85:LEU:HD22	2:H:106:MET:HE2	1.71	0.71
2:H:99:LEU:HD22	4:H:371:OZI:HM13	1.73	0.71
2:H:60(F):LYS:NZ	5:H:575:HOH:O	2.24	0.70
2:H:50:ARG:HH11	2:H:107:LYS:HD3	1.53	0.70
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.07	0.69
2:H:165:ARG:NH2	2:H:180:MET:O	2.27	0.68
2:H:126:ARG:NH2	2:H:127:GLU:OE2	2.27	0.67
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.76	0.66
2:H:50:ARG:HD3	2:H:108:LEU:O	1.94	0.66
1:L:14(A):LYS:HE2	2:H:23:GLU:CD	2.21	0.66
2:H:97:ARG:NH1	5:H:571:HOH:O	2.30	0.65
1:L:14(A):LYS:HE2	2:H:23:GLU:OE1	1.97	0.65
2:H:85:LEU:CD2	2:H:106:MET:HE2	2.27	0.65
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.05	0.64
2:H:185:LYS:HB2	2:H:186(A):ASP:OD1	1.98	0.64
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.79	0.63
2:H:221(A):ARG:CG	2:H:221(A):ARG:HH11	2.05	0.62
2:H:84:MET:HE3	3:I:63:TYS:O	2.00	0.62
2:H:66:VAL:CG2	2:H:85:LEU:HD21	2.29	0.62
2:H:20:SER:O	2:H:156:GLN:HA	2.00	0.61
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.36	0.61
2:H:221(A):ARG:HG3	2:H:221(A):ARG:NH1	2.16	0.60
2:H:235:LYS:HB3	2:H:236:LYS:HZ2	1.66	0.60
2:H:17:VAL:O	2:H:18:GLU:HB2	2.02	0.59
2:H:48:SER:OG	2:H:49:ASP:N	2.32	0.59
2:H:85:LEU:CD1	2:H:106:MET:HE3	2.32	0.59
2:H:221(A):ARG:CG	2:H:221(A):ARG:NH1	2.60	0.58
2:H:50:ARG:HH12	2:H:86:GLU:CD	2.11	0.58
2:H:191:CYS:C	4:H:371:OZI:HD2	2.28	0.58
2:H:236:LYS:HE3	2:H:236:LYS:HA	1.85	0.58
2:H:139:THR:HG22	2:H:157:VAL:HB	1.85	0.58
2:H:173:ARG:NH1	5:H:455:HOH:O	2.29	0.58
2:H:17:VAL:O	2:H:188:GLY:HA2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:58:GLU:H	3:I:58:GLU:CD	2.12	0.56
2:H:81:LYS:HD3	5:H:516:HOH:O	2.06	0.55
2:H:127:GLU:HB2	5:H:597:HOH:O	2.06	0.55
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.05	0.55
2:H:20:SER:HB3	5:H:443:HOH:O	2.05	0.55
2:H:146:GLU:OE1	2:H:221(A):ARG:NE	2.38	0.55
2:H:236:LYS:HE3	2:H:236:LYS:CA	2.37	0.55
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.10	0.52
2:H:65:LEU:HG	2:H:82:ILE:HG22	1.91	0.52
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.44	0.52
1:L:14(J):TYR:O	1:L:14(K):ILE:CB	2.49	0.52
2:H:237:TRP:O	2:H:241:VAL:HG13	2.10	0.52
2:H:35:ARG:HB3	2:H:39:GLU:HG2	1.92	0.51
2:H:81:LYS:NZ	2:H:81:LYS:CB	2.63	0.51
2:H:173:ARG:HD2	5:H:455:HOH:O	2.11	0.51
2:H:191:CYS:HA	4:H:371:OZI:HD2	1.93	0.51
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.68	0.51
2:H:60(E):ASP:HA	5:H:496:HOH:O	2.09	0.51
2:H:176:ILE:HD12	2:H:227:PHE:HE2	1.74	0.51
2:H:66:VAL:HG21	2:H:85:LEU:HD21	1.92	0.50
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.26	0.50
2:H:66:VAL:HG23	2:H:85:LEU:HD21	1.94	0.50
2:H:35:ARG:HD3	2:H:39:GLU:OE2	2.12	0.49
2:H:16:ILE:O	2:H:144:LEU:HA	2.12	0.49
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.47	0.49
1:L:1(A):ASP:CB	5:L:506:HOH:O	2.28	0.49
2:H:165:ARG:N	2:H:166:PRO:HD2	2.27	0.48
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.95	0.48
2:H:87:LYS:HD3	2:H:88:ILE:H	1.79	0.48
2:H:109:LYS:HB2	5:H:536:HOH:O	2.14	0.47
2:H:114:PHE:CD1	2:H:114:PHE:N	2.77	0.47
2:H:236:LYS:HE3	2:H:236:LYS:N	2.29	0.47
2:H:186(A):ASP:CG	2:H:186(B):GLU:N	2.72	0.47
2:H:211:GLY:HA2	2:H:229:THR:O	2.13	0.47
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.12	0.47
2:H:50:ARG:CD	2:H:108:LEU:O	2.60	0.47
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.44	0.47
1:L:14(G):LEU:N	1:L:14(G):LEU:CD2	2.78	0.47
2:H:236:LYS:HB2	5:H:530:HOH:O	2.14	0.46
2:H:34:PHE:CE2	2:H:38:GLN:HB3	2.50	0.46
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.45	0.46
2:H:94:TYR:HA	2:H:100:ASP:O	2.16	0.46
2:H:90:ILE:O	2:H:91:HIS:C	2.58	0.46
1:L:14:ASP:OD1	1:L:14:ASP:C	2.59	0.45
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.52	0.45
2:H:100:ASP:CG	2:H:177:THR:HG21	2.41	0.45
2:H:236:LYS:CE	2:H:239:GLN:NE2	2.72	0.45
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.98	0.45
2:H:99:LEU:HD22	4:H:371:OZI:CM1	2.45	0.45
2:H:114:PHE:HB3	5:H:480:HOH:O	2.17	0.45
2:H:50:ARG:NH1	2:H:108:LEU:O	2.50	0.45
2:H:235:LYS:HB3	2:H:236:LYS:NZ	2.30	0.44
2:H:94:TYR:HA	2:H:101:ARG:HB2	1.99	0.44
2:H:129:ALA:HA	2:H:210:MET:HE1	1.98	0.44
2:H:191:CYS:CA	4:H:371:OZI:HD2	2.47	0.44
2:H:70:LYS:CE	2:H:72:SER:O	2.58	0.44
2:H:36(A):SER:HA	2:H:37:PRO:C	2.42	0.43
2:H:36:LYS:HG2	2:H:65:LEU:HD22	1.99	0.43
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.81	0.43
2:H:240:LYS:HB2	5:H:595:HOH:O	2.19	0.43
4:H:371:OZI:H62	4:H:371:OZI:HA	1.79	0.43
2:H:217:GLU:O	2:H:221(A):ARG:HG3	2.19	0.43
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.99	0.43
2:H:176:ILE:CD1	2:H:227:PHE:CE2	3.01	0.43
2:H:194:ASP:O	2:H:195:SER:C	2.60	0.43
2:H:201:MET:SD	2:H:210:MET:HG3	2.59	0.43
2:H:185:LYS:CB	2:H:186(A):ASP:OD1	2.66	0.43
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.82	0.42
2:H:82:ILE:HG13	3:I:63:TYS:CD2	2.49	0.42
2:H:29:TRP:O	2:H:31:VAL:HG23	2.18	0.42
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.35	0.42
2:H:50:ARG:NH1	2:H:107:LYS:CD	2.75	0.41
2:H:232:PHE:O	2:H:235:LYS:HB2	2.21	0.41
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.56	0.41
2:H:130:LEU:HA	2:H:130:LEU:HD23	1.77	0.41
2:H:144:LEU:HD21	2:H:152:PRO:CB	2.51	0.41
3:I:60:PRO:C	3:I:62:GLU:N	2.79	0.41
2:H:228:TYR:CD1	2:H:228:TYR:N	2.89	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	L	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
2	H	244/259 (94%)	227 (93%)	16 (7%)	1 (0%)	30	38
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	275/307 (90%)	257 (94%)	17 (6%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	195	SER

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	L	24/31 (77%)	23 (96%)	1 (4%)	26	40
2	H	213/225 (95%)	191 (90%)	22 (10%)	7	8
3	I	7/10 (70%)	6 (86%)	1 (14%)	3	3
All	All	244/266 (92%)	220 (90%)	24 (10%)	7	10

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	LYS
2	H	20	SER

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Mol	Chain	Res	Type
2	H	33	LEU
2	H	41	LEU
2	H	48	SER
2	H	50	ARG
2	H	62	ASN
2	H	65	LEU
2	H	74	THR
2	H	81	LYS
2	H	82	ILE
2	H	87	LYS
2	H	90	ILE
2	H	97	ARG
2	H	97(A)	GLU
2	H	99	LEU
2	H	127	GLU
2	H	154	VAL
2	H	201	MET
2	H	233	ARG
2	H	235	LYS
2	H	236	LYS
2	H	241	VAL
3	I	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	60(G)	ASN
2	H	71	HIS
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TYS	I	63	-	15,16,17	1.70	2 (13%)	15,22,24	1.63	4 (26%)

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	TYS	I	63	-	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-S	5.32	1.68	1.58
3	I	63	TYS	OH-CZ	-3.08	1.37	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-S-O2	-3.32	97.44	107.56
3	I	63	TYS	CB-CG-CD1	-2.49	116.26	120.90
3	I	63	TYS	CD1-CE1-CZ	-2.11	117.32	119.73
3	I	63	TYS	O3-S-O2	2.02	115.63	108.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
4	OZI	H	371	-	37,37,37	3.67	16 (43%)	51,52,52	2.96	16 (31%)

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
4	OZI	H	371	-	-	5/32/42/42	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	371	OZI	S-N1	9.46	1.77	1.61
4	H	371	OZI	C1-S	9.35	1.87	1.77
4	H	371	OZI	CM2-N	7.52	1.62	1.45
4	H	371	OZI	O2S-S	6.95	1.51	1.43
4	H	371	OZI	C-N11	6.70	1.44	1.35
4	H	371	OZI	C61-N11	5.59	1.57	1.47
4	H	371	OZI	C21-N11	5.13	1.56	1.47
4	H	371	OZI	O1S-S	4.70	1.49	1.43
4	H	371	OZI	C2-C1	3.89	1.42	1.37
4	H	371	OZI	C51-C41	3.82	1.63	1.52
4	H	371	OZI	C31-C41	3.10	1.61	1.52
4	H	371	OZI	C1-C8A	-2.82	1.38	1.43
4	H	371	OZI	C5-C4A	-2.77	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	371	OZI	C8-C8A	-2.38	1.37	1.42
4	H	371	OZI	CG-CD	-2.30	1.42	1.51
4	H	371	OZI	C3-C4	2.01	1.41	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	371	OZI	CG-CB-CA	11.55	149.32	113.80
4	H	371	OZI	O2S-S-C1	10.14	125.77	108.09
4	H	371	OZI	O2S-S-O1S	-7.03	110.99	119.52
4	H	371	OZI	C61-N11-C21	5.03	122.94	112.68
4	H	371	OZI	O2S-S-N1	-4.16	99.33	106.88
4	H	371	OZI	C1'-C41-C31	-3.72	100.79	112.75
4	H	371	OZI	CM1-N-C5	3.48	124.78	114.19
4	H	371	OZI	C21-N11-C	-3.48	110.28	123.30
4	H	371	OZI	C51-C61-N11	-3.32	104.15	110.66
4	H	371	OZI	O-C-N11	-2.89	118.16	121.61
4	H	371	OZI	C51-C41-C31	2.66	115.78	109.29
4	H	371	OZI	O1S-S-C1	-2.20	104.25	108.09
4	H	371	OZI	C1-S-N1	2.13	110.37	106.96
4	H	371	OZI	CM2-N-CM1	-2.11	109.42	116.18
4	H	371	OZI	O-C-CA	2.10	123.46	119.61
4	H	371	OZI	CA-C-N11	-2.04	115.77	118.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	371	OZI	N1-CA-CB-CG
4	H	371	OZI	NE-CD-CG-CB
4	H	371	OZI	CA-C-N11-C61
4	H	371	OZI	CG-CD-NE-CZ
4	H	371	OZI	O-C-N11-C21

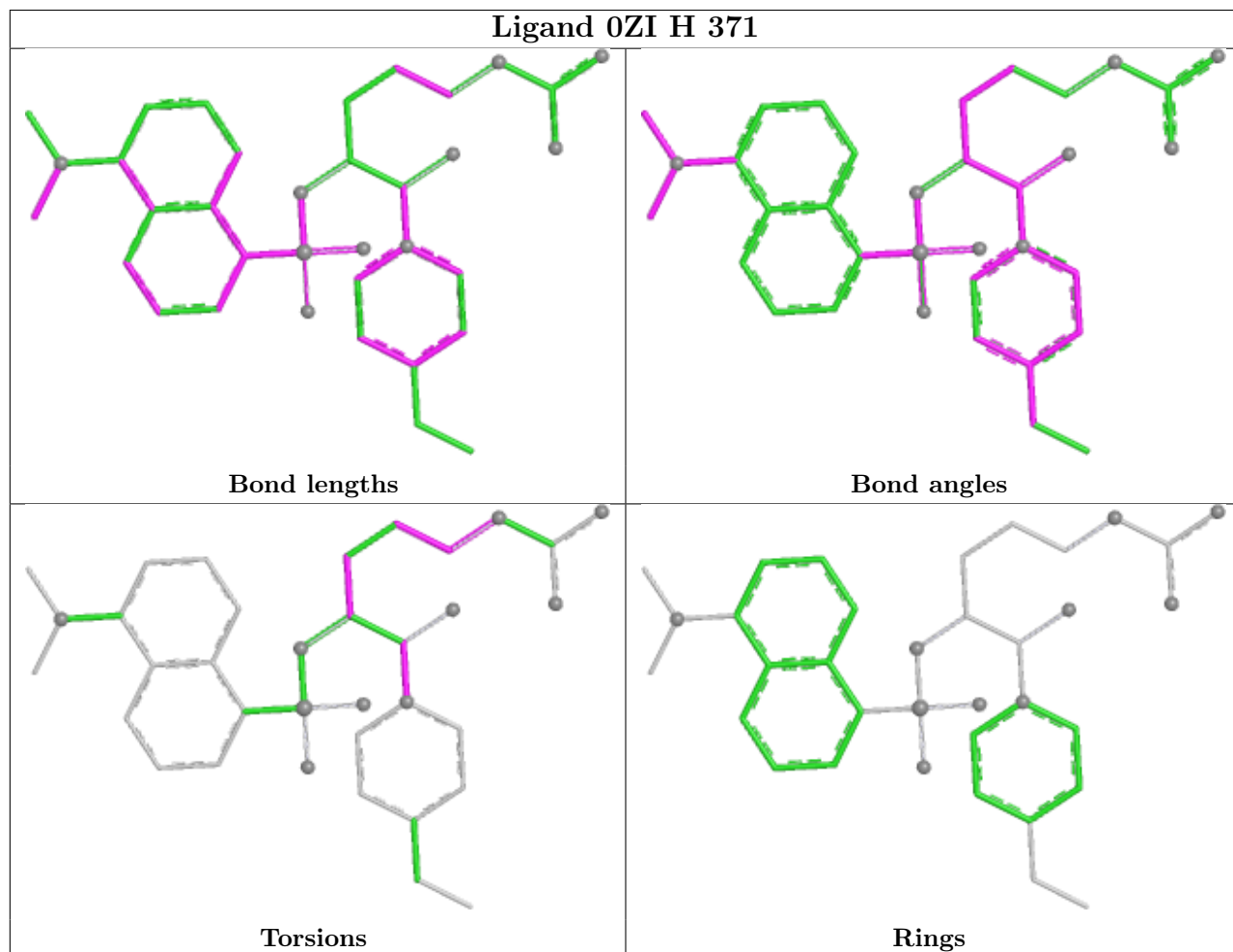
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	371	OZI	6	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

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.