



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:15 PM UTC

PDB ID : 1ABJ / pdb_00001abj
Title : STRUCTURE OF THE HIRULOG 3-THROMBIN COMPLEX AND NATURE OF THE S' SUBSITES OF SUBSTRATES AND INHIBITORS
Authors : Qiu, X.; Tulinsky, A.
Deposited on : 1992-08-24
Resolution : 2.40 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)	:	2.49

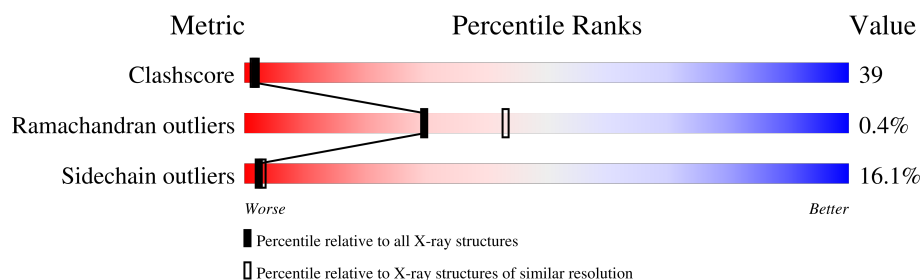
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OG6	H	1	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2531 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.

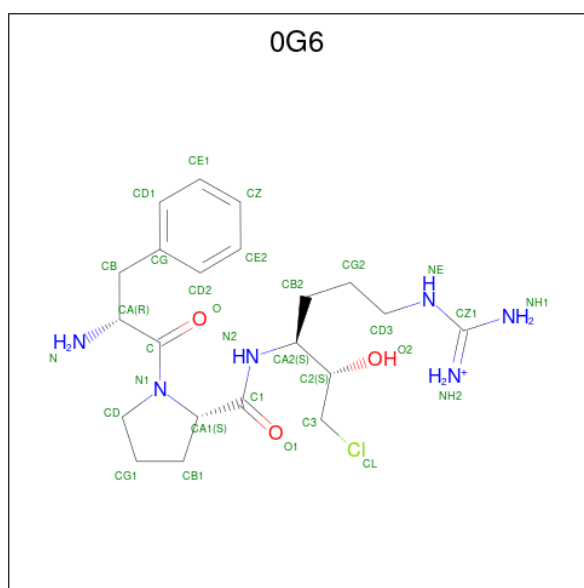
- Molecule 1 is a protein called ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	0
			2083	1329	369	371	14			

- Molecule 3 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 4 is water.

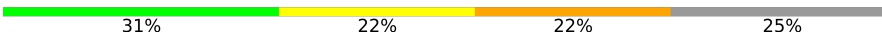
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	14	Total 14	O 14	0	0
4	H	182	Total 182	O 182	0	0

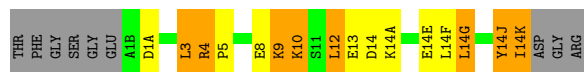
3 Residue-property plots [i](#)

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.

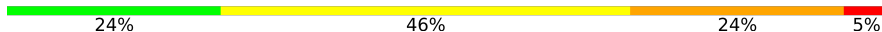
Note EDS was not executed.

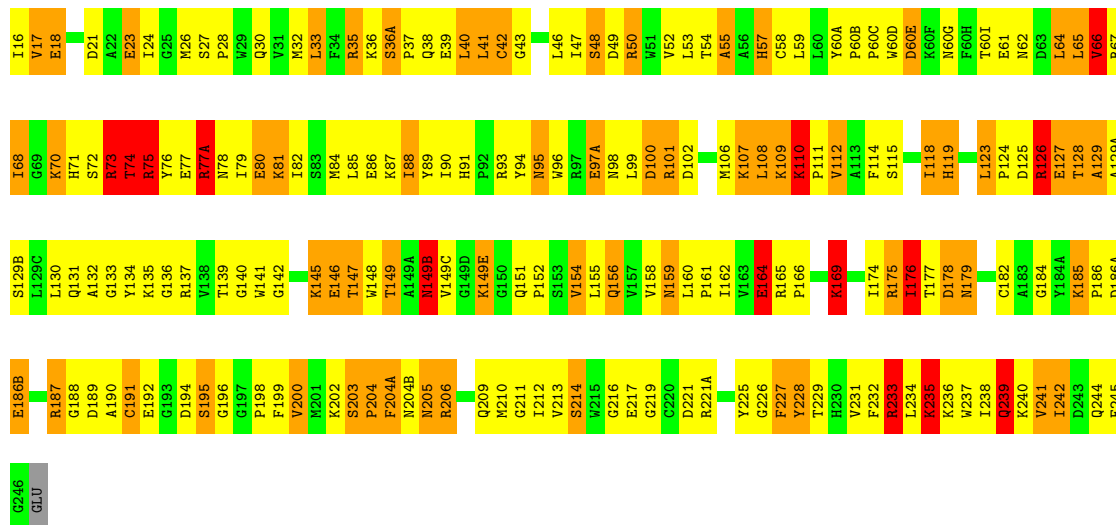
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



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 21	Depositor
Cell constants a, b, c, α , β , γ	88.26Å 68.02Å 61.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.144 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2531	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: 0G6

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	1.07	0/224	2.26	11/298 (3.7%)
2	H	1.29	1/2138 (0.0%)	2.48	149/2891 (5.2%)
All	All	1.27	1/2362 (0.0%)	2.46	160/3189 (5.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	214	SER	CA-CB	6.61	1.63	1.53

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	38	GLN	OE1-CD-NE2	12.62	135.22	122.60
2	H	239	GLN	OE1-CD-NE2	11.66	134.26	122.60
2	H	235	LYS	CA-CB-CG	10.82	135.74	114.10
2	H	62	ASN	CA-CB-CG	-10.82	101.78	112.60
2	H	73	ARG	CA-C-O	10.52	131.91	120.24
2	H	118	ILE	O-C-N	10.03	132.00	122.97
2	H	227	PHE	CA-C-N	9.50	137.18	122.94
2	H	227	PHE	C-N-CA	9.50	137.18	122.94
2	H	179	ASN	CA-CB-CG	-9.47	103.13	112.60
2	H	66	VAL	CB-CA-C	9.21	126.86	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	43	GLY	N-CA-C	-8.89	98.84	112.89
2	H	191	CYS	CA-C-O	8.89	130.30	121.14
2	H	169	LYS	O-C-N	8.84	131.18	122.07
2	H	27	SER	CB-CA-C	8.69	122.94	110.87
2	H	185	LYS	CA-C-O	-8.66	112.81	120.60
2	H	53	LEU	CA-C-O	8.64	129.80	120.38
2	H	64	LEU	N-CA-C	8.58	122.44	109.41
2	H	119	HIS	CA-CB-CG	-8.54	105.26	113.80
2	H	123	LEU	CB-CA-C	8.42	120.38	108.68
2	H	233	ARG	CD-NE-CZ	8.42	136.18	124.40
2	H	221(A)	ARG	NE-CZ-NH2	-8.32	111.71	119.20
2	H	101	ARG	CD-NE-CZ	-8.12	113.03	124.40
2	H	186(A)	ASP	CA-CB-CG	-8.07	104.53	112.60
2	H	62	ASN	CA-C-O	-7.61	112.83	120.82
2	H	57	HIS	N-CA-CB	7.60	123.69	110.39
2	H	137	ARG	NE-CZ-NH1	7.49	128.99	121.50
2	H	240	LYS	O-C-N	7.44	130.64	122.15
2	H	149	THR	N-CA-CB	7.44	125.37	111.53
2	H	18	GLU	CA-C-O	-7.42	111.67	120.57
2	H	204	PRO	N-CA-C	-7.42	104.59	113.86
1	L	1(A)	ASP	CA-C-O	7.39	126.65	118.52
2	H	229	THR	CA-CB-OG1	-7.38	98.53	109.60
2	H	231	VAL	CA-C-O	-7.31	113.67	121.27
2	H	88	ILE	O-C-N	7.25	130.73	123.18
2	H	141	TRP	CA-C-O	-7.25	110.93	119.48
1	L	14	ASP	CA-CB-CG	7.18	119.78	112.60
2	H	158	VAL	CB-CA-C	7.17	121.54	110.50
2	H	242	ILE	CA-CB-CG2	7.10	122.58	110.50
2	H	78	ASN	CA-CB-CG	-7.05	105.55	112.60
2	H	74	THR	N-CA-CB	-6.84	99.96	110.42
2	H	142	GLY	CA-C-N	6.79	130.75	121.05
2	H	142	GLY	C-N-CA	6.79	130.75	121.05
2	H	192	GLU	N-CA-C	-6.77	100.42	110.23
2	H	110	LYS	N-CA-CB	6.72	123.28	111.19
2	H	126	ARG	CA-C-N	6.67	129.45	120.65
2	H	126	ARG	C-N-CA	6.67	129.45	120.65
2	H	62	ASN	O-C-N	6.65	128.92	122.07
2	H	187	ARG	NE-CZ-NH1	6.65	128.15	121.50
2	H	141	TRP	O-C-N	6.64	130.23	122.19
2	H	115	SER	CA-C-O	-6.63	114.31	121.14
1	L	3	LEU	N-CA-CB	6.57	120.86	110.55
2	H	137	ARG	O-C-N	6.56	131.26	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	38	GLN	CB-CG-CD	-6.50	101.55	112.60
2	H	123	LEU	N-CA-C	-6.50	101.34	110.31
2	H	175	ARG	CD-NE-CZ	-6.48	115.33	124.40
2	H	234	LEU	CB-CA-C	6.46	120.88	109.65
2	H	186(B)	GLU	CB-CG-CD	6.45	123.57	112.60
2	H	194	ASP	CA-C-O	-6.44	112.07	119.60
2	H	187	ARG	NE-CZ-NH2	-6.43	113.42	119.20
1	L	1(A)	ASP	CA-CB-CG	-6.39	106.21	112.60
2	H	127	GLU	CA-C-N	6.38	128.83	120.28
2	H	127	GLU	C-N-CA	6.38	128.83	120.28
2	H	67	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	H	35	ARG	CB-CA-C	-6.37	99.46	109.84
2	H	209	GLN	N-CA-CB	6.37	120.33	110.21
2	H	227	PHE	CA-CB-CG	6.33	120.13	113.80
2	H	214	SER	N-CA-C	6.28	120.57	111.02
2	H	203	SER	N-CA-CB	6.28	118.46	110.23
2	H	241	VAL	N-CA-CB	6.28	119.56	110.52
2	H	108	LEU	CA-C-N	6.18	128.89	120.54
2	H	108	LEU	C-N-CA	6.18	128.89	120.54
2	H	147	THR	N-CA-CB	-6.18	100.03	110.41
2	H	67	ARG	CB-CA-C	6.17	120.41	110.16
2	H	64	LEU	CA-C-O	6.17	128.74	121.58
2	H	108	LEU	N-CA-CB	-6.17	101.29	110.17
2	H	149(B)	ASN	OD1-CG-ND2	6.11	128.71	122.60
2	H	195	SER	CA-CB-OG	-6.08	98.95	111.10
2	H	239	GLN	N-CA-C	6.04	118.66	111.71
2	H	26	MET	CA-C-N	-6.04	116.97	122.28
2	H	26	MET	C-N-CA	-6.04	116.97	122.28
2	H	80	GLU	CA-C-O	6.01	128.38	121.47
2	H	66	VAL	CA-C-O	5.95	127.00	120.64
2	H	73	ARG	NE-CZ-NH2	-5.93	113.87	119.20
2	H	164	GLU	CB-CG-CD	5.93	122.67	112.60
2	H	40	LEU	CA-C-O	-5.92	113.94	120.69
2	H	18	GLU	CB-CA-C	-5.90	102.24	111.39
2	H	91	HIS	CA-CB-CG	-5.88	107.92	113.80
2	H	100	ASP	CA-C-O	-5.86	113.78	120.58
2	H	241	VAL	CB-CA-C	5.85	119.71	112.04
2	H	211	GLY	CA-C-N	5.85	130.88	123.10
2	H	211	GLY	C-N-CA	5.85	130.88	123.10
2	H	159	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	L	4	ARG	CA-C-O	5.80	123.61	119.32
1	L	14(G)	LEU	CB-CA-C	5.79	121.79	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	54	THR	CA-C-O	-5.77	115.19	121.14
2	H	18	GLU	O-C-N	5.75	131.81	122.20
2	H	129(A)	ALA	N-CA-C	5.74	117.53	111.28
2	H	239	GLN	CA-CB-CG	-5.72	102.66	114.10
2	H	221(A)	ARG	NH1-CZ-NH2	5.71	126.72	119.30
2	H	129	ALA	C-N-CA	5.71	135.96	121.70
2	H	146	GLU	CA-C-O	5.70	127.14	120.98
2	H	176	ILE	CA-C-O	-5.70	113.66	120.78
1	L	14(J)	TYR	N-CA-C	-5.68	101.89	110.70
2	H	97(A)	GLU	N-CA-C	5.67	119.79	111.34
2	H	200	VAL	N-CA-C	5.66	117.75	108.97
2	H	33	LEU	CA-C-O	-5.66	114.24	120.69
2	H	75	ARG	CA-C-O	5.65	126.59	120.43
2	H	21	ASP	CA-C-O	-5.62	114.51	120.92
2	H	242	ILE	N-CA-C	5.62	116.36	110.62
2	H	55	ALA	CA-C-N	5.59	128.04	120.38
2	H	55	ALA	C-N-CA	5.59	128.04	120.38
2	H	149(B)	ASN	CA-CB-CG	-5.58	107.02	112.60
2	H	204(A)	PHE	CA-CB-CG	-5.58	108.22	113.80
2	H	149(E)	LYS	CA-CB-CG	5.56	125.21	114.10
2	H	240	LYS	CA-C-O	-5.55	114.53	120.42
2	H	129(A)	ALA	CA-C-O	5.53	126.41	120.55
2	H	77(A)	ARG	CD-NE-CZ	-5.47	116.74	124.40
2	H	42	CYS	CA-C-N	5.46	129.16	121.30
2	H	42	CYS	C-N-CA	5.46	129.16	121.30
2	H	203	SER	O-C-N	5.46	126.37	121.35
2	H	17	VAL	CA-C-O	5.44	127.02	120.65
2	H	48	SER	CA-CB-OG	5.44	121.99	111.10
1	L	1(A)	ASP	N-CA-C	-5.44	106.11	114.16
2	H	60(E)	ASP	CB-CA-C	-5.44	102.17	111.26
2	H	35	ARG	CA-C-O	-5.43	114.50	120.69
1	L	14(E)	GLU	CB-CG-CD	5.41	121.80	112.60
2	H	231	VAL	O-C-N	5.40	127.34	121.94
2	H	35	ARG	NE-CZ-NH1	5.38	126.88	121.50
2	H	95	ASN	N-CA-CB	-5.35	101.64	110.53
2	H	178	ASP	CA-CB-CG	-5.35	107.25	112.60
2	H	146	GLU	CA-C-N	5.34	131.99	121.58
2	H	146	GLU	C-N-CA	5.34	131.99	121.58
2	H	75	ARG	N-CA-C	5.33	117.94	109.24
2	H	35	ARG	O-C-N	5.33	129.28	123.04
2	H	68	ILE	CA-C-O	-5.31	114.45	120.67
2	H	23	GLU	N-CA-C	-5.28	103.42	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	ARG	CD-NE-CZ	-5.26	117.03	124.40
2	H	156	GLN	CA-CB-CG	5.26	124.62	114.10
2	H	190	ALA	N-CA-C	-5.25	102.69	110.46
2	H	60(I)	THR	CB-CA-C	5.25	119.16	109.71
2	H	228	TYR	CA-C-N	5.24	128.29	120.95
2	H	228	TYR	C-N-CA	5.24	128.29	120.95
1	L	14(E)	GLU	CA-C-O	5.24	126.50	120.90
2	H	53	LEU	O-C-N	-5.23	117.12	123.29
2	H	53	LEU	CB-CA-C	5.22	118.75	109.72
2	H	186	PRO	N-CA-CB	5.17	108.65	103.48
2	H	77(A)	ARG	CA-C-N	-5.14	114.42	122.65
2	H	77(A)	ARG	C-N-CA	-5.14	114.42	122.65
2	H	187	ARG	O-C-N	5.14	129.83	122.74
2	H	225	TYR	CA-C-N	-5.12	115.42	120.60
2	H	225	TYR	C-N-CA	-5.12	115.42	120.60
2	H	228	TYR	CA-C-O	-5.09	115.20	120.70
2	H	206	ARG	CD-NE-CZ	5.08	131.51	124.40
2	H	196	GLY	N-CA-C	-5.05	107.55	114.67
2	H	27	SER	CA-C-O	5.04	126.36	121.32
2	H	133	GLY	N-CA-C	-5.03	109.03	115.42
1	L	14(K)	ILE	N-CA-CB	-5.01	102.99	111.50
2	H	217	GLU	CA-C-O	-5.01	115.14	120.40
2	H	91	HIS	O-C-N	5.00	125.37	121.47
2	H	137	ARG	CD-NE-CZ	5.00	131.41	124.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	ARG	Sidechain
2	H	73	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	222	0	225	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2083	0	2058	167	0
3	H	30	0	30	5	0
4	H	182	0	0	12	0
4	L	14	0	0	2	0
All	All	2531	0	2313	181	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 39.

All (181) 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:5:PRO:HA	1:L:9:LYS:HB2	1.19	1.18
2:H:195:SER:HG	3:H:1:OG6:C2	1.62	1.07
2:H:50:ARG:NH1	2:H:108:LEU:O	1.92	1.01
2:H:195:SER:OG	3:H:1:OG6:C3	2.09	1.01
2:H:126:ARG:HB3	2:H:126:ARG:NH1	1.84	0.93
2:H:205:ASN:C	2:H:205:ASN:HD22	1.72	0.93
2:H:60(D):TRP:O	2:H:60(E):ASP:HB2	1.70	0.92
2:H:73:ARG:HD3	2:H:152:PRO:O	1.69	0.91
2:H:50:ARG:NH1	2:H:107:LYS:HE2	1.87	0.90
1:L:5:PRO:HA	1:L:9:LYS:CB	2.01	0.90
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.08	0.89
2:H:74:THR:HG23	2:H:75:ARG:HD3	1.56	0.88
2:H:205:ASN:O	2:H:205:ASN:ND2	2.07	0.88
2:H:60(G):ASN:ND2	4:H:528:HOH:O	2.05	0.86
1:L:10:LYS:HB3	1:L:12:LEU:HD22	1.57	0.86
1:L:5:PRO:CA	1:L:9:LYS:HB2	2.06	0.86
2:H:57:HIS:CD2	3:H:1:OG6:C3	2.58	0.85
2:H:93:ARG:O	2:H:101:ARG:HD2	1.78	0.83
1:L:10:LYS:CB	1:L:12:LEU:HD22	2.10	0.82
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.14	0.81
2:H:126:ARG:HB3	2:H:126:ARG:CZ	2.09	0.81
1:L:8:GLU:OE2	2:H:202:LYS:HE3	1.81	0.80
2:H:75:ARG:NH1	2:H:75:ARG:HG2	1.98	0.78
2:H:75:ARG:HG2	2:H:75:ARG:HH11	1.47	0.77
1:L:14(A):LYS:HB2	1:L:14(A):LYS:NZ	2.00	0.77
2:H:125:ASP:OD1	2:H:128:THR:HB	1.84	0.77
2:H:164:GLU:OE1	2:H:164:GLU:N	2.13	0.76
2:H:169:LYS:HD3	4:H:559:HOH:O	1.87	0.75
2:H:205:ASN:C	2:H:205:ASN:ND2	2.38	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:THR:CG2	2:H:75:ARG:HD3	2.17	0.75
2:H:130:LEU:HG	2:H:210:MET:HE2	1.68	0.74
2:H:76:TYR:CE2	2:H:77(A):ARG:HA	2.23	0.73
2:H:87:LYS:HG2	2:H:89:TYR:CZ	2.24	0.73
2:H:239:GLN:NE2	4:H:471:HOH:O	2.22	0.73
2:H:49:ASP:HB3	2:H:114:PHE:CE1	2.24	0.72
2:H:74:THR:HG23	2:H:75:ARG:CD	2.20	0.71
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.27	0.70
2:H:236:LYS:HB2	4:H:436:HOH:O	1.91	0.69
2:H:126:ARG:NH1	2:H:126:ARG:CB	2.55	0.69
1:L:3:LEU:HD12	1:L:9:LYS:NZ	2.09	0.67
2:H:71:HIS:CE1	2:H:154:VAL:HG13	2.30	0.67
2:H:195:SER:CB	3:H:1:OG6:C3	2.73	0.66
2:H:187:ARG:NH2	2:H:221:ASP:O	2.27	0.66
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.78	0.66
2:H:126:ARG:HG2	2:H:232:PHE:HZ	1.60	0.66
2:H:164:GLU:C	2:H:166:PRO:HD2	2.22	0.65
2:H:80:GLU:O	2:H:81:LYS:HD2	1.98	0.64
1:L:14(F):LEU:HD11	2:H:159:ASN:HB3	1.80	0.64
2:H:188:GLY:O	2:H:189:ASP:HB2	1.98	0.63
2:H:70:LYS:HE3	2:H:72:SER:O	1.98	0.62
2:H:50:ARG:O	2:H:107:LYS:HA	1.99	0.62
2:H:75:ARG:HH11	2:H:75:ARG:CG	2.12	0.62
2:H:136:GLY:HA3	2:H:199:PHE:CE1	2.33	0.62
2:H:94:TYR:HA	2:H:101:ARG:HB2	1.82	0.61
2:H:125:ASP:OD2	2:H:127:GLU:HB3	2.01	0.61
1:L:14(J):TYR:O	1:L:14(K):ILE:C	2.44	0.61
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.15	0.61
1:L:3:LEU:HD12	1:L:9:LYS:HZ1	1.64	0.60
2:H:30:GLN:O	4:H:419:HOH:O	2.15	0.59
2:H:90:ILE:HD12	4:H:525:HOH:O	2.01	0.59
2:H:49:ASP:N	2:H:49:ASP:OD1	2.33	0.58
2:H:216:GLY:O	3:H:1:OG6:N	2.37	0.58
2:H:127:GLU:HA	2:H:127:GLU:OE1	2.03	0.58
2:H:135:LYS:HA	2:H:161:PRO:HA	1.85	0.58
2:H:164:GLU:H	2:H:164:GLU:CD	2.07	0.57
2:H:176:ILE:HD13	2:H:176:ILE:N	2.18	0.57
1:L:13:GLU:OE1	4:L:442:HOH:O	2.17	0.57
2:H:213:VAL:HG13	4:H:409:HOH:O	2.04	0.57
1:L:8:GLU:OE2	2:H:202:LYS:CE	2.50	0.57
2:H:47:ILE:O	2:H:48:SER:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:ALA:O	2:H:58:CYS:HB2	2.03	0.57
2:H:85:LEU:CD2	2:H:106:MET:HB3	2.36	0.56
1:L:9:LYS:HB3	4:L:484:HOH:O	2.05	0.56
2:H:165:ARG:N	2:H:166:PRO:CD	2.68	0.56
2:H:17:VAL:O	2:H:18:GLU:HB2	2.06	0.55
2:H:49:ASP:HB2	2:H:112:VAL:O	2.07	0.55
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.22	0.55
2:H:39:GLU:HG3	2:H:41:LEU:CD1	2.37	0.55
2:H:33:LEU:HD23	2:H:66:VAL:HG23	1.88	0.54
2:H:176:ILE:HG22	2:H:177:THR:N	2.22	0.54
2:H:160:LEU:HD22	2:H:184:GLY:HA2	1.90	0.54
2:H:77(A):ARG:HH11	2:H:77(A):ARG:HG2	1.73	0.54
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.90	0.54
2:H:36(A):SER:HA	2:H:37:PRO:C	2.32	0.53
2:H:148:TRP:H	2:H:148:TRP:CD1	2.25	0.53
2:H:146:GLU:HG3	4:H:521:HOH:O	2.08	0.53
2:H:185:LYS:H	2:H:186(B):GLU:HG3	1.74	0.53
2:H:140:GLY:O	2:H:155:LEU:HD12	2.09	0.53
2:H:60(A):TYR:CE1	2:H:60(C):PRO:HG2	2.45	0.52
2:H:100:ASP:O	2:H:101:ARG:HB2	2.09	0.52
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.91	0.52
2:H:49:ASP:O	2:H:111:PRO:HA	2.09	0.51
2:H:17:VAL:O	2:H:188:GLY:HA2	2.10	0.51
2:H:16:ILE:N	4:H:403:HOH:O	2.44	0.51
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.74	0.50
2:H:70:LYS:NZ	2:H:77:GLU:OE1	2.36	0.50
2:H:80:GLU:C	2:H:81:LYS:HD2	2.36	0.50
2:H:237:TRP:O	2:H:238:ILE:C	2.51	0.49
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.48	0.49
2:H:87:LYS:HG3	2:H:88:ILE:N	2.27	0.49
2:H:97(A):GLU:CD	2:H:175:ARG:HH21	2.21	0.49
2:H:71:HIS:CE1	2:H:154:VAL:CG1	2.96	0.49
2:H:139:THR:HA	2:H:156:GLN:O	2.13	0.49
2:H:165:ARG:NH2	2:H:177:THR:O	2.37	0.49
2:H:178:ASP:O	2:H:233:ARG:HD2	2.13	0.49
2:H:244:GLN:HB3	2:H:245:PHE:CD1	2.48	0.48
2:H:97(A):GLU:HG2	2:H:98:ASN:N	2.28	0.48
2:H:124:PRO:HB3	2:H:128:THR:HG22	1.95	0.48
2:H:179:ASN:OD1	2:H:233:ARG:HD3	2.13	0.48
1:L:14(G):LEU:HD12	1:L:14(G):LEU:HA	1.55	0.48
2:H:182:CYS:HA	2:H:226:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:HD3	2:H:75:ARG:N	2.29	0.48
2:H:131:GLN:HB2	2:H:134:TYR:CD2	2.49	0.48
2:H:28:PRO:HB2	2:H:119:HIS:HB3	1.96	0.47
2:H:126:ARG:HG2	2:H:232:PHE:CZ	2.46	0.47
2:H:145:LYS:CE	2:H:149(B):ASN:HB3	2.44	0.47
2:H:154:VAL:HG13	2:H:155:LEU:N	2.30	0.47
2:H:129:ALA:HA	2:H:210:MET:HE1	1.97	0.46
1:L:14(F):LEU:CD1	2:H:159:ASN:HB3	2.42	0.46
2:H:50:ARG:HD3	2:H:111:PRO:N	2.30	0.46
2:H:50:ARG:HH12	2:H:107:LYS:HE2	1.73	0.46
2:H:165:ARG:N	2:H:166:PRO:HD2	2.30	0.46
2:H:204:PRO:HG2	2:H:204(A):PHE:CZ	2.50	0.46
2:H:32:MET:HE2	2:H:40:LEU:HD12	1.97	0.46
2:H:126:ARG:CB	2:H:126:ARG:HH11	2.29	0.46
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.46	0.46
2:H:46:LEU:HD11	2:H:48:SER:O	2.16	0.46
2:H:50:ARG:NH1	2:H:107:LYS:CE	2.71	0.46
2:H:125:ASP:OD1	2:H:128:THR:CB	2.58	0.46
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.60	0.45
2:H:42:CYS:HB3	2:H:195:SER:O	2.15	0.45
2:H:57:HIS:ND1	2:H:102:ASP:OD2	2.49	0.45
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.56	0.45
2:H:66:VAL:O	2:H:82:ILE:HA	2.16	0.45
2:H:95:ASN:HB3	2:H:100:ASP:HB3	1.99	0.45
1:L:14(J):TYR:HE2	2:H:202:LYS:O	1.99	0.45
2:H:236:LYS:N	2:H:236:LYS:HD2	2.32	0.45
2:H:77(A):ARG:HG2	2:H:77(A):ARG:NH1	2.32	0.44
2:H:100:ASP:O	2:H:101:ARG:CB	2.66	0.44
2:H:164:GLU:C	2:H:166:PRO:CD	2.90	0.44
2:H:132:ALA:HA	2:H:162:ILE:HG22	1.99	0.44
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.33	0.44
2:H:107:LYS:HE2	2:H:107:LYS:HB2	1.67	0.43
2:H:35:ARG:NH2	4:H:524:HOH:O	2.34	0.43
2:H:114:PHE:CD1	2:H:114:PHE:N	2.82	0.43
2:H:87:LYS:HG3	2:H:88:ILE:H	1.83	0.43
2:H:101:ARG:HD2	2:H:101:ARG:HH11	1.56	0.43
2:H:152:PRO:HG3	2:H:156:GLN:HG2	1.99	0.43
2:H:235:LYS:HA	2:H:238:ILE:HB	2.00	0.43
2:H:100:ASP:C	2:H:101:ARG:HG3	2.42	0.43
2:H:125:ASP:CG	2:H:128:THR:HB	2.42	0.43
2:H:235:LYS:O	2:H:236:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:ILE:O	2:H:176:ILE:HD13	2.19	0.43
2:H:57:HIS:CE1	2:H:214:SER:O	2.72	0.43
2:H:145:LYS:HE2	2:H:149(B):ASN:HB3	2.01	0.43
2:H:219:GLY:HA2	4:H:443:HOH:O	2.19	0.43
2:H:98:ASN:N	2:H:98:ASN:OD1	2.49	0.43
2:H:61:GLU:HG2	2:H:86:GLU:O	2.18	0.42
2:H:84:MET:C	2:H:109:LYS:HG2	2.44	0.42
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.97	0.42
1:L:14(A):LYS:HB2	1:L:14(A):LYS:HZ3	1.83	0.42
2:H:146:GLU:O	2:H:149(B):ASN:ND2	2.51	0.42
2:H:214:SER:HB3	2:H:227:PHE:O	2.18	0.42
2:H:68:ILE:CG2	2:H:118:ILE:HG23	2.49	0.42
2:H:136:GLY:CA	2:H:199:PHE:CZ	2.97	0.42
2:H:154:VAL:CG1	2:H:155:LEU:N	2.82	0.42
2:H:127:GLU:OE1	2:H:127:GLU:CA	2.60	0.42
2:H:129(B):SER:O	2:H:131:GLN:NE2	2.53	0.42
2:H:123:LEU:HD23	2:H:123:LEU:HA	1.83	0.42
2:H:114:PHE:HA	2:H:118:ILE:O	2.19	0.42
1:L:14(A):LYS:HZ3	2:H:23:GLU:CD	2.29	0.41
2:H:52:VAL:HB	2:H:106:MET:HB2	2.03	0.41
2:H:59:LEU:HD11	2:H:106:MET:HE3	2.01	0.41
1:L:5:PRO:C	1:L:9:LYS:HB2	2.45	0.41
2:H:131:GLN:O	2:H:134:TYR:HB2	2.20	0.41
2:H:169:LYS:HB3	4:H:559:HOH:O	2.21	0.41
2:H:212:ILE:O	2:H:228:TYR:HA	2.21	0.41
2:H:176:ILE:CG2	2:H:177:THR:N	2.84	0.40
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.56	0.40
2:H:65:LEU:HD12	2:H:65:LEU:HA	1.69	0.40
2:H:110:LYS:CB	2:H:111:PRO:HD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	25/36 (69%)	21 (84%)	4 (16%)	0	100	100
2	H	256/259 (99%)	237 (93%)	18 (7%)	1 (0%)	30	43
All	All	281/295 (95%)	258 (92%)	22 (8%)	1 (0%)	30	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	77(A)	ARG

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	L	25/31 (81%)	22 (88%)	3 (12%)	5	7
2	H	224/225 (100%)	187 (84%)	37 (16%)	2	3
All	All	249/256 (97%)	209 (84%)	40 (16%)	2	3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
1	L	10	LYS
1	L	12	LEU
2	H	24	ILE
2	H	36	LYS
2	H	36(A)	SER
2	H	41	LEU
2	H	50	ARG
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	70	LYS
2	H	74	THR
2	H	75	ARG
2	H	79	ILE

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Mol	Chain	Res	Type
2	H	81	LYS
2	H	99	LEU
2	H	107	LYS
2	H	109	LYS
2	H	110	LYS
2	H	112	VAL
2	H	128	THR
2	H	145	LYS
2	H	147	THR
2	H	149	THR
2	H	149(B)	ASN
2	H	149(C)	VAL
2	H	149(E)	LYS
2	H	151	GLN
2	H	154	VAL
2	H	164	GLU
2	H	169	LYS
2	H	176	ILE
2	H	191	CYS
2	H	205	ASN
2	H	233	ARG
2	H	235	LYS
2	H	239	GLN
2	H	241	VAL
2	H	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	78	ASN
2	H	204(B)	ASN
2	H	205	ASN
2	H	239	GLN
2	H	244	GLN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
3	0G6	H	1	2	30,31,32	2.08	3 (10%)	37,41,42	1.42	5 (13%)

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	0G6	H	1	2	1/1/8/10	2/31/41/43	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	0G6	C3-C2	-8.51	1.27	1.51
3	H	1	0G6	O2-C2	-5.61	1.28	1.43
3	H	1	0G6	CE1-CD1	2.01	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	0G6	CB-CA-C	3.03	117.52	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	0G6	O2-C2-C3	2.83	118.14	109.68
3	H	1	0G6	CE1-CD1-CG	-2.78	116.70	120.61
3	H	1	0G6	CZ-CE2-CD2	-2.66	116.96	120.24
3	H	1	0G6	CE2-CD2-CG	2.51	124.15	120.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1	0G6	C2

All (2) torsion outliers are listed below:

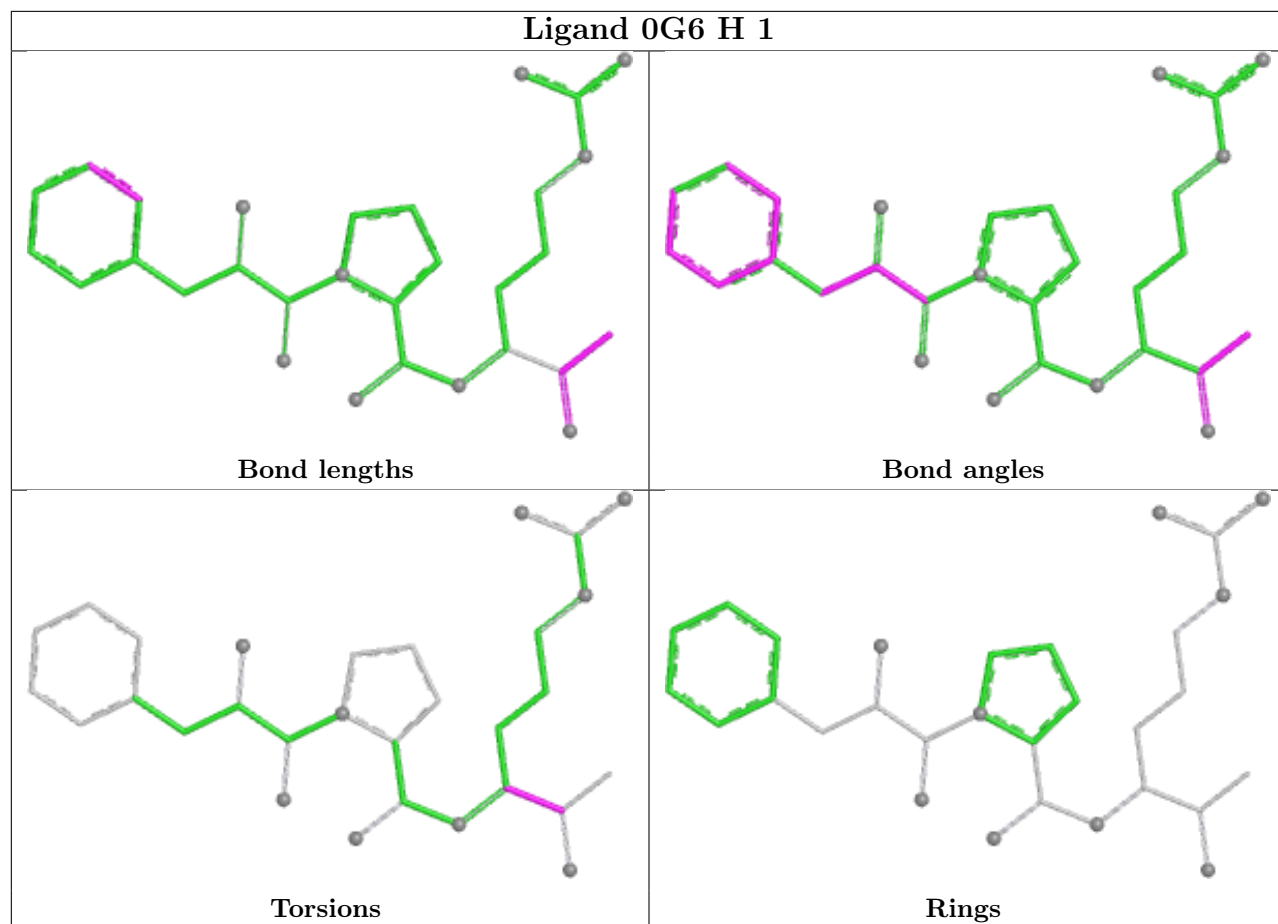
Mol	Chain	Res	Type	Atoms
3	H	1	0G6	C3-C2-CA2-N2
3	H	1	0G6	C3-C2-CA2-CB2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	0G6	5	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.