



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:39 PM UTC

PDB ID : 1B5G / pdb_00001b5g
Title : HUMAN THROMBIN COMPLEXED WITH NOVEL SYNTHETIC PEP-
TIDE MIMETIC INHIBITOR AND HIRUGEN
Authors : St Charles, R.; Tulinsky, A.; Kahn, M.
Deposited on : 1998-03-05
Resolution : 2.07 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

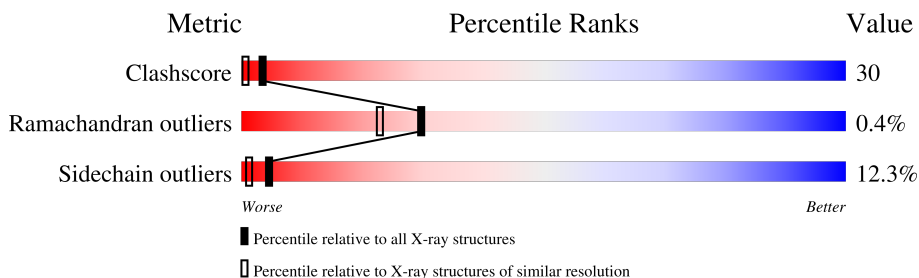
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)

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

There are 6 unique types of molecules in this entry. The entry contains 2526 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			239	149	38	51	1			

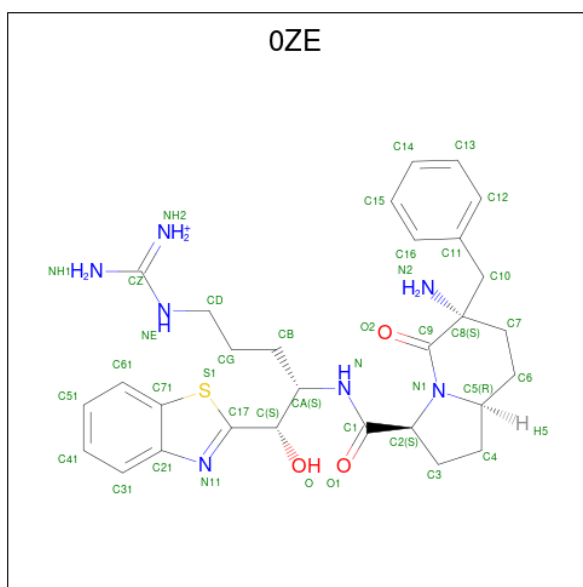
- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			2022	1290	358	360	14			

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			90	56	10	23	1			

- Molecule 4 is [[[(4S,5S)-4-[[[(3S,6S,8aR)-6-azanyl-5-oxo-6-(phenylmethyl)-1,2,3,7,8,8a-hexahydroindolizin-3-yl]carbonylamino]-5-(1,3-benzothiazol-2-yl)-5-hydroxy-pentyl]amino]-azanyl-methylidene]azanium (CCD ID: 0ZE) (formula: C₂₉H₃₈N₇O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	S	0	0
			40	29	7	3	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	11	Total	O	0	0
			11	11		
6	H	117	Total	O	0	0
			117	117		
6	I	5	Total	O	0	0
			5	5		

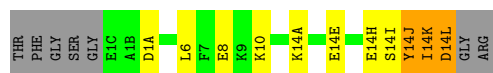
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

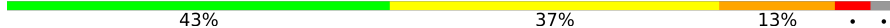
Note EDS was not executed.

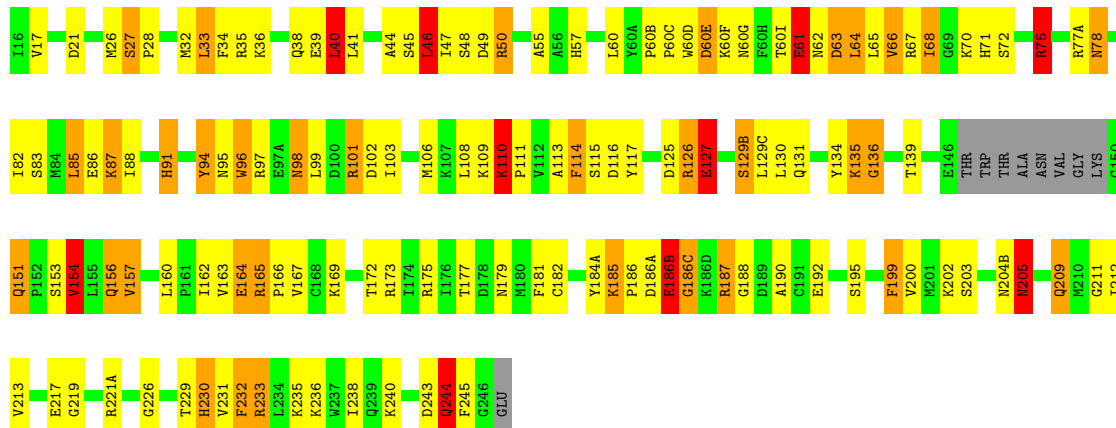
• Molecule 1: ALPHA-THROMBIN

Chain L: 



• Molecule 2: ALPHA-THROMBIN

Chain H: 



• Molecule 3: HIRUGEN

Chain I: 



4 Data and refinement statistics

Xtriage (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	70.84Å 72.08Å 73.00Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	7.00 – 2.07	Depositor
% Data completeness (in resolution range)	81.0 (7.00-2.07)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2526	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OZE, 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	1.16	0/241	2.26	10/321 (3.1%)
2	H	1.33	2/2074 (0.1%)	2.22	106/2801 (3.8%)
3	I	1.12	0/74	2.73	6/96 (6.2%)
All	All	1.31	2/2389 (0.1%)	2.24	122/3218 (3.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	136	GLY	N-CA	5.27	1.49	1.44
2	H	117	TYR	C-N	-5.12	1.27	1.33

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(J)	TYR	N-CA-C	-10.81	98.50	113.20
2	H	233	ARG	NE-CZ-NH1	10.20	131.70	121.50
2	H	230	HIS	CA-CB-CG	10.12	123.92	113.80
3	I	55	ASP	CA-CB-CG	10.10	122.70	112.60
2	H	205	ASN	OD1-CG-ND2	10.07	132.67	122.60
2	H	175	ARG	CD-NE-CZ	-9.83	110.64	124.40
1	L	14(L)	ASP	CA-CB-CG	9.75	122.35	112.60
1	L	1(A)	ASP	CA-CB-CG	-9.26	103.34	112.60
2	H	205	ASN	CA-CB-CG	-9.18	103.42	112.60
2	H	233	ARG	CD-NE-CZ	8.75	136.65	124.40
2	H	129(B)	SER	CA-C-O	-8.17	110.58	119.97
2	H	44	ALA	CA-C-O	-8.00	112.53	121.25
2	H	154	VAL	N-CA-CB	-7.91	100.56	112.35
2	H	243	ASP	CB-CA-C	7.88	124.85	109.72
2	H	165	ARG	NE-CZ-NH2	7.72	126.15	119.20
2	H	221(A)	ARG	NE-CZ-NH2	7.71	126.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	187	ARG	NE-CZ-NH1	-7.40	114.10	121.50
2	H	91	HIS	CA-CB-CG	-7.34	106.46	113.80
2	H	221(A)	ARG	NE-CZ-NH1	-7.32	114.18	121.50
2	H	28	PRO	CA-C-O	7.28	128.90	118.86
3	I	57	GLU	N-CA-CB	7.27	120.64	110.17
2	H	186(B)	GLU	CB-CG-CD	7.09	124.66	112.60
2	H	190	ALA	N-CA-C	-7.00	101.50	110.53
2	H	68	ILE	N-CA-C	6.96	118.62	108.53
2	H	233	ARG	NE-CZ-NH2	-6.72	113.15	119.20
3	I	57	GLU	N-CA-C	-6.69	101.07	110.50
2	H	186(C)	GLY	C-N-CA	6.64	138.31	121.70
2	H	186	PRO	C-N-CA	6.63	138.26	121.70
2	H	64	LEU	N-CA-C	6.57	120.33	110.14
2	H	114	PHE	CA-C-O	-6.54	114.29	121.87
2	H	60(E)	ASP	CA-CB-CG	-6.47	106.13	112.60
2	H	61	GLU	CB-CG-CD	6.46	123.59	112.60
2	H	44	ALA	O-C-N	6.44	129.74	123.04
3	I	56	PHE	CA-CB-CG	-6.42	107.38	113.80
2	H	47	ILE	CB-CA-C	6.36	117.81	110.88
2	H	151	GLN	O-C-N	6.27	127.55	121.66
2	H	231	VAL	CA-C-O	-6.25	114.54	121.17
2	H	110	LYS	O-C-N	6.24	125.70	121.71
2	H	179	ASN	OD1-CG-ND2	6.20	128.80	122.60
2	H	47	ILE	CB-CG1-CD1	6.18	126.77	113.80
2	H	175	ARG	NE-CZ-NH1	-6.09	115.41	121.50
2	H	172	THR	O-C-N	6.09	130.10	123.10
2	H	192	GLU	CA-C-O	-6.07	114.34	120.96
2	H	62	ASN	CA-C-O	6.05	126.94	120.10
2	H	232	PHE	CA-CB-CG	-6.04	107.76	113.80
2	H	177	THR	CA-C-N	6.03	130.25	120.60
2	H	177	THR	C-N-CA	6.03	130.25	120.60
2	H	232	PHE	O-C-N	-6.02	115.18	122.22
2	H	160	LEU	O-C-N	6.01	126.15	121.88
1	L	14(K)	ILE	CB-CA-C	5.98	121.09	111.29
2	H	164	GLU	CG-CD-OE2	5.98	132.15	118.40
2	H	63	ASP	O-C-N	5.97	129.61	122.27
3	I	58	GLU	CB-CG-CD	5.96	122.74	112.60
2	H	78	ASN	N-CA-CB	-5.94	107.40	114.17
2	H	66	VAL	N-CA-CB	-5.94	103.98	111.46
3	I	61	GLU	N-CA-C	5.78	117.58	111.28
2	H	127	GLU	CB-CG-CD	5.76	122.40	112.60
2	H	75	ARG	CA-C-O	-5.75	115.45	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	LYS	O-C-N	5.75	129.71	123.10
2	H	136	GLY	N-CA-C	-5.72	102.56	112.06
2	H	34	PHE	CA-C-O	5.69	126.50	120.36
2	H	27	SER	O-C-N	5.66	126.47	121.37
2	H	115	SER	CA-C-O	-5.64	115.12	121.05
2	H	40	LEU	O-C-N	5.62	129.91	122.95
2	H	181	PHE	CA-C-O	-5.62	115.26	121.33
2	H	163	VAL	CA-C-N	5.59	128.65	120.71
2	H	163	VAL	C-N-CA	5.59	128.65	120.71
2	H	213	VAL	CA-CB-CG2	5.58	119.88	110.40
2	H	101	ARG	NE-CZ-NH2	-5.57	114.19	119.20
2	H	55	ALA	CA-C-O	-5.57	114.52	120.92
2	H	164	GLU	CA-C-N	5.55	127.91	120.58
2	H	164	GLU	C-N-CA	5.55	127.91	120.58
1	L	14(L)	ASP	N-CA-CB	5.55	119.93	110.50
2	H	199	PHE	N-CA-C	-5.54	99.70	108.73
2	H	244	GLN	N-CA-C	-5.53	106.70	113.50
2	H	173	ARG	CD-NE-CZ	-5.53	116.66	124.40
2	H	46	LEU	CA-C-O	-5.50	114.27	120.43
2	H	177	THR	CA-C-O	-5.48	115.21	121.68
2	H	117	TYR	CA-C-N	5.45	130.72	122.98
2	H	117	TYR	C-N-CA	5.45	130.72	122.98
2	H	46	LEU	CA-C-N	5.43	128.31	121.85
2	H	46	LEU	C-N-CA	5.43	128.31	121.85
2	H	45	SER	CA-CB-OG	-5.42	100.25	111.10
2	H	113	ALA	O-C-N	5.36	129.46	123.19
2	H	95	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	H	114	PHE	O-C-N	5.32	128.85	122.79
2	H	185	LYS	CB-CA-C	5.30	117.80	109.37
2	H	192	GLU	O-C-N	5.29	129.41	123.06
1	L	14(J)	TYR	CA-C-N	-5.29	105.57	117.20
2	H	131	GLN	CB-CG-CD	-5.28	103.63	112.60
2	H	179	ASN	CA-CB-CG	-5.26	107.34	112.60
1	L	14(A)	LYS	CA-CB-CG	5.26	124.61	114.10
2	H	60	LEU	N-CA-CB	-5.25	102.85	110.84
2	H	94	TYR	CA-C-O	-5.24	115.25	120.96
2	H	219	GLY	N-CA-C	-5.23	101.48	112.45
2	H	40	LEU	CA-C-O	-5.22	114.97	120.92
2	H	163	VAL	O-C-N	-5.21	117.56	122.98
1	L	8	GLU	CA-C-N	5.21	128.93	120.60
1	L	8	GLU	C-N-CA	5.21	128.93	120.60
2	H	33	LEU	CB-CA-C	5.19	119.37	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	209	GLN	CA-C-O	-5.14	114.86	120.36
2	H	98	ASN	CA-C-N	5.14	129.86	122.40
2	H	98	ASN	C-N-CA	5.14	129.86	122.40
2	H	156	GLN	OE1-CD-NE2	-5.14	117.46	122.60
2	H	62	ASN	OD1-CG-ND2	5.13	127.73	122.60
2	H	115	SER	CA-C-N	5.13	127.66	120.28
2	H	115	SER	C-N-CA	5.13	127.66	120.28
2	H	116	ASP	O-C-N	5.12	128.21	122.22
2	H	165	ARG	NE-CZ-NH1	-5.11	116.39	121.50
2	H	28	PRO	CB-CA-C	5.09	119.13	111.44
2	H	172	THR	CA-C-O	-5.08	116.01	121.45
2	H	47	ILE	CA-C-O	5.08	123.37	118.90
2	H	67	ARG	CA-C-O	5.08	125.89	120.46
2	H	126	ARG	CA-C-N	5.08	127.34	120.44
2	H	126	ARG	C-N-CA	5.08	127.34	120.44
2	H	213	VAL	CA-C-O	5.08	127.13	120.78
2	H	96	TRP	O-C-N	5.06	129.44	122.46
2	H	60(E)	ASP	CA-C-O	-5.04	115.28	121.28
2	H	127	GLU	CA-CB-CG	5.02	124.14	114.10
1	L	14(E)	GLU	CB-CG-CD	5.02	121.13	112.60
2	H	46	LEU	N-CA-CB	-5.02	101.74	110.17
2	H	98	ASN	N-CA-C	5.02	119.12	112.30

There are no chirality outliers.

There are no planarity outliers.

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	239	0	235	8	1
2	H	2022	0	1997	116	2
3	I	90	0	69	13	2
4	H	40	0	37	15	0
5	H	2	0	0	0	0
6	H	117	0	0	12	0
6	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	11	0	0	2	0
All	All	2526	0	2338	140	3

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 30.

All (140) 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)
2:H:195:SER:OG	4:H:372:0ZE:C	1.84	1.26
2:H:195:SER:OG	4:H:372:0ZE:H37	0.90	1.07
2:H:151:GLN:HG2	6:H:447:HOH:O	1.55	1.06
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.36	1.03
4:H:372:0ZE:H72	4:H:372:0ZE:C12	1.85	1.03
1:L:14(J):TYR:C	1:L:14(K):ILE:HG12	1.84	1.02
2:H:165:ARG:HE	2:H:169:LYS:HE3	1.20	1.02
2:H:165:ARG:HE	2:H:169:LYS:CE	1.76	0.97
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.66	0.95
2:H:165:ARG:NE	2:H:169:LYS:HZ1	1.63	0.95
2:H:26:MET:HE3	6:H:458:HOH:O	1.67	0.93
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	1.49	0.91
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.72	0.91
2:H:195:SER:CB	4:H:372:0ZE:H37	2.01	0.91
2:H:72:SER:OG	2:H:75:ARG:HG2	1.76	0.86
2:H:165:ARG:CZ	2:H:169:LYS:HZ1	1.93	0.82
4:H:372:0ZE:H72	4:H:372:0ZE:H12	1.60	0.81
2:H:60(E):ASP:OD2	6:H:511:HOH:O	1.96	0.81
2:H:165:ARG:NE	2:H:169:LYS:NZ	2.28	0.80
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.54	0.80
1:L:10:LYS:HE2	6:L:515:HOH:O	1.81	0.79
2:H:165:ARG:CZ	2:H:169:LYS:NZ	2.46	0.79
2:H:236:LYS:HE2	6:H:540:HOH:O	1.84	0.77
2:H:35:ARG:O	2:H:38:GLN:HA	1.85	0.76
4:H:372:0ZE:H4	6:H:497:HOH:O	1.86	0.76
2:H:164:GLU:OE1	2:H:167:VAL:HG21	1.86	0.76
2:H:85:LEU:HD13	2:H:106:MET:CE	2.14	0.75
2:H:130:LEU:CD2	2:H:162:ILE:HD13	2.17	0.75
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.45	0.73
2:H:26:MET:CE	6:H:458:HOH:O	2.29	0.73
3:I:58:GLU:H	3:I:58:GLU:CD	1.96	0.71
4:H:372:0ZE:C41	6:H:497:HOH:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:46:LEU:HD22	2:H:48:SER:O	1.92	0.70
2:H:165:ARG:NE	2:H:169:LYS:HE3	2.03	0.69
2:H:130:LEU:HD23	2:H:162:ILE:CD1	2.24	0.68
2:H:195:SER:CB	4:H:372:OZE:C	2.66	0.67
2:H:165:ARG:NH2	2:H:169:LYS:HZ3	1.92	0.67
2:H:50:ARG:HD3	2:H:108:LEU:O	1.96	0.66
2:H:17:VAL:O	2:H:188:GLY:HA2	1.95	0.66
2:H:165:ARG:HE	2:H:169:LYS:NZ	1.93	0.64
2:H:70:LYS:HE3	2:H:72:SER:O	1.97	0.64
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.80	0.63
2:H:186(A):ASP:O	2:H:186(C):GLY:N	2.32	0.63
2:H:60(F):LYS:HG2	6:H:497:HOH:O	1.99	0.62
2:H:135:LYS:HE2	2:H:184(A):TYR:OH	1.98	0.62
3:I:60:PRO:HD2	3:I:63:TYS:HD2	1.81	0.62
1:L:10:LYS:CE	6:L:515:HOH:O	2.44	0.62
2:H:244:GLN:HG2	2:H:245:PHE:CD2	2.35	0.61
2:H:130:LEU:HD22	2:H:162:ILE:HD13	1.84	0.60
2:H:36:LYS:HG2	3:I:64:LEU:HD23	1.83	0.60
2:H:61:GLU:OE1	2:H:87:LYS:CA	2.47	0.60
3:I:61:GLU:C	3:I:63:TYS:N	2.59	0.59
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.01	0.59
2:H:130:LEU:CD2	2:H:162:ILE:CD1	2.79	0.59
2:H:236:LYS:HB2	6:H:517:HOH:O	2.02	0.59
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.83	0.59
2:H:165:ARG:NE	2:H:169:LYS:CE	2.55	0.59
2:H:165:ARG:NH2	2:H:169:LYS:NZ	2.50	0.59
2:H:64:LEU:HB2	2:H:85:LEU:HD11	1.84	0.58
3:I:60:PRO:HB2	3:I:62:GLU:OE2	2.03	0.58
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.09	0.57
2:H:97:ARG:NH2	6:H:498:HOH:O	2.38	0.57
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.39	0.57
2:H:164:GLU:OE1	2:H:167:VAL:CG2	2.54	0.55
2:H:165:ARG:O	2:H:169:LYS:HG3	2.06	0.55
2:H:186(A):ASP:C	2:H:186(C):GLY:H	2.15	0.55
2:H:60(D):TRP:CH2	4:H:372:OZE:H42	2.43	0.54
2:H:185:LYS:N	2:H:186(B):GLU:OE1	2.39	0.54
2:H:186(A):ASP:C	2:H:186(C):GLY:N	2.66	0.54
2:H:60(G):ASN:O	2:H:60(G):ASN:OD1	2.25	0.54
4:H:372:OZE:C12	4:H:372:OZE:C7	2.74	0.54
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.44	0.53
2:H:164:GLU:C	2:H:166:PRO:HD2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.39	0.52
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.24	0.52
3:I:60:PRO:O	3:I:63:TYS:HB3	2.10	0.52
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.45	0.52
2:H:230:HIS:CE1	2:H:233:ARG:HG3	2.45	0.51
2:H:98:ASN:OD1	2:H:98:ASN:N	2.42	0.51
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.36	0.51
2:H:57:HIS:HD2	4:H:372:OZE:H3	1.75	0.51
2:H:50:ARG:NH1	2:H:108:LEU:O	2.43	0.51
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.45	0.51
3:I:57:GLU:HG2	3:I:58:GLU:O	2.11	0.50
2:H:60(G):ASN:O	2:H:60(G):ASN:CG	2.54	0.49
2:H:244:GLN:OE1	2:H:245:PHE:CE2	2.66	0.49
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.47	0.49
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.47	0.49
2:H:139:THR:HG22	2:H:157:VAL:HG13	1.93	0.49
2:H:36:LYS:O	2:H:38:GLN:HG3	2.12	0.48
2:H:50:ARG:CD	2:H:108:LEU:O	2.61	0.48
2:H:195:SER:CB	4:H:372:OZE:O	2.60	0.48
2:H:75:ARG:N	2:H:75:ARG:HD3	2.26	0.48
2:H:60(I):THR:O	2:H:63:ASP:HB2	2.13	0.48
2:H:21:ASP:OD1	2:H:156:GLN:OE1	2.31	0.47
1:L:14(K):ILE:HD11	2:H:134:TYR:OH	2.14	0.47
2:H:217:GLU:HA	4:H:372:OZE:H16	1.95	0.47
2:H:97:ARG:HG3	6:H:438:HOH:O	2.14	0.47
2:H:165:ARG:N	2:H:166:PRO:HD2	2.29	0.47
2:H:46:LEU:CD2	2:H:48:SER:O	2.62	0.47
2:H:99:LEU:O	2:H:102:ASP:HB2	2.15	0.47
2:H:127:GLU:H	2:H:127:GLU:CD	2.23	0.47
2:H:139:THR:CG2	2:H:157:VAL:HG13	2.45	0.47
2:H:35:ARG:HD3	2:H:39:GLU:OE2	2.15	0.46
2:H:57:HIS:CD2	2:H:57:HIS:C	2.94	0.45
3:I:61:GLU:O	3:I:63:TYS:N	2.49	0.45
2:H:135:LYS:CE	2:H:184(A):TYR:OH	2.64	0.45
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.17	0.45
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.15	0.45
2:H:41:LEU:CD2	2:H:64:LEU:CD2	2.96	0.44
2:H:165:ARG:N	2:H:166:PRO:CD	2.81	0.44
2:H:230:HIS:ND1	2:H:233:ARG:HG3	2.32	0.44
2:H:103:ILE:HD11	2:H:238:ILE:HD11	1.99	0.44
2:H:182:CYS:HA	2:H:226:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:ILE:HD12	2:H:229:THR:HB	2.00	0.44
2:H:211:GLY:HA2	2:H:229:THR:O	2.17	0.43
2:H:244:GLN:CD	2:H:245:PHE:CE2	2.97	0.43
3:I:57:GLU:CG	3:I:58:GLU:N	2.82	0.43
2:H:202:LYS:HE3	2:H:205:ASN:O	2.18	0.43
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.27	0.43
3:I:61:GLU:C	3:I:63:TYR:H	2.26	0.43
3:I:57:GLU:HG2	3:I:58:GLU:N	2.34	0.42
2:H:110:LYS:HE2	6:H:529:HOH:O	2.18	0.42
2:H:195:SER:OG	4:H:372:OZE:C17	2.61	0.42
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.68	0.42
2:H:60(G):ASN:OD1	2:H:60(G):ASN:C	2.63	0.42
2:H:85:LEU:CD1	2:H:106:MET:CE	2.94	0.42
2:H:88:ILE:HG21	2:H:88:ILE:HD13	1.73	0.42
2:H:60(F):LYS:HE2	4:H:372:OZE:H51	2.02	0.42
2:H:134:TYR:N	2:H:134:TYR:HD1	2.18	0.42
2:H:50:ARG:HG2	2:H:111:PRO:HA	2.01	0.41
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.82	0.41
2:H:134:TYR:N	2:H:134:TYR:CD1	2.89	0.41
2:H:185:LYS:HG3	2:H:186(B):GLU:CD	2.45	0.41
2:H:200:VAL:HG12	2:H:209:GLN:HA	2.02	0.41
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.74	0.41
3:I:62:GLU:OE1	3:I:62:GLU:N	2.33	0.41
2:H:185:LYS:HG3	2:H:186(B):GLU:OE1	2.20	0.41
2:H:85:LEU:N	2:H:85:LEU:HD23	2.35	0.41
2:H:125:ASP:OD1	2:H:127:GLU:HB2	2.20	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:NH1	3:I:57:GLU:OE1[2_555]	1.70	0.50
2:H:75:ARG:NH2	3:I:57:GLU:CB[2_555]	2.12	0.08
1:L:14(H):GLU:OE2	1:L:14(L):ASP:OD2[2_556]	2.15	0.05

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	27/36 (75%)	22 (82%)	5 (18%)	0	100	100
2	H	246/259 (95%)	236 (96%)	9 (4%)	1 (0%)	30	23
3	I	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	280/307 (91%)	264 (94%)	15 (5%)	1 (0%)	30	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	186(B)	GLU

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	27/31 (87%)	26 (96%)	1 (4%)	30	24
2	H	218/225 (97%)	190 (87%)	28 (13%)	4	1
3	I	8/10 (80%)	6 (75%)	2 (25%)	0	0
All	All	253/266 (95%)	222 (88%)	31 (12%)	4	1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
2	H	27	SER

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Mol	Chain	Res	Type
2	H	33	LEU
2	H	40	LEU
2	H	46	LEU
2	H	50	ARG
2	H	61	GLU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	75	ARG
2	H	82	ILE
2	H	83	SER
2	H	85	LEU
2	H	86	GLU
2	H	87	LYS
2	H	109	LYS
2	H	110	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	153	SER
2	H	154	VAL
2	H	157	VAL
2	H	187	ARG
2	H	205	ASN
2	H	235	LYS
2	H	240	LYS
2	H	244	GLN
3	I	58	GLU
3	I	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	156	GLN
2	H	204(B)	ASN
2	H	230	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	3	15,16,17	1.82	3 (20%)	15,22,24	1.47	2 (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	TYS	I	63	3	-	3/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	-4.47	1.35	1.42
3	I	63	TYS	OH-S	4.25	1.66	1.58
3	I	63	TYS	CB-CA	2.13	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CB-CG-CD1	-2.68	115.91	120.90
3	I	63	TYS	O2-S-O1	2.67	122.52	112.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	63	TYS	CA-CB-CG-CD1
3	I	63	TYS	CA-CB-CG-CD2
3	I	63	TYS	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	OZE	H	372	-	42,44,44	1.80	5 (11%)	48,63,63	1.67	9 (18%)

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	OZE	H	372	-	-	2/27/57/57	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	372	OZE	O-C	-8.08	1.26	1.42
4	H	372	OZE	C17-S1	3.57	1.80	1.75
4	H	372	OZE	C-C17	3.20	1.56	1.51
4	H	372	OZE	CB-CA	2.36	1.57	1.52
4	H	372	OZE	C21-C71	-2.24	1.36	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	372	0ZE	CG-CB-CA	-5.35	103.75	113.94
4	H	372	0ZE	C8-C10-C11	-4.16	107.45	115.49
4	H	372	0ZE	O-C-CA	3.11	117.20	108.43
4	H	372	0ZE	CA-N-C1	-3.11	117.83	123.25
4	H	372	0ZE	C6-C5-N1	3.05	115.08	110.09
4	H	372	0ZE	C7-C6-C5	2.59	114.59	110.99
4	H	372	0ZE	C-CA-N	-2.59	105.12	109.93
4	H	372	0ZE	S1-C17-N11	-2.42	113.19	116.24
4	H	372	0ZE	C4-C5-N1	-2.41	99.05	101.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

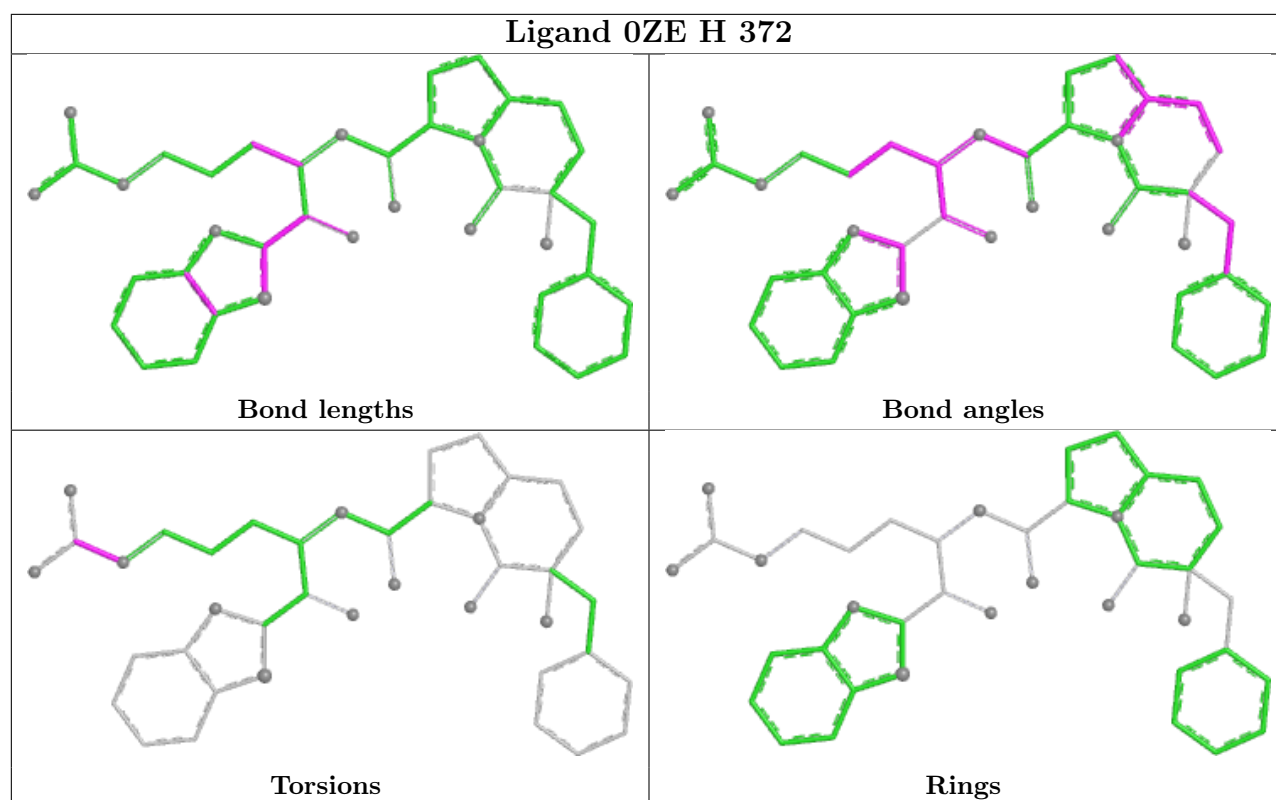
Mol	Chain	Res	Type	Atoms
4	H	372	0ZE	NH1-CZ-NE-CD
4	H	372	0ZE	NH2-CZ-NE-CD

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	372	0ZE	15	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.