



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 1A46 / pdb_00001a46
Title : THROMBIN COMPLEXED WITH HIRUGEN AND A BETA-STRAND
MIMETIC INHIBITOR
Authors : St Charles, R.; Matthews, J.H.; Zhang, E.; Tulinsky, A.; Kahn, M.
Deposited on : 1998-02-11
Resolution : 2.12 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

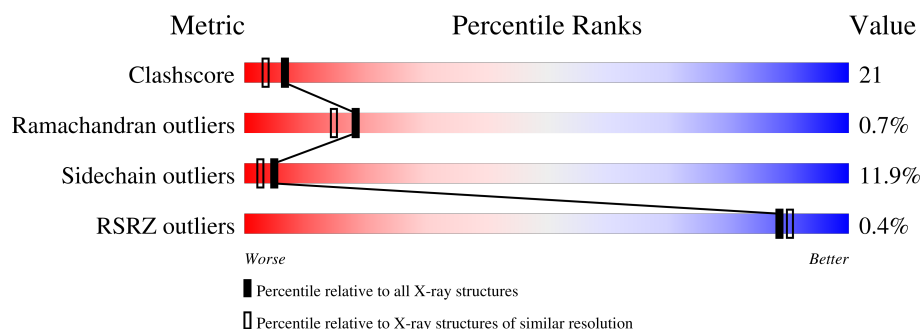
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 2503 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	26	Total	C	N	O	S	0	0	0
			214	135	34	44	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			2008	1279	355	360	14			

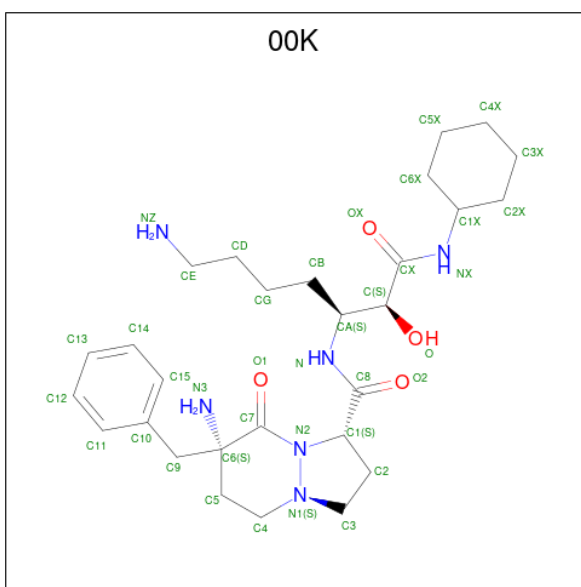
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			76	48	10	17	1			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is (1S,7S)-7-amino-N-[(2R,3S)-7-amino-1-(cyclohexylamino)-2-hydroxy-1-oxoheptan-3-yl]-7-benzyl-8-oxohexahydro-1H-pyrazolo[1,2-a]pyridazine-1-carboxamide (CCD ID: 00K) (formula: C₂₈H₄₄N₆O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			38	28	6	4		

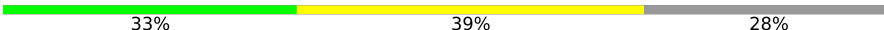
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	15	Total O 15 15	0	0
6	H	148	Total O 148 148	0	0
6	I	2	Total O 2 2	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

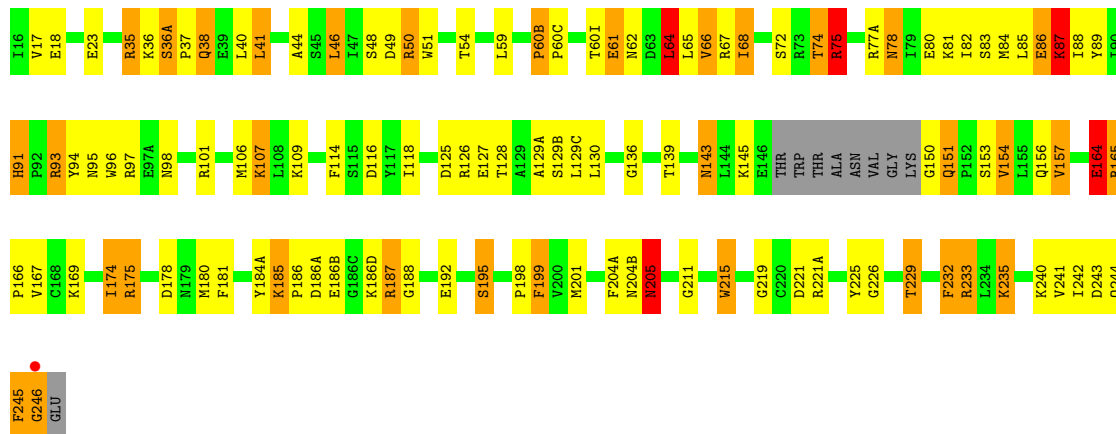
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



- Molecule 3: HIRUGEN

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.30Å 73.09Å 73.82Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	7.00 – 2.12 7.00 – 2.13	Depositor EDS
% Data completeness (in resolution range)	75.0 (7.00-2.12) 74.3 (7.00-2.13)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.155 , (Not available) 0.151 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2503	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TYS, 00K

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	1.30	0/216	2.00	5/288 (1.7%)
2	H	1.51	7/2060 (0.3%)	2.18	86/2785 (3.1%)
3	I	1.14	0/60	2.18	2/76 (2.6%)
All	All	1.48	7/2336 (0.3%)	2.16	93/3149 (3.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	174	ILE	CA-CB	6.77	1.61	1.54
2	H	226	GLY	N-CA	6.47	1.52	1.45
2	H	154	VAL	N-CA	6.41	1.53	1.46
2	H	201	MET	CA-C	5.89	1.59	1.52
2	H	199	PHE	CA-C	5.67	1.60	1.52
2	H	219	GLY	CA-C	5.31	1.58	1.52
2	H	198	PRO	CA-CB	5.22	1.59	1.54

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	61	GLU	CB-CG-CD	16.26	140.24	112.60
2	H	205	ASN	OD1-CG-ND2	13.82	136.42	122.60
2	H	205	ASN	CA-CB-CG	-10.86	101.74	112.60
2	H	35	ARG	NE-CZ-NH2	-10.07	110.14	119.20
2	H	154	VAL	N-CA-CB	-9.61	99.06	112.52
2	H	61	GLU	CA-CB-CG	8.93	131.97	114.10
1	L	1(A)	ASP	CA-CB-CG	-8.86	103.74	112.60
2	H	97	ARG	NE-CZ-NH2	-8.41	111.63	119.20
2	H	93	ARG	CD-NE-CZ	8.12	135.78	124.40
2	H	175	ARG	CD-NE-CZ	-7.80	113.47	124.40
2	H	62	ASN	CA-CB-CG	-7.79	104.81	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	157	VAL	CA-C-O	-7.66	113.16	121.28
2	H	192	GLU	CB-CG-CD	7.65	125.60	112.60
2	H	75	ARG	CA-C-O	-7.36	113.12	121.81
2	H	40	LEU	CA-C-O	-7.34	112.36	120.81
2	H	205	ASN	N-CA-CB	-7.34	101.19	113.15
2	H	50	ARG	CA-C-O	-7.29	110.58	119.18
2	H	98	ASN	OD1-CG-ND2	-7.29	115.31	122.60
2	H	98	ASN	CB-CG-ND2	7.27	127.31	116.40
2	H	164	GLU	CG-CD-OE2	7.15	134.85	118.40
2	H	116	ASP	CA-CB-CG	7.15	119.75	112.60
2	H	91	HIS	CA-C-O	7.05	125.63	119.71
2	H	44	ALA	CA-C-O	-7.01	113.78	121.28
1	L	14(B)	THR	CA-C-O	-6.99	111.72	119.34
2	H	95	ASN	OD1-CG-ND2	-6.93	115.67	122.60
2	H	151	GLN	O-C-N	6.80	127.45	121.39
2	H	68	ILE	N-CA-C	6.78	118.36	108.53
2	H	186(A)	ASP	N-CA-CB	-6.76	100.04	109.91
2	H	23	GLU	CB-CG-CD	6.73	124.04	112.60
2	H	78	ASN	OD1-CG-ND2	-6.68	115.92	122.60
3	I	360	PRO	CA-C-N	6.66	129.50	120.38
3	I	360	PRO	C-N-CA	6.66	129.50	120.38
2	H	232	PHE	CA-CB-CG	-6.66	107.14	113.80
2	H	186(D)	LYS	N-CA-C	-6.63	99.02	109.50
1	L	13	GLU	CA-C-O	-6.58	113.72	121.16
2	H	40	LEU	O-C-N	6.47	130.89	122.93
2	H	75	ARG	CA-CB-CG	-6.43	101.23	114.10
2	H	198	PRO	CB-CA-C	-6.39	100.09	110.25
2	H	246	GLY	CA-C-O	-6.39	107.38	120.80
2	H	165	ARG	CA-C-N	6.34	125.56	118.97
2	H	165	ARG	C-N-CA	6.34	125.56	118.97
2	H	82	ILE	CA-C-O	-6.34	113.75	120.53
2	H	129(A)	ALA	CA-C-O	-6.33	113.84	120.55
2	H	74	THR	CA-C-O	-6.31	112.22	118.97
2	H	54	THR	CA-C-N	6.22	130.74	121.72
2	H	54	THR	C-N-CA	6.22	130.74	121.72
2	H	154	VAL	CB-CA-C	6.14	119.90	110.82
2	H	192	GLU	CB-CA-C	5.95	119.19	109.90
2	H	87	LYS	O-C-N	5.91	130.10	123.48
2	H	164	GLU	CG-CD-OE1	-5.87	104.90	118.40
2	H	233	ARG	CD-NE-CZ	-5.87	116.19	124.40
2	H	78	ASN	N-CA-CB	-5.86	108.24	114.10
2	H	60(I)	THR	CA-CB-OG1	-5.83	100.86	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	VAL	N-CA-CB	-5.80	104.36	111.67
2	H	225	TYR	CA-C-N	-5.79	116.13	122.38
2	H	225	TYR	C-N-CA	-5.79	116.13	122.38
1	L	14	ASP	CA-C-O	5.78	128.63	121.81
2	H	221(A)	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	H	151	GLN	CB-CA-C	5.78	117.22	109.42
2	H	153	SER	N-CA-C	-5.71	106.47	113.50
2	H	186	PRO	C-N-CA	5.71	135.98	121.70
2	H	74	THR	N-CA-C	5.71	121.27	113.97
2	H	78	ASN	CB-CG-ND2	5.69	124.93	116.40
2	H	61	GLU	CG-CD-OE1	5.64	131.38	118.40
2	H	186	PRO	CA-C-O	5.64	128.55	119.64
2	H	187	ARG	CD-NE-CZ	-5.62	116.53	124.40
2	H	153	SER	N-CA-CB	5.61	118.78	110.53
2	H	143	ASN	O-C-N	5.59	129.79	122.97
2	H	60(B)	PRO	CB-CA-C	5.54	117.68	110.92
2	H	181	PHE	CA-C-O	-5.50	115.19	121.40
2	H	186(D)	LYS	CB-CA-C	5.47	120.82	109.38
2	H	50	ARG	NE-CZ-NH1	-5.42	116.08	121.50
2	H	38	GLN	CB-CG-CD	5.37	121.73	112.60
2	H	74	THR	CA-CB-OG1	-5.37	101.55	109.60
1	L	14	ASP	CB-CA-C	5.36	120.43	109.76
2	H	126	ARG	CD-NE-CZ	5.36	131.90	124.40
2	H	118	ILE	CA-C-O	-5.36	115.06	120.31
2	H	125	ASP	N-CA-C	-5.35	102.13	110.42
2	H	178	ASP	CA-CB-CG	-5.33	107.27	112.60
2	H	98	ASN	CA-C-O	-5.33	113.53	119.34
2	H	180	MET	CA-C-O	-5.29	115.42	121.40
2	H	83	SER	O-C-N	5.24	130.43	122.94
2	H	164	GLU	CA-C-N	5.21	127.45	120.58
2	H	164	GLU	C-N-CA	5.21	127.45	120.58
2	H	64	LEU	N-CA-C	5.20	117.31	109.41
2	H	215	TRP	N-CA-C	5.15	116.12	108.60
2	H	204(A)	PHE	CA-CB-CG	-5.15	108.65	113.80
2	H	128	THR	N-CA-C	-5.10	105.80	111.36
2	H	46	LEU	CA-C-N	5.09	127.90	121.85
2	H	46	LEU	C-N-CA	5.09	127.90	121.85
2	H	245	PHE	N-CA-C	5.07	119.02	111.87
2	H	243	ASP	CA-C-N	5.02	127.51	120.28
2	H	243	ASP	C-N-CA	5.02	127.51	120.28

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	214	0	211	10	0
2	H	2008	0	1962	86	1
3	I	76	0	56	5	1
4	H	2	0	0	0	0
5	H	38	0	43	7	0
6	H	148	0	0	4	0
6	I	2	0	0	0	0
6	L	15	0	0	1	0
All	All	2503	0	2272	98	1

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 21.

All (98) 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:75:ARG:HH11	2:H:75:ARG:CG	1.50	1.21
2:H:195:SER:OG	5:H:372:00K:H40	0.94	1.10
2:H:75:ARG:HH11	2:H:75:ARG:HG3	0.93	1.08
2:H:139:THR:HG22	2:H:157:VAL:HG22	1.38	1.05
2:H:75:ARG:HG3	2:H:75:ARG:NH1	1.56	0.99
2:H:50:ARG:HH21	2:H:107:LYS:HE2	1.29	0.98
2:H:50:ARG:NH2	2:H:107:LYS:HE2	1.87	0.89
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.57	0.86
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.07	0.85
2:H:244:GLN:HG2	2:H:245:PHE:CE2	2.15	0.81
2:H:75:ARG:N	2:H:75:ARG:HD3	1.94	0.81
2:H:139:THR:CG2	2:H:157:VAL:HG22	2.12	0.79
2:H:195:SER:HG	5:H:372:00K:H40	0.99	0.78
2:H:36(A):SER:HA	2:H:37:PRO:C	2.11	0.75
2:H:164:GLU:H	2:H:164:GLU:CD	1.95	0.74
1:L:14(D):ARG:NH1	1:L:14(H):GLU:OE2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ASN:HA	2:H:150:GLY:O	1.92	0.68
2:H:50:ARG:HG2	2:H:50:ARG:NH1	2.08	0.68
1:L:10:LYS:HE2	6:L:477:HOH:O	1.95	0.67
2:H:242:ILE:O	2:H:246:GLY:O	2.13	0.67
2:H:50:ARG:HH11	2:H:50:ARG:CG	2.07	0.67
2:H:93:ARG:NH1	6:H:532:HOH:O	2.29	0.66
2:H:164:GLU:N	2:H:164:GLU:OE1	2.28	0.65
2:H:244:GLN:HG2	2:H:245:PHE:CD2	2.31	0.64
2:H:75:ARG:HH11	2:H:75:ARG:HG2	1.54	0.63
2:H:75:ARG:CG	2:H:75:ARG:NH1	2.21	0.62
2:H:87:LYS:HD3	2:H:88:ILE:H	1.63	0.61
2:H:50:ARG:HE	2:H:107:LYS:CE	2.13	0.61
2:H:74:THR:O	6:H:470:HOH:O	2.16	0.61
2:H:187:ARG:NH2	2:H:221:ASP:O	2.33	0.60
2:H:35:ARG:O	2:H:38:GLN:HA	2.00	0.60
2:H:50:ARG:HG2	2:H:50:ARG:HH11	1.64	0.60
2:H:195:SER:CB	5:H:372:00K:H40	2.19	0.59
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.00	0.59
1:L:14(D):ARG:HG3	1:L:14(D):ARG:HH11	1.67	0.58
2:H:87:LYS:HD3	2:H:88:ILE:N	2.19	0.58
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE2	2.51	0.58
2:H:205:ASN:ND2	6:H:485:HOH:O	2.36	0.58
2:H:36:LYS:HG2	3:I:364:LEU:HD23	1.86	0.58
2:H:165:ARG:N	2:H:166:PRO:CD	2.68	0.57
2:H:165:ARG:N	2:H:166:PRO:HD2	2.20	0.57
2:H:36(A):SER:CA	2:H:37:PRO:C	2.78	0.56
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.87	0.56
2:H:72:SER:OG	2:H:75:ARG:HG2	2.05	0.56
2:H:85:LEU:HD11	2:H:106:MET:HE2	1.84	0.56
2:H:195:SER:CB	5:H:372:00K:C	2.81	0.56
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.05	0.55
2:H:167:VAL:HG11	2:H:185:LYS:HE2	1.88	0.55
2:H:50:ARG:CZ	2:H:107:LYS:HE2	2.36	0.55
2:H:17:VAL:O	2:H:188:GLY:HA2	2.06	0.55
2:H:195:SER:OG	5:H:372:00K:CX	2.52	0.55
2:H:164:GLU:C	2:H:166:PRO:HD2	2.33	0.54
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.08	0.54
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.43	0.53
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.17	0.53
2:H:151:GLN:OE1	6:H:544:HOH:O	2.19	0.53
2:H:17:VAL:O	2:H:18:GLU:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.47	0.50
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.69	0.49
2:H:156:GLN:C	2:H:157:VAL:HG23	2.37	0.49
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.27	0.49
2:H:244:GLN:HG2	2:H:245:PHE:CZ	2.47	0.49
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.20	0.49
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.60	0.49
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.48	0.48
2:H:80:GLU:O	2:H:81:LYS:HD3	2.14	0.48
2:H:85:LEU:CD1	2:H:106:MET:CE	2.88	0.48
2:H:215:TRP:HB2	5:H:372:00K:H11	1.96	0.47
2:H:50:ARG:NH2	2:H:86:GLU:OE1	2.47	0.47
2:H:244:GLN:NE2	2:H:245:PHE:CZ	2.83	0.47
2:H:195:SER:HG	5:H:372:00K:C	1.92	0.47
2:H:50:ARG:NE	2:H:107:LYS:CE	2.77	0.46
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.51	0.46
2:H:164:GLU:CD	2:H:164:GLU:N	2.71	0.45
2:H:150:GLY:C	2:H:151:GLN:HG3	2.40	0.44
2:H:85:LEU:HD11	2:H:106:MET:CE	2.47	0.44
3:I:359:ILE:HG21	3:I:359:ILE:HD13	1.70	0.44
1:L:14(J):TYR:O	1:L:14(K):ILE:C	2.61	0.43
2:H:74:THR:C	2:H:75:ARG:HD3	2.42	0.43
2:H:51:TRP:CZ3	2:H:107:LYS:HB3	2.54	0.43
2:H:232:PHE:O	2:H:235:LYS:HB2	2.17	0.43
2:H:50:ARG:HE	2:H:107:LYS:NZ	2.16	0.43
2:H:175:ARG:HH11	2:H:175:ARG:HD2	1.57	0.43
2:H:240:LYS:NZ	2:H:244:GLN:OE1	2.49	0.43
2:H:41:LEU:CD2	2:H:64:LEU:CD2	2.97	0.42
2:H:174:ILE:HG23	2:H:174:ILE:HD12	1.78	0.42
2:H:59:LEU:HD13	2:H:88:ILE:HD13	2.01	0.42
2:H:17:VAL:HG12	2:H:18:GLU:HG2	2.01	0.42
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.35	0.42
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.43	0.41
2:H:67:ARG:HH21	2:H:80:GLU:CD	2.27	0.41
2:H:185:LYS:HZ3	2:H:185:LYS:HG3	1.74	0.41
2:H:74:THR:HB	3:I:356:PHE:HA	2.02	0.41
2:H:84:MET:HE3	3:I:363:TYS:O	2.22	0.40
3:I:363:TYS:HD1	3:I:363:TYS:HA	1.95	0.40
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.56	0.40
2:H:184(A):TYR:HA	2:H:186(B):GLU:OE1	2.22	0.40
2:H:211:GLY:HA2	2:H:229:THR:O	2.21	0.40

All (1) 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:357:GLU:OE1[2_555]	2.02	0.18

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	246/259 (95%)	234 (95%)	10 (4%)	2 (1%)	16	12
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	277/307 (90%)	264 (95%)	11 (4%)	2 (1%)	18	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	195	SER
2	H	36(A)	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%)	22 (92%)	2 (8%)	10	7
2	H	215/225 (96%)	188 (87%)	27 (13%)	4	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	5/10 (50%)	5 (100%)	0	100	100
All	All	244/266 (92%)	215 (88%)	29 (12%)	5	2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	9	LYS
2	H	41	LEU
2	H	46	LEU
2	H	48	SER
2	H	61	GLU
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	75	ARG
2	H	86	GLU
2	H	87	LYS
2	H	107	LYS
2	H	109	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	145	LYS
2	H	154	VAL
2	H	164	GLU
2	H	169	LYS
2	H	185	LYS
2	H	205	ASN
2	H	229	THR
2	H	233	ARG
2	H	235	LYS
2	H	241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	H	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	204(B)	ASN
2	H	239	GLN

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	363	3	15,16,17	1.98	2 (13%)	15,22,24	1.44	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	363	3	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	363	TYS	OH-S	5.51	1.69	1.58
3	I	363	TYS	OH-CZ	-4.08	1.36	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	363	TYS	O2-S-O1	2.66	122.47	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	363	TYS	OH-S-O2	-2.57	99.72	107.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	363	TYS	CA-CB-CG-CD1
3	I	363	TYS	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	363	TYS	2	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
5	00K	H	372	2	37,41,41	1.68	6 (16%)	42,57,57	2.88	17 (40%)

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
5	00K	H	372	2	-	2/29/67/67	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	372	00K	O-C	-5.45	1.31	1.42
5	H	372	00K	C2-C3	3.64	1.59	1.52
5	H	372	00K	O2-C8	3.59	1.30	1.23
5	H	372	00K	O1-C7	3.35	1.27	1.22
5	H	372	00K	C12-C11	2.58	1.43	1.38
5	H	372	00K	C8-N	2.45	1.39	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	372	00K	C-CA-N	7.15	123.20	109.93
5	H	372	00K	C2-C1-C8	-6.58	97.22	111.21
5	H	372	00K	OX-CX-C	-6.45	108.62	119.99
5	H	372	00K	O2-C8-N	-5.37	113.35	122.96
5	H	372	00K	O-C-CX	-5.22	99.72	110.63
5	H	372	00K	CA-N-C8	4.45	130.99	123.25
5	H	372	00K	O-C-CA	4.17	120.19	108.43
5	H	372	00K	C-CX-NX	4.06	121.72	116.22
5	H	372	00K	CB-CA-N	3.78	115.21	110.30
5	H	372	00K	C2X-C1X-NX	3.49	117.54	110.57
5	H	372	00K	C1-C8-N	3.23	123.62	116.52
5	H	372	00K	C7-N2-N1	3.08	125.73	120.31
5	H	372	00K	OX-CX-NX	3.07	128.46	122.96
5	H	372	00K	C1-N2-C7	-2.54	121.35	124.94
5	H	372	00K	C6X-C1X-NX	2.28	115.12	110.57
5	H	372	00K	C3-N1-N2	2.06	104.42	102.46
5	H	372	00K	C13-C12-C11	2.05	122.77	120.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

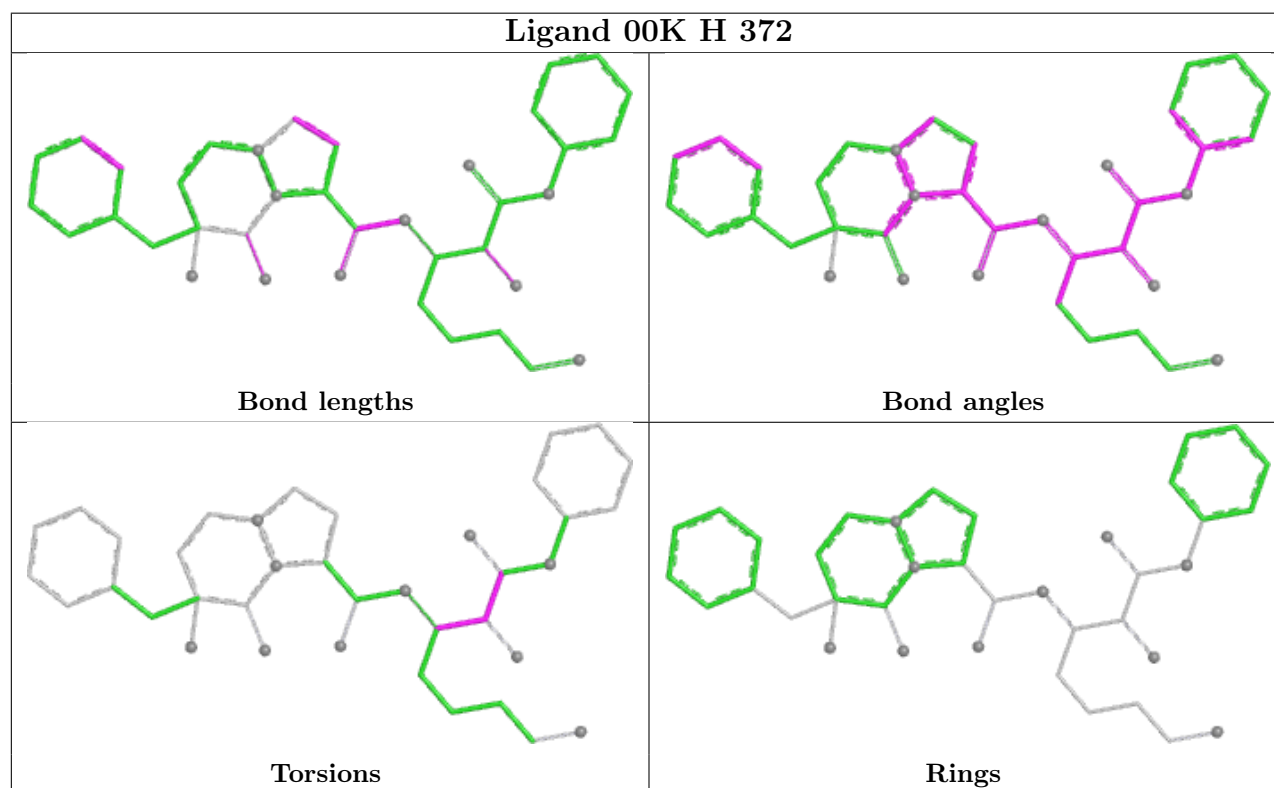
Mol	Chain	Res	Type	Atoms
5	H	372	00K	O-C-CX-OX
5	H	372	00K	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	372	00K	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	26/36 (72%)	-0.96	0 100 100	13, 19, 35, 41	0
2	H	250/259 (96%)	-0.97	1 (0%) 88 90	10, 20, 38, 49	0
3	I	9/12 (75%)	-0.35	0 100 100	41, 43, 45, 47	0
All	All	285/307 (92%)	-0.95	1 (0%) 88 90	10, 20, 41, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	246	GLY	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYS	I	363	16/17	0.96	0.06	31,35,46,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

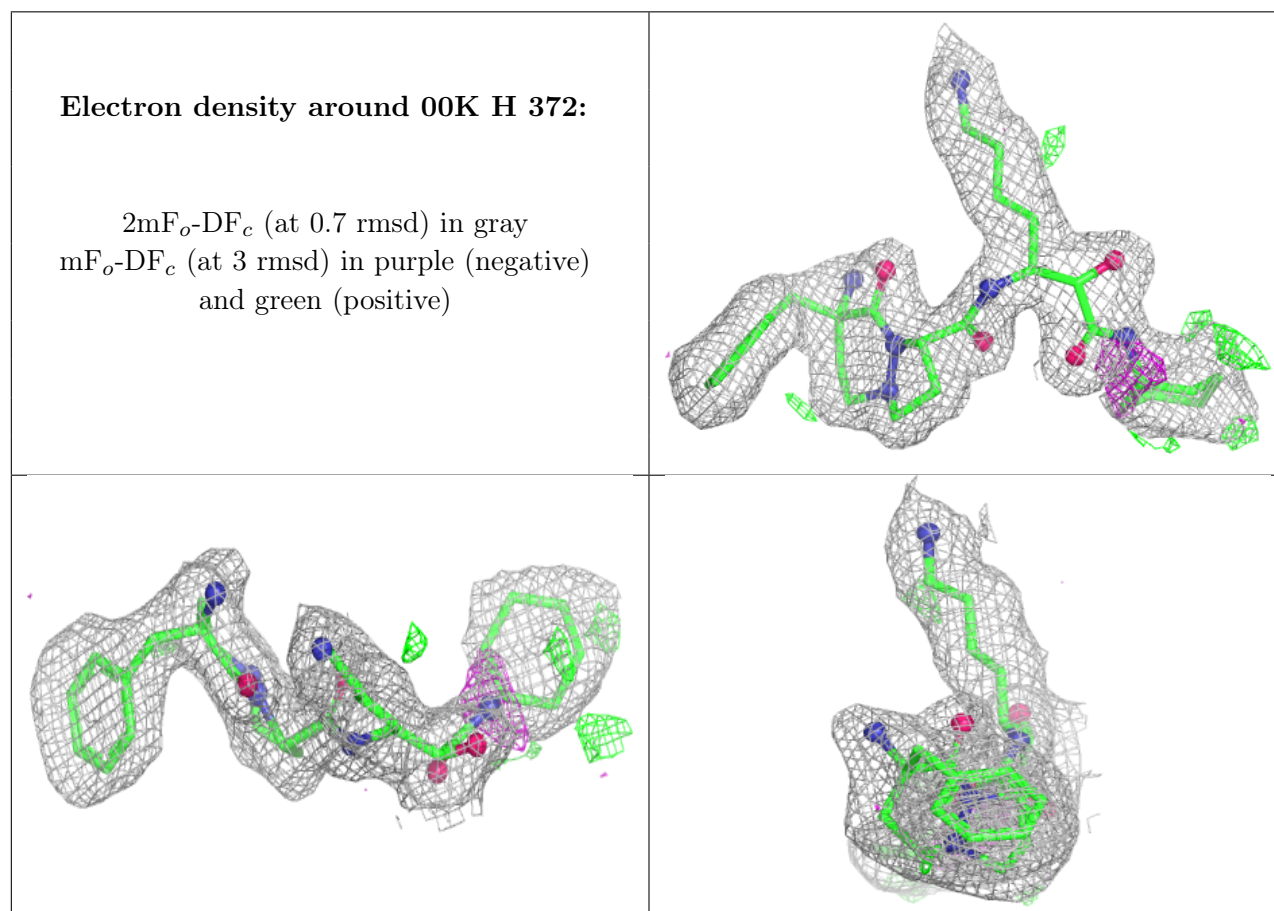
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	00K	H	372	38/38	0.93	0.05	12,21,34,34	0
4	NA	H	548	1/1	0.95	0.03	24,24,24,24	1
4	NA	H	549	1/1	0.99	0.07	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.