



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:46 PM UTC

PDB ID : 1H8D / pdb_00001h8d
Title : X-ray structure of the human alpha-thrombin complex with a tripeptide phosphonate inhibitor.
Authors : Skordalakes, E.; Dodson, G.G.; Green, D.; Deadman, J.
Deposited on : 2001-02-01
Resolution : 1.40 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)	:	2.0
EDS	:	FAILED
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

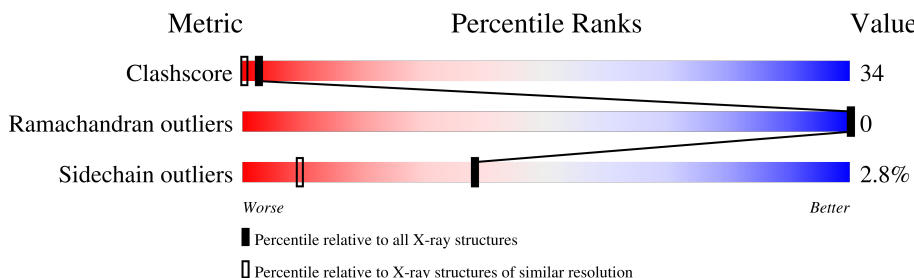
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	H	260	
2	I	10	
3	L	29	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3086 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
1	H	260	Total	C	N	O	S	0	8	9
			2030	1295	355	364	16			

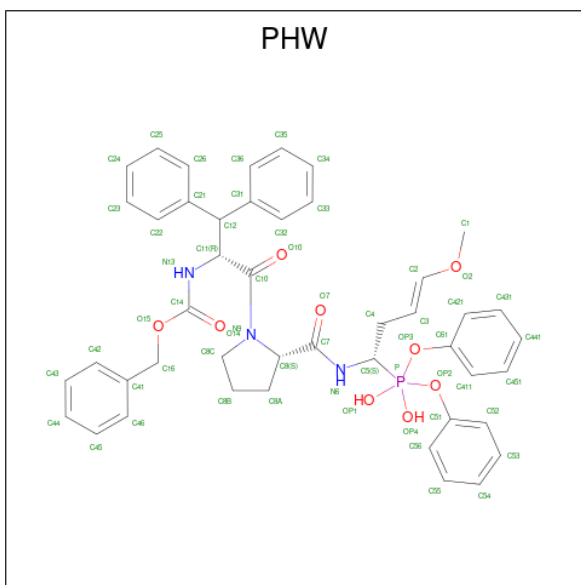
- Molecule 2 is a protein called HIRUDIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	S	0	0	0
			94	59	10	24	1			

- Molecule 3 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	29	Total	C	N	O	S	0	0	1
			225	143	36	45	1			

- Molecule 4 is N-[(benzyloxy)carbonyl]-beta-phenyl-D-phenylalanyl-N-{(1S,3E)-1-[dihydroxy(diphenoxy)-lambda 5 -phosphanyl]-4-methoxybut-3-en-1-yl}-L-prolinamide (CCD ID: PHW) (formula: C₄₅H₄₈N₃O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			53	40	3	9	1		

- Molecule 5 is water.

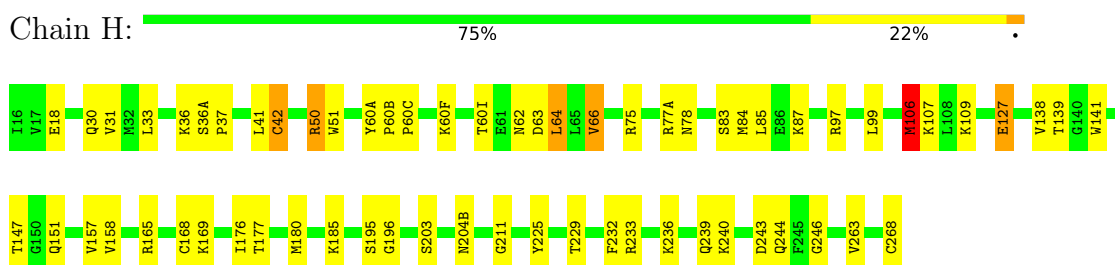
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	572	Total O 572 572	0	0
5	I	38	Total O 38 38	0	0
5	L	74	Total O 74 74	0	0

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 failed to run properly.

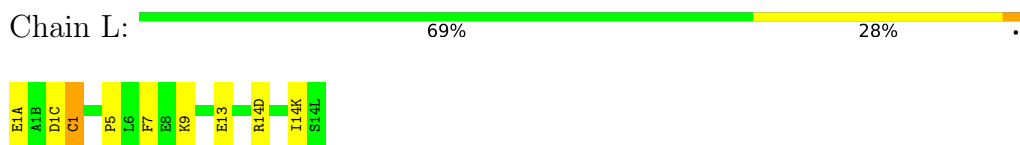
• Molecule 1: THROMBIN



• Molecule 2: HIRUDIN I



• Molecule 3: THROMBIN



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.64Å 71.60Å 71.90Å 90.00° 100.35° 90.00°	Depositor
Resolution (Å)	14.00 – 1.40	Depositor
% Data completeness (in resolution range)	95.4 (14.00-1.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.89 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.220	Depositor
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.501	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	H	0.56	0/2073	1.17	4/2802 (0.1%)
2	I	0.35	0/78	0.94	0/103
3	L	4.12	2/225 (0.9%)	1.93	3/297 (1.0%)
All	All	1.38	2/2376 (0.1%)	1.25	7/3202 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1	CYS	CA-C	55.01	2.68	1.52
3	L	1	CYS	CA-CB	27.33	2.08	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	CYS	CB-CA-C	-25.87	60.95	110.10
3	L	1	CYS	CA-CB-SG	9.61	136.49	114.40
1	H	42	CYS	CA-CB-SG	7.84	132.42	114.40
1	H	232	PHE	CA-CB-CG	-6.90	106.90	113.80
1	H	106	MET	CA-CB-CG	5.55	125.20	114.10
3	L	7	PHE	CA-CB-CG	-5.16	108.64	113.80
1	H	30	GLN	OE1-CD-NE2	5.13	127.73	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2030	0	1986	111	0
2	I	94	0	77	10	0
3	L	225	0	225	24	0
4	H	53	0	40	15	0
5	H	572	0	0	58	5
5	I	38	0	0	8	0
5	L	74	0	0	17	0
All	All	3086	0	2328	159	5

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 34.

All (159) 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:H:177:THR:H	1:H:180:MET:CE	1.22	1.49
1:H:168:CYS:HB2	1:H:268:CYS:SG	1.61	1.37
3:L:1:CYS:CA	3:L:1:CYS:CB	2.08	1.32
2:I:4:GLU:HG2	5:I:113:HOH:O	1.14	1.29
4:H:301:PHW:C52	5:H:722:HOH:O	1.80	1.26
1:H:84:MET:SD	5:I:122:HOH:O	1.94	1.24
1:H:177:THR:N	1:H:180:MET:CE	2.01	1.22
3:L:14(K):ILE:O	5:L:102:HOH:O	1.54	1.22
4:H:301:PHW:HC41	4:H:301:PHW:C61	1.72	1.19
1:H:50:ARG:HG3	5:H:590:HOH:O	1.44	1.17
1:H:165:ARG:HD3	5:H:456:HOH:O	1.47	1.12
4:H:301:PHW:H54	5:H:425:HOH:O	0.94	1.10
1:H:176:ILE:CA	1:H:180:MET:HE1	1.80	1.09
1:H:176:ILE:HA	1:H:180:MET:HE1	1.08	1.07
1:H:60(F):LYS:HB2	5:H:750:HOH:O	1.53	1.06
3:L:1(C):ASP:C	3:L:1:CYS:CA	2.29	1.05
1:H:236:LYS:CG	5:H:912:HOH:O	2.05	1.04
4:H:301:PHW:C61	4:H:301:PHW:C4	2.34	1.04
1:H:177:THR:N	1:H:180:MET:HE2	1.65	1.02
3:L:9:LYS:HG2	5:L:150:HOH:O	1.57	1.02
3:L:9:LYS:HD3	5:L:153:HOH:O	1.58	1.01
1:H:64:LEU:HD11	1:H:85:LEU:HD11	1.41	1.00
1:H:177:THR:H	1:H:180:MET:HE2	0.85	1.00
2:I:1:ASP:HB2	5:I:117:HOH:O	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:CYS:CB	1:H:268:CYS:SG	2.51	0.98
1:H:165:ARG:CG	1:H:169:LYS:NZ	2.26	0.97
1:H:165:ARG:HG2	1:H:169:LYS:NZ	1.79	0.97
1:H:84:MET:HE3	1:H:109:LYS:HD2	1.47	0.95
1:H:75:ARG:HB2	5:H:748:HOH:O	1.64	0.94
1:H:87:LYS:CE	5:H:401:HOH:O	2.15	0.94
4:H:301:PHW:O7	4:H:301:PHW:HC42	1.65	0.92
3:L:13:GLU:OE1	5:L:103:HOH:O	1.88	0.88
3:L:1:CYS:CB	3:L:1:CYS:C	2.47	0.87
1:H:165:ARG:HG2	1:H:169:LYS:HZ2	1.35	0.87
1:H:50:ARG:CG	5:H:590:HOH:O	2.09	0.86
1:H:176:ILE:HA	1:H:180:MET:CE	2.01	0.86
3:L:14(K):ILE:C	5:L:104:HOH:O	2.19	0.85
4:H:301:PHW:C53	5:H:722:HOH:O	2.09	0.83
3:L:5:PRO:HA	3:L:9:LYS:HD2	1.62	0.82
1:H:41:LEU:HD12	5:H:828:HOH:O	1.80	0.81
1:H:127:GLU:HB3	5:H:404:HOH:O	1.81	0.81
1:H:64:LEU:HD11	1:H:85:LEU:CD1	2.11	0.80
3:L:9:LYS:CD	5:L:153:HOH:O	2.23	0.78
1:H:62:ASN:HB3	5:H:410:HOH:O	1.82	0.78
1:H:50:ARG:CB	5:H:590:HOH:O	2.28	0.78
1:H:87:LYS:NZ	5:H:401:HOH:O	2.03	0.78
1:H:268:CYS:SG	5:H:695:HOH:O	2.43	0.76
3:L:1:CYS:C	3:L:1:CYS:HB2	2.10	0.76
1:H:244:GLN:CG	5:H:405:HOH:O	2.34	0.75
1:H:244:GLN:HG3	5:H:405:HOH:O	1.85	0.75
3:L:14(K):ILE:CD1	5:L:151:HOH:O	2.35	0.75
1:H:42:CYS:SG	1:H:195:SER:O	2.44	0.75
1:H:83:SER:HB2	1:H:263[A]:VAL:CG2	2.16	0.75
2:I:1:ASP:HB2	5:I:104:HOH:O	1.85	0.75
1:H:165:ARG:CG	1:H:169:LYS:HZ2	1.96	0.74
2:I:10:LEU:O	5:I:101:HOH:O	2.05	0.74
1:H:165:ARG:O	1:H:268:CYS:SG	2.46	0.73
1:H:165:ARG:CD	5:H:456:HOH:O	2.16	0.73
1:H:176:ILE:C	1:H:180:MET:HE1	2.14	0.72
1:H:50:ARG:HB2	5:H:590:HOH:O	1.90	0.71
1:H:177:THR:N	1:H:180:MET:HE1	1.97	0.71
3:L:14(K):ILE:O	5:L:104:HOH:O	2.06	0.71
1:H:87:LYS:NZ	5:H:407:HOH:O	2.23	0.71
3:L:9:LYS:HB3	5:L:153:HOH:O	1.89	0.71
1:H:84:MET:HE2	5:H:869:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:LEU:HD11	1:H:106:MET:HE1	1.74	0.69
1:H:165:ARG:HG3	1:H:268:CYS:SG	2.32	0.69
1:H:41:LEU:CD1	5:H:828:HOH:O	2.40	0.69
1:H:151:GLN:OE1	5:H:403:HOH:O	2.09	0.69
1:H:147:THR:HG22	5:H:629:HOH:O	1.93	0.69
1:H:176:ILE:CA	1:H:180:MET:CE	2.65	0.68
1:H:62:ASN:CB	5:H:410:HOH:O	2.41	0.68
1:H:240:LYS:HE3	5:H:689:HOH:O	1.93	0.68
1:H:176:ILE:C	1:H:180:MET:CE	2.67	0.67
3:L:1:CYS:CA	3:L:1:CYS:C	2.68	0.67
1:H:127:GLU:OE2	5:H:404:HOH:O	2.12	0.66
1:H:62:ASN:HB3	5:H:628:HOH:O	1.95	0.66
1:H:60(I):THR:HG22	1:H:63:ASP:OD2	1.95	0.66
4:H:301:PHW:C61	5:H:423:HOH:O	2.43	0.66
1:H:41:LEU:CG	5:H:828:HOH:O	2.44	0.65
5:H:417:HOH:O	2:I:10:LEU:HD21	1.96	0.65
1:H:64:LEU:CD1	1:H:85:LEU:HD11	2.25	0.64
1:H:165:ARG:CD	1:H:169:LYS:HZ3	2.10	0.64
1:H:165:ARG:CG	1:H:169:LYS:HZ3	2.10	0.64
1:H:244:GLN:OE1	5:H:405:HOH:O	2.15	0.64
3:L:9:LYS:HE2	5:L:150:HOH:O	1.97	0.64
1:H:165:ARG:HG2	1:H:169:LYS:HZ3	1.62	0.64
1:H:127:GLU:H	1:H:127:GLU:CD	2.06	0.63
3:L:14(D):ARG:NH2	5:L:105:HOH:O	2.31	0.63
1:H:165:ARG:CD	1:H:169:LYS:NZ	2.62	0.63
4:H:301:PHW:C61	4:H:301:PHW:HC42	2.28	0.62
1:H:165:ARG:HD3	1:H:169:LYS:HZ3	1.65	0.62
1:H:139:THR:HG22	1:H:157:VAL:HG22	1.82	0.61
3:L:14(D):ARG:NE	5:L:105:HOH:O	2.34	0.61
1:H:239:GLN:NE2	5:H:409:HOH:O	2.32	0.61
1:H:243:ASP:OD1	5:H:406:HOH:O	2.16	0.60
1:H:177:THR:H	1:H:180:MET:HE3	1.49	0.60
1:H:165:ARG:HD3	1:H:169:LYS:NZ	2.15	0.60
1:H:75:ARG:CG	5:H:792:HOH:O	2.49	0.60
4:H:301:PHW:C54	5:H:425:HOH:O	1.79	0.60
1:H:176:ILE:CG2	1:H:180:MET:HE3	2.32	0.59
1:H:18:GLU:CG	5:H:659:HOH:O	2.50	0.59
1:H:41:LEU:HG	5:H:828:HOH:O	2.03	0.59
1:H:176:ILE:HG23	1:H:180:MET:HE3	1.84	0.59
2:I:7:GLU:CD	5:I:105:HOH:O	2.46	0.59
1:H:36(A):SER:HA	1:H:37:PRO:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:LYS:HE3	1:H:246:GLY:O	2.04	0.57
3:L:14(K):ILE:HD13	5:L:151:HOH:O	2.00	0.57
2:I:1:ASP:CB	5:I:104:HOH:O	2.50	0.57
1:H:97:ARG:NH2	5:H:402:HOH:O	2.32	0.57
1:H:87:LYS:CE	5:H:407:HOH:O	2.54	0.56
2:I:1:ASP:OD1	2:I:1:ASP:O	2.24	0.56
1:H:97:ARG:NE	5:H:402:HOH:O	2.09	0.56
1:H:246:GLY:C	5:H:457:HOH:O	2.49	0.56
3:L:14(K):ILE:C	5:L:102:HOH:O	2.26	0.56
3:L:9:LYS:CB	5:L:153:HOH:O	2.53	0.55
1:H:77(A):ARG:O	1:H:78:ASN:HB2	2.05	0.55
4:H:301:PHW:C61	5:H:535:HOH:O	2.55	0.55
1:H:236:LYS:CB	5:H:912:HOH:O	2.46	0.55
3:L:1(A):GLU:CB	5:L:154:HOH:O	2.54	0.54
1:H:97:ARG:NH1	5:H:413:HOH:O	2.37	0.54
1:H:42:CYS:SG	1:H:196:GLY:HA3	2.48	0.53
1:H:169:LYS:HG3	1:H:268:CYS:SG	2.49	0.52
2:I:1:ASP:CB	5:I:117:HOH:O	2.38	0.52
1:H:31:VAL:HG13	1:H:66:VAL:HG13	1.92	0.52
1:H:127:GLU:CD	1:H:127:GLU:N	2.68	0.52
1:H:87:LYS:HD2	5:H:401:HOH:O	2.10	0.51
1:H:33:LEU:CD1	1:H:106:MET:HE1	2.40	0.51
1:H:87:LYS:CD	5:H:401:HOH:O	2.54	0.51
1:H:33:LEU:HD21	1:H:106:MET:HE3	1.94	0.49
1:H:18:GLU:HG2	5:H:659:HOH:O	2.11	0.48
1:H:18:GLU:HG3	5:H:659:HOH:O	2.13	0.48
1:H:165:ARG:HG3	1:H:169:LYS:NZ	2.24	0.48
1:H:141:TRP:HE3	5:H:697:HOH:O	1.96	0.48
3:L:5:PRO:CA	3:L:9:LYS:HD2	2.40	0.48
5:H:417:HOH:O	2:I:10:LEU:CD2	2.60	0.48
1:H:87:LYS:HE3	5:H:401:HOH:O	1.94	0.47
3:L:14(D):ARG:CZ	5:L:105:HOH:O	2.61	0.47
1:H:204(B):ASN:C	1:H:204(B):ASN:HD22	2.23	0.47
4:H:301:PHW:C61	5:H:422:HOH:O	2.65	0.45
1:H:177:THR:N	1:H:180:MET:HE3	2.14	0.45
1:H:33:LEU:HD21	1:H:106:MET:CE	2.47	0.44
1:H:60(I):THR:HG22	1:H:63:ASP:CG	2.41	0.44
1:H:85:LEU:HD22	1:H:106:MET:HB2	1.99	0.44
1:H:36:LYS:NZ	5:H:410:HOH:O	2.33	0.43
1:H:60(B):PRO:N	1:H:60(C):PRO:CD	2.82	0.43
1:H:211:GLY:HA2	1:H:229:THR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60(F):LYS:CB	5:H:750:HOH:O	2.32	0.42
4:H:301:PHW:H2	4:H:301:PHW:HC5	1.66	0.42
4:H:301:PHW:H8C	5:H:445:HOH:O	2.20	0.42
1:H:138:VAL:CG2	1:H:158:VAL:HG12	2.49	0.42
4:H:301:PHW:C26	4:H:301:PHW:H8C2	2.50	0.41
1:H:185:LYS:HG2	1:H:225:TYR:OH	2.20	0.41
1:H:84:MET:CE	5:H:869:HOH:O	2.59	0.41
1:H:51:TRP:HE1	1:H:246:GLY:C	2.29	0.41
1:H:64:LEU:CD1	1:H:85:LEU:CD1	2.90	0.41
1:H:203:SER:HB3	1:H:204(B):ASN:ND2	2.36	0.41
1:H:138:VAL:HG23	1:H:158:VAL:HG12	2.02	0.40
1:H:60(A):TYR:OH	4:H:301:PHW:H8B1	2.22	0.40

All (5) 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)
5:H:754:HOH:O	5:H:754:HOH:O[2_556]	1.46	0.74
5:H:520:HOH:O	5:H:634:HOH:O[3_545]	1.84	0.36
5:H:931:HOH:O	5:H:944:HOH:O[3_455]	1.85	0.35
5:H:801:HOH:O	5:H:801:HOH:O[2_555]	2.01	0.19
5:H:658:HOH:O	5:H:759:HOH:O[4_546]	2.17	0.03

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	H	247/260 (95%)	239 (97%)	8 (3%)	0	100	100
2	I	7/10 (70%)	7 (100%)	0	0	100	100
3	L	24/29 (83%)	23 (96%)	1 (4%)	0	100	100
All	All	278/299 (93%)	269 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	217/228 (95%)	210 (97%)	7 (3%)	34	7
2	I	9/9 (100%)	9 (100%)	0	100	100
3	L	23/27 (85%)	23 (100%)	0	100	100
All	All	249/264 (94%)	242 (97%)	7 (3%)	38	9

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	ARG
1	H	64	LEU
1	H	66	VAL
1	H	99	LEU
1	H	106	MET
1	H	127	GLU
1	H	233	ARG

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

Mol	Chain	Res	Type
1	H	30	GLN
1	H	38	GLN
1	H	151	GLN
1	H	204(B)	ASN
1	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$
2	TYS	I	9	2	15,16,17	1.07	2 (13%)	15,22,24	0.83	1 (6%)

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
2	TYS	I	9	2	-	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)
2	I	9	TYS	OH-CZ	-2.64	1.38	1.42
2	I	9	TYS	OH-S	-2.62	1.53	1.58

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	9	TYS	OH-S-O1	2.69	115.75	107.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	PHW	H	301	-	50,57,63	2.98	7 (14%)	63,79,87	1.49	10 (15%)

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	PHW	H	301	-	-	10/43/70/72	0/5/5/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	PHW	O2-C1	-12.16	1.20	1.43
4	H	301	PHW	OP3-C61	9.41	1.62	1.43
4	H	301	PHW	C4-C5	-9.14	1.38	1.53
4	H	301	PHW	C7-N6	6.04	1.47	1.34
4	H	301	PHW	C10-N9	5.44	1.46	1.34
4	H	301	PHW	C14-N13	4.89	1.46	1.34
4	H	301	PHW	O15-C14	2.64	1.40	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	PHW	C4-C5-N6	-5.31	105.17	111.36
4	H	301	PHW	C5-C4-C3	-4.60	105.09	113.69
4	H	301	PHW	C1-O2-C2	4.58	130.01	115.87
4	H	301	PHW	C8A-C8-C7	3.47	118.59	111.21
4	H	301	PHW	O14-C14-N13	-2.58	120.64	124.86
4	H	301	PHW	C25-C26-C21	-2.32	117.87	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	301	PHW	C16-O15-C14	-2.15	111.09	115.93
4	H	301	PHW	O15-C14-N13	2.14	115.03	110.45
4	H	301	PHW	P-OP2-C51	-2.11	120.59	129.03
4	H	301	PHW	C24-C25-C26	2.08	122.80	120.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

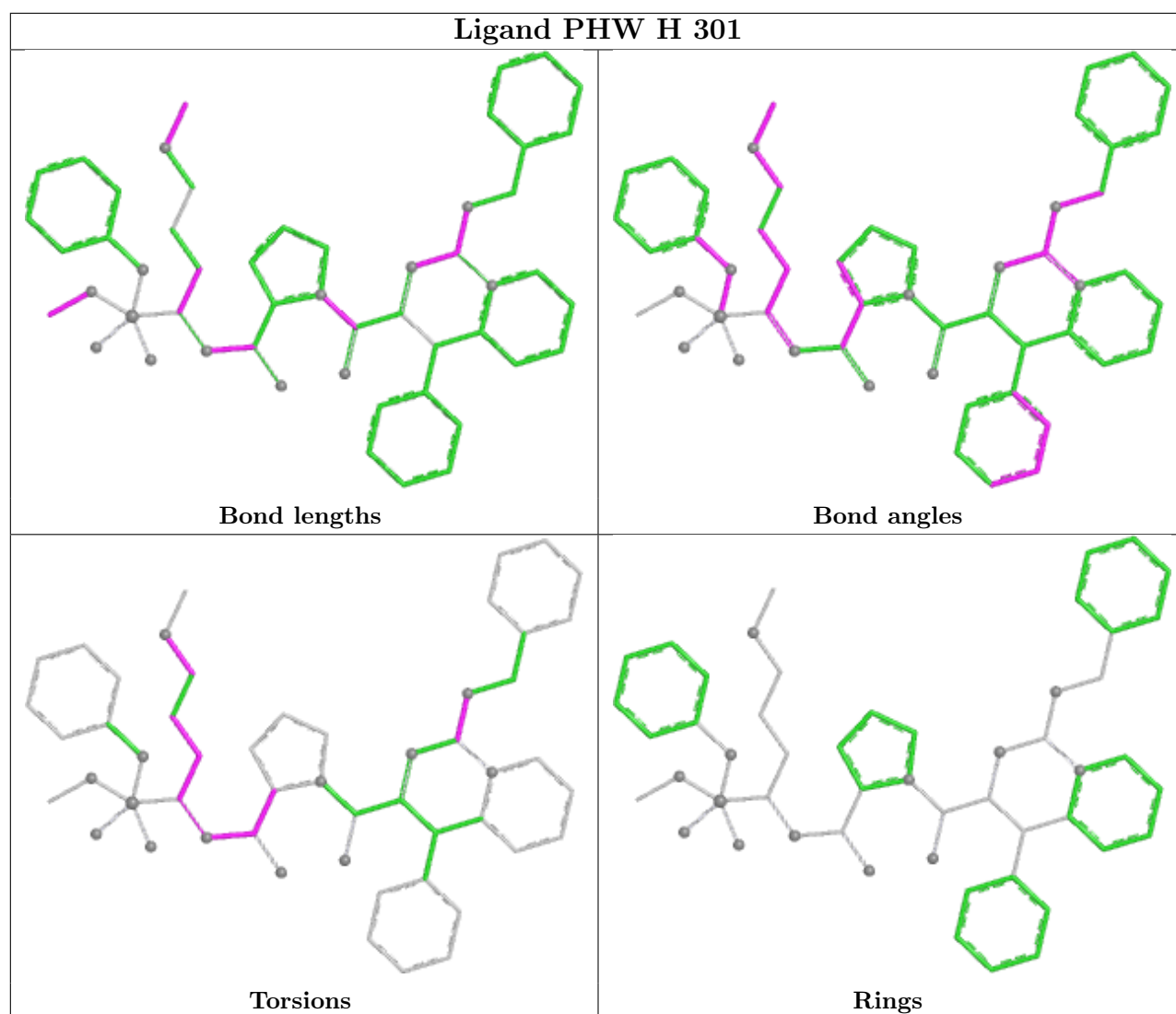
Mol	Chain	Res	Type	Atoms
4	H	301	PHW	C3-C2-O2-C1
4	H	301	PHW	C2-C3-C4-C5
4	H	301	PHW	C3-C4-C5-N6
4	H	301	PHW	C4-C5-N6-C7
4	H	301	PHW	O7-C7-C8-N9
4	H	301	PHW	O7-C7-N6-C5
4	H	301	PHW	O7-C7-C8-C8A
4	H	301	PHW	N6-C7-C8-N9
4	H	301	PHW	N6-C7-C8-C8A
4	H	301	PHW	O14-C14-O15-C16

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	PHW	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	147:THR	C	150:GLY	N	7.20

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.