



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 PM UTC

PDB ID : 1TMU / pdb_00001tmu
Title : Changes in interactions in complexes of hirudin derivatives and human alpha-thrombin due to different crystal forms
Authors : Priestle, J.P.; Gruetter, M.G.
Deposited on : 1994-05-26
Resolution : 2.50 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

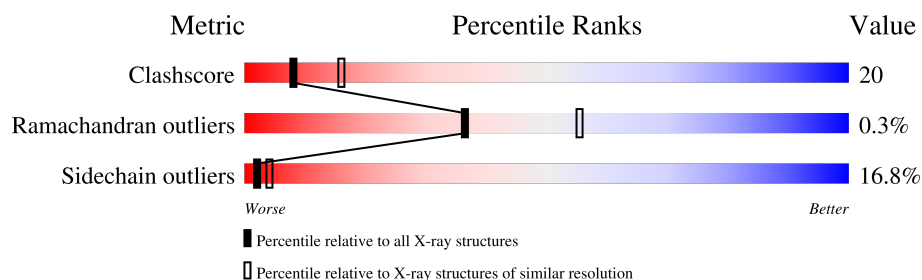
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	28	
2	H	259	
3	J	11	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2516 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	28	Total	C	N	O	S	0	0	0
			232	145	37	49	1			

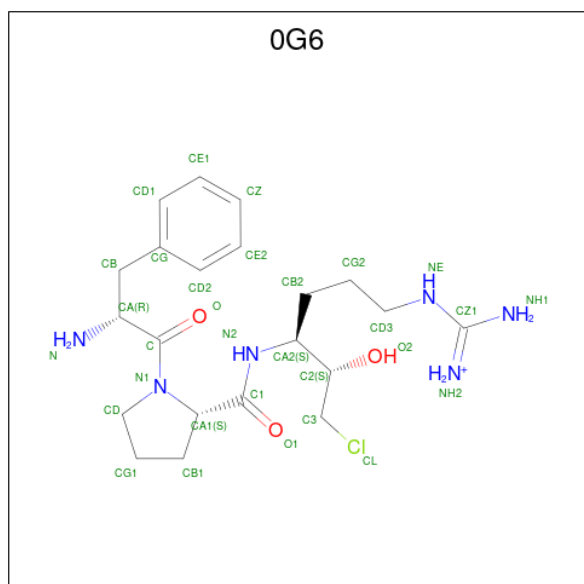
- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	257	Total	C	N	O	S	0	0	0
			2064	1316	364	370	14			

- Molecule 3 is a protein called Hirudin variant-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	11	Total	C	N	O	S	0	0	0
			104	64	12	27	1			

- Molecule 4 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
4	H	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

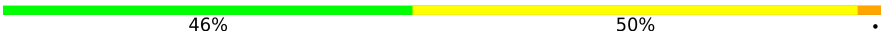
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	3	Total	O	0	0
			3	3		
6	H	69	Total	O	0	0
			69	69		

3 Residue-property plots [i](#)

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

Note EDS was not executed.

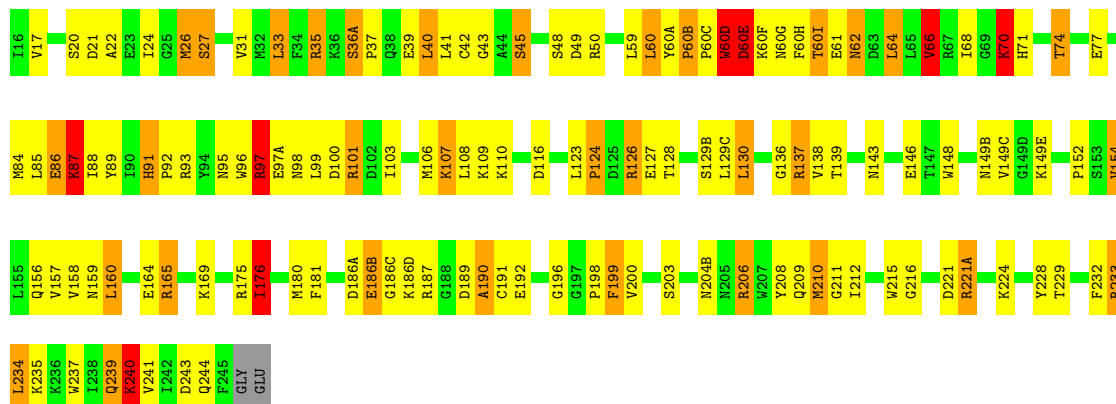
• Molecule 1: Thrombin light chain

Chain L: 

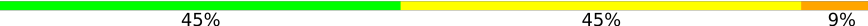


• Molecule 2: Thrombin heavy chain

Chain H: 



• Molecule 3: Hirudin variant-2

Chain J: 



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 2	Depositor
Cell constants a, b, c, α , β , γ	80.90Å 107.50Å 45.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2516	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: NAG, TYS, 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	1.50	0/234	1.97	7/310 (2.3%)
2	H	1.48	8/2119 (0.4%)	2.05	79/2871 (2.8%)
3	J	1.65	0/88	2.54	2/115 (1.7%)
All	All	1.49	8/2441 (0.3%)	2.06	88/3296 (2.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	21	ASP	CA-C	-6.89	1.43	1.52
2	H	60(D)	TRP	CA-C	-6.70	1.44	1.52
2	H	93	ARG	NE-CZ	6.51	1.40	1.33
2	H	123	LEU	C-N	-5.86	1.25	1.33
2	H	40	LEU	C-N	-5.76	1.25	1.33
2	H	160	LEU	CA-C	-5.57	1.46	1.52
2	H	60(E)	ASP	CA-C	-5.29	1.45	1.53
2	H	60(E)	ASP	N-CA	-5.11	1.38	1.46

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	55	ASP	CA-CB-CG	19.29	131.89	112.60
2	H	74	THR	N-CA-CB	-13.46	91.96	110.67
2	H	27	SER	CB-CA-C	-11.98	93.65	111.27
2	H	21	ASP	CA-CB-CG	-11.67	100.93	112.60
2	H	176	ILE	N-CA-CB	-10.29	92.27	112.24
2	H	36(A)	SER	CB-CA-C	-9.63	97.13	109.65
2	H	137	ARG	CD-NE-CZ	9.62	137.87	124.40
2	H	221	ASP	CA-CB-CG	9.58	122.18	112.60
2	H	221(A)	ARG	CA-CB-CG	-8.57	96.96	114.10
2	H	39	GLU	N-CA-CB	-8.29	96.88	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	CD-NE-CZ	7.88	135.44	124.40
2	H	64	LEU	CB-CA-C	-7.83	94.48	109.66
2	H	152	PRO	CA-C-N	-7.54	110.09	122.54
2	H	152	PRO	C-N-CA	-7.54	110.09	122.54
2	H	97	ARG	N-CA-C	7.49	120.50	111.82
2	H	45	SER	N-CA-CB	-7.38	97.91	111.13
2	H	243	ASP	CA-CB-CG	7.21	119.81	112.60
2	H	27	SER	O-C-N	7.12	127.00	121.23
2	H	124	PRO	N-CA-C	7.08	122.47	111.21
2	H	100	ASP	CA-CB-CG	6.79	119.39	112.60
2	H	186(B)	GLU	N-CA-C	-6.77	104.60	112.92
1	L	10	LYS	CB-CA-C	-6.70	99.19	110.44
2	H	60(E)	ASP	N-CA-C	6.67	120.72	112.58
2	H	240	LYS	CB-CA-C	6.60	122.07	110.85
1	L	14(I)	SER	N-CA-C	-6.51	105.15	113.23
2	H	87	LYS	N-CA-CB	-6.51	100.00	111.39
2	H	60(B)	PRO	N-CA-C	6.50	118.63	110.70
2	H	176	ILE	CB-CG1-CD1	-6.46	100.23	113.80
2	H	129(B)	SER	CB-CA-C	-6.42	99.93	110.85
2	H	124	PRO	CB-CA-C	-6.39	103.05	111.23
2	H	206	ARG	CB-CA-C	-6.29	97.86	109.37
2	H	70	LYS	N-CA-C	6.28	119.81	110.52
2	H	95	ASN	CB-CA-C	-6.27	100.74	111.41
2	H	221(A)	ARG	N-CA-C	6.18	118.76	110.35
1	L	13	GLU	N-CA-CB	-6.15	100.79	110.69
2	H	241	VAL	N-CA-C	-6.12	104.78	110.53
2	H	154	VAL	N-CA-CB	-6.10	99.50	112.00
2	H	126	ARG	CB-CA-C	-6.09	100.63	110.74
2	H	232	PHE	CA-CB-CG	-6.07	107.73	113.80
2	H	143	ASN	CA-CB-CG	6.06	118.66	112.60
2	H	74	THR	N-CA-C	6.05	121.71	113.97
2	H	143	ASN	CB-CA-C	-6.04	98.44	109.54
2	H	49	ASP	N-CA-C	6.01	120.45	113.18
2	H	190	ALA	N-CA-C	-5.96	101.12	110.36
2	H	186(A)	ASP	N-CA-C	5.95	120.39	113.20
2	H	175	ARG	NE-CZ-NH2	5.94	124.54	119.20
2	H	129(C)	LEU	N-CA-C	5.91	120.65	112.90
2	H	21	ASP	CB-CA-C	-5.82	99.70	109.65
2	H	160	LEU	O-C-N	5.81	126.00	121.88
2	H	62	ASN	N-CA-C	5.80	120.09	113.19
1	L	14	ASP	N-CA-CB	5.76	119.21	110.45
2	H	240	LYS	N-CA-C	5.74	117.62	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	148	TRP	N-CA-CB	-5.71	100.89	110.99
2	H	60	LEU	N-CA-CB	-5.70	102.00	110.90
2	H	66	VAL	N-CA-CB	-5.67	103.59	111.41
2	H	216	GLY	CA-C-O	-5.66	116.11	121.60
2	H	199	PHE	N-CA-C	-5.65	97.99	107.99
1	L	14(H)	GLU	CB-CG-CD	5.63	122.18	112.60
2	H	110	LYS	CA-C-N	5.62	125.55	119.76
2	H	110	LYS	C-N-CA	5.62	125.55	119.76
1	L	14(C)	GLU	N-CA-C	5.58	119.35	112.54
2	H	181	PHE	N-CA-CB	5.54	121.33	111.69
2	H	192	GLU	N-CA-CB	5.53	118.17	110.04
2	H	107	LYS	CB-CA-C	5.41	119.06	110.19
2	H	239	GLN	N-CA-C	5.40	117.92	111.71
2	H	116	ASP	CA-CB-CG	5.38	117.98	112.60
3	J	56	PHE	N-CA-C	5.38	117.51	108.96
2	H	149(E)	LYS	N-CA-C	-5.36	101.91	109.96
2	H	101	ARG	CA-CB-CG	-5.33	103.44	114.10
2	H	26	MET	CA-C-N	5.33	128.71	122.85
2	H	26	MET	C-N-CA	5.33	128.71	122.85
1	L	14	ASP	CA-CB-CG	5.32	117.92	112.60
2	H	39	GLU	CA-CB-CG	5.28	124.67	114.10
2	H	221(A)	ARG	CG-CD-NE	-5.28	100.38	112.00
2	H	91	HIS	N-CA-C	-5.27	102.95	109.64
2	H	40	LEU	CB-CA-C	-5.26	101.66	110.29
2	H	149(B)	ASN	CA-CB-CG	5.26	117.86	112.60
2	H	60(B)	PRO	N-CA-CB	5.23	108.15	103.08
2	H	64	LEU	CA-C-N	5.22	130.91	122.29
2	H	64	LEU	C-N-CA	5.22	130.91	122.29
2	H	237	TRP	N-CA-C	-5.21	105.49	111.07
2	H	241	VAL	N-CA-CB	-5.18	103.94	110.57
2	H	210	MET	N-CA-C	5.17	119.67	112.90
2	H	137	ARG	CG-CD-NE	5.08	123.17	112.00
2	H	60	LEU	CB-CA-C	-5.07	103.21	110.62
2	H	239	GLN	N-CA-CB	-5.04	102.47	110.22
2	H	60(D)	TRP	CB-CA-C	-5.03	102.00	110.64
2	H	136	GLY	N-CA-C	-5.02	104.29	111.42

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	232	0	231	11	0
2	H	2064	0	2011	86	0
3	J	104	0	81	5	0
4	H	30	0	30	3	0
5	H	14	0	13	0	0
6	H	69	0	0	6	0
6	L	3	0	0	0	0
All	All	2516	0	2366	94	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 20.

All (94) 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:14(F):LEU:HD21	2:H:159:ASN:HD22	1.20	1.01
1:L:14(F):LEU:CD2	2:H:159:ASN:HD22	1.91	0.84
2:H:233:ARG:HH11	2:H:233:ARG:HG2	1.42	0.83
2:H:60(I):THR:HG22	2:H:62:ASN:H	1.43	0.83
2:H:50:ARG:HH21	2:H:107:LYS:CE	1.99	0.76
2:H:186(D):LYS:NZ	2:H:186(D):LYS:HB3	2.02	0.74
1:L:14(F):LEU:HD21	2:H:159:ASN:ND2	1.99	0.73
4:H:1:OG6:HD22	6:H:264:HOH:O	1.87	0.73
2:H:146:GLU:OE1	2:H:221(A):ARG:HD2	1.90	0.71
2:H:50:ARG:HE	2:H:107:LYS:HE3	1.55	0.70
2:H:70:LYS:HB3	2:H:77:GLU:OE1	1.91	0.69
2:H:165:ARG:NH2	2:H:180:MET:O	2.26	0.68
2:H:130:LEU:HD12	2:H:210:MET:HE2	1.77	0.67
2:H:87:LYS:HG2	2:H:89:TYR:CZ	2.30	0.66
2:H:31:VAL:HG22	2:H:68:ILE:HG12	1.77	0.66
2:H:130:LEU:HD12	2:H:210:MET:CE	2.25	0.66
3:J:63:TYO	3:J:65:GLN:N	2.27	0.66
1:L:14(A):LYS:NZ	2:H:26:MET:HE1	2.14	0.62
2:H:50:ARG:HH21	2:H:107:LYS:HE2	1.62	0.62
2:H:189:ASP:OD2	6:H:292:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:ARG:HH11	2:H:233:ARG:CG	2.13	0.60
2:H:187:ARG:NH2	6:H:316:HOH:O	2.31	0.59
2:H:50:ARG:HE	2:H:107:LYS:CE	2.16	0.58
1:L:1:CYS:O	2:H:206:ARG:NH1	2.35	0.58
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.86	0.58
2:H:186(D):LYS:HB3	2:H:186(D):LYS:HZ2	1.68	0.57
1:L:14(A):LYS:HE3	2:H:26:MET:HE1	1.86	0.57
2:H:157:VAL:HG12	2:H:158:VAL:N	2.21	0.55
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.36	0.55
2:H:186(B):GLU:O	2:H:186(D):LYS:HG3	2.07	0.54
2:H:71:HIS:ND1	6:H:310:HOH:O	2.28	0.54
1:L:14(K):ILE:OXT	1:L:14(K):ILE:HG22	2.07	0.54
1:L:14(A):LYS:HE3	2:H:26:MET:CE	2.37	0.54
2:H:159:ASN:O	2:H:160:LEU:HD23	2.08	0.53
2:H:235:LYS:O	2:H:239:GLN:HG2	2.09	0.53
2:H:96:TRP:CZ2	2:H:97:ARG:NH1	2.78	0.52
1:L:14(A):LYS:CE	2:H:26:MET:HE1	2.39	0.52
2:H:59:LEU:HD13	2:H:88:ILE:HG21	1.93	0.51
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.27	0.50
2:H:86:GLU:HB3	2:H:107:LYS:O	2.12	0.50
2:H:22:ALA:HB2	2:H:157:VAL:HG23	1.94	0.49
2:H:45:SER:HB2	6:H:265:HOH:O	2.11	0.49
2:H:233:ARG:HG2	2:H:233:ARG:NH1	2.20	0.49
3:J:63:TYS:C	3:J:65:GLN:N	2.75	0.49
2:H:33:LEU:HB2	2:H:42:CYS:O	2.12	0.49
2:H:103:ILE:HG21	2:H:234:LEU:HD22	1.93	0.49
2:H:149(C):VAL:O	2:H:149(C):VAL:HG12	2.08	0.48
2:H:50:ARG:NH2	2:H:107:LYS:HE2	2.28	0.48
2:H:211:GLY:HA2	2:H:229:THR:O	2.14	0.48
2:H:35:ARG:CZ	2:H:37:PRO:HD2	2.44	0.47
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.96	0.47
2:H:43:GLY:O	2:H:196:GLY:HA3	2.15	0.47
2:H:233:ARG:CG	2:H:233:ARG:NH1	2.74	0.47
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.97	0.47
2:H:124:PRO:HD3	2:H:209:GLN:O	2.15	0.47
2:H:189:ASP:OD1	2:H:190:ALA:N	2.48	0.47
2:H:27:SER:HB2	6:H:285:HOH:O	2.14	0.46
2:H:26:MET:SD	2:H:157:VAL:HG21	2.56	0.46
2:H:35:ARG:NH1	2:H:36(A):SER:O	2.49	0.46
2:H:66:VAL:O	2:H:66:VAL:HG12	2.16	0.46
2:H:138:VAL:HG22	2:H:199:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(A):LYS:HG3	1:L:14(B):THR:HG23	1.97	0.46
2:H:176:ILE:HG22	2:H:176:ILE:O	2.15	0.46
2:H:240:LYS:HG2	2:H:244:GLN:HE22	1.80	0.46
2:H:98:ASN:O	2:H:99:LEU:HB2	2.15	0.46
2:H:186(D):LYS:HB3	2:H:186(D):LYS:HZ3	1.77	0.45
2:H:17:VAL:HG23	2:H:191:CYS:HB2	1.99	0.45
2:H:215:TRP:HA	4:H:1:OG6:HG21	1.99	0.44
2:H:137:ARG:HD3	2:H:157:VAL:HG13	2.00	0.44
3:J:58:GLU:H	3:J:58:GLU:CD	2.25	0.44
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.29	0.44
1:L:3:LEU:HA	1:L:3:LEU:HD23	1.58	0.43
2:H:91:HIS:HA	2:H:92:PRO:HD2	1.86	0.43
2:H:60(I):THR:HG22	2:H:61:GLU:N	2.32	0.43
2:H:99:LEU:HD12	2:H:215:TRP:HB3	1.99	0.43
2:H:85:LEU:HD22	2:H:106:MET:HB3	2.01	0.43
2:H:60(D):TRP:O	2:H:60(E):ASP:HB2	2.17	0.42
2:H:212:ILE:O	2:H:228:TYR:HA	2.19	0.42
2:H:101:ARG:HG2	2:H:234:LEU:HD21	2.01	0.42
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.27	0.42
2:H:50:ARG:HH21	2:H:107:LYS:NZ	2.17	0.42
2:H:60(I):THR:HG22	2:H:62:ASN:N	2.23	0.42
2:H:85:LEU:HD23	2:H:108:LEU:HD23	2.00	0.42
2:H:88:ILE:HG12	2:H:106:MET:HG2	2.01	0.41
2:H:84:MET:HE2	3:J:63:TYR:O	2.20	0.41
2:H:240:LYS:HG2	2:H:244:GLN:NE2	2.34	0.41
2:H:206:ARG:HB2	2:H:208:TYR:CE1	2.56	0.41
2:H:24:ILE:HD12	2:H:24:ILE:HG23	1.70	0.41
2:H:60(I):THR:CG2	2:H:61:GLU:N	2.83	0.41
2:H:139:THR:HA	2:H:156:GLN:O	2.21	0.41
2:H:33:LEU:HD12	2:H:42:CYS:HB2	2.03	0.41
2:H:130:LEU:HD12	2:H:210:MET:HE3	1.98	0.41
3:J:65:GLN:HA	3:J:65:GLN:OE1	2.21	0.41
2:H:215:TRP:HA	4:H:1:OG6:CG2	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	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
2	H	255/259 (98%)	243 (95%)	11 (4%)	1 (0%)	30	49
3	J	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	289/298 (97%)	274 (95%)	14 (5%)	1 (0%)	36	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	186(C)	GLY

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	26/26 (100%)	22 (85%)	4 (15%)	2	5
2	H	220/225 (98%)	182 (83%)	38 (17%)	2	4
3	J	10/10 (100%)	9 (90%)	1 (10%)	7	15
All	All	256/261 (98%)	213 (83%)	43 (17%)	2	4

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	1(A)	ASP

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Mol	Chain	Res	Type
1	L	1	CYS
1	L	6	LEU
2	H	20	SER
2	H	33	LEU
2	H	35	ARG
2	H	40	LEU
2	H	41	LEU
2	H	48	SER
2	H	60	LEU
2	H	60(A)	TYR
2	H	60(B)	PRO
2	H	60(C)	PRO
2	H	60(D)	TRP
2	H	60(E)	ASP
2	H	60(F)	LYS
2	H	60(G)	ASN
2	H	60(H)	PHE
2	H	60(I)	THR
2	H	64	LEU
2	H	66	VAL
2	H	70	LYS
2	H	74	THR
2	H	86	GLU
2	H	87	LYS
2	H	97	ARG
2	H	97(A)	GLU
2	H	109	LYS
2	H	126	ARG
2	H	127	GLU
2	H	128	THR
2	H	130	LEU
2	H	154	VAL
2	H	164	GLU
2	H	165	ARG
2	H	169	LYS
2	H	176	ILE
2	H	224	LYS
2	H	233	ARG
2	H	234	LEU
2	H	240	LYS
3	J	62	GLU

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

sidechains are listed below:

Mol	Chain	Res	Type
2	H	143	ASN
2	H	149(B)	ASN
2	H	159	ASN
2	H	204(B)	ASN
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 ⓘ

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	J	63	3	15,16,17	1.80	2 (13%)	15,22,24	1.13	0

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	J	63	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	63	TYS	OH-S	-4.58	1.49	1.58
3	J	63	TYS	OH-CZ	-3.94	1.36	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	63	TYS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	OG6	H	1	2	30,31,32	0.85	1 (3%)	37,41,42	1.28	7 (18%)
5	NAG	H	250	2	14,14,15	1.05	1 (7%)	17,19,21	1.94	7 (41%)

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	OG6	H	1	2	-	4/31/41/43	0/2/2/2
5	NAG	H	250	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	250	NAG	C1-C2	-2.53	1.48	1.52
4	H	1	0G6	CA1-N1	-2.25	1.42	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	250	NAG	C2-N2-C7	4.19	128.52	122.90
4	H	1	0G6	CD-N1-CA1	3.18	117.00	112.01
5	H	250	NAG	C6-C5-C4	-3.06	105.51	113.02
5	H	250	NAG	C3-C4-C5	-2.80	105.15	110.23
4	H	1	0G6	CB2-CA2-N2	2.63	113.71	110.30
4	H	1	0G6	CG2-CB2-CA2	-2.54	109.10	113.94
4	H	1	0G6	C2-CA2-N2	-2.51	106.34	110.90
5	H	250	NAG	O7-C7-N2	2.45	126.31	121.98
5	H	250	NAG	O5-C1-C2	-2.40	107.58	111.29
5	H	250	NAG	C8-C7-N2	-2.19	112.48	116.12
5	H	250	NAG	O4-C4-C3	2.19	115.55	110.38
4	H	1	0G6	NE-CZ1-NH2	-2.17	116.95	120.67
4	H	1	0G6	CB-CA-N	-2.14	103.19	111.40
4	H	1	0G6	CB1-CA1-C1	-2.02	106.92	111.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	0G6	NE-CD3-CG2-CB2
5	H	250	NAG	O5-C5-C6-O6
5	H	250	NAG	C4-C5-C6-O6
4	H	1	0G6	CA2-CB2-CG2-CD3
4	H	1	0G6	N2-CA2-CB2-CG2
4	H	1	0G6	O2-C2-CA2-CB2

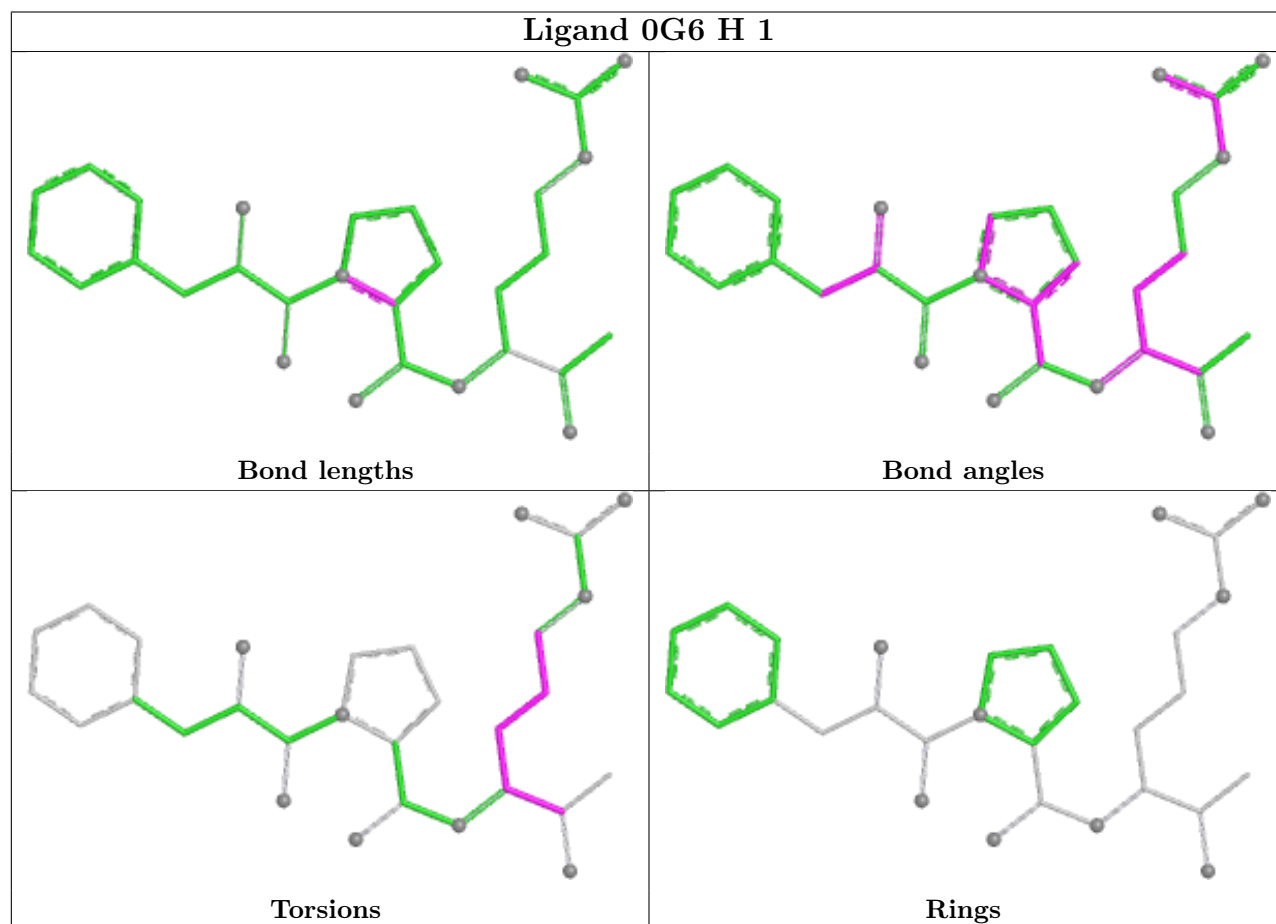
There are no ring outliers.

1 monomer is involved in 3 short contacts:

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