Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:38 PM EDT

PDB ID	:	1HAI
Title	:	THE ISOMORPHOUS STRUCTURES OF PRETHROMBIN2, HIRUGEN- AND PPACK-THROMBIN: CHANGES ACCOMPANYING ACTIVATION AND EXOSITE BINDING TO THROMBIN
Authors	:	Tulinsky, A.; Vijayalakshmi, J.
Deposited on	:	1994-06-27
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

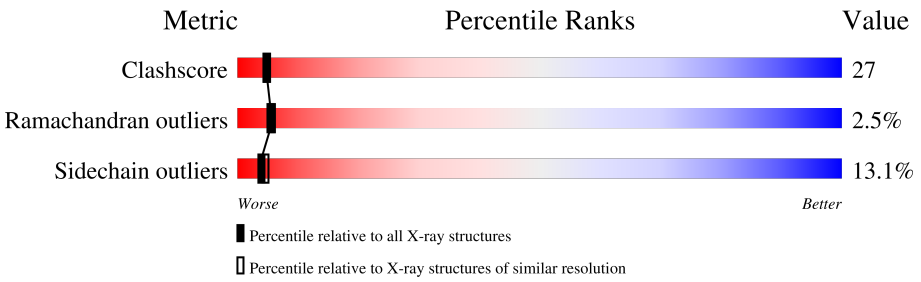
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	36% 28% 22% 14%
2	H	259	48% 31% 14% . .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2590 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.

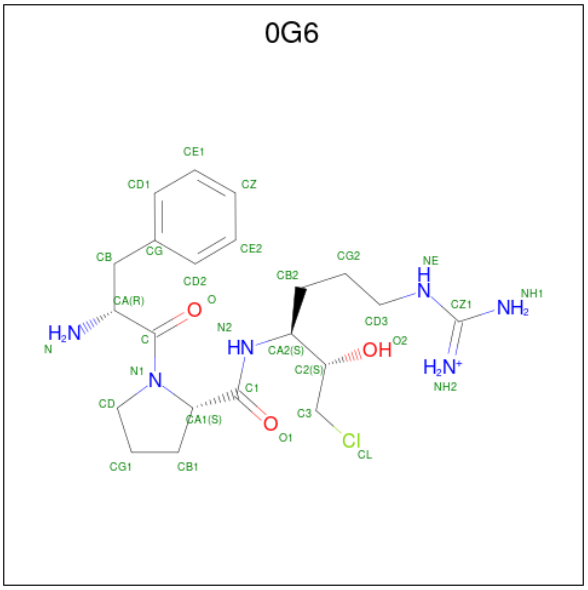
- Molecule 1 is a protein called ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	36	287	177	48	61	1	0	0	0

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

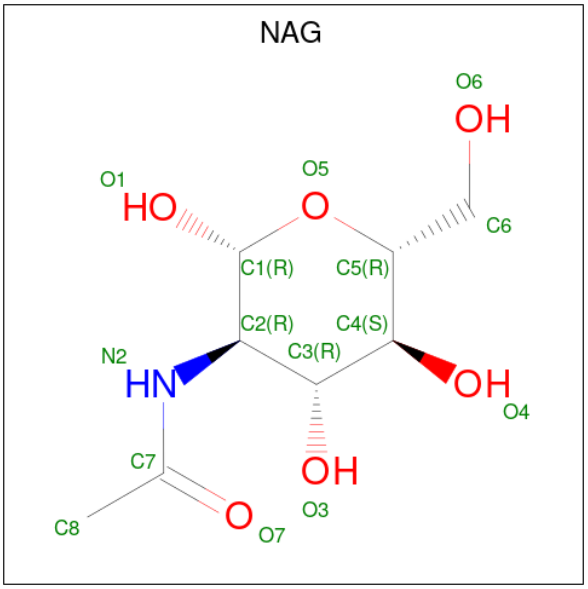
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	253	2065	1316	368	367	14	0	2	0

- Molecule 3 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	21	21	21	0	0
			Total	O		
5	H	173	173	173	0	0

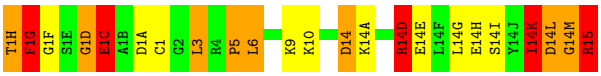
3 Residue-property plots (i)

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

Note EDS was not executed.

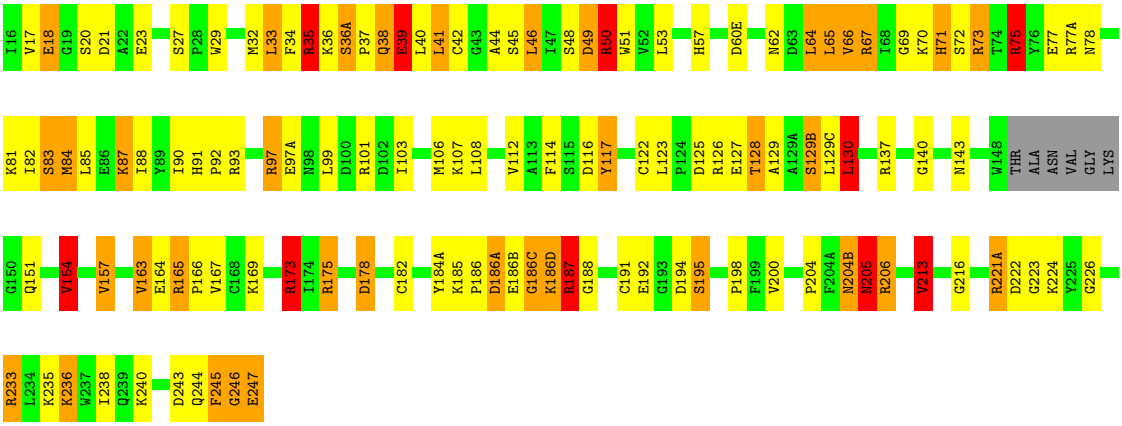
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 36% 28% 22% 14%



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 48% 31% 14%



4 Data and refinement statistics (i)

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	70.97Å 72.50Å 72.57Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.139 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2590	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	1.31	1/290 (0.3%)	2.73	18/384 (4.7%)
2	H	1.19	0/2129	2.38	91/2875 (3.2%)
All	All	1.20	1/2419 (0.0%)	2.43	109/3259 (3.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
2	H	0	5
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14(K)	ILE	C-N	10.53	1.58	1.34

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	173	ARG	NE-CZ-NH2	-25.70	107.45	120.30
2	H	173	ARG	NE-CZ-NH1	21.64	131.12	120.30
1	L	14(M)	GLY	O-C-N	19.95	154.62	122.70
2	H	221(A)	ARG	NE-CZ-NH2	18.36	129.48	120.30
2	H	97	ARG	NE-CZ-NH1	18.22	129.41	120.30
2	H	126	ARG	NE-CZ-NH1	16.87	128.73	120.30
2	H	97	ARG	NE-CZ-NH2	-16.85	111.88	120.30
1	L	15	ARG	CD-NE-CZ	15.37	145.11	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	233	ARG	NE-CZ-NH1	15.26	127.93	120.30
2	H	101	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	L	14(M)	GLY	CA-C-N	-14.89	84.44	117.20
1	L	15	ARG	NE-CZ-NH1	14.35	127.47	120.30
2	H	50[A]	ARG	NE-CZ-NH1	-14.24	113.18	120.30
2	H	50[B]	ARG	NE-CZ-NH1	-14.24	113.18	120.30
2	H	233	ARG	NE-CZ-NH2	-13.44	113.58	120.30
2	H	73	ARG	NE-CZ-NH1	12.20	126.40	120.30
2	H	67	ARG	NE-CZ-NH1	11.29	125.95	120.30
2	H	117	TYR	CB-CG-CD2	-11.18	114.29	121.00
2	H	35	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	L	15	ARG	NH1-CZ-NH2	-10.99	107.31	119.40
2	H	101	ARG	NE-CZ-NH1	10.92	125.76	120.30
2	H	221(A)	ARG	NE-CZ-NH1	-10.61	115.00	120.30
2	H	75	ARG	NE-CZ-NH2	10.40	125.50	120.30
2	H	49	ASP	CB-CG-OD2	10.35	127.61	118.30
2	H	186(A)	ASP	CB-CG-OD1	-10.01	109.29	118.30
1	L	15	ARG	NE-CZ-NH2	9.80	125.20	120.30
2	H	50[A]	ARG	CD-NE-CZ	-9.73	109.98	123.60
2	H	50[B]	ARG	CD-NE-CZ	-9.73	109.98	123.60
2	H	126	ARG	NH1-CZ-NH2	-9.51	108.94	119.40
2	H	165[A]	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	H	165[B]	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	H	178	ASP	CB-CG-OD1	9.29	126.67	118.30
2	H	117	TYR	CB-CG-CD1	8.73	126.24	121.00
2	H	35	ARG	NE-CZ-NH1	8.53	124.56	120.30
2	H	39	GLU	OE1-CD-OE2	8.51	133.51	123.30
2	H	116	ASP	CB-CG-OD1	8.40	125.86	118.30
1	L	1(C)	GLU	CG-CD-OE2	8.28	134.86	118.30
2	H	175	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	H	206	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	L	1(A)	ASP	CB-CG-OD1	-7.75	111.33	118.30
2	H	75	ARG	NH1-CZ-NH2	-7.72	110.91	119.40
2	H	164	GLU	CG-CD-OE1	7.66	133.62	118.30
2	H	243	ASP	CB-CG-OD1	7.47	125.02	118.30
2	H	187	ARG	NE-CZ-NH2	7.43	124.01	120.30
2	H	245	PHE	C-N-CA	7.39	137.81	122.30
2	H	35	ARG	CD-NE-CZ	-7.38	113.26	123.60
2	H	206	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	H	175	ARG	NE-CZ-NH2	7.15	123.88	120.30
2	H	186(A)	ASP	CB-CG-OD2	7.06	124.66	118.30
2	H	205	ASN	OD1-CG-ND2	7.02	138.05	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	50[A]	ARG	NH1-CZ-NH2	6.97	127.07	119.40
2	H	50[B]	ARG	NH1-CZ-NH2	6.97	127.07	119.40
2	H	84	MET	CA-CB-CG	-6.80	101.74	113.30
2	H	243	ASP	CB-CA-C	6.71	123.82	110.40
1	L	1(A)	ASP	CB-CG-OD2	6.50	124.15	118.30
2	H	77	GLU	OE1-CD-OE2	-6.35	115.67	123.30
2	H	75	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	H	50[A]	ARG	CB-CA-C	-6.25	97.90	110.40
2	H	50[B]	ARG	CB-CA-C	-6.25	97.90	110.40
2	H	21	ASP	CB-CG-OD1	6.23	123.91	118.30
2	H	75	ARG	CB-CG-CD	6.17	127.66	111.60
2	H	243	ASP	CB-CG-OD2	-6.17	112.75	118.30
2	H	66	VAL	CG1-CB-CG2	6.14	120.72	110.90
2	H	221(A)	ARG	CD-NE-CZ	-6.13	115.02	123.60
2	H	130	LEU	C-N-CA	6.11	136.99	121.70
2	H	178	ASP	CB-CG-OD2	-6.07	112.84	118.30
2	H	213	VAL	CA-C-O	6.07	132.84	120.10
2	H	27	SER	CB-CA-C	-6.05	98.60	110.10
2	H	20	SER	O-C-N	6.05	132.37	122.70
2	H	226	GLY	O-C-N	6.03	132.35	122.70
2	H	73	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	L	3	LEU	O-C-N	6.01	132.32	122.70
1	L	14(D)	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	H	71	HIS	CA-C-O	6.00	132.70	120.10
2	H	18	GLU	CG-CD-OE1	5.90	130.10	118.30
2	H	93	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	H	38	GLN	CB-CA-C	-5.84	98.71	110.40
2	H	60(E)	ASP	CB-CG-OD1	-5.82	113.06	118.30
2	H	125	ASP	CB-CG-OD1	5.78	123.50	118.30
2	H	128	THR	O-C-N	5.71	131.83	122.70
2	H	154	VAL	CA-CB-CG1	5.68	119.42	110.90
2	H	27	SER	N-CA-CB	5.61	118.91	110.50
2	H	67	ARG	NE-CZ-NH2	-5.53	117.54	120.30
2	H	154	VAL	N-CA-CB	-5.48	99.45	111.50
2	H	46	LEU	N-CA-CB	-5.47	99.45	110.40
2	H	129(C)	LEU	O-C-N	5.44	131.40	122.70
2	H	33	LEU	CB-CA-C	5.43	120.53	110.20
2	H	66	VAL	CB-CA-C	5.42	121.70	111.40
1	L	1(D)	GLY	N-CA-C	5.42	126.64	113.10
2	H	213	VAL	CA-CB-CG1	5.37	118.96	110.90
2	H	143	ASN	O-C-N	5.36	131.27	122.70
2	H	164	GLU	CG-CD-OE2	-5.33	107.64	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	192	GLU	OE1-CD-OE2	-5.31	116.93	123.30
2	H	62	ASN	CB-CG-OD1	-5.31	110.98	121.60
2	H	140	GLY	C-N-CA	5.26	134.86	121.70
2	H	83	SER	CA-C-N	-5.25	105.64	117.20
1	L	14	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	L	1(C)	GLU	OE1-CD-OE2	-5.22	117.04	123.30
2	H	163	VAL	CA-CB-CG2	5.20	118.69	110.90
2	H	157	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	L	14(G)	LEU	CB-CG-CD1	5.15	119.76	111.00
2	H	178	ASP	O-C-N	5.14	130.92	122.70
2	H	167	VAL	N-CA-CB	-5.13	100.22	111.50
1	L	1(C)	GLU	CG-CD-OE1	-5.12	108.05	118.30
1	L	1(A)	ASP	CA-CB-CG	-5.12	102.14	113.40
2	H	116	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	H	247	GLU	CA-C-O	-5.08	109.42	120.10
2	H	90	ILE	CB-CG1-CD1	5.05	128.03	113.90
1	L	14(K)	ILE	CA-C-N	-5.04	106.11	117.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	195	SER	Mainchain
2	H	35	ARG	Sidechain
2	H	44	ALA	Mainchain
2	H	50[A]	ARG	Sidechain
2	H	50[B]	ARG	Sidechain
1	L	15	ARG	Sidechain
1	L	5	PRO	Mainchain

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	L	287	0	278	36	0
2	H	2065	0	2036	102	0
3	H	30	0	31	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	14	0	13	0	0
5	H	173	0	0	12	1
5	L	21	0	0	4	0
All	All	2590	0	2358	128	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 27.

All (128) 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:51:TRP:HE1	2:H:247:GLU:HA	0.98	1.13
1:L:14(D):ARG:HD3	1:L:14(E):GLU:H	1.10	1.11
1:L:1(D):GLY:HA3	5:H:458:HOH:O	1.49	1.09
2:H:247:GLU:HG2	2:H:247:GLU:O	1.54	1.08
1:L:14(D):ARG:HH11	1:L:14(E):GLU:HB2	1.17	1.03
2:H:51:TRP:NE1	2:H:247:GLU:HA	1.83	0.94
1:L:14(D):ARG:HD3	1:L:14(E):GLU:N	1.83	0.94
2:H:75:ARG:HH11	2:H:75:ARG:HG3	1.33	0.91
1:L:1(G):PHE:H	1:L:1(D):GLY:HA2	1.36	0.91
1:L:14(D):ARG:NH1	1:L:14(E):GLU:HB2	1.86	0.91
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.55	0.89
2:H:173:ARG:HG3	5:H:419:HOH:O	1.72	0.89
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.04	0.88
2:H:50[B]:ARG:NH1	2:H:108:LEU:O	2.06	0.88
1:L:14(D):ARG:CD	1:L:14(E):GLU:H	1.88	0.87
2:H:186(A):ASP:N	2:H:186(A):ASP:OD1	2.07	0.85
1:L:14(D):ARG:HH11	1:L:14(E):GLU:CB	1.89	0.84
1:L:1(F):GLY:HA2	2:H:235:LYS:NZ	1.94	0.82
1:L:14(D):ARG:HG2	5:L:590:HOH:O	1.80	0.82
2:H:50[B]:ARG:HG3	2:H:50[B]:ARG:HH11	1.44	0.81
2:H:50[B]:ARG:NH1	2:H:50[B]:ARG:HG3	1.96	0.81
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.60	0.81
2:H:35:ARG:O	2:H:38:GLN:HA	1.82	0.78
2:H:236:LYS:HD3	5:H:437:HOH:O	1.84	0.77
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	1.67	0.77
2:H:81:LYS:HE3	2:H:112:VAL:HG23	1.65	0.76
1:L:14(D):ARG:CG	5:L:590:HOH:O	2.33	0.76
2:H:97:ARG:NH1	5:H:589:HOH:O	2.16	0.76
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.21	0.76
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ2	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:TRP:HE1	2:H:247:GLU:CA	1.89	0.75
2:H:50[B]:ARG:NH1	2:H:50[B]:ARG:CG	2.47	0.73
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.22	0.70
2:H:247:GLU:O	2:H:247:GLU:CG	2.34	0.67
2:H:75:ARG:HG3	2:H:75:ARG:NH1	1.97	0.67
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.94	0.67
1:L:1(G):PHE:HA	2:H:123:LEU:HD12	1.77	0.67
2:H:50[A]:ARG:HD2	2:H:247:GLU:OXT	1.96	0.66
2:H:224:LYS:HE2	5:H:566:HOH:O	1.95	0.66
2:H:195:SER:HA	2:H:213:VAL:HG22	1.80	0.64
2:H:50[A]:ARG:CD	2:H:247:GLU:OXT	2.47	0.63
2:H:67:ARG:HG2	2:H:82:ILE:HG12	1.81	0.62
2:H:50[A]:ARG:HD2	2:H:247:GLU:C	2.19	0.62
1:L:14(D):ARG:CD	1:L:14(E):GLU:N	2.55	0.62
2:H:73:ARG:CZ	2:H:151:GLN:HB3	2.29	0.62
2:H:185:LYS:O	2:H:186(B):GLU:HB2	2.01	0.61
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.67	0.60
1:L:1(H):THR:O	1:L:1(H):THR:HG22	2.02	0.60
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.06	0.59
2:H:32:MET:CG	2:H:40:LEU:HD13	2.31	0.59
2:H:99:LEU:HD11	3:H:1:0G6:HB21	1.84	0.59
2:H:165[B]:ARG:HH21	2:H:169:LYS:HE3	1.69	0.58
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.38	0.57
2:H:17:VAL:O	2:H:188:GLY:HA2	2.05	0.57
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	2.04	0.56
2:H:85:LEU:CD1	2:H:106:MET:CE	2.84	0.56
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.88	0.56
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.60	0.55
2:H:85:LEU:HD11	2:H:106:MET:HE1	1.88	0.54
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.34	0.54
2:H:36(A):SER:HA	2:H:37:PRO:C	2.29	0.54
2:H:35:ARG:HB3	2:H:39:GLU:HG3	1.88	0.53
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.08	0.53
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.70	0.53
2:H:137:ARG:HG3	2:H:157:VAL:HG23	1.91	0.52
2:H:129:ALA:O	2:H:130:LEU:HB2	2.10	0.52
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.45	0.51
2:H:97(A):GLU:CB	5:H:421:HOH:O	2.57	0.51
2:H:240:LYS:HG2	2:H:244:GLN:NE2	2.26	0.51
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.92	0.51
1:L:1(D):GLY:CA	5:H:458:HOH:O	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97(A):GLU:OE1	5:H:421:HOH:O	2.20	0.50
2:H:41:LEU:CD2	2:H:64:LEU:CD2	2.90	0.49
1:L:14(D):ARG:HD2	1:L:14(D):ARG:H	1.77	0.49
3:H:1:0G6:CD1	3:H:1:0G6:HD3	2.41	0.49
2:H:221(A):ARG:HG3	5:H:417:HOH:O	2.10	0.49
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.10	0.49
1:L:1(G):PHE:CA	2:H:123:LEU:HD12	2.41	0.49
2:H:186(A):ASP:O	2:H:186(C):GLY:N	2.46	0.49
2:H:97(A):GLU:HB2	5:H:421:HOH:O	2.14	0.48
1:L:14(D):ARG:CG	1:L:14(E):GLU:N	2.77	0.48
2:H:65:LEU:CD1	2:H:84:MET:HG2	2.43	0.48
1:L:1(G):PHE:HA	2:H:123:LEU:CD1	2.42	0.47
2:H:35:ARG:HD3	2:H:39:GLU:OE2	2.15	0.47
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.96	0.46
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.68	0.46
2:H:87:LYS:HD3	2:H:88:ILE:N	2.31	0.46
1:L:1(C):GLU:OE1	2:H:48:SER:HA	2.17	0.45
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.64	0.45
2:H:29:TRP:O	2:H:45:SER:HA	2.17	0.45
1:L:15:ARG:HB2	2:H:204:PRO:O	2.17	0.44
2:H:221(A):ARG:HH11	2:H:221(A):ARG:HD2	1.38	0.44
2:H:65:LEU:HD12	2:H:84:MET:HG2	2.00	0.44
2:H:85:LEU:HD13	2:H:106:MET:CE	2.33	0.44
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.85	0.44
1:L:14(D):ARG:HG3	5:L:590:HOH:O	2.12	0.44
2:H:57:HIS:CE1	2:H:195:SER:OG	2.70	0.44
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.78	0.44
1:L:1(G):PHE:N	1:L:1(D):GLY:HA2	2.18	0.43
2:H:127:GLU:O	2:H:129(B):SER:OG	2.35	0.43
1:L:6:LEU:HD12	1:L:6:LEU:HA	1.85	0.43
2:H:178:ASP:O	2:H:233:ARG:HD2	2.18	0.43
2:H:75:ARG:HB3	5:H:576:HOH:O	2.17	0.43
2:H:72:SER:OG	2:H:75:ARG:HG2	2.18	0.43
1:L:14(D):ARG:HD2	1:L:14(D):ARG:N	2.33	0.43
2:H:49:ASP:O	2:H:112:VAL:HG12	2.18	0.43
2:H:191:CYS:O	2:H:194:ASP:HB2	2.18	0.43
2:H:245:PHE:HE2	5:H:569:HOH:O	2.01	0.43
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.35	0.42
2:H:236:LYS:O	2:H:236:LYS:HG2	2.15	0.42
1:L:1:CYS:O	2:H:206:ARG:HD3	2.20	0.42
2:H:107:LYS:NZ	2:H:246:GLY:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:216:GLY:O	3:H:1:0G6:N	2.53	0.42
1:L:1:CYS:C	2:H:122:CYS:SG	2.99	0.41
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.19	0.41
2:H:165[B]:ARG:NH2	2:H:169:LYS:CE	2.83	0.41
2:H:186:PRO:HG3	2:H:223:GLY:H	1.85	0.41
2:H:103:ILE:HD11	2:H:238:ILE:HD11	2.02	0.41
2:H:73:ARG:NE	2:H:151:GLN:HB3	2.36	0.41
1:L:3:LEU:O	1:L:9:LYS:NZ	2.54	0.41
2:H:184(A):TYR:CZ	2:H:186(D):LYS:HD2	2.55	0.41
2:H:53:LEU:HD11	2:H:103:ILE:HD11	2.02	0.41
2:H:175:ARG:HH11	2:H:175:ARG:HD2	1.59	0.41
2:H:42:CYS:HB3	2:H:195:SER:O	2.21	0.41
2:H:69:GLY:HA2	2:H:117:TYR:O	2.21	0.41
1:L:10:LYS:NZ	5:L:524:HOH:O	2.54	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)
5:H:415:HOH:O	5:H:415:HOH:O[2_555]	2.19	0.01

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	34/36 (94%)	24 (71%)	6 (18%)	4 (12%)	0 0
2	H	251/259 (97%)	236 (94%)	12 (5%)	3 (1%)	13 19
All	All	285/295 (97%)	260 (91%)	18 (6%)	7 (2%)	5 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(G)	PHE
1	L	1(C)	GLU
1	L	14(M)	GLY
2	H	246	GLY
1	L	14(L)	ASP
2	H	186(D)	LYS
2	H	186(C)	GLY

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	31/31 (100%)	23 (74%)	8 (26%)	0 0
2	H	223/225 (99%)	197 (88%)	26 (12%)	5 7
All	All	254/256 (99%)	220 (87%)	34 (13%)	4 4

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(H)	THR
1	L	1(G)	PHE
1	L	1(C)	GLU
1	L	6	LEU
1	L	14	ASP
1	L	14(D)	ARG
1	L	14(K)	ILE
1	L	15	ARG
2	H	33	LEU
2	H	36	LYS
2	H	36(A)	SER
2	H	39	GLU
2	H	41	LEU
2	H	46	LEU
2	H	50[A]	ARG
2	H	50[B]	ARG
2	H	64	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	65	LEU
2	H	66	VAL
2	H	75	ARG
2	H	83	SER
2	H	87	LYS
2	H	128	THR
2	H	129(B)	SER
2	H	130	LEU
2	H	154	VAL
2	H	163	VAL
2	H	173	ARG
2	H	182	CYS
2	H	187	ARG
2	H	204(B)	ASN
2	H	205	ASN
2	H	213	VAL
2	H	236	LYS

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	78	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	0G6	H	1	2	30,31,32	0.89	1 (3%)	37,41,42	1.61	8 (21%)
4	NAG	H	400	2	14,14,15	1.12	1 (7%)	17,19,21	2.22	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0G6	H	1	2	-	2/31/41/43	0/2/2/2
4	NAG	H	400	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)
3	H	1	0G6	O-C	2.23	1.26	1.22
4	H	400	NAG	O7-C7	2.18	1.28	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	400	NAG	C2-N2-C7	6.13	131.62	122.90
3	H	1	0G6	CB2-CA2-N2	4.71	116.53	110.33
4	H	400	NAG	O7-C7-N2	-4.38	113.91	121.95
3	H	1	0G6	CA2-N2-C1	3.65	129.52	123.07
4	H	400	NAG	O3-C3-C4	-3.61	102.01	110.35
3	H	1	0G6	CB-CA-N	-2.83	100.47	111.46
3	H	1	0G6	CG-CB-CA	-2.77	108.37	114.13
3	H	1	0G6	NE-CZ1-NH2	2.23	124.61	120.70
3	H	1	0G6	O1-C1-N2	-2.12	119.01	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	0G6	CG1-CB1-CA1	2.07	108.51	104.18
3	H	1	0G6	CB-CA-C	2.07	114.22	109.27
4	H	400	NAG	C8-C7-N2	-2.06	112.61	116.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAG	C8-C7-N2-C2
4	H	400	NAG	O7-C7-N2-C2
3	H	1	0G6	C3-C2-CA2-N2
3	H	1	0G6	NH1-CZ1-NE-CD3

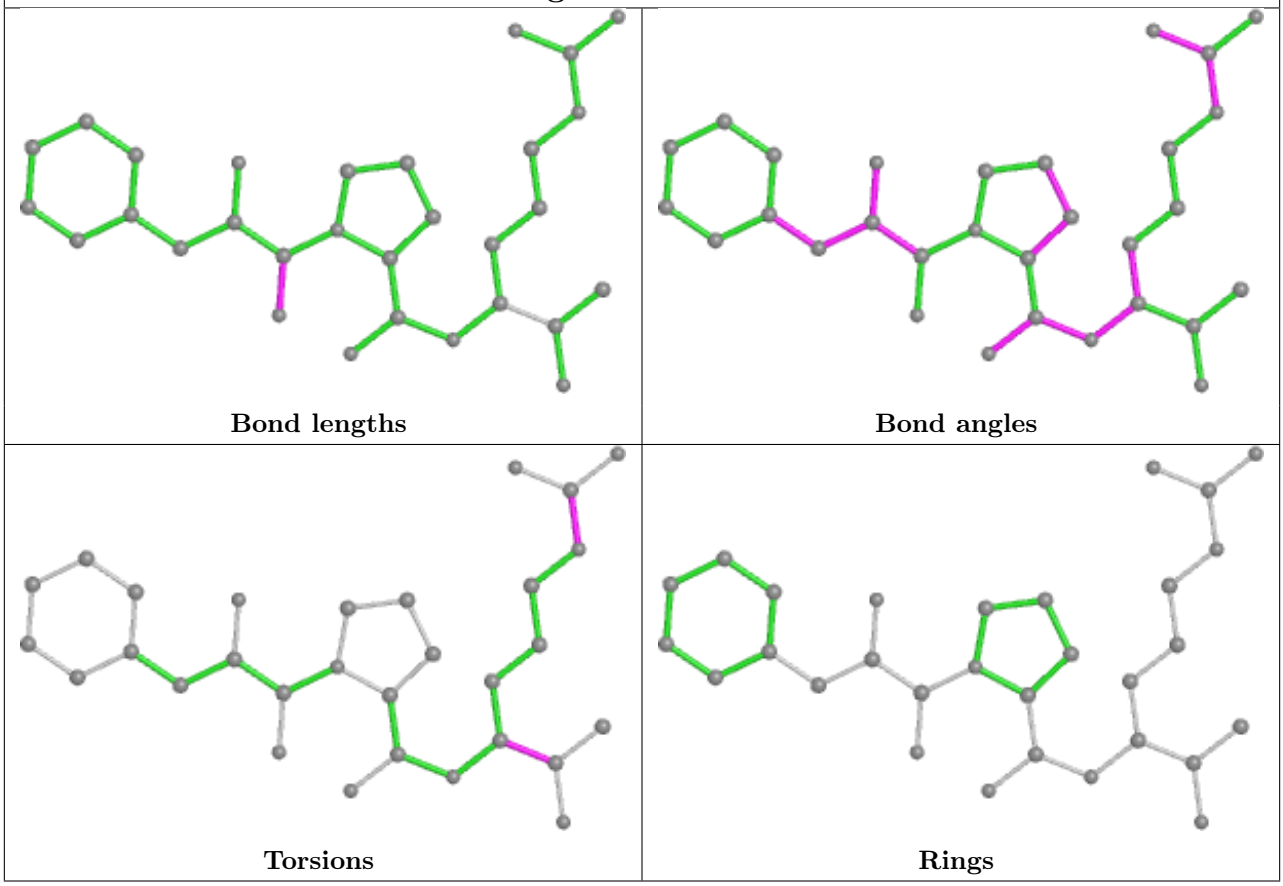
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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 then 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.

Ligand 0G6 H 1



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.