



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 09:32 AM EST

PDB ID : 1HAH  
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 : unknown  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

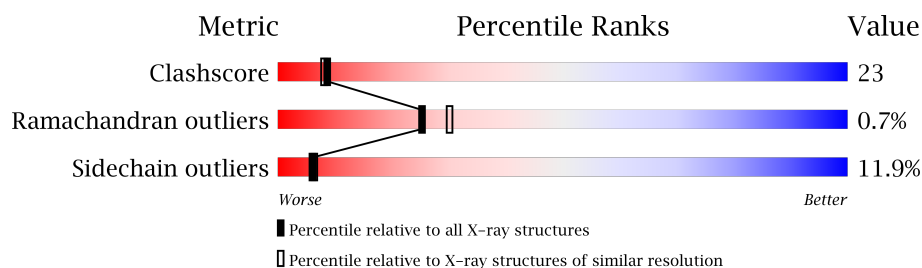
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	10	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2664 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	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	0	2	0
			2064	1315	368	367	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
			95	59	10	25	1			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is water.

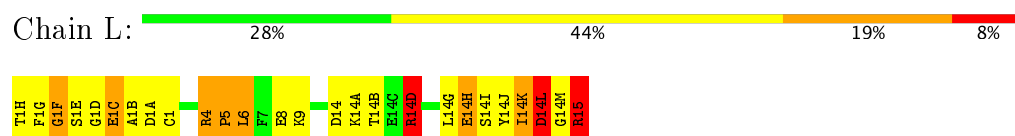
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	24	Total	O	0	0
			24	24		
5	H	178	Total	O	0	0
			178	178		
5	I	2	Total	O	0	0
			2	2		

### 3 Residue-property plots [i](#)

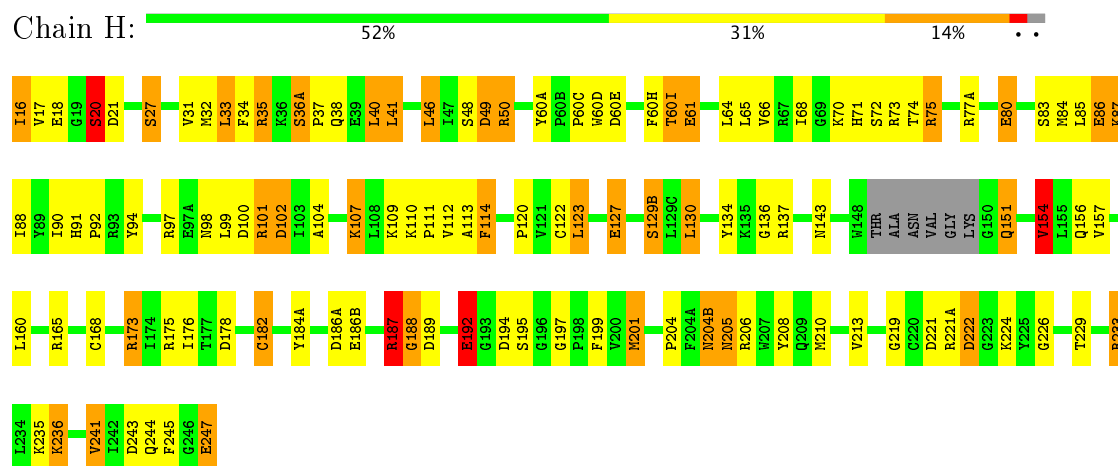
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

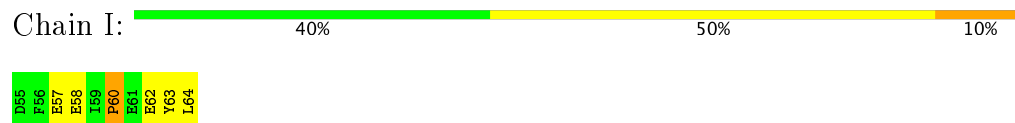
#### • Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)



#### • Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)



#### • Molecule 3: HIRUGEN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.75Å 72.39Å 73.52Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.114 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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

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	1.43	2/290 (0.7%)	3.09	20/384 (5.2%)
2	H	1.33	4/2129 (0.2%)	2.28	94/2874 (3.3%)
3	I	1.20	0/79	1.85	2/103 (1.9%)
All	All	1.33	6/2498 (0.2%)	2.38	116/3361 (3.5%)

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	3
2	H	0	7
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	219	GLY	N-CA	6.21	1.55	1.46
1	L	15	ARG	CZ-NH1	6.05	1.41	1.33
1	L	14(D)	ARG	CZ-NH1	5.63	1.40	1.33
2	H	61	GLU	CB-CG	5.55	1.62	1.52
2	H	168	CYS	C-O	5.36	1.33	1.23
2	H	80	GLU	CD-OE1	-5.25	1.19	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	15	ARG	NE-CZ-NH1	29.87	135.24	120.30
1	L	15	ARG	NE-CZ-NH2	-20.91	109.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	233	ARG	NE-CZ-NH1	17.18	128.89	120.30
2	H	101	ARG	NE-CZ-NH1	15.96	128.28	120.30
2	H	137	ARG	NE-CZ-NH1	-15.62	112.49	120.30
2	H	97	ARG	NE-CZ-NH2	-15.54	112.53	120.30
2	H	101	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	L	15	ARG	CD-NE-CZ	14.21	143.49	123.60
2	H	35	ARG	NE-CZ-NH2	-13.97	113.31	120.30
2	H	233	ARG	NE-CZ-NH2	-13.97	113.32	120.30
2	H	97	ARG	NE-CZ-NH1	12.64	126.62	120.30
2	H	21	ASP	CB-CG-OD2	-11.34	108.10	118.30
1	L	14(D)	ARG	NE-CZ-NH2	10.65	125.62	120.30
2	H	137	ARG	NE-CZ-NH2	10.32	125.46	120.30
2	H	60(A)	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	L	14(M)	GLY	C-N-CA	9.79	146.17	121.70
1	L	1(A)	ASP	CB-CG-OD1	-9.73	109.54	118.30
2	H	100	ASP	CB-CG-OD2	-9.48	109.76	118.30
2	H	184(A)	TYR	CB-CG-CD1	-9.23	115.46	121.00
2	H	175	ARG	NE-CZ-NH2	9.15	124.87	120.30
2	H	175	ARG	NE-CZ-NH1	-9.12	115.74	120.30
2	H	134	TYR	CB-CG-CD2	-9.08	115.55	121.00
2	H	173	ARG	NE-CZ-NH1	9.01	124.80	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-8.89	115.86	120.30
2	H	61	GLU	OE1-CD-OE2	8.72	133.77	123.30
2	H	27	SER	N-CA-CB	8.64	123.47	110.50
2	H	33	LEU	CB-CG-CD2	-8.40	96.71	111.00
2	H	102	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	L	1(A)	ASP	CB-CG-OD2	8.27	125.74	118.30
2	H	221	ASP	CB-CG-OD2	8.05	125.55	118.30
2	H	49	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	L	4	ARG	NE-CZ-NH2	7.74	124.17	120.30
2	H	243	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	L	14(H)	GLU	OE1-CD-OE2	7.58	132.40	123.30
1	L	14(D)	ARG	CD-NE-CZ	7.55	134.17	123.60
2	H	186(B)	GLU	C-N-CA	-7.25	107.08	122.30
2	H	60(I)	THR	CA-CB-CG2	7.06	122.29	112.40
2	H	154	VAL	N-CA-CB	-6.98	96.15	111.50
2	H	20	SER	N-CA-CB	6.92	120.88	110.50
2	H	241	VAL	CA-CB-CG1	6.75	121.02	110.90
1	L	1(F)	GLY	CA-C-O	-6.70	108.55	120.60
2	H	73	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	H	187	ARG	NE-CZ-NH2	6.67	123.63	120.30
2	H	205	ASN	OD1-CG-ND2	6.64	137.16	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75[A]	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	H	75[B]	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	H	157	VAL	CB-CA-C	-6.59	98.88	111.40
2	H	75[A]	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	H	75[B]	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	H	221(A)	ARG	CD-NE-CZ	6.51	132.71	123.60
2	H	94	TYR	CB-CG-CD2	-6.49	117.10	121.00
2	H	60(H)	PHE	CB-CG-CD1	-6.45	116.29	120.80
2	H	21	ASP	CB-CG-OD1	6.43	124.09	118.30
2	H	113	ALA	O-C-N	6.34	132.85	122.70
2	H	192	GLU	OE1-CD-OE2	6.32	130.89	123.30
2	H	66	VAL	C-N-CA	6.31	137.48	121.70
2	H	80	GLU	CG-CD-OE2	-6.25	105.80	118.30
2	H	60(A)	TYR	CB-CG-CD2	6.25	124.75	121.00
2	H	18	GLU	CG-CD-OE2	-6.24	105.81	118.30
2	H	134	TYR	CD1-CE1-CZ	-6.23	114.19	119.80
2	H	77(A)	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	H	84	MET	CA-CB-CG	-6.14	102.86	113.30
2	H	195	SER	CA-C-O	-6.14	107.21	120.10
2	H	233	ARG	CD-NE-CZ	6.12	132.16	123.60
2	H	33	LEU	CB-CA-C	6.09	121.76	110.20
2	H	60(E)	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	L	4	ARG	NH1-CZ-NH2	-6.06	112.74	119.40
1	L	14(K)	ILE	C-N-CA	6.04	136.79	121.70
2	H	127	GLU	CA-CB-CG	6.03	126.66	113.40
2	H	247	GLU	CG-CD-OE1	-5.97	106.36	118.30
2	H	201	MET	CG-SD-CE	-5.90	90.76	100.20
2	H	213	VAL	CA-C-O	5.86	132.41	120.10
2	H	61	GLU	N-CA-CB	-5.80	100.15	110.60
1	L	6	LEU	CB-CG-CD1	5.79	120.84	111.00
2	H	60(I)	THR	CA-CB-OG1	-5.73	96.97	109.00
2	H	243	ASP	CB-CA-C	5.73	121.86	110.40
2	H	187	ARG	CD-NE-CZ	5.72	131.60	123.60
1	L	1(F)	GLY	O-C-N	5.70	131.81	122.70
2	H	229	THR	OG1-CB-CG2	5.69	123.10	110.00
2	H	165	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	H	83	SER	CA-C-N	-5.62	104.83	117.20
2	H	104	ALA	O-C-N	5.60	131.65	122.70
2	H	27	SER	CB-CA-C	-5.56	99.54	110.10
2	H	205	ASN	CA-CB-CG	-5.50	101.29	113.40
2	H	50[A]	ARG	CB-CA-C	-5.50	99.40	110.40
2	H	50[B]	ARG	CB-CA-C	-5.50	99.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	MET	CA-CB-CG	-5.49	103.96	113.30
2	H	151	GLN	CA-CB-CG	-5.48	101.34	113.40
2	H	192	GLU	N-CA-CB	-5.48	100.74	110.60
1	L	4	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	H	20	SER	O-C-N	5.38	131.32	122.70
2	H	173	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	I	64	LEU	CA-C-O	-5.37	108.82	120.10
1	L	14(K)	ILE	CB-CA-C	5.36	122.32	111.60
2	H	154	VAL	CB-CA-C	5.34	121.56	111.40
2	H	40	LEU	O-C-N	5.32	131.22	122.70
3	I	64	LEU	CB-CA-C	5.32	120.30	110.20
2	H	60(E)	ASP	OD1-CG-OD2	5.29	133.35	123.30
2	H	123	LEU	CA-CB-CG	5.29	127.46	115.30
2	H	208	TYR	CD1-CE1-CZ	-5.28	115.05	119.80
1	L	14(G)	LEU	CB-CA-C	5.27	120.22	110.20
2	H	129(B)	SER	N-CA-CB	5.24	118.36	110.50
2	H	247	GLU	OE1-CD-OE2	5.24	129.59	123.30
2	H	107	LYS	CA-CB-CG	5.20	124.84	113.40
2	H	208	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	H	175	ARG	O-C-N	-5.18	114.42	122.70
2	H	60(E)	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	H	99	LEU	O-C-N	-5.13	114.49	122.70
2	H	129(B)	SER	CB-CA-C	-5.12	100.38	110.10
2	H	80	GLU	CG-CD-OE1	5.11	128.53	118.30
2	H	197	GLY	CA-C-O	5.09	129.75	120.60
2	H	114	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	L	14(B)	THR	CA-C-O	-5.03	109.54	120.10
2	H	184(A)	TYR	CB-CG-CD2	5.02	124.01	121.00
2	H	86	GLU	CG-CD-OE1	5.01	128.32	118.30
1	L	14(G)	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	101	ARG	Sidechain
2	H	102	ASP	Sidechain
2	H	16	ILE	Mainchain
2	H	160	LEU	Mainchain
2	H	173	ARG	Sidechain
2	H	187	ARG	Sidechain
2	H	188	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	L	14(D)	ARG	Sidechain
1	L	15	ARG	Sidechain
1	L	5	PRO	Mainchain

## 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	287	0	277	32	0
2	H	2064	0	2032	91	0
3	I	95	0	73	9	0
4	H	14	0	13	0	0
5	H	178	0	0	10	1
5	I	2	0	0	0	0
5	L	24	0	0	0	0
All	All	2664	0	2395	108	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 23.

All (108) 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:1(F):GLY:HA2	2:H:235:LYS:NZ	1.73	1.03
1:L:1(E):SER:HA	2:H:123:LEU:O	1.63	0.99
2:H:50[A]:ARG:HH11	2:H:50[A]:ARG:HG2	1.32	0.93
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ3	1.34	0.88
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.59	0.85
1:L:1(E):SER:CA	2:H:123:LEU:O	2.28	0.81
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.64	0.78
3:I:58:GLU:CD	3:I:58:GLU:H	1.86	0.76
1:L:1(D):GLY:CA	2:H:123:LEU:H	1.98	0.76
2:H:244:GLN:HB2	5:H:595:HOH:O	1.88	0.74
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.88	0.72
2:H:236:LYS:HG2	5:H:509:HOH:O	1.93	0.69
1:L:1(D):GLY:N	2:H:123:LEU:H	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:GLN:OE1	5:H:581:HOH:O	2.10	0.68
2:H:36(A):SER:HA	2:H:37:PRO:C	2.15	0.67
3:I:60:PRO:HG2	3:I:63:TYS:CE2	2.24	0.67
2:H:86:GLU:HB3	2:H:107:LYS:HG3	1.76	0.66
2:H:35:ARG:O	2:H:38:GLN:HA	1.97	0.65
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.12	0.64
2:H:110:LYS:O	5:H:529:HOH:O	2.15	0.63
2:H:75[B]:ARG:NH1	3:I:57:GLU:CB	2.60	0.63
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ1	1.62	0.63
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.02	0.63
2:H:178:ASP:O	2:H:233:ARG:HD2	2.01	0.60
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.22	0.60
2:H:110:LYS:NZ	5:H:604:HOH:O	2.30	0.59
2:H:201:MET:SD	2:H:210:MET:HG3	2.42	0.58
1:L:1(H):THR:O	1:L:1(H):THR:HG22	2.03	0.58
2:H:143:ASN:ND2	2:H:192:GLU:CB	2.66	0.58
2:H:75[B]:ARG:NH1	3:I:57:GLU:HB3	2.19	0.58
1:L:15:ARG:HB2	2:H:204:PRO:O	2.03	0.58
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.86	0.58
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.25	0.56
2:H:87:LYS:HD3	2:H:88:ILE:H	1.69	0.56
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.41	0.56
2:H:224:LYS:HE2	5:H:472:HOH:O	2.05	0.56
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.09	0.55
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.74	0.55
2:H:86:GLU:HB3	2:H:107:LYS:CG	2.36	0.55
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.23	0.54
2:H:75[B]:ARG:HH11	3:I:57:GLU:HB3	1.73	0.54
2:H:46:LEU:HD22	2:H:48:SER:O	2.08	0.52
2:H:64:LEU:HB2	2:H:85:LEU:HD12	1.91	0.52
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.10	0.52
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.62	0.52
2:H:75[A]:ARG:NH2	5:H:520:HOH:O	2.42	0.52
2:H:143:ASN:HD22	2:H:192:GLU:HB2	1.76	0.51
2:H:72:SER:OG	2:H:75[A]:ARG:HG2	2.11	0.51
2:H:50[A]:ARG:HE	2:H:107:LYS:CE	2.24	0.50
2:H:74:THR:O	2:H:75[B]:ARG:NH1	2.44	0.50
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.12	0.50
1:L:1(D):GLY:HA3	2:H:122:CYS:CA	2.39	0.49
2:H:17:VAL:O	2:H:188:GLY:HA2	2.11	0.49
2:H:87:LYS:CD	2:H:88:ILE:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:ASP:C	1:L:14:ASP:OD1	2.51	0.49
2:H:75[B]:ARG:HH12	3:I:57:GLU:N	2.10	0.49
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.94	0.48
1:L:1(H):THR:OG1	2:H:48:SER:CB	2.62	0.48
2:H:75[B]:ARG:NH1	3:I:57:GLU:HB2	2.28	0.47
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	1.95	0.47
2:H:50[B]:ARG:HD2	2:H:111:PRO:HB3	1.96	0.47
2:H:98:ASN:OD1	2:H:98:ASN:N	2.47	0.47
2:H:49:ASP:OD2	2:H:111:PRO:CB	2.63	0.47
2:H:72:SER:OG	2:H:75[B]:ARG:HG2	2.14	0.47
1:L:1(H):THR:HG21	2:H:247:GLU:OE1	2.15	0.47
2:H:87:LYS:CD	2:H:88:ILE:N	2.78	0.46
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.51	0.46
2:H:49:ASP:O	2:H:112:VAL:HG12	2.15	0.46
1:L:1(H):THR:OG1	2:H:48:SER:HB2	2.16	0.46
1:L:1(C):GLU:HG3	2:H:120:PRO:HG2	1.96	0.46
2:H:222:ASP:OD1	2:H:222:ASP:N	2.47	0.46
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.75	0.45
2:H:182:CYS:HA	2:H:226:GLY:O	2.16	0.45
2:H:61:GLU:HG2	2:H:61:GLU:H	1.03	0.45
1:L:1(D):GLY:CA	5:H:442:HOH:O	2.64	0.45
2:H:188:GLY:O	2:H:189:ASP:HB2	2.15	0.45
2:H:50[A]:ARG:HE	2:H:107:LYS:HE2	1.80	0.45
1:L:1(B):ALA:H	1:L:1:CYS:H	1.65	0.45
1:L:1(H):THR:CG2	1:L:1(H):THR:O	2.63	0.45
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.46	0.45
2:H:50[A]:ARG:NH1	2:H:50[A]:ARG:HG2	2.08	0.44
2:H:50[A]:ARG:HH12	2:H:110:LYS:HA	1.83	0.44
1:L:4:ARG:HB2	1:L:8:GLU:OE1	2.17	0.44
2:H:35:ARG:HG2	5:H:464:HOH:O	2.17	0.44
1:L:1(F):GLY:CA	2:H:235:LYS:HZ1	2.28	0.43
2:H:64:LEU:HB2	2:H:85:LEU:CD1	2.47	0.43
1:L:1:CYS:O	2:H:206:ARG:HD3	2.18	0.43
2:H:41:LEU:HD23	2:H:64:LEU:HD21	1.99	0.43
2:H:244:GLN:OE1	2:H:245:PHE:CE2	2.72	0.42
2:H:50[A]:ARG:HH12	2:H:110:LYS:CA	2.33	0.42
1:L:1(D):GLY:HA2	5:H:442:HOH:O	2.20	0.42
2:H:60(C):PRO:O	2:H:60(D):TRP:HD1	2.02	0.42
2:H:107:LYS:HE3	2:H:107:LYS:HB2	1.64	0.41
2:H:187:ARG:HA	2:H:187:ARG:HD2	1.90	0.41
2:H:236:LYS:HG2	2:H:236:LYS:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:PRO:O	1:L:9:LYS:HB2	2.19	0.41
2:H:114:PHE:CD1	2:H:114:PHE:N	2.89	0.41
2:H:20:SER:O	2:H:156:GLN:HA	2.20	0.41
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.56	0.41
2:H:16:ILE:HD13	2:H:194:ASP:OD2	2.21	0.41
1:L:1(F):GLY:HA2	2:H:235:LYS:CE	2.46	0.41
2:H:70:LYS:HB3	2:H:70:LYS:HE3	1.69	0.40
2:H:87:LYS:HD2	2:H:88:ILE:N	2.36	0.40
1:L:1(E):SER:N	2:H:235:LYS:HZ1	2.18	0.40
2:H:176:ILE:HA	2:H:176:ILE:HD13	1.79	0.40
2:H:31:VAL:HG12	2:H:32:MET:N	2.37	0.40
2:H:74:THR:OG1	2:H:75[B]:ARG:CZ	2.69	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:434:HOH:O	5:H:434:HOH:O[2_555]	1.85	0.35

## 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	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	2	1
2	H	251/259 (97%)	234 (93%)	17 (7%)	0	100	100
3	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	292/305 (96%)	267 (91%)	23 (8%)	2 (1%)	25	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(G)	PHE
1	L	14(L)	ASP

### 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	31/31 (100%)	26 (84%)	5 (16%)	3	3
2	H	223/225 (99%)	198 (89%)	25 (11%)	7	7
3	I	9/9 (100%)	8 (89%)	1 (11%)	7	8
All	All	263/265 (99%)	232 (88%)	31 (12%)	6	6

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

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	6	LEU
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(L)	ASP
2	H	20	SER
2	H	27	SER
2	H	33	LEU
2	H	36(A)	SER
2	H	41	LEU
2	H	46	LEU
2	H	60(I)	THR
2	H	65	LEU
2	H	68	ILE
2	H	80	GLU
2	H	87	LYS
2	H	90	ILE
2	H	109	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	130	LEU

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Mol	Chain	Res	Type
2	H	154	VAL
2	H	182	CYS
2	H	186(A)	ASP
2	H	187	ARG
2	H	192	GLU
2	H	204(B)	ASN
2	H	222	ASP
2	H	236	LYS
2	H	241	VAL
3	I	60	PRO

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

Mol	Chain	Res	Type
2	H	143	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TYS	I	63	3	16,16,17	1.45	2 (12%)	19,22,24	2.11	8 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the



Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	I	63	3	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	-3.79	1.36	1.42
3	I	63	TYS	OH-S	3.09	1.69	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-S-O2	-4.70	94.40	107.59
3	I	63	TYS	CD1-CE1-CZ	-3.17	115.77	119.74
3	I	63	TYS	CG-CB-CA	-2.73	108.80	114.29
3	I	63	TYS	OH-CZ-CE2	-2.68	113.78	118.73
3	I	63	TYS	O-C-CA	-2.52	118.07	125.02
3	I	63	TYS	CE2-CZ-CE1	2.03	123.38	120.19
3	I	63	TYS	OH-CZ-CE1	2.22	122.84	118.73
3	I	63	TYS	O2-S-O1	2.99	125.17	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	NAG	H	400	2	14,14,15	0.83	0	15,19,21	2.34	3 (20%)

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	NAG	H	400	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	O3-C3-C4	-5.88	97.56	110.36
4	H	400	NAG	C2-N2-C7	-5.04	115.59	122.94
4	H	400	NAG	O7-C7-C8	2.17	126.02	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.