



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:52 PM GMT

PDB ID : 5GDS  
Title : HIRUNORMS ARE TRUE HIRUDIN MIMETICS. THE CRYSTAL STRUCTURE OF HUMAN ALPHA-THROMBIN:HIRUNORMV COMPLEX  
Authors : De Simone, G.; Lombardi, A.; Galdiero, S.; Nastri, F.; Della Morte, R.; Staliano, N.; Pedone, C.; Bolognesi, M.; Pavone, V.  
Deposited on : 1997-07-17  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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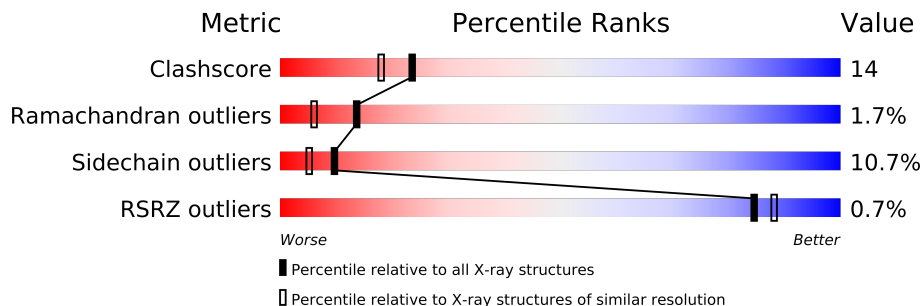
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	26	

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2629 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	77	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	119	1	0
			2059	1313	365	367	14			

- Molecule 3 is a protein called HIRUNORM V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	15	Total	C	N	O	39	0	0
			136	95	15	26			

- Molecule 4 is SUGAR (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	14	0
			14	8	1	5		

- Molecule 5 is water.

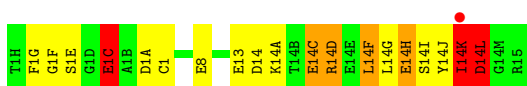
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	120	Total	O	0	0
			120	120		
5	I	3	Total	O	0	0
			3	3		
5	L	10	Total	O	0	0
			10	10		

### 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 errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

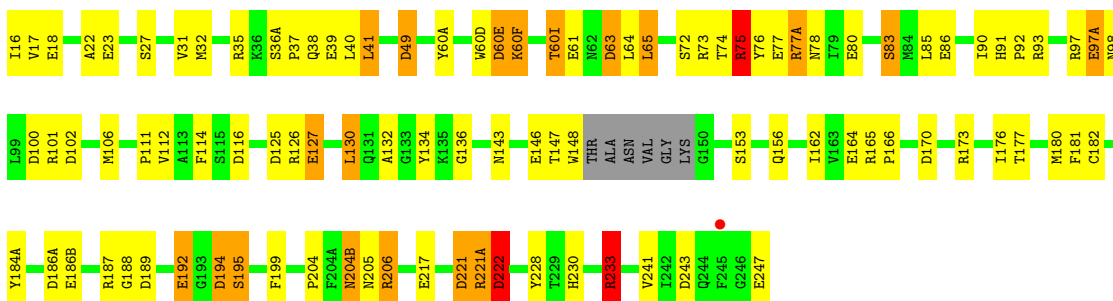
- Molecule 1: ALPHA-THROMBIN

Chain L:



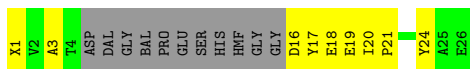
- Molecule 2: ALPHA-THROMBIN

Chain H:



- Molecule 3: HIRUNORM V

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.90Å 72.80Å 73.30Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.10) 99.2 (19.91-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.41 (at 2.09Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.176 , (Not available) 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 116.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 21609 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, CHG, ALC, NAL, DGL, AIB

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	1.41	5/290 (1.7%)	1.63	6/384 (1.6%)
2	H	1.27	19/2118 (0.9%)	1.67	47/2860 (1.6%)
3	I	1.45	2/79 (2.5%)	1.63	2/105 (1.9%)
All	All	1.29	26/2487 (1.0%)	1.66	55/3349 (1.6%)

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
2	H	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	61	GLU	CD-OE2	9.03	1.35	1.25
2	H	97(A)	GLU	CD-OE2	8.20	1.34	1.25
3	I	18	GLU	CD-OE2	7.90	1.34	1.25
1	L	14(C)	GLU	CD-OE2	7.58	1.33	1.25
2	H	164	GLU	CD-OE2	7.13	1.33	1.25
2	H	23	GLU	CD-OE2	6.84	1.33	1.25
2	H	80	GLU	CD-OE1	6.57	1.32	1.25
2	H	217	GLU	CD-OE2	6.50	1.32	1.25
2	H	75[A]	ARG	CB-CG	6.44	1.70	1.52
2	H	75[B]	ARG	CB-CG	6.44	1.70	1.52
1	L	8	GLU	CD-OE2	6.22	1.32	1.25
2	H	86	GLU	CD-OE2	5.50	1.31	1.25
2	H	101	ARG	CZ-NH1	5.46	1.40	1.33
2	H	127	GLU	CD-OE2	5.43	1.31	1.25
2	H	186(B)	GLU	CD-OE2	5.42	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	19	GLU	CD-OE2	5.33	1.31	1.25
2	H	39	GLU	CD-OE2	5.31	1.31	1.25
2	H	195	SER	CA-CB	5.28	1.60	1.52
2	H	146	GLU	CD-OE2	5.23	1.31	1.25
2	H	247	GLU	CD-OE2	5.17	1.31	1.25
1	L	13	GLU	CD-OE2	5.13	1.31	1.25
1	L	14(H)	GLU	CD-OE2	5.11	1.31	1.25
2	H	153	SER	CA-CB	5.07	1.60	1.52
1	L	1(C)	GLU	CD-OE1	5.03	1.31	1.25
2	H	77	GLU	CD-OE2	-5.03	1.20	1.25
2	H	18	GLU	CD-OE2	5.02	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	77(A)	ARG	NE-CZ-NH1	12.58	126.59	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-12.35	114.12	120.30
2	H	206	ARG	NE-CZ-NH1	11.05	125.82	120.30
2	H	101	ARG	NE-CZ-NH1	10.36	125.48	120.30
2	H	100	ASP	CB-CG-OD2	-10.00	109.30	118.30
2	H	101	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	H	49	ASP	CB-CG-OD2	-9.47	109.78	118.30
2	H	102	ASP	CB-CG-OD2	-9.45	109.79	118.30
2	H	206	ARG	NE-CZ-NH2	-8.33	116.13	120.30
2	H	100	ASP	CB-CG-OD1	8.32	125.79	118.30
2	H	97	ARG	NE-CZ-NH1	7.67	124.13	120.30
2	H	27	SER	N-CA-CB	7.65	121.98	110.50
2	H	125	ASP	CB-CG-OD2	-7.55	111.50	118.30
2	H	97	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	L	14	ASP	CB-CG-OD2	-7.07	111.94	118.30
2	H	49	ASP	CB-CG-OD1	7.04	124.64	118.30
2	H	60(E)	ASP	CB-CG-OD2	-6.74	112.23	118.30
2	H	170	ASP	CB-CG-OD1	6.71	124.34	118.30
1	L	1(A)	ASP	CB-CG-OD2	-6.66	112.31	118.30
3	I	16	ASP	CB-CG-OD1	6.51	124.16	118.30
2	H	125	ASP	CB-CG-OD1	6.39	124.06	118.30
2	H	221(A)	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	H	93	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	H	186(A)	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	L	14	ASP	CB-CG-OD1	6.03	123.73	118.30
2	H	221	ASP	CB-CG-OD1	6.01	123.71	118.30
2	H	243	ASP	CB-CG-OD2	-5.93	112.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	16	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	H	204	PRO	N-CA-CB	5.84	110.31	103.30
1	L	14(L)	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	H	116	ASP	CB-CG-OD2	-5.71	113.16	118.30
2	H	73	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	H	22	ALA	N-CA-CB	-5.59	102.28	110.10
2	H	116	ASP	CB-CG-OD1	5.58	123.32	118.30
2	H	63	ASP	CB-CG-OD2	-5.53	113.33	118.30
2	H	181	PHE	N-CA-CB	5.53	120.54	110.60
2	H	75[A]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	H	75[B]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	H	83	SER	N-CA-CB	5.52	118.78	110.50
1	L	1(A)	ASP	N-CA-CB	-5.50	100.70	110.60
2	H	222	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	L	14(L)	ASP	CB-CG-OD1	5.44	123.20	118.30
2	H	194	ASP	CB-CG-OD2	-5.41	113.43	118.30
2	H	102	ASP	CB-CG-OD1	5.35	123.12	118.30
2	H	170	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	H	243	ASP	CB-CG-OD1	5.30	123.07	118.30
2	H	184(A)	TYR	CB-CG-CD1	-5.28	117.83	121.00
2	H	189	ASP	CB-CG-OD1	5.28	123.05	118.30
2	H	233	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	H	205	ASN	CA-CB-CG	-5.24	101.88	113.40
2	H	132	ALA	N-CA-CB	5.23	117.42	110.10
2	H	189	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	H	228	TYR	CG-CD2-CE2	-5.16	117.17	121.30
2	H	153	SER	N-CA-CB	5.08	118.12	110.50
2	H	22	ALA	CB-CA-C	-5.08	102.49	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	156	GLN	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	287	0	278	8	1
2	H	2059	0	2028	53	1
3	I	136	0	126	6	0
4	H	14	0	11	0	0
5	H	120	0	0	3	0
5	I	3	0	0	0	0
5	L	10	0	0	0	0
All	All	2629	0	2443	64	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:74:THR:OG1	2:H:75[A]:ARG:NH1	1.93	1.01
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.66	0.95
2:H:72:SER:OG	2:H:75[A]:ARG:HG3	1.74	0.87
2:H:75[B]:ARG:HG3	2:H:76:TYR:N	1.89	0.85
2:H:176:ILE:N	2:H:176:ILE:HD13	2.07	0.68
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.93	0.68
2:H:60(I):THR:N	2:H:63:ASP:OD2	2.27	0.66
2:H:75[A]:ARG:HG2	2:H:75[A]:ARG:HH11	1.64	0.62
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.01	0.62
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.21	0.61
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.82	0.59
3:I:1:CHG:H3A	3:I:3:NAL:C5	2.34	0.58
1:L:1(C):GLU:H	1:L:1:CYS:HB3	1.69	0.57
2:H:72:SER:OG	2:H:75[A]:ARG:CG	2.50	0.57
2:H:36(A):SER:HA	2:H:37:PRO:C	2.26	0.56
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.08	0.56
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.89	0.54
2:H:75[A]:ARG:NH1	2:H:75[A]:ARG:HG2	2.23	0.53
2:H:60(F):LYS:HE2	5:H:516:HOH:O	2.09	0.53
2:H:97(A):GLU:HG2	2:H:98:ASN:N	2.23	0.52
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.11	0.51
2:H:35:ARG:O	2:H:38:GLN:HA	2.09	0.51
2:H:60(D):TRP:O	2:H:60(E):ASP:HB2	2.09	0.50
2:H:17:VAL:O	2:H:188:GLY:HA2	2.11	0.50
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	2.12	0.50
2:H:49:ASP:O	2:H:112:VAL:HG12	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:74:THR:CB	2:H:75[A]:ARG:HH12	2.23	0.49
2:H:187:ARG:NH2	2:H:221:ASP:O	2.44	0.49
3:I:20:ILE:HD12	3:I:21:PRO:O	2.13	0.49
2:H:41:LEU:HA	2:H:41:LEU:HD12	1.65	0.47
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.44	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.50	0.46
2:H:230:HIS:CG	2:H:233:ARG:HG3	2.51	0.46
2:H:134:TYR:O	2:H:162:ILE:HG12	2.16	0.46
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.16	0.46
3:I:20:ILE:HD12	3:I:20:ILE:C	2.37	0.46
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.31	0.45
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.51	0.45
2:H:134:TYR:N	2:H:134:TYR:CD1	2.84	0.45
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.97	0.45
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.32	0.45
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	2.16	0.45
2:H:134:TYR:HD1	2:H:134:TYR:N	2.16	0.44
2:H:31:VAL:HG12	2:H:32:MET:N	2.30	0.44
2:H:60(D):TRP:CD1	2:H:60(D):TRP:N	2.85	0.44
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.69	0.44
2:H:85:LEU:CD1	2:H:106:MET:CE	2.96	0.43
2:H:176:ILE:HG23	2:H:176:ILE:HD12	1.56	0.43
2:H:74:THR:HG1	2:H:75[A]:ARG:NH1	2.13	0.43
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.49	0.43
2:H:60(F):LYS:CE	5:H:516:HOH:O	2.67	0.42
2:H:130:LEU:HA	2:H:130:LEU:HD23	1.80	0.42
2:H:222:ASP:N	2:H:222:ASP:OD1	2.51	0.42
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.72	0.42
2:H:60(F):LYS:HE2	5:H:487:HOH:O	2.20	0.42
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.18	0.42
2:H:85:LEU:HD23	2:H:85:LEU:HA	1.86	0.41
2:H:60(A):TYR:CZ	3:I:1:CHG:H4	2.55	0.41
2:H:16:ILE:N	2:H:194:ASP:OD2	2.54	0.41
2:H:165:ARG:NH2	2:H:177:THR:O	2.54	0.40
2:H:74:THR:HA	3:I:17:TYR:CD1	2.56	0.40
2:H:65:LEU:HD12	2:H:65:LEU:HA	1.48	0.40
2:H:114:PHE:CD1	2:H:114:PHE:N	2.85	0.40
2:H:74:THR:HA	3:I:17:TYR:HD1	1.87	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	Distance(Å)	Clash(Å)
1:L:14(L):ASP:O	2:H:173:ARG:NH2[4_556]	1.75	0.45

## 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%)	4 (12%)	4 (12%)	1	0
2	H	250/259 (96%)	240 (96%)	10 (4%)	0	100	100
3	I	7/26 (27%)	6 (86%)	0	1 (14%)	0	0
All	All	291/321 (91%)	272 (94%)	14 (5%)	5 (2%)	14	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(F)	GLY
3	I	24	TYR
1	L	14(L)	ASP
1	L	1(E)	SER
1	L	14(K)	ILE

### 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%)	25 (81%)	6 (19%)	2	1
2	H	222/225 (99%)	199 (90%)	23 (10%)	10	6
3	I	9/14 (64%)	9 (100%)	0	100	100
All	All	262/270 (97%)	233 (89%)	29 (11%)	10	5

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

Mol	Chain	Res	Type
1	L	1(G)	PHE
1	L	1(C)	GLU
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(F)	LEU
1	L	14(K)	ILE
2	H	41	LEU
2	H	60(F)	LYS
2	H	60(I)	THR
2	H	64	LEU
2	H	65	LEU
2	H	75[A]	ARG
2	H	75[B]	ARG
2	H	83	SER
2	H	90	ILE
2	H	126	ARG
2	H	127	GLU
2	H	130	LEU
2	H	147	THR
2	H	148	TRP
2	H	180	MET
2	H	182	CYS
2	H	192	GLU
2	H	195	SER
2	H	204(B)	ASN
2	H	221(A)	ARG
2	H	222	ASP
2	H	233	ARG
2	H	241	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	204(B)	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues 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	CHG	I	1	3	10,10,11	7.71	1 (10%)	10,12,14	1.77	3 (30%)
3	AIB	I	22	3	5,5,6	8.31	2 (40%)	5,7,9	0.80	0
3	AIB	I	23	3	5,5,6	8.53	2 (40%)	5,7,9	0.32	0
3	ALC	I	25	3	10,10,12	0.67	0	10,12,15	1.56	3 (30%)
3	DGL	I	26	3	9,9,9	0.71	0	11,11,11	1.00	1 (9%)
3	NAL	I	3	3	16,16,17	6.13	3 (18%)	19,21,23	2.18	3 (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
3	CHG	I	1	3	-	0/4/14/16	0/1/1/1
3	AIB	I	22	3	-	0/0/3/6	0/0/0/0
3	AIB	I	23	3	-	0/0/3/6	0/0/0/0
3	ALC	I	25	3	-	0/4/12/16	0/1/1/1
3	DGL	I	26	3	-	0/9/9/9	0/0/0/0
3	NAL	I	3	3	-	0/4/6/8	0/0/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	CHG	O-C	24.27	1.28	1.11
3	I	3	NAL	O-C	24.04	1.28	1.11
3	I	23	AIB	O-C	18.74	1.24	1.11
3	I	22	AIB	O-C	18.17	1.23	1.11
3	I	23	AIB	CA-C	3.35	1.55	1.48
3	I	22	AIB	CB2-CA	-2.95	1.50	1.53
3	I	3	NAL	CA-C	2.63	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	NAL	C9-C2	-2.60	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	NAL	C-CA-N	-7.75	106.09	113.83
3	I	3	NAL	C2-C9-CA	-3.77	105.52	114.42
3	I	1	CHG	C5-C6-C1	-3.25	106.87	111.92
3	I	25	ALC	CE1-CD1-CG	-3.13	107.10	112.23
3	I	25	ALC	CE2-CD2-CG	-2.88	107.51	112.23
3	I	1	CHG	C1-CA-N	2.73	117.47	110.69
3	I	26	DGL	OXT-C-O	-2.50	118.42	124.07
3	I	1	CHG	C3-C2-C1	-2.42	108.17	111.92
3	I	3	NAL	C9-C2-C3	-2.37	116.26	120.90
3	I	25	ALC	CG-CB-CA	-2.13	112.46	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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	NAG	H	400	2	12,14,15	1.41	1 (8%)	15,19,21	5.54	12 (80%)

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	2/2/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	400	NAG	C2-N2	3.90	1.50	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	O5-C5-C6	14.02	121.69	106.98
4	H	400	NAG	C3-C2-N2	7.75	123.56	111.76
4	H	400	NAG	C3-C4-C5	5.99	120.90	110.20
4	H	400	NAG	O3-C3-C2	5.97	121.63	109.09
4	H	400	NAG	O7-C7-N2	-5.61	110.18	121.90
4	H	400	NAG	O7-C7-C8	-5.37	111.56	122.04
4	H	400	NAG	O4-C4-C3	3.86	119.00	110.35
4	H	400	NAG	C2-N2-C7	3.67	129.25	123.09
4	H	400	NAG	O4-C4-C5	3.64	118.88	109.28
4	H	400	NAG	O6-C6-C5	3.35	122.87	111.36
4	H	400	NAG	O3-C3-C4	2.68	116.37	110.35
4	H	400	NAG	O5-C5-C4	2.65	114.02	110.65

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	400	NAG	C4
4	H	400	NAG	C2

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	28/36 (77%)	-0.36	1 (3%) 41 45	24, 34, 58, 87	6 (21%)
2	H	251/259 (96%)	-0.46	1 (0%) 90 92	20, 34, 56, 80	32 (12%)
3	I	12/26 (46%)	0.04	0 100 100	40, 60, 75, 75	4 (33%)
All	All	291/321 (90%)	-0.43	2 (0%) 84 88	20, 35, 60, 87	42 (14%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	14(K)	ILE	3.2
2	H	245	PHE	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DGL	I	26	10/10	-	-	20,38,76,77	10
3	AIB	I	22	6/7	0.23	-	42,73,80,81	1
3	CHG	I	1	10/11	0.10	-	31,41,58,74	0
3	NAL	I	3	15/16	0.10	-	28,40,54,60	0
3	AIB	I	23	6/7	0.15	-	69,78,80,81	3
3	ALC	I	25	10/12	-	-	28,38,69,86	10

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	400	14/15	-	-	55,55,55,55	14

### 6.5 Other polymers

There are no such residues in this entry.