



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:11 AM GMT

PDB ID : 1HGT  
Title : STRUCTURE OF THE HIRUGEN AND HIRULOG 1 COMPLEXES OF  
ALPHA-THROMBIN  
Authors : Tulinsky, A.; Skrzypczak-Jankun, E.  
Deposited on : 1991-06-03  
Resolution : 2.20 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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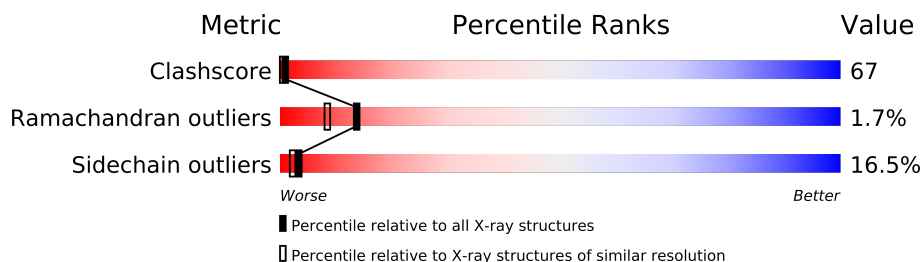
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.20 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	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	12	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2678 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 (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	0	0
			2053	1310	362	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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	54	GLU	GLY	CONFLICT	UNP P09945

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	191	Total	O	0	0
			191	191		
4	I	15	Total	O	0	0
			15	15		
4	L	37	Total	O	0	0
			37	37		

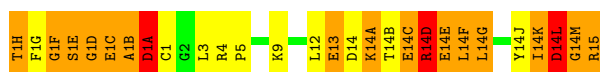
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

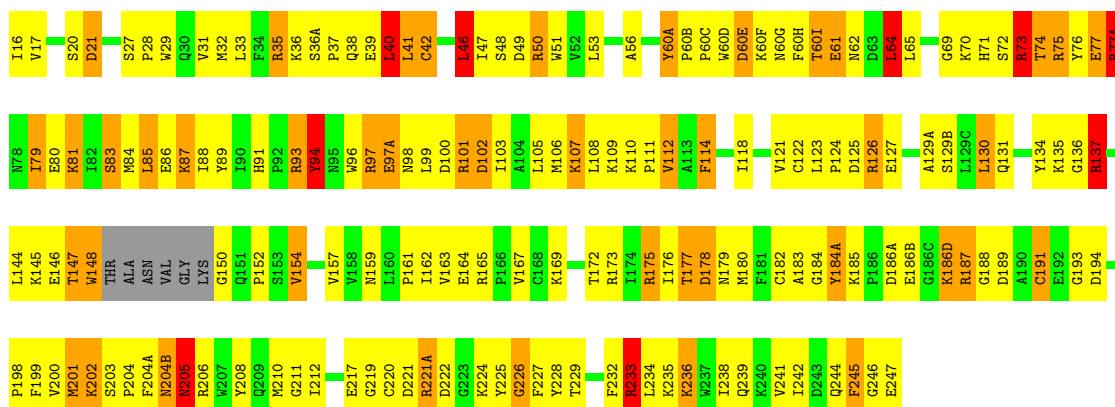
#### • Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



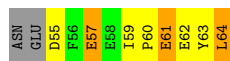
#### • Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



#### • Molecule 3: HIRUGEN

Chain I: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.80Å 71.80Å 72.60Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: 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	1.39	1/290 (0.3%)	2.62	16/384 (4.2%)
2	H	1.21	0/2107	2.32	69/2846 (2.4%)
3	I	1.21	0/79	2.08	4/103 (3.9%)
All	All	1.23	1/2476 (0.0%)	2.35	89/3333 (2.7%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	15	ARG	CZ-NH1	5.18	1.39	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	137	ARG	NE-CZ-NH1	24.33	132.47	120.30
2	H	101	ARG	NE-CZ-NH2	-23.36	108.62	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-17.90	111.35	120.30
2	H	137	ARG	NE-CZ-NH2	-15.77	112.42	120.30
2	H	75	ARG	NE-CZ-NH1	15.73	128.16	120.30
2	H	101	ARG	NE-CZ-NH1	15.21	127.91	120.30
2	H	97	ARG	NE-CZ-NH2	-14.18	113.21	120.30
2	H	233	ARG	NE-CZ-NH2	-14.03	113.28	120.30
1	L	15	ARG	NE-CZ-NH2	-13.88	113.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	NE-CZ-NH1	13.71	127.15	120.30
1	L	15	ARG	NE-CZ-NH1	-13.45	113.58	120.30
2	H	35	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	L	15	ARG	NH1-CZ-NH2	12.40	133.04	119.40
2	H	137	ARG	CD-NE-CZ	12.19	140.67	123.60
2	H	75	ARG	NE-CZ-NH2	-12.19	114.20	120.30
2	H	35	ARG	NE-CZ-NH1	11.67	126.14	120.30
2	H	221(A)	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	L	1(A)	ASP	CB-CG-OD1	-11.22	108.20	118.30
1	L	14(D)	ARG	CD-NE-CZ	11.17	139.24	123.60
2	H	233	ARG	NE-CZ-NH1	11.07	125.83	120.30
2	H	60(A)	TYR	CB-CG-CD1	-10.53	114.68	121.00
2	H	97	ARG	NE-CZ-NH1	10.23	125.42	120.30
2	H	77(A)	ARG	NE-CZ-NH1	10.03	125.32	120.30
2	H	187	ARG	NE-CZ-NH2	9.93	125.27	120.30
2	H	73	ARG	NE-CZ-NH1	9.83	125.22	120.30
2	H	175	ARG	NE-CZ-NH2	-9.79	115.40	120.30
2	H	50	ARG	NE-CZ-NH1	9.17	124.89	120.30
2	H	221(A)	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	L	15	ARG	CD-NE-CZ	-8.57	111.59	123.60
2	H	126	ARG	NE-CZ-NH2	-8.49	116.06	120.30
2	H	76	TYR	CB-CG-CD2	-8.47	115.92	121.00
2	H	50	ARG	NE-CZ-NH2	-8.08	116.26	120.30
2	H	41	LEU	CB-CA-C	7.79	125.00	110.20
2	H	187	ARG	CD-NE-CZ	-7.75	112.75	123.60
2	H	93	ARG	NE-CZ-NH2	7.75	124.18	120.30
2	H	60(E)	ASP	CB-CG-OD2	-7.69	111.38	118.30
2	H	201	MET	CA-CB-CG	-7.27	100.94	113.30
2	H	27	SER	N-CA-CB	-7.26	99.61	110.50
2	H	191	CYS	CB-CA-C	7.19	124.78	110.40
1	L	1(A)	ASP	CB-CG-OD2	7.11	124.70	118.30
2	H	46	LEU	CA-CB-CG	7.05	131.52	115.30
2	H	102	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	L	14(D)	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	H	206	ARG	NE-CZ-NH2	-6.91	116.85	120.30
2	H	64	LEU	N-CA-C	6.79	129.34	111.00
2	H	126	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	L	12	LEU	C-N-CA	6.47	137.87	121.70
2	H	36	LYS	CA-CB-CG	6.45	127.58	113.40
2	H	110	LYS	N-CA-CB	6.31	121.97	110.60
1	L	1(A)	ASP	CA-CB-CG	-6.30	99.53	113.40
2	H	137	ARG	CG-CD-NE	6.29	125.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	64	LEU	N-CA-CB	-6.26	97.87	110.40
3	I	61	GLU	N-CA-CB	6.21	121.78	110.60
1	L	14(G)	LEU	CB-CA-C	6.19	121.97	110.20
2	H	94	TYR	CB-CG-CD2	-6.10	117.34	121.00
2	H	184(A)	TYR	CB-CG-CD1	-6.09	117.34	121.00
2	H	64	LEU	CB-CG-CD2	-6.01	100.79	111.00
2	H	40	LEU	O-C-N	6.00	132.29	122.70
2	H	225	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	H	173	ARG	CD-NE-CZ	5.96	131.95	123.60
1	L	1(D)	GLY	CA-C-O	5.96	131.33	120.60
2	H	42	CYS	N-CA-CB	-5.89	100.00	110.60
2	H	60(E)	ASP	OD1-CG-OD2	5.81	134.34	123.30
2	H	114	PHE	O-C-N	5.79	131.96	122.70
3	I	61	GLU	CA-CB-CG	5.77	126.10	113.40
2	H	21	ASP	CB-CG-OD2	-5.75	113.12	118.30
2	H	173	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	L	13	GLU	CB-CA-C	-5.71	98.98	110.40
1	L	1(E)	SER	C-N-CA	5.70	134.27	122.30
1	L	14(C)	GLU	CA-CB-CG	5.66	125.84	113.40
2	H	134	TYR	CB-CG-CD2	-5.56	117.67	121.00
2	H	193	GLY	O-C-N	5.54	131.57	122.70
2	H	64	LEU	CB-CA-C	-5.49	99.77	110.20
2	H	100	ASP	O-C-N	5.49	131.48	122.70
2	H	205	ASN	CB-CA-C	5.47	121.34	110.40
2	H	178	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	H	233	ARG	CB-CA-C	-5.32	99.76	110.40
2	H	75	ARG	CB-CA-C	5.31	121.02	110.40
2	H	97(A)	GLU	CG-CD-OE2	-5.31	107.69	118.30
2	H	226	GLY	O-C-N	5.31	131.19	122.70
2	H	65	LEU	CB-CG-CD2	-5.30	102.00	111.00
2	H	21	ASP	CB-CG-OD1	5.24	123.02	118.30
1	L	14(C)	GLU	CB-CA-C	-5.23	99.94	110.40
2	H	225	TYR	CB-CG-CD1	5.08	124.05	121.00
2	H	50	ARG	CA-CB-CG	-5.07	102.24	113.40
2	H	73	ARG	CD-NE-CZ	5.07	130.69	123.60
2	H	77	GLU	CA-C-O	5.04	130.69	120.10
3	I	57	GLU	CA-CB-CG	5.01	124.43	113.40
3	I	64	LEU	CA-C-O	-5.01	109.58	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	H	233	ARG	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	70	2
2	H	2053	0	2020	259	3
3	I	95	0	73	30	0
4	H	191	0	0	30	1
4	I	15	0	0	4	0
4	L	37	0	0	8	0
All	All	2678	0	2371	320	3

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 67.

All (320) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:1(E):SER:HA	2:H:123:LEU:O	1.43	1.16
2:H:60(I):THR:CG2	2:H:62:ASN:HB2	1.75	1.15
2:H:199:PHE:HE1	2:H:201:MET:HE2	0.99	1.15
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.16	1.11
1:L:1(G):PHE:HA	2:H:123:LEU:HD12	1.32	1.10
1:L:1(H):THR:HG23	2:H:242:ILE:HD13	1.26	1.09
2:H:33:LEU:HD22	2:H:64:LEU:HD21	1.26	1.08
2:H:145:LYS:HD3	2:H:148:TRP:HB3	1.30	1.07
2:H:199:PHE:CE1	2:H:201:MET:HE2	1.90	1.05
2:H:50:ARG:NH2	2:H:108:LEU:O	1.91	1.03
2:H:199:PHE:HE1	2:H:201:MET:CE	1.71	1.03
1:L:1(B):ALA:HB3	4:L:645:HOH:O	1.56	1.03
2:H:85:LEU:HD13	2:H:106:MET:CE	1.90	1.02
2:H:33:LEU:CD2	2:H:64:LEU:HD21	1.90	1.01
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.58	1.01
3:I:61:GLU:CG	3:I:64:LEU:HB2	1.91	0.99
3:I:55:ASP:HB3	4:I:625:HOH:O	1.60	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:1(H):THR:HG21	2:H:242:ILE:HG21	1.45	0.98
3:I:59:ILE:HG12	3:I:64:LEU:HD21	1.44	0.98
2:H:50:ARG:NH2	2:H:86:GLU:OE1	1.96	0.97
1:L:15:ARG:HB2	2:H:204:PRO:O	1.63	0.97
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.46	0.95
2:H:185:LYS:CB	2:H:186(A):ASP:OD1	2.13	0.95
1:L:14(D):ARG:HD3	4:L:901:HOH:O	1.67	0.94
2:H:148:TRP:CE3	2:H:148:TRP:N	2.35	0.93
3:I:61:GLU:HG2	3:I:64:LEU:HB2	1.51	0.92
2:H:79:ILE:HD11	4:H:662:HOH:O	1.69	0.91
3:I:59:ILE:HD11	3:I:64:LEU:HD23	1.52	0.91
3:I:59:ILE:CG1	3:I:64:LEU:HD21	2.00	0.90
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.68	0.90
2:H:147:THR:HA	2:H:148:TRP:CE3	2.06	0.90
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.00	0.90
2:H:60(I):THR:HG23	2:H:62:ASN:HB2	1.50	0.89
2:H:87:LYS:HD2	2:H:88:ILE:N	1.87	0.89
3:I:59:ILE:HD11	3:I:64:LEU:CD2	2.03	0.89
1:L:9:LYS:HG2	4:L:753:HOH:O	1.72	0.89
2:H:148:TRP:HE3	2:H:148:TRP:N	1.68	0.89
2:H:147:THR:HA	2:H:148:TRP:CZ3	2.08	0.88
2:H:126:ARG:HB2	2:H:232:PHE:CZ	2.10	0.87
2:H:185:LYS:HB3	2:H:186(A):ASP:OD1	1.74	0.87
2:H:185:LYS:HB2	2:H:186(A):ASP:OD1	1.76	0.86
1:L:3:LEU:O	1:L:9:LYS:HE2	1.76	0.85
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.12	0.84
2:H:172:THR:HG21	2:H:176:ILE:HD11	1.58	0.83
2:H:165:ARG:NH2	2:H:177:THR:O	2.10	0.83
2:H:85:LEU:CD1	2:H:106:MET:CE	2.55	0.82
1:L:1(E):SER:CA	2:H:123:LEU:O	2.27	0.82
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.48	0.82
2:H:97(A):GLU:OE1	2:H:175:ARG:NH1	2.13	0.82
1:L:1(G):PHE:O	1:L:1(D):GLY:N	2.13	0.81
2:H:51:TRP:HE1	2:H:247:GLU:H	1.29	0.80
2:H:35:ARG:O	2:H:38:GLN:HA	1.79	0.80
2:H:236:LYS:HD2	4:H:864:HOH:O	1.81	0.80
3:I:61:GLU:HG3	3:I:64:LEU:HB2	1.63	0.80
1:L:1(H):THR:CG2	2:H:242:ILE:HD13	2.12	0.78
2:H:60(I):THR:HG23	2:H:62:ASN:H	1.48	0.78
3:I:61:GLU:HA	3:I:64:LEU:HG	1.66	0.77
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.65	0.77
2:H:124:PRO:HG3	2:H:210:MET:HE2	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:3:LEU:O	1:L:9:LYS:CE	2.33	0.76
2:H:87:LYS:CD	2:H:88:ILE:H	1.98	0.76
1:L:1(G):PHE:HA	2:H:123:LEU:CD1	2.15	0.75
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.05	0.75
1:L:1(H):THR:N	1:L:1(C):GLU:HA	2.01	0.75
2:H:41:LEU:HD13	4:H:603:HOH:O	1.86	0.74
2:H:199:PHE:CE1	2:H:201:MET:CE	2.58	0.74
1:L:1(G):PHE:CA	2:H:123:LEU:HD12	2.13	0.73
1:L:15:ARG:O	1:L:15:ARG:CG	2.34	0.73
2:H:217:GLU:O	2:H:221(A):ARG:HD2	1.88	0.73
1:L:1(E):SER:H	2:H:235:LYS:NZ	1.87	0.72
1:L:1(C):GLU:N	4:L:523:HOH:O	2.21	0.72
1:L:1(E):SER:HG	2:H:208:TYR:HE1	1.37	0.72
1:L:1(E):SER:H	2:H:235:LYS:HZ1	1.37	0.72
3:I:63:TYS:O1	3:I:63:TYS:HE2	1.88	0.72
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.91	0.71
2:H:221(A):ARG:HD3	4:H:763:HOH:O	1.91	0.71
1:L:5:PRO:N	1:L:9:LYS:HD2	2.05	0.71
2:H:221(A):ARG:HG3	4:H:702:HOH:O	1.88	0.71
3:I:59:ILE:CD1	3:I:64:LEU:HD21	2.20	0.70
2:H:41:LEU:HB2	4:H:603:HOH:O	1.91	0.70
1:L:1(C):GLU:HG3	2:H:48:SER:HA	1.74	0.70
2:H:145:LYS:CD	2:H:148:TRP:HB3	2.15	0.70
2:H:87:LYS:HD2	2:H:88:ILE:H	1.53	0.69
2:H:87:LYS:CD	2:H:88:ILE:N	2.55	0.69
2:H:77:GLU:HB2	2:H:80:GLU:HG2	1.73	0.69
2:H:147:THR:C	2:H:148:TRP:HE3	1.95	0.69
2:H:126:ARG:HB2	2:H:232:PHE:HZ	1.54	0.69
3:I:61:GLU:HB2	3:I:64:LEU:HD12	1.74	0.69
1:L:15:ARG:O	1:L:15:ARG:HG2	1.92	0.69
2:H:217:GLU:HB2	2:H:224:LYS:HD2	1.75	0.69
2:H:60(B):PRO:HG2	2:H:96:TRP:CD2	2.27	0.69
2:H:75:ARG:HB3	3:I:57:GLU:OE2	1.91	0.69
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ3	1.58	0.68
2:H:77(A):ARG:HD3	4:H:949:HOH:O	1.92	0.68
1:L:1(C):GLU:OE1	4:L:645:HOH:O	2.11	0.68
1:L:14(J):TYR:O	1:L:14(K):ILE:CG1	2.37	0.68
3:I:59:ILE:CD1	3:I:64:LEU:CD2	2.71	0.68
3:I:63:TYS:C	3:I:64:LEU:O	2.36	0.68
1:L:1(C):GLU:HB2	4:L:523:HOH:O	1.92	0.68
1:L:1(B):ALA:HB2	4:L:692:HOH:O	1.95	0.67
2:H:208:TYR:HB3	2:H:210:MET:HE1	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.25	0.66
2:H:60(I):THR:HG23	4:H:805:HOH:O	1.94	0.66
2:H:224:LYS:HD2	4:H:763:HOH:O	1.94	0.66
3:I:63:TYS:O1	3:I:63:TYS:CE2	2.40	0.66
2:H:244:GLN:NE2	2:H:245:PHE:CZ	2.65	0.65
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.59	0.65
2:H:97(A):GLU:OE1	4:H:710:HOH:O	2.14	0.65
2:H:147:THR:CA	2:H:148:TRP:CE3	2.77	0.65
1:L:14(F):LEU:HD12	2:H:135:LYS:HB3	1.77	0.65
2:H:81:LYS:HD3	2:H:118:ILE:CD1	2.26	0.65
2:H:60(D):TRP:O	2:H:60(E):ASP:HB2	1.97	0.65
2:H:179:ASN:OD1	2:H:233:ARG:HD3	1.97	0.64
1:L:1(H):THR:HA	2:H:48:SER:HB3	1.80	0.64
2:H:49:ASP:O	2:H:112:VAL:HG13	1.98	0.64
2:H:35:ARG:HB3	2:H:39:GLU:H	1.62	0.64
2:H:81:LYS:HD2	4:H:607:HOH:O	1.97	0.64
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.32	0.64
2:H:60(F):LYS:HG3	2:H:60(H):PHE:CE2	2.33	0.64
1:L:1(F):GLY:HA2	2:H:235:LYS:NZ	2.13	0.63
1:L:1(A):ASP:OD2	1:L:9:LYS:NZ	2.17	0.63
2:H:33:LEU:CD2	2:H:64:LEU:CD2	2.71	0.63
2:H:74:THR:HG23	4:I:817:HOH:O	1.98	0.63
1:L:14(M):GLY:HA2	2:H:204:PRO:HB3	1.80	0.63
2:H:163:VAL:HG13	2:H:185:LYS:HE2	1.82	0.62
2:H:105:LEU:HD12	2:H:241:VAL:HG21	1.81	0.62
2:H:165:ARG:NH1	4:H:833:HOH:O	2.32	0.62
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.12	0.62
2:H:36(A):SER:HA	2:H:37:PRO:C	2.19	0.62
1:L:4:ARG:C	1:L:9:LYS:HD2	2.20	0.62
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.30	0.62
3:I:60:PRO:HB2	3:I:62:GLU:HG2	1.81	0.61
2:H:227:PHE:HE1	4:H:890:HOH:O	1.82	0.61
3:I:61:GLU:HG2	3:I:64:LEU:CB	2.27	0.61
2:H:84:MET:CE	3:I:63:TYS:O	2.49	0.60
2:H:60(I):THR:HG21	2:H:62:ASN:HB2	1.74	0.60
2:H:164:GLU:HA	4:H:782:HOH:O	2.00	0.60
2:H:69:GLY:O	2:H:79:ILE:HD11	2.03	0.59
2:H:147:THR:CA	2:H:148:TRP:HE3	2.14	0.59
2:H:17:VAL:O	2:H:188:GLY:HA2	2.02	0.59
2:H:114:PHE:HB3	4:H:503:HOH:O	2.03	0.59
2:H:105:LEU:CD1	2:H:241:VAL:HG22	2.33	0.58
2:H:60(H):PHE:CE2	4:H:603:HOH:O	2.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:1(H):THR:H2	1:L:1(C):GLU:HA	1.69	0.58
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.39	0.58
1:L:14(D):ARG:HH21	1:L:14(E):GLU:HB3	1.69	0.58
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.37	0.58
2:H:208:TYR:HB3	2:H:210:MET:CE	2.33	0.57
2:H:236:LYS:CD	4:H:864:HOH:O	2.47	0.57
1:L:1(H):THR:HG23	2:H:242:ILE:CD1	2.18	0.57
2:H:87:LYS:HD3	2:H:88:ILE:H	1.68	0.57
2:H:50:ARG:CZ	2:H:108:LEU:O	2.53	0.57
2:H:50:ARG:HD2	2:H:111:PRO:HD3	1.86	0.57
3:I:61:GLU:HA	3:I:64:LEU:H	1.69	0.57
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.86	0.56
2:H:164:GLU:OE2	4:H:760:HOH:O	2.18	0.56
2:H:97:ARG:HG3	4:H:742:HOH:O	2.05	0.56
2:H:35:ARG:HB3	2:H:39:GLU:HG3	1.88	0.56
2:H:182:CYS:HA	2:H:226:GLY:O	2.06	0.56
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.35	0.56
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.40	0.56
2:H:129(A):ALA:HB3	4:H:874:HOH:O	2.05	0.56
2:H:97(A):GLU:CD	2:H:175:ARG:HH11	2.08	0.56
2:H:32:MET:SD	2:H:40:LEU:HD12	2.47	0.55
2:H:187:ARG:HH21	2:H:222:ASP:CG	2.08	0.55
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.22	0.55
2:H:31:VAL:HG12	2:H:32:MET:N	2.21	0.55
2:H:201:MET:CE	2:H:210:MET:HG3	2.37	0.55
1:L:1(H):THR:HG22	1:L:1(G):PHE:N	2.22	0.55
2:H:60(I):THR:CG2	2:H:62:ASN:CB	2.67	0.54
1:L:1(E):SER:N	2:H:235:LYS:HZ1	2.03	0.54
1:L:1(H):THR:CG2	2:H:242:ILE:HG21	2.29	0.54
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.43	0.54
2:H:129(B):SER:O	2:H:131:GLN:NE2	2.41	0.53
2:H:46:LEU:HD22	2:H:48:SER:O	2.09	0.53
1:L:14(J):TYR:C	1:L:14(K):ILE:HG12	2.29	0.53
2:H:60(I):THR:CG2	4:H:805:HOH:O	2.53	0.53
2:H:211:GLY:HA2	2:H:229:THR:O	2.09	0.53
3:I:60:PRO:C	3:I:62:GLU:H	2.11	0.53
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.44	0.53
2:H:185:LYS:HG2	2:H:186(B):GLU:OE2	2.09	0.52
2:H:31:VAL:CG1	2:H:32:MET:N	2.72	0.52
2:H:85:LEU:HD11	2:H:106:MET:HE1	1.92	0.52
3:I:59:ILE:CG1	3:I:64:LEU:CD2	2.80	0.52
1:L:5:PRO:CA	1:L:9:LYS:HD2	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:61:GLU:HG2	3:I:64:LEU:C	2.29	0.52
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.91	0.52
1:L:14(B):THR:HA	1:L:14(D):ARG:NE	2.25	0.52
2:H:49:ASP:O	2:H:111:PRO:HA	2.10	0.51
2:H:16:ILE:N	2:H:194:ASP:OD2	2.44	0.51
2:H:217:GLU:OE1	2:H:224:LYS:HD3	2.10	0.51
1:L:1(G):PHE:O	1:L:1(D):GLY:CA	2.59	0.51
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.42	0.51
2:H:94:TYR:HA	2:H:101:ARG:HB2	1.91	0.51
2:H:107:LYS:HZ2	2:H:246:GLY:HA2	1.76	0.50
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.93	0.50
2:H:178:ASP:O	2:H:233:ARG:HD2	2.12	0.50
2:H:145:LYS:HD3	2:H:148:TRP:CB	2.21	0.49
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.94	0.49
1:L:14(G):LEU:HD21	2:H:202:LYS:HD2	1.94	0.49
2:H:188:GLY:O	2:H:189:ASP:HB2	2.12	0.49
2:H:162:ILE:HD11	2:H:199:PHE:HZ	1.69	0.49
2:H:204(B):ASN:HD22	2:H:204(B):ASN:C	2.16	0.49
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.11	0.49
2:H:73:ARG:HD3	2:H:152:PRO:O	2.12	0.49
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.43	0.49
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.27	0.49
2:H:60(I):THR:HG22	2:H:62:ASN:HB2	1.85	0.48
2:H:122:CYS:HB2	2:H:208:TYR:CD1	2.48	0.48
2:H:126:ARG:CB	2:H:232:PHE:CZ	2.89	0.48
2:H:81:LYS:HD3	2:H:118:ILE:HD11	1.95	0.48
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.75	0.48
2:H:93:ARG:NH1	2:H:101:ARG:NH2	2.61	0.48
2:H:184:GLY:HA3	4:H:708:HOH:O	2.13	0.48
2:H:105:LEU:CD1	2:H:241:VAL:CG2	2.92	0.48
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.74	0.47
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.50	0.47
2:H:60(D):TRP:O	2:H:60(E):ASP:CB	2.63	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.49	0.47
3:I:55:ASP:HA	4:I:778:HOH:O	2.14	0.47
1:L:14(L):ASP:O	1:L:14(M):GLY:O	2.33	0.47
2:H:187:ARG:HB3	2:H:221:ASP:OD2	2.14	0.47
2:H:87:LYS:NZ	2:H:88:ILE:O	2.35	0.46
2:H:71:HIS:NE2	2:H:154:VAL:HG22	2.30	0.46
2:H:81:LYS:HE3	4:H:547:HOH:O	2.15	0.46
2:H:51:TRP:HZ2	2:H:246:GLY:CA	2.27	0.46
2:H:73:ARG:NH2	3:I:55:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:89:TYR:CE2	2:H:245:PHE:CE1	3.04	0.46
1:L:5:PRO:HA	1:L:9:LYS:CD	2.45	0.46
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.51	0.46
2:H:177:THR:HG23	2:H:180:MET:CE	2.46	0.46
2:H:79:ILE:HG13	2:H:80:GLU:N	2.31	0.46
1:L:1(C):GLU:CB	1:L:1:CYS:HB3	2.46	0.46
2:H:70:LYS:HE3	2:H:72:SER:O	2.16	0.45
2:H:56:ALA:HB2	2:H:103:ILE:O	2.16	0.45
2:H:124:PRO:HG3	2:H:210:MET:CE	2.42	0.45
2:H:88:ILE:HD11	2:H:106:MET:CE	2.46	0.45
2:H:64:LEU:HD22	2:H:85:LEU:HD11	1.98	0.45
2:H:203:SER:O	2:H:205:ASN:HA	2.16	0.45
2:H:244:GLN:HB3	2:H:245:PHE:CD1	2.51	0.45
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.16	0.45
2:H:62:ASN:HB3	4:H:658:HOH:O	2.17	0.45
1:L:13:GLU:HA	1:L:14(C):GLU:OE2	2.16	0.45
2:H:187:ARG:NH1	2:H:221:ASP:O	2.48	0.45
3:I:61:GLU:HA	3:I:64:LEU:CG	2.43	0.45
2:H:61:GLU:HG2	2:H:61:GLU:H	1.20	0.45
2:H:61:GLU:OE1	2:H:87:LYS:HD3	2.17	0.45
2:H:126:ARG:HA	2:H:232:PHE:CE1	2.52	0.45
1:L:1(G):PHE:O	2:H:123:LEU:HB2	2.16	0.45
2:H:74:THR:CG2	4:I:817:HOH:O	2.61	0.44
2:H:126:ARG:CA	2:H:232:PHE:CZ	3.00	0.44
2:H:32:MET:CG	2:H:40:LEU:HD12	2.47	0.44
1:L:14(J):TYR:HE2	2:H:202:LYS:O	2.00	0.44
2:H:130:LEU:HD23	2:H:201:MET:HE3	1.99	0.44
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.42	0.44
1:L:1(H):THR:HA	2:H:47:ILE:O	2.17	0.44
2:H:75:ARG:HA	3:I:57:GLU:HB2	2.00	0.44
1:L:14(D):ARG:HE	1:L:14(E):GLU:H	1.66	0.44
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.80	0.44
2:H:236:LYS:CE	4:H:864:HOH:O	2.66	0.44
2:H:164:GLU:H	2:H:164:GLU:CD	2.22	0.44
2:H:187:ARG:HD3	2:H:221:ASP:OD2	2.18	0.44
2:H:199:PHE:CE1	2:H:201:MET:HE1	2.48	0.43
2:H:79:ILE:CD1	4:H:662:HOH:O	2.45	0.43
2:H:144:LEU:HD12	2:H:150:GLY:C	2.39	0.43
2:H:147:THR:HA	2:H:148:TRP:HZ3	1.74	0.43
2:H:107:LYS:HE3	2:H:107:LYS:HB2	1.61	0.43
1:L:15:ARG:NH1	2:H:204(A):PHE:O	2.52	0.43
2:H:187:ARG:NH1	2:H:221:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:32:MET:CE	2:H:40:LEU:CD1	2.96	0.43
2:H:84:MET:HE1	3:I:63:TYS:O	2.19	0.43
1:L:1(C):GLU:CB	4:L:523:HOH:O	2.60	0.43
2:H:33:LEU:HB2	2:H:42:CYS:O	2.19	0.43
2:H:84:MET:HE3	3:I:63:TYS:O	2.17	0.43
2:H:164:GLU:OE1	2:H:167:VAL:HG21	2.19	0.43
1:L:1(H):THR:H2	1:L:1(C):GLU:CA	2.32	0.43
2:H:60(I):THR:HG23	2:H:62:ASN:CB	2.36	0.43
2:H:187:ARG:HH11	2:H:187:ARG:HD3	1.48	0.43
2:H:29:TRP:CG	2:H:121:VAL:HB	2.54	0.43
2:H:99:LEU:O	2:H:102:ASP:HB2	2.19	0.43
2:H:183:ALA:HB3	2:H:228:TYR:CE1	2.54	0.43
2:H:212:ILE:O	2:H:228:TYR:HA	2.19	0.43
2:H:200:VAL:HA	2:H:208:TYR:O	2.19	0.42
2:H:21:ASP:OD1	2:H:154:VAL:HG12	2.19	0.42
2:H:179:ASN:HB3	2:H:234:LEU:HD11	2.00	0.42
2:H:130:LEU:CD2	2:H:201:MET:HE3	2.49	0.42
2:H:17:VAL:HG23	2:H:191:CYS:HB2	2.00	0.42
2:H:103:ILE:HD11	2:H:238:ILE:HD11	2.02	0.42
2:H:148:TRP:CD2	2:H:148:TRP:N	2.83	0.42
2:H:86:GLU:HB3	2:H:107:LYS:HG3	2.01	0.42
2:H:137:ARG:HD3	2:H:159:ASN:OD1	2.18	0.42
2:H:224:LYS:O	4:H:540:HOH:O	2.21	0.42
2:H:47:ILE:HG21	2:H:123:LEU:HD21	2.01	0.42
2:H:129(B):SER:HG	2:H:204(A):PHE:HE2	1.64	0.42
2:H:53:LEU:HD11	2:H:103:ILE:HD11	2.02	0.42
2:H:161:PRO:HG3	2:H:184(A):TYR:CE1	2.55	0.42
2:H:130:LEU:HA	2:H:130:LEU:HD23	1.87	0.41
2:H:217:GLU:OE1	2:H:224:LYS:CD	2.68	0.41
2:H:71:HIS:CD2	2:H:154:VAL:CG2	3.03	0.41
2:H:74:THR:CG2	2:H:75:ARG:HG3	2.33	0.41
2:H:167:VAL:HG23	2:H:167:VAL:H	1.59	0.41
2:H:98:ASN:O	2:H:99:LEU:HB2	2.19	0.41
1:L:14(A):LYS:HG3	4:H:846:HOH:O	2.20	0.41
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.55	0.41
1:L:1(B):ALA:H	1:L:1:CYS:H	1.69	0.41
2:H:182:CYS:HB3	2:H:227:PHE:CE2	2.55	0.41
2:H:96:TRP:HA	2:H:99:LEU:HD23	2.03	0.41
1:L:14(C):GLU:OE1	2:H:202:LYS:HE3	2.21	0.41
2:H:175:ARG:HH11	2:H:175:ARG:HD3	1.66	0.41
2:H:35:ARG:HB2	2:H:41:LEU:HD23	2.03	0.41
2:H:35:ARG:HD3	2:H:39:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:135:LYS:HZ1	2:H:186(D):LYS:HZ1	1.68	0.41
2:H:17:VAL:HG21	2:H:220:CYS:HB3	2.02	0.41
2:H:191:CYS:O	2:H:194:ASP:HB2	2.21	0.41
2:H:60(G):ASN:ND2	4:H:696:HOH:O	2.53	0.41
3:I:60:PRO:C	3:I:62:GLU:N	2.75	0.41
1:L:1(D):GLY:N	2:H:123:LEU:H	2.19	0.40
2:H:83:SER:HB3	4:H:537:HOH:O	2.21	0.40
2:H:145:LYS:O	2:H:146:GLU:C	2.59	0.40
1:L:15:ARG:HH11	1:L:15:ARG:HD2	1.55	0.40

All (3) 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:15:ARG:NH1	2:H:169:LYS:O[4.556]	2.11	0.09
2:H:186(A):ASP:CA	4:H:733:HOH:O[4.546]	2.12	0.08
1:L:15:ARG:NH1	2:H:172:THR:O[4.556]	2.13	0.07

## 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	249/259 (96%)	237 (95%)	11 (4%)	1 (0%)	43	45
3	I	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	290/307 (94%)	269 (93%)	16 (6%)	5 (2%)	14	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(M)	GLY
1	L	1(F)	GLY
1	L	1(B)	ALA
2	H	77(A)	ARG

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Mol	Chain	Res	Type
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%)	22 (71%)	9 (29%)	0	0
2	H	221/225 (98%)	187 (85%)	34 (15%)	4	3
3	I	9/11 (82%)	9 (100%)	0	100	100
All	All	261/267 (98%)	218 (84%)	43 (16%)	3	2

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

Mol	Chain	Res	Type
1	L	1(H)	THR
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(E)	GLU
1	L	14(F)	LEU
1	L	14(K)	ILE
1	L	14(L)	ASP
2	H	20	SER
2	H	40	LEU
2	H	46	LEU
2	H	60(I)	THR
2	H	61	GLU
2	H	64	LEU
2	H	73	ARG
2	H	74	THR
2	H	77(A)	ARG
2	H	79	ILE
2	H	81	LYS
2	H	83	SER
2	H	85	LEU

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Mol	Chain	Res	Type
2	H	87	LYS
2	H	94	TYR
2	H	107	LYS
2	H	109	LYS
2	H	112	VAL
2	H	125	ASP
2	H	127	GLU
2	H	130	LEU
2	H	137	ARG
2	H	147	THR
2	H	148	TRP
2	H	154	VAL
2	H	157	VAL
2	H	177	THR
2	H	186(D)	LYS
2	H	202	LYS
2	H	204(B)	ASN
2	H	205	ASN
2	H	236	LYS
2	H	239	GLN
2	H	245	PHE

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	38	GLN
2	H	156	GLN
2	H	204(B)	ASN
2	H	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	5.52	4 (25%)	20,22,24	1.39	4 (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
3	TYS	I	63	3	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	O-C	19.85	1.25	1.11
3	I	63	TYS	OH-S	-7.90	1.49	1.63
3	I	63	TYS	OH-CZ	-4.17	1.37	1.42
3	I	63	TYS	CA-C	2.08	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CZ-OH-S	-3.45	113.80	118.98
3	I	63	TYS	OH-CZ-CE2	-2.35	114.80	118.70
3	I	63	TYS	CD1-CE1-CZ	-2.24	116.76	119.76
3	I	63	TYS	OH-CZ-CE1	2.04	122.08	118.70

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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.