



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:14 PM GMT

PDB ID : 1C4Y  
Title : SELECTIVE NON-ELECTROPHILIC THROMBIN INHIBITORS  
Authors : Krishnan, R.; Mochalkin, I.; Arni, R.K.; Tulinsky, A.  
Deposited on : 1999-10-05  
Resolution : 2.70 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:

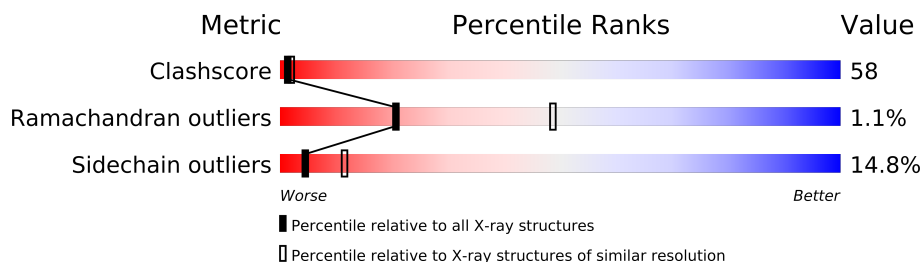
MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683



# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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	1	36	
2	2	259	
3	3	13	



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2426 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 THROMBIN:SHORT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	27	Total	C	N	O	S	0	0	0
			211	132	33	45	1			

- Molecule 2 is a protein called THROMBIN:LONG CHAIN.

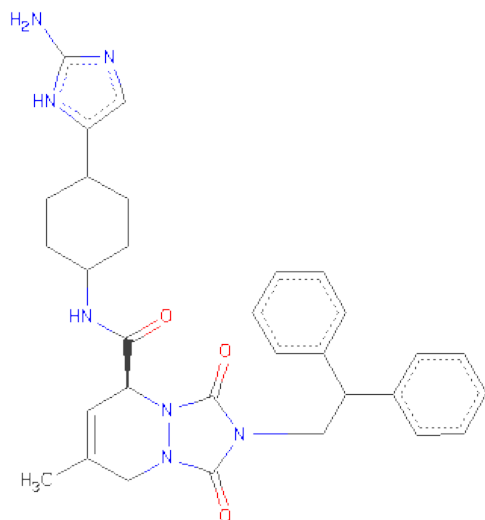
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	254	Total	C	N	O	S	0	0	0
			2049	1309	360	366	14			

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	S	0	0	0
			85	53	10	21	1			

- Molecule 4 is 2-(2,2-DIPHENYL-ETHYL)-7-METHYL-1,3-DIOXO-2,3,5,8-TETRAHYDR O-1H-[1,2,4]TRIAZOLO[1,2-A]PYRIDAZINE-5-CARBOXYLICACID [4-(2-AMINO-3H-IM IDAZOL-4-YL)-CYCLOHEXYL]-AMIDE (three-letter code: IH3) (formula: C<sub>31</sub>H<sub>35</sub>N<sub>7</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	2	1	41	31	7	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	40	Total	O	0	0
			40	40		



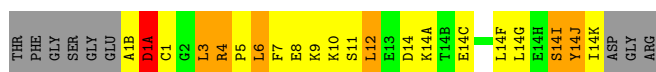
### 3 Residue-property plots

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.

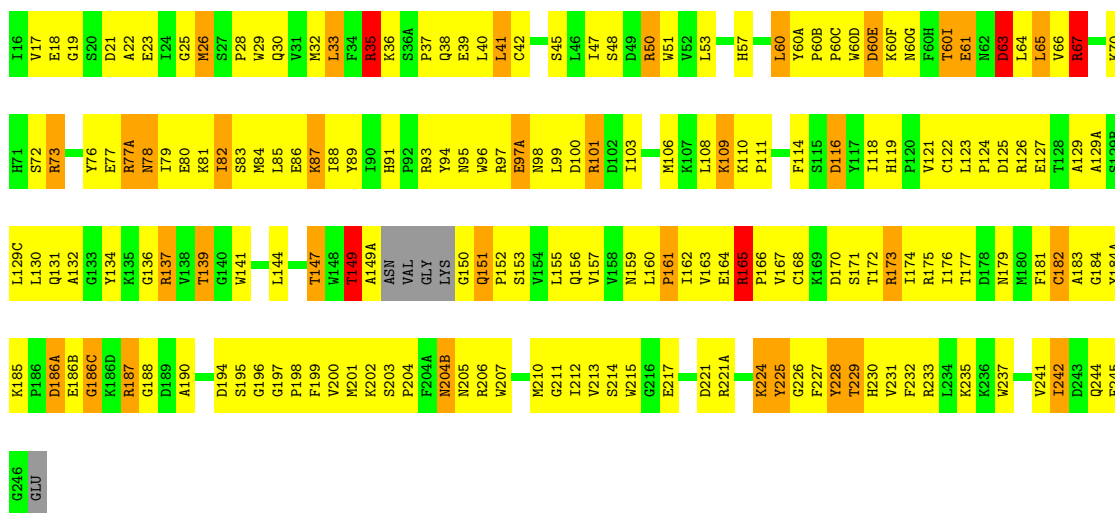
#### • Molecule 1: THROMBIN:SHORT CHAIN

Chain 1: 



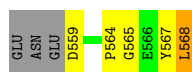
#### • Molecule 2: THROMBIN:LONG CHAIN

Chain 2: 



#### • Molecule 3: HIRUGEN

Chain 3: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.10Å 93.10Å 95.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.70	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.70)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.144 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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: IH3, 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	1	1.02	0/213	2.15	7/283 (2.5%)
2	2	0.92	1/2103 (0.0%)	1.78	33/2844 (1.2%)
3	3	0.93	0/69	1.67	0/89
All	All	0.93	1/2385 (0.0%)	1.82	40/3216 (1.2%)

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	1	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	229	THR	CA-CB	5.21	1.66	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	101	ARG	NE-CZ-NH1	23.75	132.18	120.30
1	1	4	ARG	NE-CZ-NH1	14.95	127.77	120.30
2	2	165	ARG	NE-CZ-NH1	13.32	126.96	120.30
2	2	101	ARG	NE-CZ-NH2	-12.64	113.98	120.30
2	2	101	ARG	CD-NE-CZ	11.59	139.83	123.60
1	1	4	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	2	35	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	2	165	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	2	116	ASP	CB-CG-OD1	8.15	125.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1(A)	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	1	1(A)	ASP	CA-CB-CG	-8.05	95.69	113.40
2	2	147	THR	N-CA-CB	7.22	124.02	110.30
2	2	175	ARG	CD-NE-CZ	7.13	133.58	123.60
1	1	4	ARG	CD-NE-CZ	7.09	133.52	123.60
2	2	228	TYR	CB-CG-CD2	-6.96	116.83	121.00
2	2	173	ARG	NE-CZ-NH2	-6.91	116.84	120.30
2	2	187	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	2	141	TRP	CA-CB-CG	6.85	126.72	113.70
2	2	63	ASP	CB-CG-OD1	6.65	124.29	118.30
2	2	67	ARG	NE-CZ-NH2	-6.51	117.05	120.30
2	2	170	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	2	221(A)	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	2	86	GLU	CG-CD-OE2	-6.19	105.92	118.30
2	2	60(E)	ASP	CB-CG-OD1	6.19	123.87	118.30
2	2	137	ARG	NE-CZ-NH2	6.11	123.35	120.30
2	2	116	ASP	CA-CB-CG	5.99	126.58	113.40
2	2	73	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	2	186(A)	ASP	CB-CG-OD1	5.91	123.61	118.30
2	2	125	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	2	60(E)	ASP	CB-CG-OD2	-5.75	113.12	118.30
2	2	97(A)	GLU	CG-CD-OE2	-5.69	106.92	118.30
2	2	225	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	1	14(G)	LEU	CB-CA-C	5.26	120.20	110.20
2	2	194	ASP	CB-CG-OD1	5.21	122.99	118.30
2	2	101	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
2	2	149	THR	CA-CB-OG1	-5.17	98.15	109.00
2	2	60	LEU	O-C-N	5.11	130.88	122.70
2	2	33	LEU	CB-CA-C	5.11	119.90	110.20
2	2	228	TYR	CB-CG-CD1	5.09	124.05	121.00
1	1	8	GLU	CG-CD-OE1	5.02	128.35	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1(A)	ASP	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	1	211	0	203	35	0
2	2	2049	0	2015	244	0
3	3	85	0	67	3	0
4	2	41	0	35	14	0
5	2	40	0	0	28	0
All	All	2426	0	2320	273	0

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 58.

All (273) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:2:370:IH3:C22	4:2:370:IH3:N20	1.72	1.52
1:1:10:LYS:HB2	1:1:12:LEU:HD12	1.26	1.16
2:2:150:GLY:HA2	5:2:570:HOH:O	1.54	1.07
2:2:228:TYR:OH	5:2:566:HOH:O	1.71	1.06
4:2:370:IH3:O19	5:2:575:HOH:O	1.75	1.04
2:2:165:ARG:NH2	2:2:177:THR:O	1.89	1.04
2:2:70:LYS:HE3	2:2:72:SER:O	1.58	1.03
2:2:139:THR:HG22	2:2:156:GLN:O	1.57	1.03
2:2:215:TRP:HB2	5:2:573:HOH:O	1.65	0.95
2:2:214:SER:O	5:2:572:HOH:O	1.85	0.93
1:1:14(J):TYR:HE2	2:2:202:LYS:O	1.55	0.89
2:2:57:HIS:CE1	5:2:572:HOH:O	2.31	0.84
1:1:14(J):TYR:HD2	2:2:204:PRO:HG3	1.42	0.84
2:2:149:THR:O	2:2:149(A):ALA:CB	2.25	0.84
2:2:151:GLN:H	2:2:152:PRO:CD	1.90	0.84
2:2:244:GLN:HB3	2:2:245:PHE:CD1	2.15	0.81
2:2:91:HIS:HB2	2:2:103:ILE:HG22	1.60	0.81
2:2:91:HIS:HB2	2:2:103:ILE:CG2	2.09	0.81
2:2:95:ASN:N	2:2:100:ASP:O	2.14	0.81
2:2:144:LEU:CD1	2:2:151:GLN:HB3	2.10	0.81
2:2:78:ASN:HD22	2:2:78:ASN:N	1.77	0.80
2:2:126:ARG:O	2:2:129(A):ALA:HB2	1.83	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:195:SER:OG	5:2:584:HOH:O	1.99	0.79
2:2:131:GLN:O	2:2:134:TYR:HB2	1.82	0.79
3:3:565:GLY:HA2	3:3:568:LEU:HD12	1.62	0.79
2:2:124:PRO:HG2	2:2:232:PHE:HB2	1.64	0.77
2:2:57:HIS:NE2	5:2:572:HOH:O	2.18	0.75
2:2:35:ARG:HD3	2:2:39:GLU:CG	2.17	0.74
2:2:134:TYR:O	2:2:162:ILE:HG13	1.88	0.74
2:2:139:THR:CG2	2:2:156:GLN:O	2.35	0.74
2:2:203:SER:HB3	2:2:204(B):ASN:ND2	2.03	0.73
1:1:1(A):ASP:O	2:2:119:HIS:NE2	2.17	0.73
1:1:14:ASP:HB2	2:2:23:GLU:OE2	1.88	0.73
2:2:151:GLN:H	2:2:152:PRO:HD2	1.52	0.73
2:2:160:LEU:CD2	2:2:184:GLY:HA2	2.18	0.73
2:2:95:ASN:HB3	2:2:100:ASP:HB3	1.70	0.72
1:1:14(A):LYS:HZ2	1:1:14(A):LYS:HB2	1.55	0.71
2:2:176:ILE:CD1	2:2:227:PHE:CE2	2.73	0.71
2:2:139:THR:HG23	2:2:157:VAL:HG22	1.72	0.71
2:2:176:ILE:CD1	2:2:215:TRP:HZ2	2.04	0.71
4:2:370:IH3:HC62	5:2:584:HOH:O	1.90	0.71
2:2:168:CYS:O	2:2:171:SER:HB3	1.91	0.71
2:2:217:GLU:HG3	5:2:577:HOH:O	1.89	0.70
2:2:149:THR:O	2:2:149(A):ALA:HB2	1.89	0.70
1:1:10:LYS:HB2	1:1:12:LEU:CD1	2.16	0.69
1:1:1(B):ALA:O	1:1:1:CYS:N	2.26	0.69
1:1:14(A):LYS:HB2	1:1:14(A):LYS:NZ	2.07	0.69
1:1:4:ARG:HD3	2:2:29:TRP:CH2	2.29	0.68
2:2:244:GLN:HB3	2:2:245:PHE:CE1	2.29	0.68
2:2:230:HIS:HB3	2:2:233:ARG:HB2	1.76	0.68
2:2:97:ARG:HG2	2:2:97:ARG:HH11	1.58	0.68
2:2:110:LYS:HB2	2:2:111:PRO:HD2	1.76	0.67
2:2:171:SER:O	2:2:224:LYS:NZ	2.24	0.67
2:2:144:LEU:HG	2:2:151:GLN:HB3	1.77	0.66
2:2:17:VAL:O	2:2:188:GLY:HA2	1.96	0.66
1:1:5:PRO:HA	1:1:9:LYS:HB2	1.77	0.66
2:2:160:LEU:HD22	2:2:184:GLY:HA2	1.78	0.65
2:2:215:TRP:CZ3	5:2:577:HOH:O	2.49	0.65
2:2:176:ILE:HD12	2:2:227:PHE:CE2	2.33	0.64
2:2:78:ASN:ND2	2:2:78:ASN:N	2.44	0.64
2:2:22:ALA:HB2	2:2:157:VAL:HG23	1.80	0.64
2:2:85:LEU:HD21	2:2:106:MET:HB3	1.79	0.64
2:2:50:ARG:NH2	5:2:574:HOH:O	2.20	0.64
4:2:370:IH3:C23	4:2:370:IH3:N20	2.59	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:85:LEU:HD11	2:2:106:MET:CE	2.28	0.63
2:2:36:LYS:HD3	2:2:65:LEU:HD22	1.79	0.63
1:1:14(A):LYS:CB	1:1:14(A):LYS:NZ	2.62	0.63
2:2:35:ARG:HD3	2:2:39:GLU:HG3	1.78	0.63
2:2:203:SER:HB3	2:2:204(B):ASN:HD21	1.64	0.63
2:2:176:ILE:CD1	2:2:215:TRP:CZ2	2.81	0.63
2:2:66:VAL:HG23	2:2:66:VAL:O	1.98	0.62
2:2:165:ARG:CB	2:2:166:PRO:HD3	2.30	0.62
2:2:137:ARG:HB2	2:2:159:ASN:OD1	1.99	0.62
2:2:18:GLU:HB2	2:2:188:GLY:HA2	1.82	0.62
2:2:187:ARG:NE	2:2:221:ASP:OD2	2.26	0.61
4:2:370:IH3:C21	4:2:370:IH3:C22	2.74	0.61
2:2:60(D):TRP:O	2:2:60(E):ASP:HB2	2.00	0.61
2:2:121:VAL:HG22	2:2:122:CYS:N	2.15	0.61
1:1:14:ASP:O	1:1:14(C):GLU:HG2	2.00	0.61
2:2:77:GLU:O	2:2:80:GLU:HG2	2.01	0.60
2:2:165:ARG:CB	2:2:166:PRO:CD	2.80	0.60
2:2:96:TRP:N	5:2:553:HOH:O	2.34	0.60
2:2:63:ASP:OD2	2:2:63:ASP:N	2.34	0.60
2:2:126:ARG:O	2:2:129(A):ALA:CB	2.49	0.60
2:2:176:ILE:HD11	2:2:215:TRP:CZ2	2.37	0.59
2:2:61:GLU:OE1	2:2:88:ILE:HD12	2.03	0.59
2:2:144:LEU:CG	2:2:151:GLN:HB3	2.33	0.59
2:2:204(B):ASN:O	2:2:205:ASN:HB2	2.00	0.59
2:2:84:MET:O	2:2:109:LYS:N	2.31	0.59
2:2:95:ASN:O	2:2:99:LEU:N	2.35	0.59
2:2:211:GLY:HA2	2:2:231:VAL:HG23	1.83	0.59
2:2:98:ASN:N	2:2:98:ASN:OD1	2.36	0.58
2:2:60(A):TYR:CZ	2:2:60(C):PRO:HG2	2.38	0.58
2:2:41:LEU:HD12	2:2:64:LEU:HD22	1.85	0.58
2:2:60(B):PRO:HG2	2:2:96:TRP:CE2	2.38	0.58
2:2:60(I):THR:HG23	2:2:63:ASP:OD1	2.03	0.57
2:2:165:ARG:HB2	2:2:166:PRO:HD3	1.85	0.57
2:2:70:LYS:NZ	2:2:77:GLU:OE2	2.26	0.57
2:2:144:LEU:HD12	2:2:151:GLN:HB3	1.86	0.57
4:2:370:IH3:C22	4:2:370:IH3:C19	2.75	0.57
4:2:370:IH3:H222	5:2:555:HOH:O	2.04	0.57
2:2:126:ARG:NH2	5:2:556:HOH:O	2.39	0.56
2:2:114:PHE:HD1	2:2:118:ILE:HG22	1.68	0.56
2:2:244:GLN:HG2	2:2:245:PHE:CZ	2.40	0.56
2:2:121:VAL:HG22	2:2:122:CYS:H	1.69	0.56
2:2:76:TYR:CE2	2:2:77(A):ARG:HB3	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:18:GLU:HB2	2:2:188:GLY:CA	2.36	0.56
2:2:149:THR:O	2:2:149(A):ALA:HB3	2.05	0.55
2:2:32:MET:HG3	2:2:40:LEU:CD1	2.36	0.55
1:1:1(B):ALA:C	1:1:1:CYS:H	2.10	0.55
2:2:47:ILE:HG21	2:2:53:LEU:HB2	1.88	0.55
1:1:14(J):TYR:CE2	2:2:202:LYS:O	2.47	0.55
2:2:202:LYS:O	2:2:204:PRO:HD3	2.06	0.55
2:2:85:LEU:HD11	2:2:106:MET:HE2	1.88	0.54
2:2:66:VAL:CG2	2:2:66:VAL:O	2.55	0.54
2:2:97:ARG:NH1	2:2:97:ARG:HG2	2.22	0.54
2:2:66:VAL:HG21	2:2:108:LEU:HD21	1.87	0.54
2:2:215:TRP:HE3	5:2:573:HOH:O	1.90	0.54
2:2:51:TRP:HZ3	2:2:89:TYR:CE1	2.26	0.54
2:2:197:GLY:O	2:2:213:VAL:HG23	2.06	0.54
2:2:211:GLY:HA2	2:2:229:THR:O	2.06	0.54
2:2:23:GLU:HG3	2:2:26:MET:CE	2.38	0.53
2:2:203:SER:CB	2:2:204(B):ASN:ND2	2.71	0.53
2:2:91:HIS:CE1	2:2:101:ARG:HD3	2.44	0.53
2:2:35:ARG:O	2:2:38:GLN:HA	2.07	0.53
2:2:129:ALA:O	2:2:130:LEU:HB2	2.09	0.52
2:2:137:ARG:NH2	5:2:583:HOH:O	2.35	0.52
1:1:3:LEU:CD2	2:2:206:ARG:HG2	2.39	0.52
4:2:370:IH3:O21	5:2:573:HOH:O	2.19	0.52
2:2:85:LEU:CD2	2:2:106:MET:HB3	2.40	0.52
2:2:84:MET:O	2:2:109:LYS:HB2	2.09	0.52
2:2:36:LYS:HG2	2:2:65:LEU:HD22	1.92	0.52
2:2:60(C):PRO:HD3	2:2:96:TRP:CZ3	2.44	0.52
2:2:81:LYS:CE	5:2:560:HOH:O	2.57	0.51
4:2:370:IH3:HC23	5:2:573:HOH:O	2.10	0.51
2:2:85:LEU:HD11	2:2:106:MET:HE3	1.92	0.51
2:2:179:ASN:OD1	2:2:233:ARG:HD2	2.11	0.50
2:2:73:ARG:HG2	2:2:73:ARG:NH2	2.26	0.50
2:2:215:TRP:HZ3	5:2:577:HOH:O	1.92	0.50
2:2:60:LEU:HG	2:2:60(B):PRO:HD3	1.93	0.50
2:2:212:ILE:HD12	2:2:229:THR:HB	1.92	0.50
2:2:77(A):ARG:HB2	2:2:78:ASN:ND2	2.27	0.50
2:2:215:TRP:O	2:2:227:PHE:HB2	2.12	0.50
2:2:228:TYR:CZ	5:2:566:HOH:O	2.52	0.49
2:2:171:SER:OG	5:2:565:HOH:O	2.05	0.49
2:2:19:GLY:HA3	2:2:157:VAL:O	2.12	0.49
2:2:127:GLU:O	2:2:129(A):ALA:HB3	2.12	0.49
2:2:176:ILE:HD11	2:2:215:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:3:LEU:HD21	2:2:206:ARG:HG2	1.93	0.49
2:2:98:ASN:OD1	2:2:100:ASP:HB2	2.11	0.49
2:2:95:ASN:CB	2:2:100:ASP:HB3	2.39	0.49
2:2:130:LEU:HD23	2:2:162:ILE:HD12	1.93	0.49
2:2:174:ILE:CD1	4:2:370:IH3:C32	2.91	0.49
2:2:139:THR:HG23	2:2:157:VAL:CG2	2.40	0.49
2:2:73:ARG:HH12	3:3:559:ASP:CG	2.16	0.49
2:2:185:LYS:HB2	2:2:186(A):ASP:OD2	2.13	0.49
1:1:1(A):ASP:OD2	1:1:9:LYS:NZ	2.37	0.49
2:2:136:GLY:HA3	2:2:199:PHE:CZ	2.48	0.49
1:1:3:LEU:O	1:1:9:LYS:HE3	2.13	0.48
2:2:67:ARG:HH21	2:2:80:GLU:CD	2.17	0.48
1:1:14(J):TYR:CD2	2:2:204:PRO:HG3	2.34	0.48
2:2:60(D):TRP:CH2	4:2:370:IH3:H161	2.48	0.48
2:2:163:VAL:HG11	2:2:167:VAL:CG1	2.43	0.48
2:2:19:GLY:CA	2:2:157:VAL:O	2.61	0.48
2:2:17:VAL:HA	2:2:144:LEU:O	2.13	0.48
2:2:91:HIS:HE1	2:2:93:ARG:HG3	1.78	0.48
2:2:41:LEU:CD1	2:2:64:LEU:HD22	2.43	0.48
2:2:130:LEU:HD23	2:2:162:ILE:CD1	2.44	0.48
2:2:81:LYS:NZ	5:2:560:HOH:O	2.22	0.48
2:2:77(A):ARG:HE	2:2:78:ASN:ND2	2.12	0.48
2:2:182:CYS:SG	2:2:225:TYR:HB2	2.53	0.48
2:2:41:LEU:HD12	2:2:64:LEU:CD2	2.44	0.47
1:1:10:LYS:CB	1:1:12:LEU:HD12	2.19	0.47
2:2:17:VAL:HG22	2:2:144:LEU:O	2.15	0.47
1:1:5:PRO:HA	1:1:9:LYS:HD2	1.96	0.47
2:2:36:LYS:CD	2:2:65:LEU:HD22	2.44	0.47
1:1:14(I):SER:C	1:1:14(K):ILE:H	2.17	0.47
2:2:211:GLY:CA	2:2:231:VAL:HG23	2.44	0.47
2:2:70:LYS:CE	2:2:72:SER:O	2.47	0.46
1:1:1(B):ALA:HB3	2:2:206:ARG:HH12	1.79	0.46
1:1:1(B):ALA:CB	2:2:206:ARG:HH12	2.28	0.46
1:1:6:LEU:HD23	2:2:25:GLY:HA3	1.96	0.46
2:2:21:ASP:OD1	2:2:156:GLN:OE1	2.32	0.46
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.45	0.46
2:2:45:SER:HB3	2:2:198:PRO:HG3	1.98	0.46
2:2:163:VAL:HG12	2:2:164:GLU:N	2.31	0.46
2:2:60(B):PRO:HG2	2:2:96:TRP:CZ2	2.50	0.46
2:2:57:HIS:NE2	2:2:195:SER:HB3	2.31	0.46
2:2:204(B):ASN:ND2	2:2:206:ARG:H	2.13	0.46
2:2:185:LYS:C	2:2:186(A):ASP:H	2.18	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:103:ILE:HG23	2:2:237:TRP:CZ3	2.51	0.45
2:2:28:PRO:HB2	2:2:119:HIS:HB3	1.97	0.45
2:2:94:TYR:HE1	2:2:99:LEU:CD2	2.29	0.45
2:2:182:CYS:SG	2:2:225:TYR:CB	3.05	0.45
2:2:204(B):ASN:OD1	2:2:206:ARG:HD2	2.16	0.45
2:2:65:LEU:HG	2:2:82:ILE:HG22	1.98	0.45
2:2:66:VAL:HG21	2:2:108:LEU:CD2	2.46	0.45
2:2:77(A):ARG:HE	2:2:78:ASN:HD21	1.64	0.45
1:1:7:PHE:C	1:1:9:LYS:N	2.70	0.45
2:2:91:HIS:CE1	2:2:93:ARG:H	2.33	0.45
2:2:95:ASN:HB3	2:2:100:ASP:CB	2.40	0.45
2:2:190:ALA:CB	2:2:213:VAL:HG11	2.46	0.45
2:2:200:VAL:HG23	2:2:207:TRP:CE3	2.52	0.45
1:1:1(B):ALA:CB	2:2:206:ARG:NH1	2.79	0.45
2:2:70:LYS:HZ1	2:2:77:GLU:HG3	1.82	0.45
2:2:182:CYS:HA	2:2:226:GLY:O	2.17	0.45
3:3:564:PRO:O	3:3:567:TYS:HD2	2.16	0.45
2:2:60:LEU:HA	2:2:60(F):LYS:O	2.16	0.45
2:2:185:LYS:C	2:2:186(A):ASP:N	2.70	0.45
2:2:79:ILE:HG21	5:2:550:HOH:O	2.17	0.44
2:2:185:LYS:CB	2:2:186(A):ASP:OD2	2.65	0.44
2:2:204(B):ASN:O	2:2:205:ASN:CB	2.65	0.44
2:2:139:THR:CG2	2:2:157:VAL:HG22	2.45	0.44
2:2:176:ILE:HD11	2:2:227:PHE:CE2	2.53	0.44
2:2:196:GLY:HA2	2:2:212:ILE:CG2	2.47	0.44
2:2:165:ARG:O	2:2:168:CYS:N	2.50	0.44
1:1:1(B):ALA:HB1	2:2:206:ARG:NH1	2.33	0.44
2:2:70:LYS:NZ	2:2:77:GLU:HG3	2.32	0.44
2:2:91:HIS:CE1	2:2:93:ARG:HG3	2.52	0.44
2:2:230:HIS:CB	2:2:233:ARG:HB2	2.47	0.44
2:2:45:SER:O	2:2:53:LEU:N	2.40	0.44
2:2:163:VAL:HG23	2:2:183:ALA:HA	1.99	0.43
2:2:41:LEU:O	2:2:42:CYS:SG	2.76	0.43
2:2:230:HIS:ND1	2:2:233:ARG:HB2	2.34	0.43
2:2:174:ILE:CD1	4:2:370:IH3:C31	2.97	0.43
2:2:139:THR:CG2	2:2:157:VAL:CG2	2.97	0.43
2:2:163:VAL:HG11	2:2:167:VAL:HG11	1.99	0.43
2:2:172:THR:OG1	2:2:173:ARG:N	2.51	0.43
2:2:70:LYS:HA	2:2:77:GLU:OE2	2.19	0.43
2:2:57:HIS:CD2	4:2:370:IH3:HC13	2.54	0.43
2:2:50:ARG:NH1	2:2:109:LYS:O	2.52	0.43
2:2:47:ILE:CG2	2:2:53:LEU:HB2	2.47	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:136:GLY:HA2	2:2:201:MET:HG2	2.00	0.43
2:2:165:ARG:N	2:2:166:PRO:HD2	2.34	0.43
2:2:17:VAL:O	2:2:188:GLY:CA	2.65	0.43
2:2:215:TRP:CE3	5:2:577:HOH:O	2.69	0.42
2:2:130:LEU:HA	2:2:130:LEU:HD23	1.86	0.42
2:2:201:MET:SD	2:2:210:MET:HG3	2.59	0.42
2:2:186(B):GLU:O	2:2:186(C):GLY:C	2.57	0.42
2:2:60:LEU:HD12	2:2:60(G):ASN:HB2	2.02	0.42
1:1:6:LEU:HD12	1:1:10:LYS:HE3	2.01	0.42
2:2:23:GLU:HB2	2:2:26:MET:HB2	2.02	0.42
2:2:30:GLN:HG2	2:2:155:LEU:CD2	2.50	0.42
2:2:103:ILE:HG12	2:2:237:TRP:HZ3	1.85	0.42
2:2:94:TYR:CE1	2:2:99:LEU:CD2	3.03	0.42
1:1:6:LEU:HD12	1:1:6:LEU:HA	1.88	0.42
2:2:94:TYR:CE1	2:2:99:LEU:HD23	2.55	0.41
1:1:1:CYS:O	2:2:206:ARG:NH2	2.52	0.41
2:2:35:ARG:NE	2:2:37:PRO:HD2	2.35	0.41
2:2:161:PRO:HG3	2:2:184(A):TYR:CE2	2.55	0.41
2:2:94:TYR:HA	2:2:100:ASP:O	2.20	0.41
2:2:97:ARG:NH1	2:2:97:ARG:CG	2.81	0.41
2:2:190:ALA:HB1	2:2:213:VAL:HG11	2.02	0.41
2:2:73:ARG:CG	2:2:73:ARG:HH21	2.32	0.41
2:2:132:ALA:HA	2:2:162:ILE:O	2.21	0.41
2:2:160:LEU:HD22	2:2:184:GLY:CA	2.49	0.41
2:2:32:MET:CE	2:2:70:LYS:HD3	2.50	0.41
2:2:156:GLN:HB2	5:2:580:HOH:O	2.21	0.41
2:2:77(A):ARG:C	2:2:79:ILE:H	2.23	0.41
2:2:51:TRP:CZ3	2:2:89:TYR:CE1	3.07	0.41
1:1:6:LEU:HD13	2:2:116:ASP:HB3	2.03	0.40
2:2:153:SER:HB3	5:2:587:HOH:O	2.21	0.40
2:2:123:LEU:HD23	2:2:123:LEU:HA	1.82	0.40
2:2:99:LEU:HA	2:2:99:LEU:HD23	1.99	0.40
1:1:14(C):GLU:O	1:1:14(F):LEU:HB2	2.22	0.40
2:2:160:LEU:HA	2:2:161:PRO:HD3	1.93	0.40
2:2:30:GLN:HG2	2:2:155:LEU:HD21	2.02	0.40
2:2:95:ASN:HD21	2:2:97(A):GLU:HB3	1.86	0.40
2:2:60(D):TRP:CZ3	4:2:370:IH3:H161	2.57	0.40
2:2:187:ARG:HB2	2:2:188:GLY:H	1.70	0.40
2:2:87:LYS:HD3	2:2:88:ILE:H	1.86	0.40
2:2:73:ARG:HG2	2:2:73:ARG:HH21	1.85	0.40
2:2:241:VAL:O	2:2:242:ILE:C	2.60	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	25/36 (69%)	16 (64%)	8 (32%)	1 (4%)	5	9
2	2	250/259 (96%)	229 (92%)	19 (8%)	2 (1%)	27	58
3	3	7/13 (54%)	7 (100%)	0	0	100	100
All	All	282/308 (92%)	252 (89%)	27 (10%)	3 (1%)	21	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	1(A)	ASP
2	2	151	GLN
2	2	186(C)	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	23/31 (74%)	16 (70%)	7 (30%)	0	1
2	2	220/225 (98%)	191 (87%)	29 (13%)	6	14
3	3	7/10 (70%)	6 (86%)	1 (14%)	5	12
All	All	250/266 (94%)	213 (85%)	37 (15%)	4	11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1(A)	ASP
1	1	3	LEU
1	1	6	LEU

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Mol	Chain	Res	Type
1	1	11	SER
1	1	12	LEU
1	1	14(I)	SER
1	1	14(J)	TYR
2	2	26	MET
2	2	33	LEU
2	2	35	ARG
2	2	41	LEU
2	2	48	SER
2	2	50	ARG
2	2	60(I)	THR
2	2	61	GLU
2	2	63	ASP
2	2	65	LEU
2	2	67	ARG
2	2	77(A)	ARG
2	2	78	ASN
2	2	82	ILE
2	2	83	SER
2	2	87	LYS
2	2	109	LYS
2	2	129(C)	LEU
2	2	139	THR
2	2	147	THR
2	2	149	THR
2	2	161	PRO
2	2	165	ARG
2	2	181	PHE
2	2	182	CYS
2	2	204(B)	ASN
2	2	224	LYS
2	2	235	LYS
2	2	242	ILE
3	3	568	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	78	ASN
2	2	156	GLN
2	2	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 ⓘ

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	3	567	3	16,16,17	4.21	2 (12%)	20,22,24	2.23	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	TYS	3	567	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	3	567	TYS	O-C	15.94	1.22	1.11
3	3	567	TYS	OH-CZ	-4.78	1.36	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	CZ-OH-S	6.56	128.82	118.98
3	3	567	TYS	C-CA-N	-5.14	108.70	113.83
3	3	567	TYS	OH-CZ-CE1	3.56	124.62	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

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	IH3	2	370	-	46,46,46	5.00	28 (60%)	56,66,66	2.53	20 (35%)

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	IH3	2	370	-	-	0/21/46/46	0/4/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	370	IH3	C22-N20	21.26	1.72	1.48
4	2	370	IH3	C8-N10	-11.02	1.24	1.46
4	2	370	IH3	C35-C30	9.64	1.55	1.39
4	2	370	IH3	C32-C31	9.25	1.60	1.39
4	2	370	IH3	C29-C24	7.56	1.52	1.39
4	2	370	IH3	C12-C11	-7.54	1.46	1.53
4	2	370	IH3	C16-N17	-5.90	1.40	1.46
4	2	370	IH3	C34-C35	5.49	1.51	1.39
4	2	370	IH3	C12-C13	4.70	1.54	1.50
4	2	370	IH3	C28-C29	4.35	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	370	IH3	C31-C30	4.06	1.46	1.39
4	2	370	IH3	C6-C7	3.90	1.63	1.52
4	2	370	IH3	C16-C14	3.90	1.54	1.50
4	2	370	IH3	C27-C26	3.88	1.49	1.37
4	2	370	IH3	C26-C25	3.49	1.47	1.39
4	2	370	IH3	C7-C8	3.22	1.60	1.51
4	2	370	IH3	C28-C27	3.01	1.46	1.37
4	2	370	IH3	N18-N17	2.97	1.43	1.38
4	2	370	IH3	C25-C24	2.78	1.43	1.39
4	2	370	IH3	C33-C32	2.77	1.45	1.37
4	2	370	IH3	C19-N17	2.68	1.40	1.35
4	2	370	IH3	C12-N18	-2.46	1.40	1.46
4	2	370	IH3	C1-C5	-2.44	1.45	1.50
4	2	370	IH3	C13-C14	2.13	1.37	1.32
4	2	370	IH3	C34-C33	2.11	1.44	1.37
4	2	370	IH3	C15-C14	2.10	1.56	1.50
4	2	370	IH3	C4-C5	2.03	1.59	1.53
4	2	370	IH3	C22-C23	-2.03	1.49	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	370	IH3	NC-C3-NA	-8.38	107.61	111.08
4	2	370	IH3	C8-N10-C11	-6.06	113.41	123.18
4	2	370	IH3	C9-C8-N10	-5.51	100.46	110.57
4	2	370	IH3	C16-N17-N18	5.12	123.44	119.03
4	2	370	IH3	C4-C9-C8	4.96	118.33	111.47
4	2	370	IH3	C5-C1-NC	3.88	125.70	121.54
4	2	370	IH3	C23-C22-N20	-3.71	106.95	112.19
4	2	370	IH3	C2-NA-C3	3.64	110.00	103.54
4	2	370	IH3	C15-C14-C16	3.63	119.11	113.31
4	2	370	IH3	C7-C6-C5	3.40	117.14	110.34
4	2	370	IH3	C15-C14-C13	-3.35	116.96	122.38
4	2	370	IH3	C11-C12-N18	2.97	116.07	110.81
4	2	370	IH3	C35-C30-C31	-2.58	114.91	118.33
4	2	370	IH3	C7-C8-N10	-2.56	105.88	110.57
4	2	370	IH3	C33-C32-C31	2.50	124.34	120.17
4	2	370	IH3	C4-C5-C1	-2.50	108.76	112.45
4	2	370	IH3	C16-N17-C19	2.49	128.39	124.06
4	2	370	IH3	C34-C35-C30	2.43	123.84	120.61
4	2	370	IH3	C16-C14-C13	2.35	123.93	116.88
4	2	370	IH3	C35-C30-C23	2.02	126.92	120.79



There are no chirality outliers.

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 ⓘ

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.