



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:30 PM UTC

PDB ID : 1C4Y / pdb_00001c4y
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

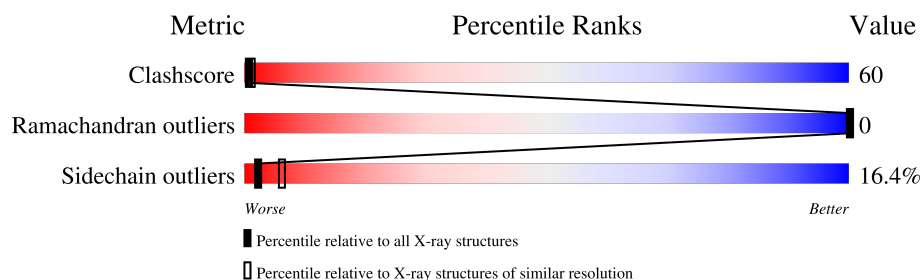
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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 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 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			

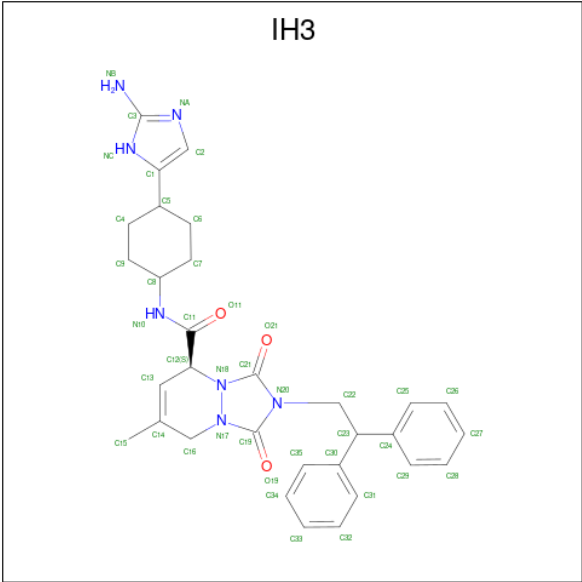
- Molecule 2 is a protein called THROMBIN:LONG CHAIN.

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-CARBOXYLIC ACID [4-(2-AMINO-3H-I MIDAZOL-4-YL)-CYCLOHEXYL]-AMIDE (CCD ID: IH3) (formula: C₃₁H₃₅N₇O₃).



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

- Molecule 5 is water.

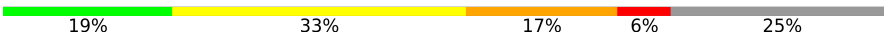
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	40	Total	O	0	0
			40	40		

3 Residue-property plots [i](#)

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

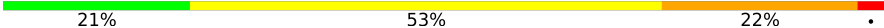
Note EDS was not executed.

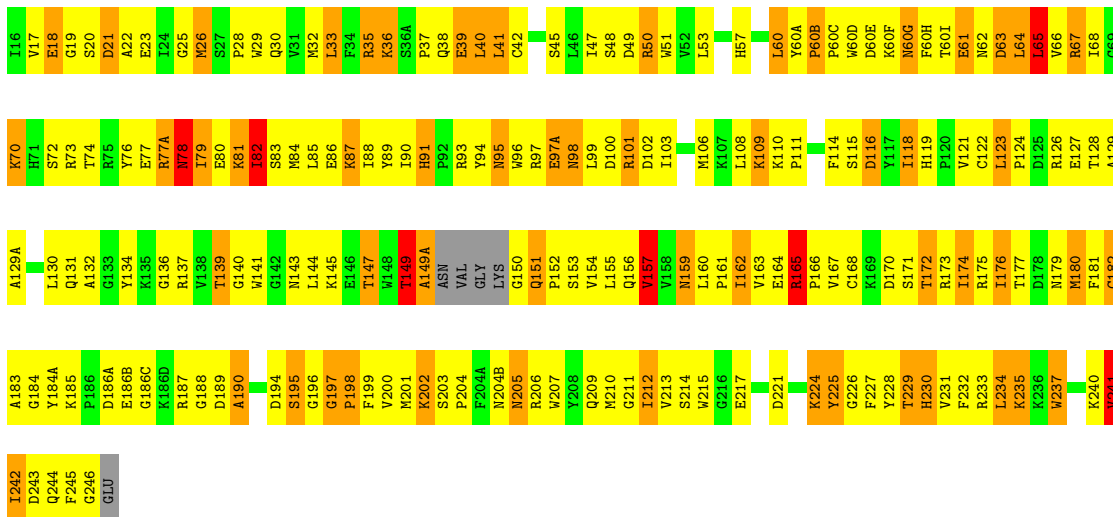
• Molecule 1: THROMBIN:SHORT CHAIN

Chain 1: 



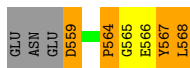
• Molecule 2: THROMBIN:LONG CHAIN

Chain 2: 



• Molecule 3: HIRUGEN

Chain 3: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	19.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.07	0/213	2.27	7/283 (2.5%)
2	2	1.17	5/2103 (0.2%)	2.09	82/2844 (2.9%)
3	3	0.98	0/69	2.40	4/89 (4.5%)
All	All	1.16	5/2385 (0.2%)	2.11	93/3216 (2.9%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	212	ILE	CA-CB	9.82	1.66	1.54
2	2	229	THR	CA-CB	8.27	1.66	1.53
2	2	36	LYS	CA-CB	6.88	1.64	1.53
2	2	212	ILE	CA-C	5.51	1.59	1.52
2	2	118	ILE	CA-CB	5.02	1.60	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1(A)	ASP	CA-CB-CG	-16.91	95.69	112.60
2	2	116	ASP	CA-CB-CG	13.98	126.58	112.60
2	2	189	ASP	CA-CB-CG	11.49	124.09	112.60
2	2	101	ARG	CD-NE-CZ	11.02	139.83	124.40
2	2	101	ARG	NE-CZ-NH1	10.68	132.18	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	564	PRO	CA-C-N	8.85	129.94	120.03
3	3	564	PRO	C-N-CA	8.85	129.94	120.03
2	2	205	ASN	CA-CB-CG	-8.27	104.33	112.60
2	2	205	ASN	OD1-CG-ND2	8.18	130.78	122.60
2	2	230	HIS	CA-CB-CG	-7.74	106.06	113.80
2	2	149	THR	CA-CB-OG1	-7.63	98.15	109.60
2	2	123	LEU	CB-CA-C	7.22	119.66	108.61
2	2	170	ASP	CA-C-N	7.11	131.48	120.82
2	2	170	ASP	C-N-CA	7.11	131.48	120.82
2	2	74	THR	N-CA-C	7.08	122.28	112.45
2	2	65	LEU	CA-C-O	-7.03	111.62	120.20
2	2	147	THR	N-CA-CB	6.95	124.02	111.37
2	2	147	THR	CA-CB-OG1	-6.91	99.23	109.60
2	2	141	TRP	CA-CB-CG	6.90	126.72	113.60
2	2	240	LYS	N-CA-C	6.74	118.42	111.14
2	2	181	PHE	CA-CB-CG	6.68	120.48	113.80
2	2	91	HIS	CA-CB-CG	-6.66	107.14	113.80
2	2	60(G)	ASN	CA-CB-CG	6.59	119.19	112.60
2	2	234	LEU	CA-C-N	6.58	129.10	120.28
2	2	234	LEU	C-N-CA	6.58	129.10	120.28
2	2	175	ARG	CD-NE-CZ	6.56	133.58	124.40
1	1	4	ARG	CD-NE-CZ	6.51	133.52	124.40
2	2	115	SER	CA-C-O	-6.28	113.91	121.32
1	1	4	ARG	NE-CZ-NH1	6.27	127.77	121.50
2	2	18	GLU	CB-CA-C	-6.21	101.76	111.39
1	1	3	LEU	O-C-N	6.21	130.44	123.05
1	1	10	LYS	N-CA-C	-6.20	104.88	112.88
2	2	39	GLU	N-CA-C	6.18	118.69	108.99
2	2	98	ASN	CA-CB-CG	-6.12	106.47	112.60
2	2	128	THR	CA-CB-OG1	-6.08	100.47	109.60
2	2	60(B)	PRO	CB-CA-C	6.01	118.26	110.92
3	3	559	ASP	CA-CB-CG	6.01	118.61	112.60
2	2	64	LEU	N-CA-CB	-5.99	101.21	110.56
2	2	225	TYR	CA-C-N	5.91	127.39	120.71
2	2	225	TYR	C-N-CA	5.91	127.39	120.71
2	2	159	ASN	CA-CB-CG	5.91	118.51	112.60
2	2	101	ARG	NE-CZ-NH2	-5.80	113.98	119.20
2	2	81	LYS	CA-C-O	5.77	126.36	120.24
2	2	95	ASN	OD1-CG-ND2	5.68	128.28	122.60
2	2	172	THR	N-CA-C	5.68	118.04	109.41
2	2	209	GLN	CB-CG-CD	-5.67	102.95	112.60
2	2	145	LYS	CA-C-O	-5.63	114.85	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	14(A)	LYS	CA-C-O	-5.60	113.00	119.61
1	1	14(G)	LEU	CB-CA-C	5.60	120.20	110.68
2	2	194	ASP	O-C-N	5.58	129.22	122.35
2	2	18	GLU	CA-C-O	-5.53	113.94	120.57
2	2	202	LYS	N-CA-C	5.49	117.70	108.96
2	2	33	LEU	CB-CA-C	5.47	119.90	110.77
2	2	60(G)	ASN	CB-CA-C	5.46	118.86	111.70
2	2	165	ARG	NE-CZ-NH1	5.46	126.96	121.50
2	2	229	THR	CA-CB-OG1	-5.46	101.42	109.60
2	2	86	GLU	CG-CD-OE2	-5.42	105.92	118.40
2	2	237	TRP	O-C-N	5.39	128.37	122.11
2	2	151	GLN	O-C-N	5.36	127.49	121.32
2	2	229	THR	CA-C-N	5.36	130.83	122.26
2	2	229	THR	C-N-CA	5.36	130.83	122.26
2	2	149(A)	ALA	CA-C-O	-5.35	111.70	120.80
2	2	172	THR	CA-C-N	5.33	131.33	122.54
2	2	172	THR	C-N-CA	5.33	131.33	122.54
2	2	241	VAL	N-CA-C	-5.33	105.52	110.53
2	2	147	THR	CA-C-N	-5.28	115.37	123.07
2	2	147	THR	C-N-CA	-5.28	115.37	123.07
2	2	77(A)	ARG	N-CA-CB	5.27	118.02	110.06
2	2	49	ASP	CA-CB-CG	5.27	117.87	112.60
2	2	180	MET	CA-C-O	-5.26	115.47	121.58
2	2	60(H)	PHE	CA-C-O	-5.23	114.91	120.92
2	2	102	ASP	CA-CB-CG	5.22	117.82	112.60
3	3	566	GLU	CB-CG-CD	5.19	121.43	112.60
2	2	212	ILE	CA-CB-CG1	5.17	119.19	110.40
2	2	209	GLN	OE1-CD-NE2	5.14	127.74	122.60
2	2	190	ALA	N-CA-C	-5.14	102.88	110.48
2	2	21	ASP	CA-CB-CG	-5.13	107.47	112.60
2	2	189	ASP	O-C-N	5.13	128.08	123.26
2	2	97(A)	GLU	N-CA-C	5.12	119.14	112.13
2	2	60	LEU	O-C-N	5.11	130.88	122.70
2	2	157	VAL	N-CA-CB	-5.11	102.47	111.93
2	2	40	LEU	CB-CA-C	5.10	118.37	109.65
2	2	70	LYS	N-CA-CB	5.09	118.19	110.45
2	2	235	LYS	CA-CB-CG	5.08	124.27	114.10
2	2	143	ASN	OD1-CG-ND2	5.08	127.68	122.60
2	2	20	SER	O-C-N	5.04	128.90	123.10
2	2	147	THR	N-CA-C	-5.04	101.54	109.50
2	2	82	ILE	N-CA-CB	-5.03	105.24	110.72
2	2	198	PRO	CA-C-N	5.02	130.71	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	198	PRO	C-N-CA	5.02	130.71	123.13
2	2	140	GLY	O-C-N	5.01	129.48	123.67
2	2	78	ASN	CB-CA-C	5.01	117.27	110.06
2	2	197	GLY	CA-C-O	-5.00	117.61	122.46

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 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	1	211	0	203	37	0
2	2	2049	0	2015	251	0
3	3	85	0	67	4	0
4	2	41	0	35	14	0
5	2	40	0	0	28	0
All	All	2426	0	2320	282	0

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 60.

All (282) 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)
4:2:370:IH3:N20	4:2:370:IH3:C22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:23:GLU:HG3	2:2:26:MET:HE3	1.50	0.92
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:N	2:2:78:ASN:HD22	1.77	0.80
2:2:126:ARG:O	2:2:129(A):ALA:HB2	1.83	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
2:2:129:ALA:HA	2:2:210:MET:HE1	1.64	0.77
1:1:14(A):LYS:HB2	1:1:14(A):LYS:HZ2	1.50	0.77
2:2:228:TYR:OH	5:2:566:HOH:O	1.71	0.76
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
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
2:2:168:CYS:O	2:2:171:SER:HB3	1.91	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
2:2:217: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:97:ARG:HG2	2:2:97:ARG:HH11	1.58	0.68
2:2:230:HIS:HB3	2:2:233:ARG:HB2	1.76	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
1:1:5:PRO:HA	1:1:9:LYS:HB2	1.77	0.66
2:2:17:VAL:O	2:2:188:GLY:HA2	1.96	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
2:2:78:ASN:N	2:2:78:ASN:ND2	2.44	0.64
2:2:176:ILE:HD12	2:2:227:PHE:CE2	2.33	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:N20	4:2:370:IH3:C23	2.59	0.63
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:NZ	1:1:14(A):LYS:CB	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:O	2:2:66:VAL:HG23	1.98	0.62
2:2:137:ARG:HB2	2:2:159:ASN:OD1	1.99	0.62
2:2:165:ARG:CB	2:2:166:PRO:HD3	2.30	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:C22	4:2:370:IH3:C21	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
2:2:85:LEU:HD11	2:2:106:MET:HE3	1.82	0.61
2:2:77:GLU:O	2:2:80:GLU:HG2	2.01	0.60
2:2:96:TRP:N	5:2:553:HOH:O	2.34	0.60
2:2:165:ARG:CB	2:2:166:PRO:CD	2.80	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
1:1:1(B):ALA:C	1:1:1:CYS:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:84:MET:O	2:2:109:LYS:N	2.31	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
2:2:95: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
2:2:60(A):TYR:CZ	2:2:60(C):PRO:HG2	2.38	0.58
2:2:98:ASN:OD1	2:2:98:ASN:N	2.36	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
2:2:195:SER:OG	5:2:584:HOH:O	1.99	0.58
2:2:60(I):THR:HG23	2:2:63:ASP:OD1	2.03	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
2:2:165:ARG:HB2	2:2:166:PRO:HD3	1.85	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
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
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
2:2:66:VAL:O	2:2:66:VAL:CG2	2.55	0.54
2:2:97:ARG:HG2	2:2:97:ARG:NH1	2.22	0.54
2:2:66:VAL:HG21	2:2:108:LEU:HD21	1.87	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
2:2:215:TRP:HE3	5:2:573:HOH:O	1.90	0.54
2:2:211:GLY:HA2	2:2:229:THR:O	2.06	0.54
2:2:67:ARG:HH21	2:2:80:GLU:CD	2.17	0.53
2:2:203:SER:CB	2:2:204(B):ASN:ND2	2.71	0.53
2:2:98:ASN:HB2	2:2:180:MET:HE1	1.91	0.53
2:2:35:ARG:O	2:2:38:GLN:HA	2.07	0.53
2:2:91:HIS:CE1	2:2:101:ARG:HD3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:36:LYS:HG2	2:2:65:LEU:HD22	1.92	0.52
2:2:73:ARG:HH12	3:3:559:ASP:CG	2.16	0.52
2:2:84:MET:O	2:2:109:LYS:HB2	2.09	0.52
1:1:14(I):SER:C	1:1:14(K):ILE:H	2.17	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
2:2:73:ARG:HG2	2:2:73:ARG:NH2	2.26	0.50
2:2:179:ASN:OD1	2:2:233:ARG:HD2	2.11	0.50
2:2:185:LYS:C	2:2:186(A):ASP:H	2.18	0.50
2:2:60:LEU:HG	2:2:60(B):PRO:HD3	1.93	0.50
2:2:215:TRP:HZ3	5:2:577:HOH:O	1.92	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
2:2:19: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
2:2:171:SER:OG	5:2:565:HOH:O	2.05	0.49
2:2:176:ILE:HD11	2:2:215:TRP:CH2	2.47	0.49
1:1:3:LEU:HD21	2:2:206:ARG:HG2	1.93	0.49
2:2:95:ASN:CB	2:2:100:ASP:HB3	2.39	0.49
2:2:98:ASN:OD1	2:2:100:ASP:HB2	2.11	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
2:2:185: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
1:1:7:PHE:C	1:1:9:LYS:N	2.70	0.48
1:1:14(J):TYR:CD2	2:2:204:PRO:HG3	2.34	0.48
2:2:228:TYR:CZ	5:2:566:HOH:O	2.52	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
2:2:17:VAL:HA	2:2:144:LEU:O	2.13	0.48
2:2:19:GLY:CA	2:2:157:VAL:O	2.61	0.48
2:2:41:LEU:CD1	2:2:64:LEU:HD22	2.43	0.48
2:2:91:HIS:HE1	2:2:93:ARG:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:81:LYS:NZ	5:2:560:HOH:O	2.22	0.48
2:2:130:LEU:HD23	2:2:162:ILE:CD1	2.44	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
2:2:185:LYS:C	2:2:186(A):ASP:N	2.70	0.47
1:1:5:PRO:HA	1:1:9:LYS:HD2	1.96	0.47
2:2:17:VAL:HG22	2:2:144:LEU:O	2.15	0.47
2:2:36:LYS:CD	2:2:65:LEU:HD22	2.44	0.47
2:2:186(B):GLU:O	2:2:186(C):GLY:C	2.57	0.47
2:2:211:GLY:CA	2:2:231:VAL:HG23	2.44	0.47
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
2:2:70:LYS:CE	2:2:72:SER:O	2.47	0.46
1:1:6:LEU:HD23	2:2:25:GLY:HA3	1.96	0.46
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.45	0.46
2:2:21:ASP:OD1	2:2:156:GLN:OE1	2.32	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
2:2:28:PRO:HB2	2:2:119:HIS:HB3	1.97	0.45
2:2:103:ILE:HG23	2:2:237:TRP:CZ3	2.51	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
2:2:65: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:C	2:2:79:ILE:H	2.23	0.45
2:2:204(B):ASN:OD1	2:2:206:ARG:HD2	2.16	0.45
2:2:77(A):ARG:HE	2:2:78:ASN:HD21	1.64	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
2:2:241:VAL:O	2:2:242:ILE:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:60:LEU:HA	2:2:60(F):LYS:O	2.16	0.45
2:2:242:ILE:O	2:2:246:GLY:C	2.60	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
2:2:45:SER:O	2:2:53:LEU:N	2.40	0.44
2:2:84:MET:HE2	3:3:567:TYS:O	2.18	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
2:2:85:LEU:HD11	2:2:106:MET:HE2	1.99	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
2:2:139: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
2:2:174:ILE:CD1	4:2:370:IH3:C31	2.97	0.43
2:2:70:LYS:HA	2:2:77:GLU:OE2	2.19	0.43
2:2:47:ILE:CG2	2:2:53:LEU:HB2	2.47	0.43
2:2:50:ARG:NH1	2:2:109:LYS:O	2.52	0.43
2:2:57:HIS:CD2	4:2:370:IH3:HC13	2.54	0.43
2:2:136:GLY:HA2	2:2:201:MET:HG2	2.00	0.43
2:2:17:VAL:O	2:2:188:GLY:CA	2.65	0.43
2:2:165:ARG:N	2:2:166:PRO:HD2	2.34	0.43
2:2:215:TRP:CE3	5:2:577:HOH:O	2.69	0.42
2:2:130:LEU:HD23	2:2:130:LEU:HA	1.86	0.42
2:2:243:ASP:C	2:2:243:ASP:OD1	2.62	0.42
2:2:201:MET:SD	2:2:210:MET:HG3	2.59	0.42
1:1:7:PHE:C	1:1:9:LYS:H	2.28	0.42
1:1:14(I):SER:C	1:1:14(K):ILE:N	2.78	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
2:2:94:TYR:CE1	2:2:99:LEU:CD2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:ILE:HG12	2:2:237:TRP:HZ3	1.85	0.42
1:1:6:LEU:HD12	1:1:6:LEU:HA	1.88	0.42
2:2:154:VAL:O	2:2:155:LEU:C	2.62	0.42
1:1:1:CYS:O	2:2:206:ARG:NH2	2.52	0.41
2:2:94:TYR:CE1	2:2:99:LEU:HD23	2.55	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
2:2:51:TRP:CZ3	2:2:89:TYR:CE1	3.07	0.41
2:2:156:GLN:HB2	5:2:580:HOH:O	2.21	0.41
2:2:187:ARG:HE	2:2:221:ASP:CG	2.23	0.41
1:1:6:LEU:HD13	2:2:116:ASP:HB3	2.03	0.40
2:2:123:LEU:HD23	2:2:123:LEU:HA	1.82	0.40
2:2:153:SER:HB3	5:2:587:HOH:O	2.21	0.40
2:2:99:LEU:HD23	2:2:99:LEU:HA	1.99	0.40
1:1:14(C):GLU:O	1:1:14(F):LEU:HB2	2.22	0.40
2:2:30:GLN:HG2	2:2:155:LEU:HD21	2.02	0.40
2:2:160:LEU:HA	2:2:161:PRO:HD3	1.93	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
2:2:73:ARG:HG2	2:2:73:ARG:HH21	1.85	0.40
2:2:87:LYS:HD3	2:2:88:ILE:H	1.86	0.40
2:2:187:ARG:HB2	2:2:188:GLY:H	1.70	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	
2	2	39/259 (15%)	36 (92%)	3 (8%)	0	100	100
3	3	7/13 (54%)	7 (100%)	0	0	100	100
All	All	46/272 (17%)	43 (94%)	3 (6%)	0	100	100

There are no Ramachandran outliers to report.

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%)	17 (74%)	6 (26%)	0	2
2	2	220/225 (98%)	186 (84%)	34 (16%)	2	7
3	3	7/10 (70%)	6 (86%)	1 (14%)	3	8
All	All	250/266 (94%)	209 (84%)	41 (16%)	2	6

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1(A)	ASP
1	1	1	CYS
1	1	3	LEU
1	1	6	LEU
1	1	11	SER
1	1	12	LEU
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	61	GLU
2	2	62	ASN
2	2	63	ASP
2	2	65	LEU
2	2	67	ARG

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Mol	Chain	Res	Type
2	2	68	ILE
2	2	78	ASN
2	2	79	ILE
2	2	82	ILE
2	2	83	SER
2	2	87	LYS
2	2	90	ILE
2	2	109	LYS
2	2	139	THR
2	2	147	THR
2	2	149	THR
2	2	157	VAL
2	2	162	ILE
2	2	165	ARG
2	2	174	ILE
2	2	176	ILE
2	2	182	CYS
2	2	195	SER
2	2	224	LYS
2	2	234	LEU
2	2	235	LYS
2	2	241	VAL
2	2	242	ILE
3	3	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	30	GLN
2	2	78	ASN
2	2	156	GLN
2	2	204(B)	ASN
2	2	239	GLN

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	3	567	3	15,16,17	1.43	2 (13%)	15,22,24	1.27	1 (6%)

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	-	0/10/11/13	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	OH-S	3.78	1.65	1.58
3	3	567	TYS	OH-CZ	-3.63	1.36	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	OH-CZ-CE1	3.02	124.62	118.70

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	3	567	TYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	IH3	2	370	-	42,46,46	4.70	25 (59%)	55,66,66	2.27	18 (32%)

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	-	-	4/24/46/46	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	370	IH3	C32-C31	12.60	1.60	1.38
4	2	370	IH3	C22-N20	11.88	1.72	1.47
4	2	370	IH3	C8-N10	-11.04	1.24	1.46
4	2	370	IH3	C35-C30	10.50	1.55	1.39
4	2	370	IH3	C29-C24	8.21	1.52	1.39
4	2	370	IH3	C34-C35	7.51	1.51	1.38
4	2	370	IH3	C28-C29	5.95	1.49	1.38
4	2	370	IH3	C27-C26	4.95	1.49	1.38
4	2	370	IH3	C26-C25	4.79	1.47	1.38
4	2	370	IH3	C31-C30	4.35	1.46	1.39
4	2	370	IH3	C16-C14	4.33	1.54	1.50
4	2	370	IH3	C6-C7	4.17	1.63	1.52
4	2	370	IH3	C16-N17	-3.89	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	370	IH3	C28-C27	3.81	1.46	1.38
4	2	370	IH3	C7-C8	3.60	1.60	1.52
4	2	370	IH3	C33-C32	3.49	1.45	1.38
4	2	370	IH3	C19-N17	3.15	1.40	1.37
4	2	370	IH3	C12-N18	-3.05	1.40	1.47
4	2	370	IH3	C25-C24	2.95	1.43	1.39
4	2	370	IH3	C13-C14	2.67	1.37	1.32
4	2	370	IH3	C34-C33	2.62	1.44	1.38
4	2	370	IH3	C4-C5	2.39	1.59	1.53
4	2	370	IH3	O19-C19	2.31	1.26	1.22
4	2	370	IH3	C5-C1	-2.30	1.45	1.51
4	2	370	IH3	C15-C14	2.21	1.56	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	370	IH3	C4-C9-C8	6.24	118.33	111.49
4	2	370	IH3	C8-N10-C11	-6.14	113.41	123.29
4	2	370	IH3	NC-C3-NA	-5.23	107.61	112.36
4	2	370	IH3	C9-C8-N10	-5.06	100.46	110.57
4	2	370	IH3	C15-C14-C13	-4.38	116.96	122.46
4	2	370	IH3	O19-C19-N17	4.22	129.47	126.69
4	2	370	IH3	C1-C2-NA	-3.41	107.87	111.46
4	2	370	IH3	C7-C6-C5	3.39	117.14	111.18
4	2	370	IH3	C33-C32-C31	3.33	124.34	120.24
4	2	370	IH3	C35-C30-C31	-2.74	114.91	118.30
4	2	370	IH3	NB-C3-NC	2.71	126.52	122.63
4	2	370	IH3	C34-C35-C30	2.67	123.84	120.65
4	2	370	IH3	C27-C26-C25	2.44	123.25	120.24
4	2	370	IH3	C7-C8-N10	-2.35	105.88	110.57
4	2	370	IH3	C35-C30-C23	2.21	126.92	120.83
4	2	370	IH3	C12-N18-N17	2.17	123.79	115.06
4	2	370	IH3	C34-C33-C32	-2.15	116.93	119.87
4	2	370	IH3	C12-C11-N10	2.04	117.20	114.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	2	370	IH3	C23-C22-N20-C19
4	2	370	IH3	N10-C11-C12-N18
4	2	370	IH3	N10-C11-C12-C13

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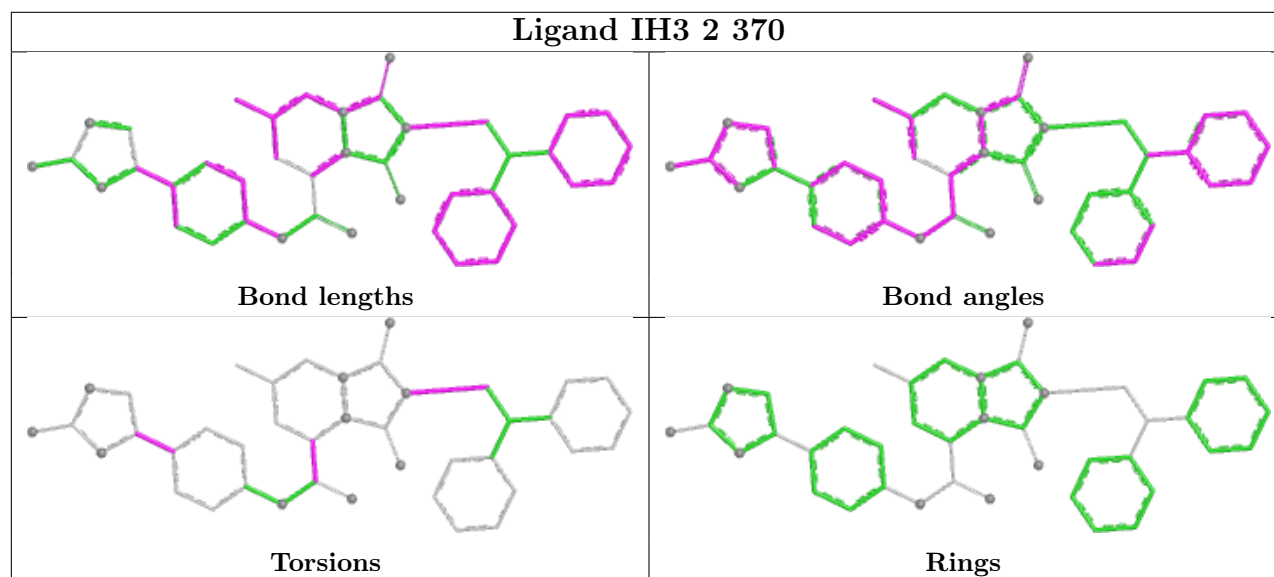
Mol	Chain	Res	Type	Atoms
4	2	370	IH3	NC-C1-C5-C4

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	2	370	IH3	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 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.