



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:41 AM UTC

PDB ID : 1QHR / pdb_00001qhr
Title : NOVEL COVALENT ACTIVE SITE THROMBIN INHIBITORS
Authors : Jhoti, H.; Cleasby, A.; Reid, S.; Thomas, P.; Wonacott, A.
Deposited on : 1999-05-26
Resolution : 2.20 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
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

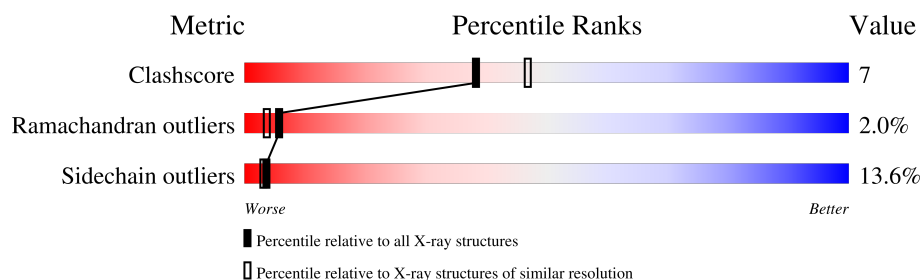
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	A	36	
2	B	259	
3	I	10	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA THROMBIN.

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

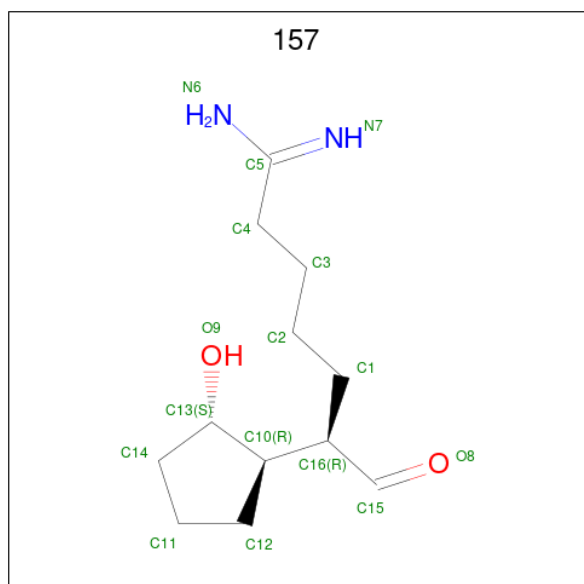
- Molecule 2 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2093	1334	370	375	14			

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			95	59	10	25	1			

- Molecule 4 is 6-(2-HYDROXY-CYCLOPENTYL)-7-OXO-HEPTANAMIDINE (CCD ID: 157) (formula: C₁₂H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	164	Total	O	0	0
			164	164		
5	I	6	Total	O	0	0
			6	6		

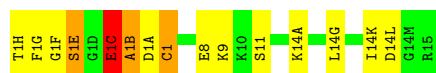
3 Residue-property plots [i](#)

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.

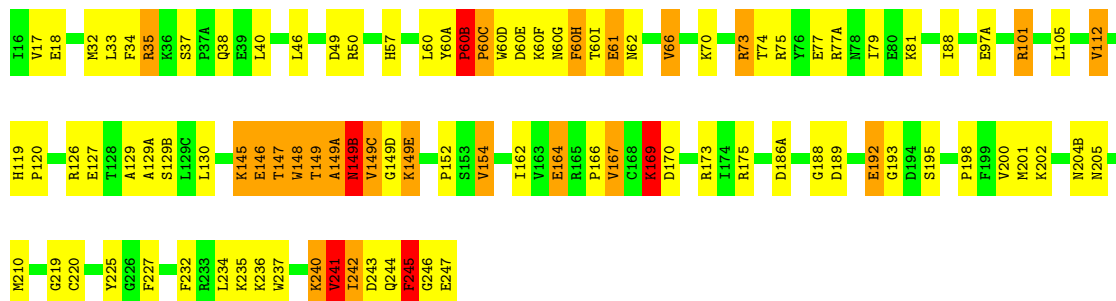
• Molecule 1: ALPHA THROMBIN

Chain A: 



• Molecule 2: ALPHA THROMBIN

Chain B: 



• Molecule 3: HIRUGEN

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.70Å 72.00Å 73.00Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2696	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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, 157

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	A	1.10	0/290	1.87	5/384 (1.3%)
2	B	1.22	2/2148 (0.1%)	1.99	61/2903 (2.1%)
3	I	0.99	0/79	1.93	4/103 (3.9%)
All	All	1.20	2/2517 (0.1%)	1.98	70/3390 (2.1%)

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	A	0	1
2	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	SER	CB-OG	-9.91	1.22	1.42
2	B	119	HIS	CE1-NE2	6.13	1.38	1.32

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77(A)	ARG	CA-C-N	-11.49	104.40	122.67
2	B	77(A)	ARG	C-N-CA	-11.49	104.40	122.67
2	B	66	VAL	N-CA-CB	-8.66	101.28	110.72
2	B	34	PHE	CA-C-N	-8.61	109.35	122.09
2	B	34	PHE	C-N-CA	-8.61	109.35	122.09
2	B	192	GLU	CA-CB-CG	-8.17	97.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129(B)	SER	CB-CA-C	-8.14	97.28	110.79
2	B	244	GLN	N-CA-C	8.06	120.98	111.71
2	B	245	PHE	N-CA-C	8.06	120.62	107.32
2	B	129(B)	SER	N-CA-C	8.05	120.06	111.28
2	B	77(A)	ARG	N-CA-C	7.89	120.57	111.11
2	B	149(B)	ASN	N-CA-C	7.76	122.18	110.14
2	B	146	GLU	N-CA-C	7.64	121.77	110.30
2	B	149(A)	ALA	N-CA-C	7.28	121.41	110.64
2	B	70	LYS	N-CA-C	7.25	120.33	110.55
2	B	186(A)	ASP	N-CA-C	6.81	119.72	111.82
2	B	18	GLU	CA-C-N	-6.79	116.39	122.43
2	B	18	GLU	C-N-CA	-6.79	116.39	122.43
2	B	129(A)	ALA	N-CA-C	6.67	118.21	111.07
2	B	169	LYS	CB-CA-C	6.65	121.82	110.79
2	B	62	ASN	CA-CB-CG	-6.55	106.05	112.60
2	B	243	ASP	N-CA-C	6.45	118.39	111.36
2	B	60(B)	PRO	N-CA-C	6.45	118.57	110.70
2	B	57	HIS	N-CA-C	6.42	120.21	112.38
2	B	147	THR	N-CA-C	6.42	122.06	113.72
2	B	170	ASP	N-CA-C	6.37	120.77	113.19
2	B	205	ASN	N-CA-C	6.37	120.63	112.86
2	B	126	ARG	CA-CB-CG	6.27	126.64	114.10
2	B	241	VAL	N-CA-C	6.21	118.86	111.09
2	B	201	MET	CA-C-N	-6.16	114.22	122.72
2	B	201	MET	C-N-CA	-6.16	114.22	122.72
1	A	9	LYS	N-CA-C	6.05	119.76	112.38
2	B	148	TRP	CA-C-N	6.04	133.07	121.54
2	B	148	TRP	C-N-CA	6.04	133.07	121.54
2	B	154	VAL	N-CA-CB	-6.03	99.43	111.91
3	I	56	PHE	CA-CB-CG	-5.94	107.86	113.80
2	B	192	GLU	N-CA-C	5.91	118.80	110.23
2	B	232	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	1	CYS	N-CA-C	5.76	117.73	110.24
2	B	242	ILE	CA-CB-CG1	5.59	119.91	110.40
2	B	35	ARG	CA-C-O	5.58	127.34	120.92
1	A	1(C)	GLU	N-CA-C	5.58	119.02	110.20
2	B	74	THR	N-CA-C	5.55	120.33	113.50
2	B	175	ARG	N-CA-C	5.54	117.14	109.15
2	B	112	VAL	CB-CA-C	-5.54	103.98	111.63
3	I	61	GLU	CA-C-N	-5.48	111.84	121.70
3	I	61	GLU	C-N-CA	-5.48	111.84	121.70
2	B	127	GLU	N-CA-C	5.47	118.17	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	LYS	CA-CB-CG	5.44	124.98	114.10
2	B	241	VAL	CA-C-N	-5.44	111.72	120.64
2	B	241	VAL	C-N-CA	-5.44	111.72	120.64
2	B	235	LYS	N-CA-C	5.40	117.92	111.71
1	A	14(A)	LYS	N-CA-CB	-5.39	101.92	110.22
3	I	60	PRO	N-CA-C	5.33	119.94	111.26
2	B	60(H)	PHE	CA-C-O	5.32	127.12	121.05
2	B	97(A)	GLU	N-CA-C	5.27	119.04	111.02
1	A	8	GLU	N-CA-C	5.25	117.69	111.33
2	B	164	GLU	CB-CA-C	-5.24	101.98	109.84
2	B	173	ARG	CB-CA-C	-5.23	99.68	109.72
2	B	189	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	66	VAL	N-CA-C	5.20	116.07	108.58
2	B	35	ARG	N-CA-C	5.16	118.62	109.96
2	B	79	ILE	N-CA-CB	-5.14	107.42	111.64
2	B	164	GLU	N-CA-C	5.12	117.77	110.24
2	B	225	TYR	CA-C-N	-5.11	114.94	120.71
2	B	225	TYR	C-N-CA	-5.11	114.94	120.71
2	B	101	ARG	CA-CB-CG	-5.08	103.93	114.10
2	B	227	PHE	CA-C-O	5.08	126.10	120.71
2	B	61	GLU	N-CA-C	5.04	117.16	111.11
2	B	49	ASP	N-CA-C	5.03	119.05	113.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1(E)	SER	Peptide
2	B	73	ARG	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	A	287	0	278	6	0
2	B	2093	0	2063	30	0
3	I	95	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	20	0	0
5	A	35	0	0	1	0
5	B	164	0	0	0	0
5	I	6	0	0	0	0
All	All	2696	0	2435	34	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 7.

All (34) 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)
2:B:75:ARG:HD2	2:B:77:GLU:HG2	1.53	0.91
1:A:1(C):GLU:HA	1:A:1(B):ALA:HB3	1.69	0.75
2:B:166:PRO:HA	2:B:169:LYS:HD2	1.76	0.67
2:B:32:MET:HG3	2:B:40:LEU:HD12	1.77	0.66
2:B:148:TRP:CZ3	2:B:220:CYS:SG	2.92	0.63
2:B:164:GLU:HB2	2:B:167:VAL:HG13	1.82	0.61
1:A:1(C):GLU:HG2	2:B:120:PRO:HG3	1.86	0.58
2:B:130:LEU:HD23	2:B:162:ILE:HD13	1.87	0.56
2:B:147:THR:HA	2:B:149(A):ALA:HA	1.87	0.55
2:B:146:GLU:O	2:B:149(B):ASN:HB2	2.07	0.55
2:B:35:ARG:O	2:B:38:GLN:HA	2.08	0.53
2:B:145:LYS:HB3	2:B:149(B):ASN:HB3	1.95	0.49
2:B:101:ARG:HG2	2:B:234:LEU:HD21	1.93	0.49
2:B:61:GLU:HG3	2:B:88:ILE:HG13	1.95	0.48
2:B:129:ALA:HA	2:B:210:MET:HE1	1.95	0.48
1:A:1(C):GLU:HA	1:A:1(B):ALA:CB	2.43	0.47
2:B:204(B):ASN:C	2:B:204(B):ASN:HD22	2.22	0.47
1:A:14(G):LEU:HD21	2:B:202:LYS:HD3	1.95	0.46
2:B:240:LYS:HB2	2:B:240:LYS:NZ	2.30	0.46
2:B:245:PHE:HA	2:B:246:GLY:HA3	1.76	0.46
2:B:148:TRP:CH2	2:B:220:CYS:SG	3.09	0.45
2:B:73:ARG:HD3	2:B:152:PRO:O	2.16	0.45
1:A:14(K):ILE:HA	5:A:372:HOH:O	2.16	0.44
2:B:145:LYS:HE2	2:B:149(D):GLY:HA3	2.00	0.44
2:B:242:ILE:HD13	2:B:242:ILE:HG21	1.68	0.43
2:B:17:VAL:O	2:B:188:GLY:HA2	2.19	0.43
2:B:148:TRP:HZ3	2:B:219:GLY:C	2.27	0.42
2:B:192:GLU:HG2	2:B:193:GLY:N	2.33	0.42
2:B:60(B):PRO:O	2:B:60(C):PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:TRP:O	2:B:241:VAL:HG13	2.20	0.41
2:B:164:GLU:HB3	2:B:166:PRO:HD2	2.02	0.41
2:B:105:LEU:HD13	2:B:241:VAL:HG22	2.03	0.41
2:B:198:PRO:HB2	2:B:200:VAL:HG13	2.01	0.41
1:A:1(F):GLY:HA3	1:A:1(C):GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	34/36 (94%)	25 (74%)	7 (21%)	2 (6%)	1	0
2	B	257/259 (99%)	242 (94%)	11 (4%)	4 (2%)	7	6
3	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	298/305 (98%)	274 (92%)	18 (6%)	6 (2%)	6	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14(L)	ASP
2	B	37	SER
2	B	149	THR
2	B	149(E)	LYS
1	A	1(B)	ALA
2	B	149(C)	VAL

5.3.2 Protein sidechains [i](#)

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	A	31/31 (100%)	24 (77%)	7 (23%)	1	0
2	B	225/225 (100%)	196 (87%)	29 (13%)	4	4
3	I	9/9 (100%)	9 (100%)	0	100	100
All	All	265/265 (100%)	229 (86%)	36 (14%)	3	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(H)	THR
1	A	1(G)	PHE
1	A	1(E)	SER
1	A	1(C)	GLU
1	A	1(A)	ASP
1	A	1	CYS
1	A	11	SER
2	B	33	LEU
2	B	46	LEU
2	B	50	ARG
2	B	60	LEU
2	B	60(A)	TYR
2	B	60(B)	PRO
2	B	60(C)	PRO
2	B	60(D)	TRP
2	B	60(E)	ASP
2	B	60(F)	LYS
2	B	60(G)	ASN
2	B	60(H)	PHE
2	B	60(I)	THR
2	B	66	VAL
2	B	81	LYS
2	B	112	VAL
2	B	145	LYS
2	B	149	THR
2	B	149(B)	ASN
2	B	149(C)	VAL
2	B	149(E)	LYS
2	B	154	VAL
2	B	167	VAL

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Mol	Chain	Res	Type
2	B	169	LYS
2	B	236	LYS
2	B	240	LYS
2	B	241	VAL
2	B	245	PHE
2	B	247	GLU

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

Mol	Chain	Res	Type
2	B	143	ASN
2	B	149(B)	ASN
2	B	204(B)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYS	I	63	3	15,16,17	0.98	2 (13%)	15,22,24	0.81	0

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	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	2.29	1.46	1.42
3	I	63	TYS	OH-S	-2.00	1.54	1.58

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	63	TYS	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

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	157	B	500	2	16,16,16	0.85	0	13,20,20	1.34	1 (7%)

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	157	B	500	2	-	3/13/23/23	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	157	O8-C15-C16	-3.63	117.02	125.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	500	157	C2-C1-C16-C10
4	B	500	157	C2-C1-C16-C15
4	B	500	157	C16-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.