



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:58 AM GMT

PDB ID : 1FPC  
Title : ACTIVE SITE MIMETIC INHIBITION OF THROMBIN  
Authors : Tulinsky, A.; Mathews, I.I.  
Deposited on : 1994-10-16  
Resolution : 2.30 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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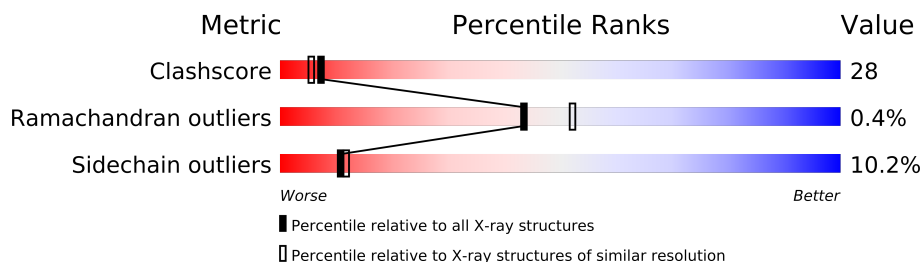
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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 5 unique types of molecules in this entry. The entry contains 2527 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	26	Total	C	N	O	S	0	0	0
			212	135	32	44	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	248	Total	C	N	O	S	0	0	0
			1993	1270	353	356	14			

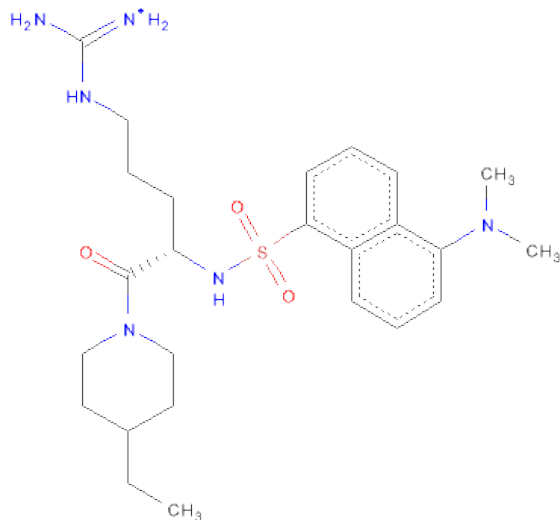
- Molecule 3 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			86	54	10	21	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	53	ASN	ASP	CONFLICT	UNP P28504

- Molecule 4 is AMINO{[(4S)-4-({[5-(DIMETHYLAMINO)NAPHTHALEN-1-YL]SULFONYL}AMINO)-5-(4-ETHYLPYPERIDIN-1-YL)-5-OXOPENTYL]AMINO}METHANIMINIUM (three-letter code: 0ZI) (formula: C<sub>25</sub>H<sub>39</sub>N<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	S	0	0
			35	25	6	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	19	Total	O	0	0
			19	19		
5	H	180	Total	O	0	0
			180	180		
5	I	2	Total	O	0	0
			2	2		

### 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.

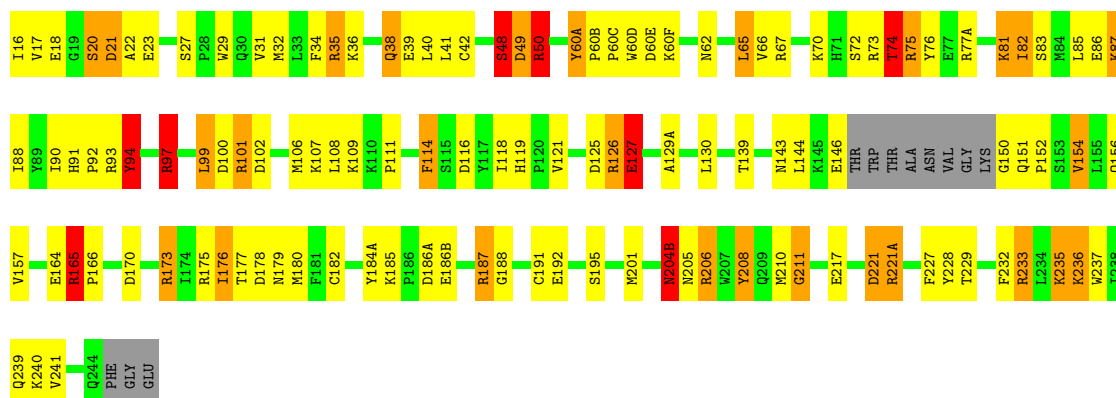
- Molecule 1: thrombin

Chain L: 



- Molecule 2: thrombin

Chain H: 



- Molecule 3: Hirudin

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, $\alpha$ , $\beta$ , $\gamma$	72.10Å 72.60Å 73.80Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.147 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: 0ZI, 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	1.18	0/214	1.95	7/285 (2.5%)
2	H	1.14	0/2044	2.27	72/2765 (2.6%)
3	I	0.98	0/70	1.71	1/91 (1.1%)
All	All	1.14	0/2328	2.23	80/3141 (2.5%)

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	3

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	CD-NE-CZ	40.19	179.86	123.60
2	H	221(A)	ARG	NE-CZ-NH1	-20.32	110.14	120.30
2	H	35	ARG	NE-CZ-NH2	-15.10	112.75	120.30
2	H	187	ARG	NE-CZ-NH2	-13.65	113.48	120.30
2	H	101	ARG	NE-CZ-NH2	-13.49	113.56	120.30
2	H	60(A)	TYR	CB-CG-CD1	-12.77	113.34	121.00
2	H	233	ARG	NE-CZ-NH2	-12.65	113.97	120.30
2	H	187	ARG	NE-CZ-NH1	12.43	126.51	120.30
2	H	173	ARG	NE-CZ-NH1	11.98	126.29	120.30
2	H	50	ARG	NE-CZ-NH1	11.97	126.28	120.30
2	H	101	ARG	NE-CZ-NH1	11.85	126.22	120.30
2	H	67	ARG	NE-CZ-NH2	11.06	125.83	120.30
2	H	165	ARG	NE-CZ-NH2	-11.05	114.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	175	ARG	NE-CZ-NH1	-10.49	115.06	120.30
2	H	77(A)	ARG	CA-C-N	9.47	138.03	117.20
2	H	102	ASP	CB-CG-OD2	-9.14	110.07	118.30
2	H	77(A)	ARG	CA-C-O	-9.06	101.08	120.10
2	H	60(A)	TYR	CB-CG-CD2	8.73	126.24	121.00
2	H	125	ASP	CB-CG-OD1	-8.65	110.51	118.30
2	H	126	ARG	NE-CZ-NH2	8.64	124.62	120.30
2	H	77(A)	ARG	NE-CZ-NH1	-8.50	116.05	120.30
2	H	165	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	H	49	ASP	CB-CG-OD2	8.13	125.62	118.30
2	H	221(A)	ARG	CD-NE-CZ	-7.94	112.49	123.60
2	H	233	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	H	94	TYR	CB-CG-CD2	-7.80	116.32	121.00
2	H	208	TYR	CB-CG-CD1	-7.78	116.33	121.00
2	H	125	ASP	CB-CG-OD2	7.67	125.20	118.30
2	H	129(A)	ALA	N-CA-CB	7.28	120.29	110.10
2	H	116	ASP	CB-CG-OD1	7.26	124.83	118.30
2	H	77(A)	ARG	N-CA-CB	6.92	123.05	110.60
2	H	73	ARG	NE-CZ-NH2	6.83	123.71	120.30
2	H	192	GLU	CA-CB-CG	6.82	128.40	113.40
2	H	74	THR	N-CA-CB	-6.62	97.71	110.30
2	H	97	ARG	NE-CZ-NH1	-6.61	117.00	120.30
2	H	97	ARG	CD-NE-CZ	-6.57	114.41	123.60
2	H	35	ARG	NH1-CZ-NH2	6.49	126.54	119.40
2	H	173	ARG	CD-NE-CZ	6.45	132.63	123.60
2	H	221(A)	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	H	176	ILE	CA-CB-CG2	6.35	123.59	110.90
2	H	21	ASP	CB-CG-OD1	6.31	123.98	118.30
2	H	221(A)	ARG	NH1-CZ-NH2	6.29	126.32	119.40
2	H	184(A)	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	H	22	ALA	N-CA-CB	-6.19	101.43	110.10
1	L	4	ARG	CD-NE-CZ	6.09	132.13	123.60
2	H	221	ASP	CB-CG-OD1	5.97	123.68	118.30
2	H	127	GLU	CA-CB-CG	5.82	126.20	113.40
2	H	102	ASP	CB-CG-OD1	5.82	123.53	118.30
3	I	58	GLU	CB-CG-CD	5.82	129.90	114.20
2	H	67	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
2	H	114	PHE	CB-CG-CD1	-5.78	116.76	120.80
1	L	14(A)	LYS	CA-CB-CG	5.76	126.08	113.40
2	H	211	GLY	C-N-CA	5.76	136.09	121.70
2	H	83	SER	O-C-N	5.76	131.91	122.70
2	H	119	HIS	N-CA-CB	-5.75	100.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(G)	LEU	CB-CA-C	5.75	121.12	110.20
2	H	170	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	H	77(A)	ARG	C-N-CA	-5.55	107.82	121.70
1	L	14(C)	GLU	CG-CD-OE1	-5.50	107.31	118.30
2	H	178	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	H	154	VAL	N-CA-CB	-5.49	99.43	111.50
1	L	10	LYS	CB-CG-CD	5.48	125.85	111.60
1	L	14(A)	LYS	N-CA-CB	5.47	120.44	110.60
2	H	179	ASN	CA-C-O	-5.46	108.64	120.10
1	L	13	GLU	CA-CB-CG	5.43	125.34	113.40
2	H	164	GLU	CB-CG-CD	5.42	128.83	114.20
2	H	170	ASP	O-C-N	5.40	131.34	122.70
2	H	48	SER	CA-C-O	-5.30	108.96	120.10
2	H	27	SER	CB-CA-C	5.27	120.11	110.10
2	H	233	ARG	CD-NE-CZ	5.27	130.97	123.60
2	H	204(B)	ASN	CB-CA-C	5.24	120.88	110.40
2	H	75	ARG	CB-CG-CD	5.21	125.14	111.60
2	H	94	TYR	CB-CG-CD1	5.20	124.12	121.00
2	H	76	TYR	CB-CG-CD2	-5.18	117.89	121.00
2	H	93	ARG	NE-CZ-NH1	-5.13	117.74	120.30
2	H	118	ILE	CG1-CB-CG2	5.10	122.63	111.40
2	H	154	VAL	CA-CB-CG1	5.09	118.54	110.90
2	H	42	CYS	CA-CB-SG	5.07	123.13	114.00
2	H	60(D)	TRP	CA-C-O	-5.06	109.47	120.10
2	H	119	HIS	CB-CA-C	5.03	120.45	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	ARG	Sidechain
2	H	233	ARG	Mainchain
2	H	94	TYR	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	212	0	211	11	0
2	H	1993	0	1952	119	0
3	I	86	0	64	2	0
4	H	35	0	38	6	0
5	H	180	0	0	16	0
5	I	2	0	0	0	0
5	L	19	0	0	2	0
All	All	2527	0	2265	129	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 28.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:1(A):ASP:HB3	5:L:506:HOH:O	1.51	1.09
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.55	1.04
2:H:236:LYS:HE2	2:H:239:GLN:HE22	1.28	0.97
2:H:18:GLU:HG3	2:H:187:ARG:HG3	1.44	0.96
1:L:14(J):TYR:O	1:L:14(K):ILE:HB	1.67	0.93
2:H:81:LYS:HB3	2:H:81:LYS:NZ	1.86	0.91
2:H:38:GLN:HB2	5:H:491:HOH:O	1.69	0.91
2:H:236:LYS:HE2	2:H:239:GLN:NE2	1.87	0.90
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.73	0.89
2:H:35:ARG:O	2:H:38:GLN:HA	1.75	0.87
2:H:205:ASN:HB3	5:H:499:HOH:O	1.76	0.85
2:H:50:ARG:NH1	2:H:107:LYS:HD3	1.92	0.84
2:H:208:TYR:HB2	5:H:461:HOH:O	1.78	0.83
2:H:70:LYS:HE3	2:H:72:SER:O	1.79	0.82
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.13	0.81
2:H:49:ASP:OD2	2:H:111:PRO:HB3	1.82	0.79
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.52	0.74
2:H:143:ASN:HA	2:H:150:GLY:O	1.86	0.74
2:H:81:LYS:HB3	2:H:81:LYS:HZ3	1.55	0.72
2:H:99:LEU:HD22	4:H:371:OZI:HM13	1.73	0.71
2:H:50:ARG:HH11	2:H:107:LYS:HD3	1.53	0.70
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.07	0.69
2:H:60(F):LYS:NZ	5:H:575:HOH:O	2.24	0.68
2:H:165:ARG:NH2	2:H:180:MET:O	2.27	0.68
2:H:126:ARG:NH2	2:H:127:GLU:OE2	2.27	0.67
2:H:50:ARG:HD3	2:H:108:LEU:O	1.94	0.66
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.76	0.66
2:H:81:LYS:HB3	2:H:81:LYS:HZ2	1.62	0.65
2:H:97:ARG:NH1	5:H:571:HOH:O	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:14(A):LYS:HE2	2:H:23:GLU:OE1	1.97	0.65
2:H:185:LYS:HB2	2:H:186(A):ASP:OD1	1.98	0.64
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.79	0.63
2:H:221(A):ARG:HH11	2:H:221(A):ARG:CG	2.05	0.62
2:H:66:VAL:CG2	2:H:85:LEU:HD21	2.29	0.62
2:H:20:SER:O	2:H:156:GLN:HA	2.00	0.61
1:L:14(A):LYS:HE2	2:H:23:GLU:CD	2.21	0.61
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.36	0.61
2:H:221(A):ARG:HG3	2:H:221(A):ARG:NH1	2.16	0.60
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.05	0.60
2:H:17:VAL:O	2:H:18:GLU:HB2	2.02	0.59
2:H:48:SER:OG	2:H:49:ASP:N	2.32	0.59
2:H:221(A):ARG:CG	2:H:221(A):ARG:NH1	2.60	0.58
2:H:236:LYS:HE3	2:H:236:LYS:HA	1.85	0.58
2:H:139:THR:HG22	2:H:157:VAL:HB	1.85	0.58
2:H:173:ARG:NH1	5:H:455:HOH:O	2.29	0.58
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.85	0.58
2:H:17:VAL:O	2:H:188:GLY:HA2	2.05	0.57
2:H:81:LYS:HD3	5:H:516:HOH:O	2.06	0.55
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.05	0.55
2:H:127:GLU:HB2	5:H:597:HOH:O	2.06	0.55
2:H:235:LYS:HB3	2:H:236:LYS:HZ2	1.72	0.55
2:H:20:SER:HB3	5:H:443:HOH:O	2.05	0.55
2:H:236:LYS:HE3	2:H:236:LYS:CA	2.37	0.55
2:H:146:GLU:OE1	2:H:221(A):ARG:NE	2.38	0.55
2:H:50:ARG:HH12	2:H:86:GLU:CD	2.11	0.54
2:H:191:CYS:C	4:H:371:OZI:HD2	2.28	0.53
1:L:14(C):GLU:O	1:L:14(G):LEU:HD23	2.10	0.52
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.44	0.52
2:H:65:LEU:HG	2:H:82:ILE:HG22	1.91	0.52
1:L:14(J):TYR:O	1:L:14(K):ILE:CB	2.49	0.52
2:H:237:TRP:O	2:H:241:VAL:HG13	2.10	0.52
2:H:35:ARG:HB3	2:H:39:GLU:HG2	1.92	0.51
3:I:58:GLU:H	3:I:58:GLU:CD	2.12	0.51
2:H:191:CYS:HA	4:H:371:OZI:HD2	1.93	0.51
2:H:173:ARG:HD2	5:H:455:HOH:O	2.11	0.51
2:H:60(E):ASP:HA	5:H:496:HOH:O	2.09	0.51
2:H:176:ILE:HD12	2:H:227:PHE:HE2	1.74	0.51
2:H:66:VAL:HG21	2:H:85:LEU:HD21	1.92	0.50
2:H:87:LYS:NZ	5:H:568:HOH:O	2.44	0.50
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.26	0.50
2:H:66:VAL:HG23	2:H:85:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:81:LYS:CB	2:H:81:LYS:HZ2	2.22	0.49
2:H:35:ARG:HD3	2:H:39:GLU:OE2	2.12	0.49
2:H:16:ILE:O	2:H:144:LEU:HA	2.12	0.49
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.47	0.49
1:L:1(A):ASP:CB	5:L:506:HOH:O	2.28	0.49
2:H:165:ARG:N	2:H:166:PRO:HD2	2.27	0.48
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.95	0.48
2:H:87:LYS:HD3	2:H:88:ILE:H	1.79	0.48
2:H:236:LYS:N	2:H:236:LYS:HE3	2.29	0.47
2:H:114:PHE:CD1	2:H:114:PHE:N	2.77	0.47
2:H:109:LYS:HB2	5:H:536:HOH:O	2.14	0.47
2:H:211:GLY:HA2	2:H:229:THR:O	2.13	0.47
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.12	0.47
2:H:85:LEU:HD22	2:H:106:MET:HE2	1.96	0.47
2:H:50:ARG:CD	2:H:108:LEU:O	2.60	0.47
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.44	0.47
2:H:235:LYS:HB3	2:H:236:LYS:NZ	2.30	0.47
1:L:14(G):LEU:N	1:L:14(G):LEU:CD2	2.78	0.47
2:H:236:LYS:HB2	5:H:530:HOH:O	2.14	0.46
2:H:34:PHE:CE2	2:H:38:GLN:HB3	2.50	0.46
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.45	0.46
2:H:94:TYR:HA	2:H:100:ASP:O	2.16	0.46
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.68	0.46
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.52	0.45
2:H:236:LYS:CE	2:H:239:GLN:NE2	2.72	0.45
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.98	0.45
2:H:99:LEU:HD22	4:H:371:OZI:CM1	2.45	0.45
2:H:114:PHE:HB3	5:H:480:HOH:O	2.17	0.45
2:H:50:ARG:NH1	2:H:108:LEU:O	2.50	0.45
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.47	0.44
2:H:94:TYR:HA	2:H:101:ARG:HB2	1.99	0.44
2:H:191:CYS:CA	4:H:371:OZI:HD2	2.47	0.44
2:H:70:LYS:CE	2:H:72:SER:O	2.58	0.44
2:H:36:LYS:HG2	2:H:65:LEU:HD22	1.99	0.43
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.81	0.43
2:H:240:LYS:HB2	5:H:595:HOH:O	2.19	0.43
4:H:371:OZI:HA	4:H:371:OZI:H62	1.79	0.43
2:H:217:GLU:O	2:H:221(A):ARG:HG3	2.19	0.43
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.99	0.43
2:H:186(A):ASP:CG	2:H:186(B):GLU:N	2.72	0.43
2:H:176:ILE:CD1	2:H:227:PHE:CE2	3.01	0.43
2:H:201:MET:SD	2:H:210:MET:HG3	2.59	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:185:LYS:CB	2:H:186(A):ASP:OD1	2.66	0.43
2:H:151:GLN:HA	2:H:152:PRO:HD3	1.82	0.42
2:H:82:ILE:HG13	3:I:63:TYS:CD2	2.49	0.42
2:H:29:TRP:O	2:H:31:VAL:HG23	2.18	0.42
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.35	0.42
2:H:50:ARG:NH1	2:H:107:LYS:CD	2.75	0.41
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.40	0.41
2:H:232:PHE:O	2:H:235:LYS:HB2	2.21	0.41
2:H:90:ILE:O	2:H:91:HIS:C	2.58	0.41
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.56	0.41
1:L:14:ASP:C	1:L:14:ASP:OD1	2.59	0.41
2:H:144:LEU:HD21	2:H:152:PRO:CB	2.51	0.41
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.77	0.41
2:H:100:ASP:CG	2:H:177:THR:HG21	2.41	0.40
2:H:85:LEU:CD2	2:H:106:MET:CE	2.98	0.40
2:H:228:TYR:CD1	2:H:228:TYR:N	2.89	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	L	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
2	H	244/259 (94%)	227 (93%)	16 (7%)	1 (0%)	43	52
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	275/307 (90%)	257 (94%)	17 (6%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	195	SER

### 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	24/31 (77%)	18 (75%)	6 (25%)	1	0
2	H	213/225 (95%)	195 (92%)	18 (8%)	15	18
3	I	7/10 (70%)	6 (86%)	1 (14%)	5	4
All	All	244/266 (92%)	219 (90%)	25 (10%)	11	12

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(A)	ASP
1	L	9	LYS
1	L	10	LYS
1	L	11	SER
1	L	14(F)	LEU
1	L	14(K)	ILE
2	H	20	SER
2	H	38	GLN
2	H	48	SER
2	H	50	ARG
2	H	62	ASN
2	H	65	LEU
2	H	74	THR
2	H	81	LYS
2	H	82	ILE
2	H	87	LYS
2	H	94	TYR
2	H	97	ARG
2	H	99	LEU
2	H	127	GLU
2	H	182	CYS
2	H	204(B)	ASN
2	H	235	LYS
2	H	236	LYS
3	I	58	GLU

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	239	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	-	16,16,17	5.26	3 (18%)	20,22,24	1.66	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	I	63	-	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	O-C	20.32	1.25	1.11
3	I	63	TYS	OH-CZ	-4.00	1.37	1.42
3	I	63	TYS	OH-S	2.76	1.68	1.63

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CG-CB-CA	-3.65	105.81	114.42
3	I	63	TYS	OH-S-O2	-3.53	97.44	107.64
3	I	63	TYS	CB-CG-CD1	-2.37	116.26	120.90

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	0ZI	H	371	-	37,37,37	3.69	16 (43%)	52,52,52	3.00	15 (28%)

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	0ZI	H	371	-	-	0/32/42/42	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	371	0ZI	S-N1	10.23	1.77	1.61
4	H	371	0ZI	C1-S	9.16	1.87	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	371	OZI	O2S-S	7.33	1.51	1.43
4	H	371	OZI	CM2-N	6.53	1.62	1.45
4	H	371	OZI	C-N11	5.93	1.44	1.34
4	H	371	OZI	C61-N11	5.54	1.57	1.47
4	H	371	OZI	C21-N11	5.09	1.56	1.47
4	H	371	OZI	O1S-S	4.98	1.49	1.43
4	H	371	OZI	C51-C41	4.17	1.63	1.52
4	H	371	OZI	C2-C1	4.14	1.42	1.37
4	H	371	OZI	C1-C8A	-3.43	1.38	1.43
4	H	371	OZI	C31-C41	3.39	1.61	1.52
4	H	371	OZI	C5-C4A	-2.37	1.37	1.42
4	H	371	OZI	CZ-NH1	2.29	1.36	1.32
4	H	371	OZI	C8-C8A	-2.25	1.37	1.42
4	H	371	OZI	CG-CD	-2.04	1.42	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	371	OZI	CG-CB-CA	10.97	149.32	114.03
4	H	371	OZI	O2S-S-C1	10.31	125.77	108.08
4	H	371	OZI	O2S-S-O1S	-6.36	110.99	119.55
4	H	371	OZI	C61-N11-C21	5.46	122.94	112.52
4	H	371	OZI	C51-C61-N11	-4.70	104.15	111.23
4	H	371	OZI	CD-NE-CZ	4.68	134.74	124.55
4	H	371	OZI	C1'-C41-C31	-4.29	100.79	112.29
4	H	371	OZI	O2S-S-N1	-4.11	99.33	106.84
4	H	371	OZI	C21-N11-C	-3.51	110.28	123.24
4	H	371	OZI	CM1-N-C5	3.43	124.78	114.00
4	H	371	OZI	O-C-N11	-2.93	118.16	121.65
4	H	371	OZI	C51-C41-C31	2.83	115.78	109.19
4	H	371	OZI	O1S-S-C1	-2.23	104.25	108.08
4	H	371	OZI	C8-C8A-C1	-2.11	120.94	123.81
4	H	371	OZI	CA-C-N11	-2.02	115.77	119.50

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.