



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1VR1 / pdb_00001vr1
Title : Specifity for Plasminogen Activator Inhibitor-1
Authors : Dekker, R.J.; Eichinger, A.; Stoop, A.A.; Bode, W.; Pannekoek, H.; Horrevoets, A.J.G.
Deposited on : 1998-12-11
Resolution : 1.90 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

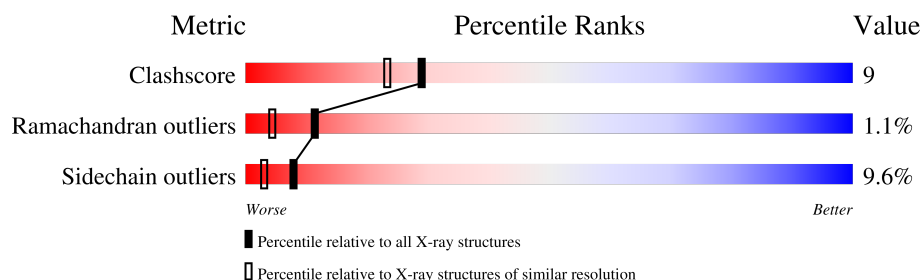
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	L	27	
2	H	261	
3	I	10	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2398 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	11	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	247	Total	C	N	O	S	33	0	0
			2001	1277	355	355	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	35	ALA	-	conflict	UNP P00734
H	36	LYS	-	conflict	UNP P00734
H	37	HIS	-	conflict	UNP P00734
H	37B	ARG	LYS	conflict	UNP P00734
H	37E	GLY	GLN	conflict	UNP P00734
H	39	ARG	-	conflict	UNP P00734
H	40	PHE	LEU	conflict	UNP P00734
H	184	TYR	GLY	conflict	UNP P00734

- Molecule 3 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	2	0	0
			94	59	10	24	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	70	Total	O	0	0
			70	70		
4	I	3	Total	O	0	0
			3	3		

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.

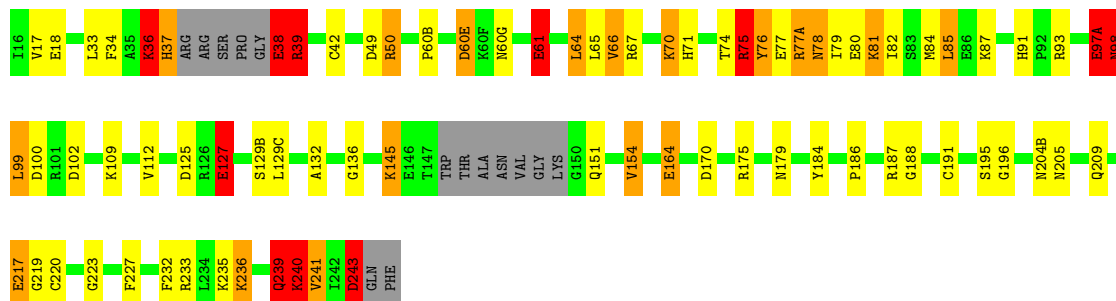
- Molecule 1: thrombin

Chain L:  78% 22%

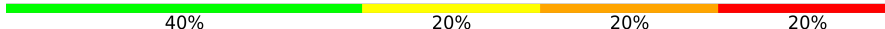


- Molecule 2: thrombin

Chain H:  64% 19% 7% 5%



- Molecule 3: Hirudin

Chain I:  40% 20% 20% 20%



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	70.88Å 71.96Å 73.04Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	19.90 – 1.90	Depositor
% Data completeness (in resolution range)	92.2 (19.90-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2398	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	L	1.17	3/224 (1.3%)	1.81	3/298 (1.0%)
2	H	1.84	26/2052 (1.3%)	2.19	70/2770 (2.5%)
3	I	1.19	1/78 (1.3%)	2.28	5/103 (4.9%)
All	All	1.77	30/2354 (1.3%)	2.16	78/3171 (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
1	L	1	0
2	H	0	13
3	I	0	1
All	All	1	14

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	50	ARG	CZ-NH2	33.80	1.77	1.33
2	H	60(E)	ASP	CG-OD2	29.22	1.80	1.25
2	H	50	ARG	CZ-NH1	25.55	1.68	1.32
2	H	97(A)	GLU	CB-CG	-23.35	0.82	1.52
2	H	50	ARG	NE-CZ	-21.39	1.09	1.33
2	H	97(A)	GLU	CD-OE1	17.11	1.57	1.25
2	H	97(A)	GLU	CD-OE2	-17.08	0.93	1.25
2	H	74	THR	C-N	-15.56	1.11	1.33
2	H	39	ARG	C-N	11.45	1.49	1.33
2	H	97(A)	GLU	CG-CD	11.19	1.80	1.52
2	H	70	LYS	C-N	-10.80	1.18	1.33
2	H	60(E)	ASP	CG-OD1	-10.61	1.05	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14(K)	ILE	CB-CG2	-9.08	1.22	1.52
2	H	77(A)	ARG	C-N	8.28	1.45	1.33
2	H	217	GLU	CG-CD	8.06	1.72	1.52
2	H	76	TYR	C-N	7.54	1.46	1.33
2	H	98	ASN	CA-CB	7.51	1.65	1.53
1	L	10	LYS	CE-NZ	-7.36	1.27	1.49
2	H	33	LEU	CG-CD2	7.36	1.76	1.52
1	L	14(K)	ILE	CB-CG1	7.27	1.68	1.53
2	H	145	LYS	CG-CD	7.03	1.73	1.52
2	H	145	LYS	C-N	-6.84	1.24	1.33
2	H	151	GLN	CA-CB	-6.39	1.43	1.53
2	H	236	LYS	CG-CD	6.21	1.71	1.52
3	I	61	GLU	C-O	-6.12	1.16	1.24
2	H	33	LEU	CG-CD1	-6.10	1.32	1.52
2	H	38	GLU	C-N	-5.90	1.26	1.33
2	H	36	LYS	C-N	-5.59	1.25	1.33
2	H	243	ASP	CA-C	-5.47	1.41	1.52
2	H	78	ASN	C-N	5.21	1.40	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	ARG	NH1-CZ-NH2	-26.73	84.55	119.30
2	H	76	TYR	CA-C-N	-19.29	94.59	123.14
2	H	76	TYR	C-N-CA	-19.29	94.59	123.14
2	H	97(A)	GLU	CB-CG-CD	19.25	145.33	112.60
2	H	36	LYS	O-C-N	-18.26	99.49	122.68
2	H	78	ASN	O-C-N	-17.66	95.41	121.91
2	H	236	LYS	CB-CG-CD	15.47	146.89	111.30
2	H	60(E)	ASP	CB-CG-OD1	15.01	152.92	118.40
2	H	74	THR	CA-C-N	14.48	144.28	121.26
2	H	74	THR	C-N-CA	14.48	144.28	121.26
2	H	98	ASN	N-CA-C	13.76	130.32	113.12
2	H	50	ARG	NE-CZ-NH2	-13.31	107.22	119.20
2	H	97(A)	GLU	CA-CB-CG	12.96	140.01	114.10
2	H	243	ASP	CB-CA-C	12.95	134.71	110.10
2	H	98	ASN	CA-CB-CG	-12.56	100.04	112.60
1	L	14(K)	ILE	CA-CB-CG2	11.98	130.87	110.50
2	H	75	ARG	O-C-N	-11.85	106.83	123.07
2	H	239	GLN	CG-CD-NE2	-11.44	99.25	116.40
2	H	50	ARG	NE-CZ-NH1	10.93	132.43	121.50
2	H	154	VAL	N-CA-CB	-9.82	98.77	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	55	ASP	CA-C-N	9.73	140.13	121.54
3	I	55	ASP	C-N-CA	9.73	140.13	121.54
2	H	60(E)	ASP	OD1-CG-OD2	-9.59	99.89	122.90
2	H	75	ARG	CA-C-N	9.46	134.16	120.82
2	H	75	ARG	C-N-CA	9.46	134.16	120.82
2	H	93	ARG	CD-NE-CZ	9.15	137.22	124.40
2	H	217	GLU	CG-CD-OE2	-8.98	97.75	118.40
2	H	151	GLN	CG-CD-OE1	-8.73	103.34	120.80
2	H	80	GLU	N-CA-CB	8.68	122.77	110.36
2	H	60(E)	ASP	CB-CG-OD2	-8.62	98.58	118.40
2	H	151	GLN	CG-CD-NE2	8.59	129.28	116.40
2	H	39	ARG	O-C-N	-8.48	114.19	123.52
2	H	33	LEU	CB-CG-CD1	8.17	135.22	110.70
2	H	78	ASN	CA-C-N	7.90	136.19	121.97
2	H	78	ASN	C-N-CA	7.90	136.19	121.97
2	H	50	ARG	CD-NE-CZ	7.89	135.45	124.40
2	H	98	ASN	N-CA-CB	-7.76	98.55	110.42
2	H	136	GLY	N-CA-C	-7.24	101.13	111.42
2	H	97(A)	GLU	CG-CD-OE1	-7.22	101.80	118.40
2	H	74	THR	O-C-N	-7.12	112.25	122.36
2	H	61	GLU	CA-CB-CG	7.00	128.10	114.10
2	H	232	PHE	CA-CB-CG	-6.96	106.84	113.80
1	L	14(D)	ARG	CD-NE-CZ	6.83	133.96	124.40
2	H	205	ASN	CA-CB-CG	-6.79	105.81	112.60
1	L	1(A)	ASP	N-CA-C	-6.59	102.58	111.87
2	H	64	LEU	N-CA-C	6.56	119.69	109.52
2	H	60(B)	PRO	N-CA-C	6.54	118.68	110.70
2	H	240	LYS	CA-CB-CG	6.54	127.19	114.10
2	H	195	SER	CB-CA-C	-6.50	99.23	109.70
3	I	56	PHE	N-CA-CB	6.40	121.31	110.49
2	H	80	GLU	CA-CB-CG	6.32	126.74	114.10
2	H	132	ALA	CA-C-O	-6.31	114.08	120.96
2	H	209	GLN	OE1-CD-NE2	6.25	128.85	122.60
2	H	127	GLU	CB-CG-CD	6.17	123.09	112.60
2	H	33	LEU	CA-C-N	-6.12	113.31	122.74
2	H	33	LEU	C-N-CA	-6.12	113.31	122.74
2	H	241	VAL	N-CA-CB	6.06	119.68	110.58
2	H	151	GLN	CB-CA-C	5.81	116.72	108.76
2	H	179	ASN	CA-CB-CG	-5.75	106.84	112.60
2	H	91	HIS	CA-CB-CG	-5.64	108.16	113.80
2	H	74	THR	N-CA-C	5.62	120.27	113.41
3	I	55	ASP	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	125	ASP	CA-CB-CG	5.47	118.07	112.60
2	H	145	LYS	CA-C-O	-5.44	115.41	121.51
2	H	227	PHE	CA-CB-CG	-5.37	108.44	113.80
2	H	49	ASP	CA-CB-CG	5.32	117.92	112.60
2	H	66	VAL	CA-CB-CG1	5.29	119.40	110.40
2	H	75	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	H	127	GLU	CA-CB-CG	5.29	124.67	114.10
2	H	170	ASP	CA-CB-CG	-5.22	107.38	112.60
2	H	76	TYR	O-C-N	5.18	129.38	122.95
2	H	50	ARG	N-CA-CB	-5.12	103.57	110.95
2	H	196	GLY	CA-C-O	-5.10	113.96	119.27
2	H	219	GLY	N-CA-C	-5.09	103.10	112.62
2	H	98	ASN	CB-CA-C	-5.08	101.18	109.56
2	H	145	LYS	CB-CG-CD	-5.06	99.67	111.30
2	H	99	LEU	N-CA-C	-5.04	105.99	113.40
3	I	61	GLU	N-CA-C	5.02	117.64	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	14(K)	ILE	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	127	GLU	Sidechain
2	H	217	GLU	Sidechain
2	H	239	GLN	Sidechain
2	H	36	LYS	Peptide,Mainchain
2	H	39	ARG	Mainchain
2	H	50	ARG	Sidechain
2	H	60(E)	ASP	Sidechain
2	H	70	LYS	Mainchain
2	H	75	ARG	Mainchain
2	H	77(A)	ARG	Mainchain
2	H	78	ASN	Mainchain
2	H	97(A)	GLU	Sidechain
3	I	63	TYS	Peptide

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	L	222	0	225	0	0
2	H	2001	0	1976	33	5
3	I	94	0	72	2	1
4	H	70	0	0	2	0
4	I	3	0	0	0	1
4	L	8	0	0	0	0
All	All	2398	0	2273	35	5

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 9.

All (35) 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:H:37:HIS:H	2:H:37:HIS:CD2	1.87	0.88
2:H:191:CYS:HG	2:H:220:CYS:HG	0.81	0.79
3:I:55:ASP:CG	3:I:56:PHE:H	1.99	0.71
2:H:243:ASP:HA	4:H:311:HOH:O	1.91	0.70
2:H:34:PHE:CZ	2:H:38:GLU:HB2	2.27	0.69
2:H:235:LYS:HE2	2:H:239:GLN:HE21	1.58	0.68
2:H:235:LYS:HE2	2:H:239:GLN:NE2	2.11	0.65
2:H:37:HIS:CD2	2:H:37:HIS:N	2.64	0.63
2:H:98:ASN:HB3	2:H:100:ASP:H	1.64	0.62
2:H:71:HIS:HD2	4:H:281:HOH:O	1.83	0.62
2:H:34:PHE:CE2	2:H:38:GLU:HB3	2.40	0.57
2:H:34:PHE:CZ	2:H:38:GLU:CB	2.90	0.53
2:H:84:MET:HE3	2:H:109:LYS:HD2	1.89	0.53
2:H:37:HIS:ND1	2:H:38:GLU:HG2	2.24	0.51
2:H:39:ARG:HB2	2:H:39:ARG:NH1	2.26	0.50
2:H:37:HIS:H	2:H:37:HIS:HD2	1.51	0.47
2:H:18:GLU:HG3	2:H:187:ARG:HG3	1.96	0.47
2:H:60(G):ASN:C	2:H:60(G):ASN:HD22	2.23	0.47
2:H:67:ARG:HG2	2:H:82:ILE:HG12	1.96	0.46
2:H:99:LEU:O	2:H:102:ASP:HB2	2.16	0.46
2:H:81:LYS:HG2	2:H:112:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:ARG:CB	2:H:39:ARG:HH11	2.29	0.45
2:H:164:GLU:H	2:H:164:GLU:CD	2.23	0.44
2:H:240:LYS:O	2:H:243:ASP:HB3	2.17	0.44
2:H:98:ASN:O	2:H:99:LEU:HB2	2.18	0.44
2:H:17:VAL:O	2:H:188:GLY:HA2	2.17	0.43
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.27	0.43
2:H:61:GLU:H	2:H:61:GLU:CD	2.27	0.42
2:H:36:LYS:HB3	2:H:65:LEU:HG	2.01	0.42
2:H:186:PRO:HG3	2:H:223:GLY:H	1.84	0.42
3:I:63:TYS:HE2	3:I:63:TYS:O3	2.19	0.41
2:H:36:LYS:HG3	2:H:36:LYS:O	2.20	0.41
2:H:64:LEU:HB2	2:H:85:LEU:HD23	2.02	0.41
2:H:97(A):GLU:CD	2:H:175:ARG:HH12	2.29	0.41
2:H:71:HIS:N	2:H:77:GLU:OE2	2.53	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:NH2	2:H:76:TYR:O[2_555]	0.97	1.23
2:H:75:ARG:NH2	2:H:76:TYR:C[2_555]	1.47	0.73
2:H:75:ARG:CG	2:H:75:ARG:NE[2_555]	1.99	0.21
2:H:75:ARG:NH1	3:I:57:GLU:OE1[2_555]	2.01	0.19
2:H:75:ARG:CD	4:I:67:HOH:O[2_555]	2.01	0.19

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	L	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
2	H	241/261 (92%)	229 (95%)	10 (4%)	2 (1%)	16	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	7/10 (70%)	5 (71%)	1 (14%)	1 (14%)	0	0
All	All	273/298 (92%)	258 (94%)	12 (4%)	3 (1%)	11	4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	184	TYR
3	I	56	PHE
2	H	79	ILE

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	L	25/25 (100%)	23 (92%)	2 (8%)	11	5
2	H	215/227 (95%)	195 (91%)	20 (9%)	8	3
3	I	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	249/261 (95%)	225 (90%)	24 (10%)	8	3

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
1	L	9	LYS
2	H	37	HIS
2	H	38	GLU
2	H	42	CYS
2	H	61	GLU
2	H	66	VAL
2	H	81	LYS
2	H	85	LEU
2	H	87	LYS
2	H	98	ASN
2	H	127	GLU

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Mol	Chain	Res	Type
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	145	LYS
2	H	154	VAL
2	H	164	GLU
2	H	233	ARG
2	H	236	LYS
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
3	I	61	GLU
3	I	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	37	HIS
2	H	60(G)	ASN
2	H	71	HIS
2	H	78	ASN
2	H	98	ASN
2	H	151	GLN
2	H	204(B)	ASN
2	H	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	I	63	3	15,16,17	1.99	3 (20%)	15,22,24	1.99	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	I	63	3	-	0/10/11/13	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	OH-S	-5.47	1.47	1.58
3	I	63	TYS	OH-CZ	-3.86	1.36	1.42
3	I	63	TYS	CB-CA	2.49	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	OH-S-O2	5.29	123.69	107.56
3	I	63	TYS	OH-S-O1	-4.97	92.40	107.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2
3	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	70:LYS	C	71:HIS	N	1.18
1	I	63:TYS	C	64:LEU	N	1.12
1	H	74:THR	C	75:ARG	N	1.11

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.