



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3HAT
Title : ACTIVE SITE MIMETIC INHIBITION OF THROMBIN
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-10-16
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

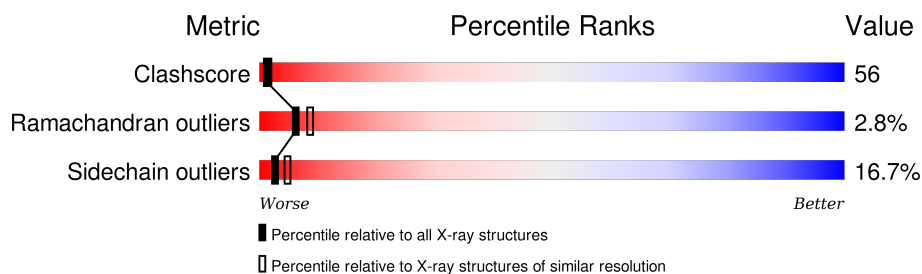
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	12	
4	T	6	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2575 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 (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			281	174	45	61	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			1996	1271	355	356	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
			87	56	10	20	1			

- Molecule 4 is a protein called FPAM (FIBRINOPEPTIDE A MIMIC).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	4	Total	C	N	O	0	0	0
			32	19	8	5			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	23	Total	O	0	0
			23	23		
5	H	146	Total	O	0	0
			146	146		
5	I	8	Total	O	0	0
			8	8		
5	T	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.

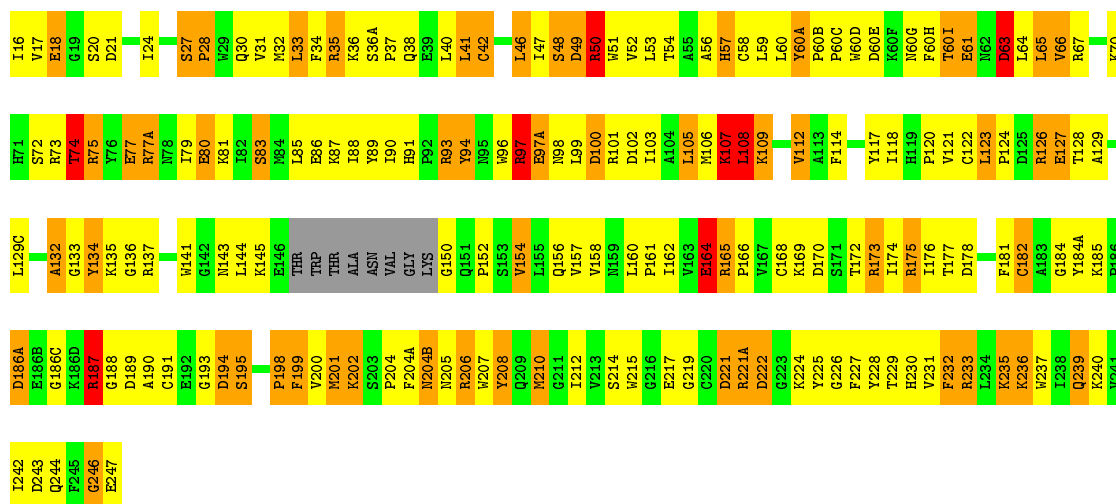
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 




• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRUGEN

Chain I: 



• Molecule 4: FPAM (FIBRINOPEPTIDE A MIMIC)

Chain T: 

YEN	YEN
7303	6304
Y305	Y306

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, α , β , γ	71.10 Å 72.40 Å 73.00 Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.140 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: RNG, 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	1.31	1/284 (0.4%)	2.76	21/377 (5.6%)
2	H	1.19	2/2047 (0.1%)	2.65	128/2764 (4.6%)
3	I	1.15	0/71	2.15	1/93 (1.1%)
4	T	1.53	0/22	3.22	3/26 (11.5%)
All	All	1.21	3/2424 (0.1%)	2.65	153/3260 (4.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	27	SER	CB-OG	-5.84	1.34	1.42
2	H	58	CYS	CB-SG	-5.53	1.72	1.81
1	L	14(C)	GLU	CD-OE2	-5.44	1.19	1.25

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75	ARG	NE-CZ-NH1	24.86	132.73	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-23.46	108.57	120.30
2	H	173	ARG	NE-CZ-NH2	21.25	130.92	120.30
1	L	4	ARG	NE-CZ-NH1	19.51	130.05	120.30
2	H	126	ARG	CD-NE-CZ	19.50	150.90	123.60
2	H	221(A)	ARG	NE-CZ-NH1	18.03	129.32	120.30
2	H	233	ARG	NE-CZ-NH1	17.67	129.14	120.30
2	H	173	ARG	NE-CZ-NH1	-17.19	111.71	120.30
2	H	187	ARG	NE-CZ-NH2	-15.08	112.76	120.30
2	H	187	ARG	NE-CZ-NH1	14.71	127.66	120.30
2	H	77(A)	ARG	CD-NE-CZ	13.53	142.54	123.60
2	H	77(A)	ARG	NE-CZ-NH1	13.34	126.97	120.30
2	H	75	ARG	CD-NE-CZ	13.09	141.93	123.60
2	H	233	ARG	CD-NE-CZ	12.79	141.50	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	102	ASP	CB-CG-OD2	-12.67	106.90	118.30
2	H	67	ARG	NE-CZ-NH2	11.98	126.29	120.30
2	H	49	ASP	CB-CG-OD2	11.54	128.69	118.30
2	H	164	GLU	OE1-CD-OE2	-11.45	109.56	123.30
2	H	165	ARG	NE-CZ-NH2	11.14	125.87	120.30
2	H	75	ARG	NH1-CZ-NH2	-11.12	107.16	119.40
2	H	221(A)	ARG	NE-CZ-NH2	-10.98	114.81	120.30
2	H	117	TYR	CB-CG-CD2	-10.90	114.46	121.00
1	L	4	ARG	NE-CZ-NH2	-10.74	114.93	120.30
2	H	175	ARG	NE-CZ-NH2	-10.68	114.96	120.30
2	H	206	ARG	NE-CZ-NH2	-10.59	115.01	120.30
2	H	33	LEU	CB-CA-C	10.52	130.18	110.20
1	L	14(H)	GLU	OE1-CD-OE2	10.51	135.91	123.30
2	H	50	ARG	NE-CZ-NH1	10.04	125.32	120.30
2	H	97(A)	GLU	OE1-CD-OE2	10.03	135.34	123.30
2	H	126	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	L	15	ARG	CD-NE-CZ	9.76	137.26	123.60
2	H	194	ASP	CB-CG-OD2	9.73	127.06	118.30
2	H	73	ARG	CD-NE-CZ	9.47	136.86	123.60
2	H	93	ARG	NE-CZ-NH1	-9.42	115.59	120.30
2	H	94	TYR	CB-CG-CD2	-9.36	115.39	121.00
2	H	67	ARG	CD-NE-CZ	9.21	136.50	123.60
2	H	60(A)	TYR	CB-CG-CD1	-9.07	115.56	121.00
2	H	170	ASP	CB-CG-OD1	9.04	126.44	118.30
2	H	60(E)	ASP	CB-CG-OD2	8.90	126.31	118.30
2	H	221	ASP	CB-CG-OD2	8.84	126.26	118.30
2	H	67	ARG	NH1-CZ-NH2	-8.49	110.06	119.40
2	H	178	ASP	CB-CG-OD2	-8.42	110.72	118.30
2	H	165	ARG	NH1-CZ-NH2	-8.40	110.16	119.40
2	H	243	ASP	CB-CG-OD2	-8.32	110.81	118.30
2	H	173	ARG	CG-CD-NE	8.16	128.94	111.80
2	H	21	ASP	CB-CG-OD2	-8.14	110.97	118.30
4	T	306	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	H	85	LEU	O-C-N	7.76	135.11	122.70
2	H	165	ARG	CD-NE-CZ	7.74	134.43	123.60
1	L	4	ARG	CG-CD-NE	7.68	127.92	111.80
2	H	93	ARG	NE-CZ-NH2	7.68	124.14	120.30
2	H	50	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	H	60(E)	ASP	CB-CG-OD1	-7.46	111.58	118.30
2	H	102	ASP	OD1-CG-OD2	7.43	137.41	123.30
2	H	230	HIS	CA-CB-CG	7.38	126.14	113.60
1	L	14(A)	LYS	CA-CB-CG	7.36	129.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	170	ASP	CB-CG-OD2	-7.28	111.74	118.30
2	H	165	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	L	14(K)	ILE	CB-CA-C	7.18	125.95	111.60
1	L	1(G)	PHE	O-C-N	7.05	135.19	123.20
1	L	14(K)	ILE	C-N-CA	7.05	139.33	121.70
2	H	233	ARG	NH1-CZ-NH2	-6.96	111.74	119.40
2	H	175	ARG	NH1-CZ-NH2	6.93	127.03	119.40
2	H	60(A)	TYR	CB-CG-CD2	6.93	125.16	121.00
2	H	77(A)	ARG	C-N-CA	-6.92	104.40	121.70
2	H	63	ASP	CB-CG-OD1	-6.87	112.11	118.30
2	H	181	PHE	N-CA-CB	6.73	122.71	110.60
2	H	67	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	H	228	TYR	CB-CG-CD2	6.64	124.99	121.00
2	H	207	TRP	O-C-N	6.61	133.28	122.70
2	H	108	LEU	CA-CB-CG	6.57	130.41	115.30
2	H	165	ARG	CG-CD-NE	6.50	125.46	111.80
1	L	1(E)	SER	CB-CA-C	6.48	122.41	110.10
2	H	74	THR	N-CA-C	6.42	128.35	111.00
2	H	60	LEU	CB-CG-CD2	-6.40	100.12	111.00
2	H	114	PHE	CB-CG-CD1	-6.39	116.33	120.80
1	L	15	ARG	NE-CZ-NH1	6.37	123.48	120.30
2	H	117	TYR	CB-CG-CD1	6.31	124.79	121.00
2	H	64	LEU	O-C-N	6.31	132.79	122.70
2	H	141	TRP	CA-CB-CG	6.26	125.60	113.70
1	L	14(H)	GLU	CG-CD-OE1	-6.25	105.80	118.30
2	H	244	GLN	N-CA-CB	6.23	121.82	110.60
2	H	73	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	H	74	THR	OG1-CB-CG2	6.22	124.31	110.00
2	H	63	ASP	O-C-N	6.21	132.64	122.70
1	L	14(B)	THR	O-C-N	6.19	132.60	122.70
2	H	173	ARG	CD-NE-CZ	-6.14	115.01	123.60
2	H	83	SER	N-CA-CB	6.06	119.58	110.50
2	H	77(A)	ARG	CA-C-O	-6.04	107.41	120.10
1	L	2	GLY	CA-C-O	-6.00	109.81	120.60
2	H	80	GLU	CA-CB-CG	5.99	126.57	113.40
2	H	129	ALA	CB-CA-C	5.98	119.07	110.10
2	H	134	TYR	CD1-CE1-CZ	-5.98	114.42	119.80
2	H	201	MET	O-C-N	5.97	132.25	122.70
2	H	243	ASP	CB-CG-OD1	5.96	123.67	118.30
2	H	94	TYR	CB-CG-CD1	5.96	124.58	121.00
2	H	198	PRO	CB-CA-C	-5.95	97.13	112.00
2	H	73	ARG	C-N-CA	5.88	136.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1(D)	GLY	CA-C-O	-5.88	110.02	120.60
2	H	164	GLU	CA-CB-CG	5.88	126.33	113.40
2	H	54	THR	CA-CB-CG2	5.70	120.38	112.40
2	H	225	TYR	CB-CG-CD1	-5.69	117.59	121.00
1	L	14(K)	ILE	CA-C-O	5.68	132.03	120.10
2	H	18	GLU	CB-CA-C	-5.66	99.08	110.40
2	H	194	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	L	1(G)	PHE	CB-CA-C	5.65	121.69	110.40
2	H	77	GLU	OE1-CD-OE2	5.64	130.07	123.30
2	H	199	PHE	CB-CA-C	5.64	121.68	110.40
2	H	157	VAL	O-C-N	5.58	131.62	122.70
2	H	189	ASP	CB-CG-OD2	5.54	123.29	118.30
2	H	59	LEU	C-N-CA	5.53	135.52	121.70
2	H	97	ARG	C-N-CA	-5.50	107.94	121.70
2	H	210	MET	CG-SD-CE	-5.50	91.40	100.20
2	H	157	VAL	CA-C-O	-5.49	108.57	120.10
2	H	108	LEU	CB-CA-C	5.48	120.61	110.20
1	L	14(M)	GLY	N-CA-C	5.48	126.79	113.10
2	H	49	ASP	CB-CG-OD1	-5.46	113.38	118.30
2	H	126	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	H	186(A)	ASP	CB-CG-OD2	-5.44	113.40	118.30
2	H	24	ILE	C-N-CA	5.44	133.72	122.30
2	H	123	LEU	CB-CG-CD2	-5.41	101.80	111.00
4	T	306	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
2	H	232	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	L	14(B)	THR	N-CA-CB	5.39	120.55	110.30
2	H	107	LYS	CA-CB-CG	5.39	125.27	113.40
2	H	105	LEU	CB-CG-CD2	-5.33	101.93	111.00
2	H	164	GLU	CB-CG-CD	5.33	128.59	114.20
2	H	117	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
2	H	35	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	H	106	MET	CA-CB-CG	-5.29	104.31	113.30
1	L	1(A)	ASP	CA-C-N	-5.28	105.58	117.20
2	H	222	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	H	231	VAL	CB-CA-C	5.28	121.42	111.40
1	L	1(H)	THR	CA-C-N	-5.26	105.64	117.20
2	H	208	TYR	CB-CG-CD2	-5.23	117.86	121.00
3	I	58	GLU	N-CA-CB	5.21	119.99	110.60
2	H	132	ALA	C-N-CA	-5.17	111.44	122.30
2	H	63	ASP	CA-C-O	-5.13	109.32	120.10
2	H	193	GLY	C-N-CA	5.13	134.52	121.70
2	H	135	LYS	C-N-CA	5.12	133.05	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	LYS	O-C-N	5.08	130.84	122.70
2	H	94	TYR	CA-CB-CG	5.08	123.06	113.40
4	T	304	GLY	O-C-N	5.08	130.83	122.70
2	H	50	ARG	CG-CD-NE	5.07	122.46	111.80
2	H	74	THR	CA-CB-OG1	-5.07	98.35	109.00
2	H	42	CYS	CA-CB-SG	5.07	123.12	114.00
2	H	154	VAL	N-CA-CB	-5.05	100.39	111.50
2	H	100	ASP	O-C-N	5.05	130.78	122.70
2	H	137	ARG	O-C-N	5.05	130.77	122.70
2	H	225	TYR	CA-CB-CG	-5.03	103.85	113.40
2	H	77	GLU	CA-C-O	5.03	130.65	120.10
2	H	199	PHE	N-CA-C	-5.01	97.46	111.00
2	H	225	TYR	CD1-CE1-CZ	-5.01	115.29	119.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	281	0	267	68	3
2	H	1996	0	1955	223	3
3	I	87	0	68	9	0
4	T	32	0	34	16	0
5	H	146	0	0	19	0
5	I	8	0	0	1	0
5	L	23	0	0	2	0
5	T	2	0	0	0	0
All	All	2575	0	2324	263	3

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 56.

All (263) 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:224:LYS:HE2	5:H:465:HOH:O	1.40	1.19
1:L:1(F):GLY:O	1:L:1(E):SER:HB3	1.46	1.14
1:L:15:ARG:NH1	2:H:204(A):PHE:O	1.83	1.08
1:L:1(H):THR:HG22	1:L:1(D):GLY:O	1.51	1.08
2:H:201:MET:CE	2:H:210:MET:HG3	1.82	1.08
2:H:240:LYS:HD2	5:H:605:HOH:O	1.56	1.03
1:L:1(D):GLY:H	2:H:123:LEU:N	1.57	1.02
2:H:165:ARG:HE	2:H:169:LYS:HZ1	1.02	1.00
2:H:201:MET:HE2	2:H:210:MET:HG3	1.42	0.98
2:H:60(I):THR:HG23	2:H:63:ASP:OD1	1.62	0.98
1:L:1(D):GLY:N	2:H:123:LEU:H	1.62	0.97
2:H:235:LYS:HZ1	2:H:239:GLN:NE2	1.62	0.97
1:L:1(D):GLY:HA3	2:H:121:VAL:O	1.66	0.95
2:H:51:TRP:HE1	2:H:247:GLU:CA	1.78	0.95
1:L:1(G):PHE:HB2	5:L:703:HOH:O	1.67	0.92
2:H:235:LYS:HZ1	2:H:239:GLN:HE22	1.18	0.92
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.52	0.91
2:H:240:LYS:CD	5:H:605:HOH:O	2.13	0.90
2:H:81:LYS:HD2	5:H:463:HOH:O	1.72	0.89
2:H:17:VAL:O	2:H:188:GLY:HA2	1.71	0.88
2:H:160:LEU:HG	5:H:480:HOH:O	1.74	0.87
1:L:1(D):GLY:H	2:H:123:LEU:H	0.89	0.87
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.75	0.86
1:L:15:ARG:HD2	2:H:204:PRO:O	1.76	0.84
2:H:236:LYS:HD2	2:H:236:LYS:H	1.41	0.84
2:H:165:ARG:NE	2:H:169:LYS:HZ1	1.75	0.84
2:H:201:MET:HE3	2:H:210:MET:HG3	1.58	0.84
2:H:195:SER:OG	4:T:306:ARG:C	2.16	0.83
1:L:1(D):GLY:N	2:H:122:CYS:HA	1.92	0.82
1:L:1(E):SER:N	2:H:123:LEU:O	2.12	0.82
2:H:236:LYS:H	2:H:236:LYS:CD	1.93	0.82
2:H:97(A):GLU:OE2	2:H:175:ARG:NH1	2.13	0.81
2:H:165:ARG:HE	2:H:169:LYS:NZ	1.77	0.81
2:H:158:VAL:HG22	5:H:480:HOH:O	1.83	0.79
1:L:1(E):SER:CA	2:H:123:LEU:O	2.31	0.79
2:H:124:PRO:HG3	2:H:210:MET:HE2	1.64	0.78
1:L:1(H):THR:CG2	1:L:1(G):PHE:H	1.95	0.78
2:H:235:LYS:NZ	2:H:239:GLN:NE2	2.32	0.78
1:L:1(E):SER:H	2:H:123:LEU:HB2	1.48	0.77
1:L:14(J):TYR:O	1:L:14(K):ILE:HG12	1.83	0.77
2:H:74:THR:HG22	2:H:75:ARG:HD3	1.66	0.77
1:L:1(H):THR:HG23	1:L:1(G):PHE:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(F):GLY:N	2:H:235:LYS:HZ2	1.84	0.75
2:H:208:TYR:HB3	2:H:210:MET:CE	2.18	0.74
2:H:46:LEU:HD22	2:H:48:SER:O	1.86	0.74
2:H:242:ILE:O	2:H:246:GLY:HA2	1.88	0.73
2:H:75:ARG:NH2	5:H:809:HOH:O	2.22	0.72
1:L:1(F):GLY:N	2:H:235:LYS:NZ	2.37	0.72
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.68	0.72
1:L:1(G):PHE:CD1	2:H:239:GLN:OE1	2.42	0.72
2:H:160:LEU:CG	5:H:480:HOH:O	2.32	0.72
2:H:41:LEU:HD11	2:H:60(H):PHE:CE2	2.23	0.72
1:L:1(H):THR:CG2	1:L:1(G):PHE:N	2.53	0.72
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.90	0.71
2:H:195:SER:HB2	4:T:306:ARG:O	1.90	0.71
2:H:224:LYS:O	5:H:429:HOH:O	2.07	0.71
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.93	0.71
2:H:160:LEU:CD2	5:H:480:HOH:O	2.37	0.71
2:H:235:LYS:NZ	2:H:239:GLN:HE22	1.89	0.71
1:L:14(E):GLU:HB2	5:L:505:HOH:O	1.89	0.70
2:H:165:ARG:NE	2:H:169:LYS:CE	2.55	0.70
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.27	0.69
3:I:61:GLU:HA	3:I:64:LEU:HD23	1.74	0.69
2:H:74:THR:HG22	2:H:75:ARG:N	2.08	0.69
1:L:1(F):GLY:CA	2:H:235:LYS:HZ2	2.06	0.68
2:H:195:SER:CB	4:T:306:ARG:O	2.41	0.68
2:H:87:LYS:HD3	2:H:88:ILE:H	1.59	0.68
1:L:1(E):SER:HA	2:H:123:LEU:N	2.09	0.67
2:H:208:TYR:HB3	2:H:210:MET:HE1	1.77	0.66
2:H:60(I):THR:CG2	2:H:63:ASP:OD1	2.41	0.66
2:H:70:LYS:HE3	2:H:72:SER:O	1.93	0.66
1:L:14(M):GLY:HA2	2:H:204:PRO:HB3	1.77	0.66
2:H:160:LEU:HD21	5:H:480:HOH:O	1.96	0.66
2:H:70:LYS:NZ	2:H:80:GLU:OE2	2.27	0.66
2:H:49:ASP:O	2:H:112:VAL:HG12	1.96	0.65
3:I:60:PRO:HB2	3:I:62:GLU:OE2	1.97	0.65
2:H:143:ASN:HA	2:H:150:GLY:O	1.97	0.65
2:H:35:ARG:O	2:H:38:GLN:HA	1.95	0.65
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.79	0.64
1:L:14(M):GLY:CA	2:H:204:PRO:HB3	2.27	0.64
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.97	0.64
2:H:98:ASN:N	2:H:98:ASN:OD1	2.27	0.64
3:I:60:PRO:O	3:I:63:TYS:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:NE	2:H:169:LYS:NZ	2.42	0.63
2:H:50:ARG:HH11	2:H:107:LYS:HG3	1.63	0.63
2:H:182:CYS:HA	2:H:226:GLY:O	1.98	0.63
2:H:161:PRO:HG3	2:H:184(A):TYR:CE1	2.34	0.62
1:L:14(G):LEU:HD12	1:L:14(M):GLY:HA3	1.82	0.62
3:I:60:PRO:HG2	3:I:63:TYS:HE2	1.81	0.62
1:L:1(H):THR:HG23	1:L:1(G):PHE:H	1.58	0.61
2:H:236:LYS:N	2:H:236:LYS:HD2	2.13	0.61
2:H:165:ARG:N	2:H:166:PRO:HD2	2.14	0.61
1:L:1(G):PHE:O	1:L:1(E):SER:N	2.34	0.61
2:H:100:ASP:O	2:H:101:ARG:HB2	2.01	0.61
2:H:201:MET:CE	2:H:210:MET:CG	2.71	0.61
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.16	0.60
1:L:1(C):GLU:N	1:L:1:CYS:HB3	2.17	0.60
2:H:17:VAL:O	2:H:18:GLU:HB2	2.01	0.60
2:H:187:ARG:NH1	2:H:221:ASP:O	2.34	0.60
1:L:1(F):GLY:HA2	2:H:235:LYS:HZ2	1.66	0.59
2:H:56:ALA:HB2	2:H:103:ILE:O	2.02	0.59
1:L:1(E):SER:CA	2:H:123:LEU:H	2.15	0.59
1:L:1(F):GLY:H	2:H:239:GLN:HE22	1.49	0.59
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.35	0.59
2:H:86:GLU:HG3	2:H:109:LYS:HG3	1.84	0.59
2:H:57:HIS:NE2	4:T:306:ARG:OXT	2.27	0.59
2:H:195:SER:CB	4:T:306:ARG:C	2.71	0.59
2:H:239:GLN:HA	2:H:239:GLN:OE1	2.03	0.59
2:H:66:VAL:HG12	2:H:83:SER:HB2	1.85	0.58
2:H:198:PRO:HB2	2:H:200:VAL:HG13	1.83	0.58
2:H:63:ASP:N	2:H:63:ASP:OD1	2.34	0.58
2:H:50:ARG:HH11	2:H:107:LYS:CG	2.16	0.58
2:H:174:ILE:HG13	4:T:303:RNG:HG2	1.85	0.58
2:H:81:LYS:HE2	2:H:118:ILE:HD12	1.86	0.57
1:L:1(H):THR:O	1:L:1(G):PHE:HD1	1.87	0.57
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.58	0.57
1:L:1(H):THR:N	1:L:1(D):GLY:HA2	2.18	0.57
1:L:14(J):TYR:HE2	2:H:202:LYS:O	1.88	0.57
2:H:72:SER:OG	2:H:75:ARG:HG2	2.05	0.57
2:H:99:LEU:HD11	4:T:305:VAL:HB	1.86	0.57
2:H:132:ALA:HA	2:H:162:ILE:O	2.04	0.56
1:L:3:LEU:HB2	1:L:9:LYS:HE2	1.87	0.56
2:H:103:ILE:HD12	2:H:212:ILE:HD11	1.87	0.56
2:H:49:ASP:N	2:H:49:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(C):GLU:HB2	2:H:120:PRO:CG	2.36	0.56
1:L:1(E):SER:HA	2:H:123:LEU:O	2.04	0.56
2:H:36:LYS:HD2	2:H:65:LEU:HD13	1.86	0.56
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.88	0.56
2:H:81:LYS:HE2	2:H:118:ILE:CD1	2.35	0.56
2:H:191:CYS:O	2:H:194:ASP:HB2	2.05	0.55
2:H:20:SER:O	2:H:156:GLN:HA	2.06	0.55
2:H:236:LYS:N	2:H:236:LYS:CD	2.68	0.55
2:H:60(A):TYR:CZ	4:T:305:VAL:HG11	2.42	0.55
1:L:14(A):LYS:HG3	5:H:705:HOH:O	2.07	0.54
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.41	0.54
2:H:201:MET:HE3	2:H:210:MET:CG	2.33	0.54
2:H:60(B):PRO:O	2:H:60(C):PRO:C	2.40	0.54
2:H:160:LEU:HD22	2:H:184:GLY:HA2	1.89	0.54
2:H:66:VAL:HG11	2:H:108:LEU:HD22	1.89	0.54
2:H:174:ILE:HG13	4:T:303:RNG:CG	2.38	0.54
2:H:165:ARG:HH21	2:H:169:LYS:NZ	2.06	0.54
2:H:158:VAL:CG2	5:H:480:HOH:O	2.46	0.54
1:L:1(E):SER:CA	2:H:123:LEU:N	2.71	0.53
1:L:1(C):GLU:CB	2:H:120:PRO:HG2	2.38	0.53
2:H:36(A):SER:HA	2:H:37:PRO:C	2.28	0.53
2:H:16:ILE:N	2:H:194:ASP:OD2	2.41	0.53
2:H:17:VAL:HG11	2:H:221:ASP:HB3	1.89	0.53
2:H:165:ARG:HH21	2:H:169:LYS:HZ3	1.56	0.53
2:H:42:CYS:HB3	2:H:195:SER:O	2.08	0.52
1:L:4:ARG:HB2	1:L:8:GLU:OE1	2.10	0.52
2:H:165:ARG:NH2	2:H:169:LYS:NZ	2.58	0.52
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.87	0.52
2:H:47:ILE:HD11	2:H:105:LEU:HD21	1.92	0.52
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.72	0.52
2:H:87:LYS:CD	2:H:88:ILE:H	2.21	0.51
1:L:3:LEU:CB	1:L:9:LYS:HE2	2.41	0.51
2:H:215:TRP:CE3	4:T:303:RNG:HH	2.45	0.51
1:L:1(F):GLY:CA	2:H:235:LYS:NZ	2.72	0.50
2:H:165:ARG:N	2:H:166:PRO:CD	2.74	0.50
1:L:1(E):SER:HA	2:H:122:CYS:HB3	1.92	0.50
2:H:165:ARG:CZ	2:H:169:LYS:NZ	2.74	0.50
1:L:1(H):THR:H2	2:H:123:LEU:HD11	1.76	0.50
2:H:134:TYR:HD1	2:H:134:TYR:N	2.10	0.50
2:H:237:TRP:HB2	5:H:937:HOH:O	2.11	0.49
2:H:165:ARG:HE	2:H:169:LYS:CE	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.09	0.49
1:L:1(H):THR:H1	1:L:1(D):GLY:HA2	1.77	0.49
2:H:60(G):ASN:ND2	5:H:521:HOH:O	2.38	0.49
2:H:165:ARG:O	2:H:168:CYS:HB2	2.13	0.49
2:H:97:ARG:HH11	2:H:97:ARG:HG2	1.78	0.49
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.96	0.48
2:H:165:ARG:CZ	2:H:169:LYS:HZ1	2.24	0.48
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.43	0.48
1:L:1(D):GLY:N	2:H:122:CYS:CA	2.70	0.48
2:H:61:GLU:HG2	2:H:61:GLU:H	1.27	0.48
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.79	0.47
2:H:49:ASP:O	2:H:112:VAL:CG1	2.61	0.47
2:H:18:GLU:HG3	2:H:187:ARG:CB	2.36	0.47
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.49	0.47
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.50	0.47
2:H:164:GLU:CD	2:H:185:LYS:HZ1	2.18	0.47
1:L:5:PRO:O	1:L:9:LYS:HB2	2.15	0.47
2:H:36:LYS:O	2:H:38:GLN:HG2	2.15	0.46
1:L:14(G):LEU:O	1:L:14(L):ASP:HA	2.16	0.46
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.68	0.46
2:H:144:LEU:HD11	2:H:152:PRO:HA	1.97	0.46
2:H:56:ALA:CB	2:H:90:ILE:HG23	2.46	0.46
2:H:74:THR:HB	5:H:902:HOH:O	2.14	0.46
2:H:161:PRO:HD3	2:H:184(A):TYR:CZ	2.50	0.46
2:H:240:LYS:HD3	5:H:605:HOH:O	1.94	0.46
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.98	0.46
2:H:187:ARG:HB3	2:H:221:ASP:OD1	2.15	0.46
2:H:134:TYR:N	2:H:134:TYR:CD1	2.84	0.46
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.46	0.46
2:H:100:ASP:CG	2:H:177:THR:HG21	2.36	0.46
1:L:1(C):GLU:HB2	2:H:120:PRO:HG2	1.97	0.45
2:H:186(A):ASP:C	2:H:186(C):GLY:N	2.69	0.45
2:H:165:ARG:NE	2:H:169:LYS:HE3	2.30	0.45
2:H:195:SER:HB2	4:T:306:ARG:C	2.36	0.45
2:H:164:GLU:C	2:H:166:PRO:HD2	2.37	0.45
1:L:1(H):THR:N	2:H:123:LEU:CD1	2.80	0.45
1:L:1(D):GLY:CA	2:H:122:CYS:HA	2.46	0.44
2:H:128:THR:HG23	2:H:129(C):LEU:HD12	1.98	0.44
2:H:186(A):ASP:O	2:H:186(C):GLY:N	2.50	0.44
2:H:57:HIS:CE1	2:H:195:SER:OG	2.71	0.44
2:H:60(B):PRO:HG2	2:H:96:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:SER:OG	4:T:306:ARG:O	2.35	0.44
1:L:1(E):SER:C	2:H:123:LEU:H	2.18	0.44
1:L:1(D):GLY:H	2:H:122:CYS:CA	2.30	0.44
2:H:217:GLU:O	2:H:221(A):ARG:HD2	2.18	0.44
2:H:16:ILE:HD13	2:H:190:ALA:HA	2.00	0.44
2:H:165:ARG:HB3	2:H:166:PRO:HD3	1.99	0.44
2:H:30:GLN:HG3	2:H:31:VAL:N	2.33	0.43
2:H:41:LEU:HD22	2:H:41:LEU:HA	1.84	0.43
2:H:61:GLU:OE1	2:H:87:LYS:CA	2.55	0.43
3:I:59:ILE:O	3:I:60:PRO:C	2.56	0.43
2:H:91:HIS:CE1	2:H:101:ARG:HD2	2.54	0.43
2:H:60(A):TYR:OH	4:T:305:VAL:HG11	2.18	0.43
1:L:14(A):LYS:HB2	1:L:14(A):LYS:HE3	1.68	0.43
2:H:161:PRO:HG3	2:H:184(A):TYR:CD1	2.54	0.43
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.17	0.43
2:H:129(C):LEU:HD21	2:H:204:PRO:HD3	2.00	0.43
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	2.00	0.43
2:H:144:LEU:HD11	2:H:152:PRO:CA	2.49	0.42
2:H:97(A):GLU:CD	2:H:175:ARG:HH12	2.22	0.42
3:I:64:LEU:N	3:I:64:LEU:HD22	2.33	0.42
3:I:58:GLU:HB2	5:I:426:HOH:O	2.19	0.42
2:H:81:LYS:CE	2:H:118:ILE:HD12	2.48	0.42
3:I:63:TYR:HD1	3:I:63:TYR:HA	1.80	0.42
2:H:173:ARG:NE	5:H:733:HOH:O	2.52	0.42
2:H:87:LYS:HB3	2:H:89:TYR:HE1	1.83	0.42
4:T:305:VAL:O	4:T:305:VAL:HG22	2.20	0.42
2:H:133:GLY:N	2:H:162:ILE:O	2.47	0.42
1:L:1(H):THR:H2	2:H:123:LEU:CD1	2.32	0.42
2:H:60(I):THR:HG22	2:H:63:ASP:OD2	2.19	0.42
1:L:1(F):GLY:N	2:H:239:GLN:HE22	2.16	0.41
3:I:61:GLU:CD	3:I:61:GLU:H	2.23	0.41
2:H:66:VAL:HG11	2:H:108:LEU:CD2	2.50	0.41
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.94	0.41
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.55	0.41
2:H:165:ARG:CZ	2:H:169:LYS:HE2	2.50	0.41
2:H:242:ILE:O	2:H:246:GLY:CA	2.64	0.41
2:H:60(D):TRP:CH2	4:T:305:VAL:HG22	2.56	0.41
2:H:236:LYS:O	2:H:240:LYS:HB3	2.20	0.41
2:H:165:ARG:CZ	2:H:169:LYS:CE	2.98	0.41
4:T:305:VAL:O	4:T:305:VAL:CG2	2.68	0.41
1:L:1(G):PHE:HA	2:H:239:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(G):PHE:O	1:L:1(E):SER:C	2.59	0.41
2:H:46:LEU:CD2	2:H:48:SER:O	2.64	0.41
2:H:49:ASP:HA	2:H:112:VAL:HG13	2.02	0.41
2:H:57:HIS:HE1	2:H:214:SER:O	2.03	0.41
2:H:52:VAL:HG23	2:H:108:LEU:HD21	2.03	0.41
1:L:15:ARG:O	1:L:15:ARG:HG3	2.21	0.41
2:H:124:PRO:HG3	2:H:210:MET:CE	2.44	0.41
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	2.20	0.41
2:H:51:TRP:NE1	2:H:247:GLU:CA	2.63	0.41
1:L:1(C):GLU:H	1:L:1:CYS:HB3	1.83	0.40
2:H:93:ARG:HH11	2:H:93:ARG:HD3	1.72	0.40
2:H:103:ILE:HB	2:H:229:THR:HG21	2.04	0.40
2:H:127:GLU:HB3	5:H:715:HOH:O	2.21	0.40
2:H:165:ARG:NH2	2:H:169:LYS:HZ3	2.18	0.40
2:H:50:ARG:HA	2:H:108:LEU:HD12	2.04	0.40
1:L:14(J):TYR:HD2	2:H:204:PRO:HG3	1.86	0.40

All (3) 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)
1:L:14(L):ASP:O	2:H:173:ARG:NH1[4_556]	2.07	0.13
1:L:14(M):GLY:O	2:H:173:ARG:NH1[4_556]	2.09	0.11
1:L:15:ARG:CZ	2:H:172:THR:O[4_556]	2.18	0.02

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	34/36 (94%)	21 (62%)	7 (21%)	6 (18%)	0	0
2	H	247/259 (95%)	228 (92%)	17 (7%)	2 (1%)	24	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	7/12 (58%)	7 (100%)	0	0	100	100
4	T	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	290/313 (93%)	257 (89%)	25 (9%)	8 (3%)	6	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(F)	GLY
1	L	1(E)	SER
1	L	1(D)	GLY
1	L	1(C)	GLU
1	L	14(M)	GLY
2	H	246	GLY
2	H	77(A)	ARG
1	L	14(K)	ILE

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	30/31 (97%)	23 (77%)	7 (23%)	1	1
2	H	212/225 (94%)	178 (84%)	34 (16%)	3	5
3	I	7/10 (70%)	6 (86%)	1 (14%)	4	7
4	T	2/2 (100%)	2 (100%)	0	100	100
All	All	251/268 (94%)	209 (83%)	42 (17%)	3	5

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(E)	SER
1	L	6	LEU
1	L	10	LYS
1	L	14	ASP

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Mol	Chain	Res	Type
1	L	14(F)	LEU
1	L	14(K)	ILE
1	L	14(L)	ASP
2	H	27	SER
2	H	28	PRO
2	H	33	LEU
2	H	41	LEU
2	H	46	LEU
2	H	48	SER
2	H	50	ARG
2	H	57	HIS
2	H	60(I)	THR
2	H	61	GLU
2	H	63	ASP
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	77	GLU
2	H	79	ILE
2	H	94	TYR
2	H	97	ARG
2	H	107	LYS
2	H	108	LEU
2	H	109	LYS
2	H	112	VAL
2	H	127	GLU
2	H	154	VAL
2	H	164	GLU
2	H	182	CYS
2	H	187	ARG
2	H	195	SER
2	H	202	LYS
2	H	204(B)	ASN
2	H	233	ARG
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
3	I	62	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	60(G)	ASN
2	H	95	ASN
2	H	156	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	1.59	2 (13%)	16,22,24	1.92	5 (31%)

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	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-CZ	-4.39	1.35	1.42
3	I	63	TYS	OH-S	3.36	1.70	1.63

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CG-CB-CA	-4.07	105.01	114.21
3	I	63	TYS	O-C-CA	-2.50	118.98	125.49
3	I	63	TYS	CB-CG-CD1	-2.18	116.35	120.90
3	I	63	TYS	CD2-CG-CD1	2.12	121.52	118.13
3	I	63	TYS	O2-S-O1	3.74	128.75	112.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.