



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 AM UTC

PDB ID : 1FAK / pdb_00001fak
Title : HUMAN TISSUE FACTOR COMPLEXED WITH COAGULATION FACTOR VIIA INHIBITED WITH A BPTI-MUTANT
Authors : Zhang, E.; St Charles, R.; Tulinsky, A.
Deposited on : 1998-12-28
Resolution : 2.10 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

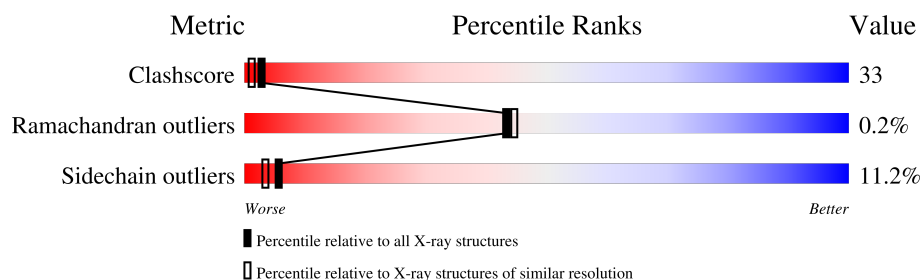
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	152	26% 33% 9% • 29%
2	H	254	37% 41% 19% ••
3	T	206	26% 44% 18% • 11%
4	I	55	9% 56% 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLC	L	600	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5079 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 PROTEIN (BLOOD COAGULATION FACTOR VIIA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	108	Total	C	N	O	S	0	0	0
			827	504	143	167	13			

- Molecule 2 is a protein called PROTEIN (BLOOD COAGULATION FACTOR VIIA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			1955	1242	348	352	13			

- Molecule 3 is a protein called PROTEIN (SOLUBLE TISSUE FACTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	183	Total	C	N	O	S	0	0	0
			1495	957	240	293	5			

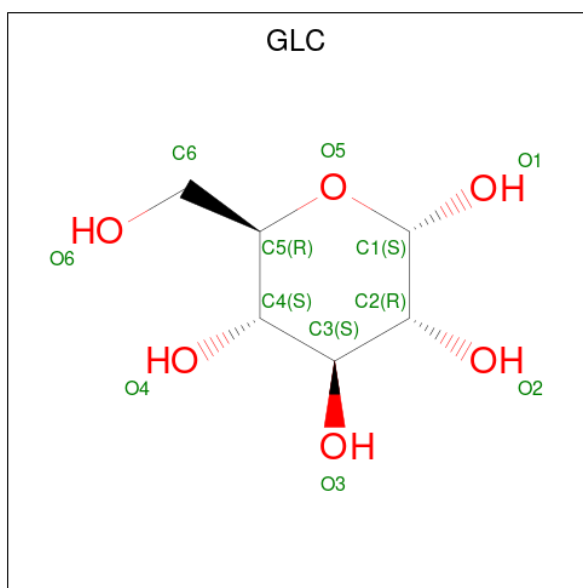
- Molecule 4 is a protein called PROTEIN (5L15).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	55	Total	C	N	O	S	0	0	0
			439	277	75	80	7			

There are 8 discrepancies between the modelled and reference sequences:

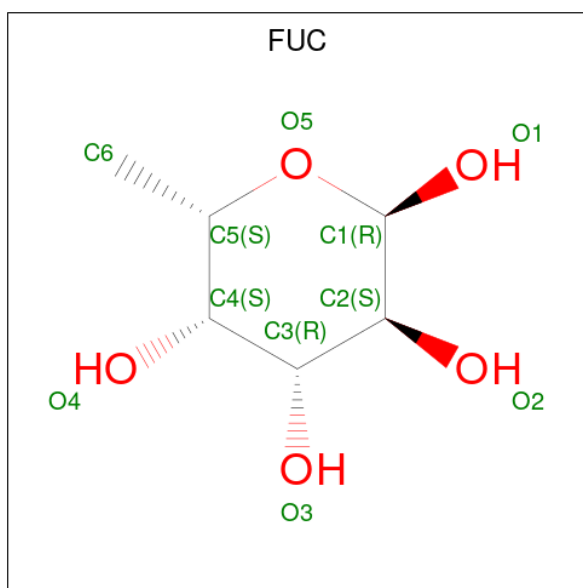
Chain	Residue	Modelled	Actual	Comment	Reference
I	11	ASP	THR	conflict	UNP P00974
I	15	ARG	LYS	conflict	UNP P00974
I	17	LEU	ARG	conflict	UNP P00974
I	18	HIS	ILE	conflict	UNP P00974
I	19	LEU	ILE	conflict	UNP P00974
I	34	TYR	VAL	conflict	UNP P00974
I	39	LEU	ARG	conflict	UNP P00974
I	46	GLU	LYS	conflict	UNP P00974

- Molecule 5 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total 1	Ca 1	0	0
7	H	1	Total 1	Ca 1	0	0

- Molecule 8 is water.

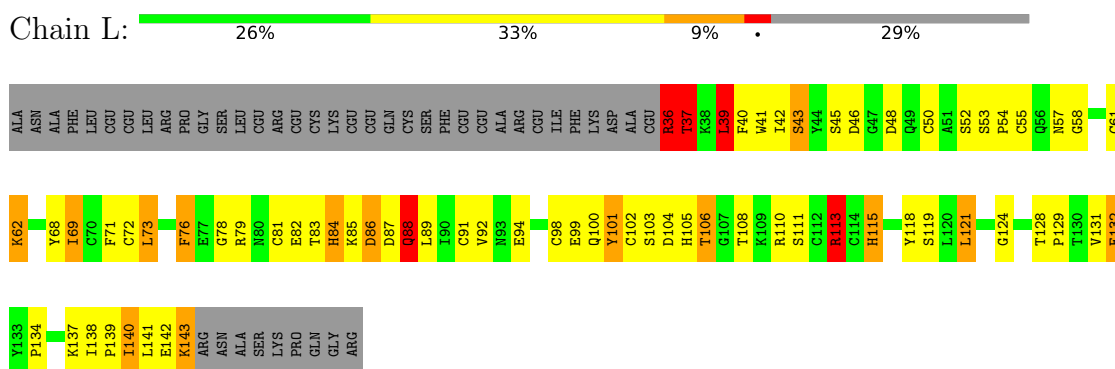
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	78	Total 78	O 78	0	0
8	H	164	Total 164	O 164	0	0
8	T	75	Total 75	O 75	0	0
8	I	23	Total 23	O 23	0	0

3 Residue-property plots

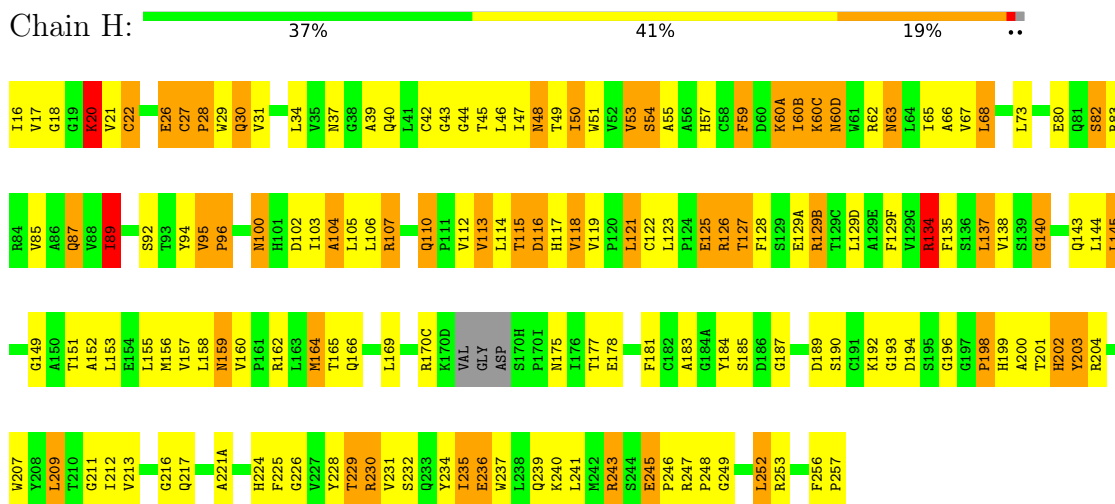
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

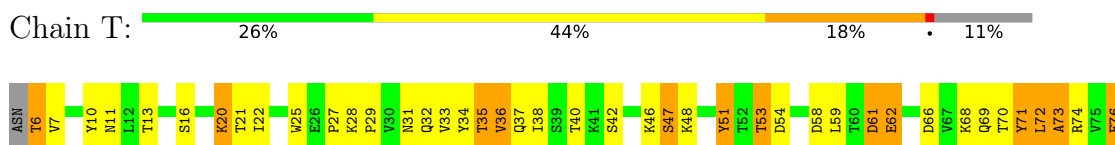
- Molecule 1: PROTEIN (BLOOD COAGULATION FACTOR VIIA)

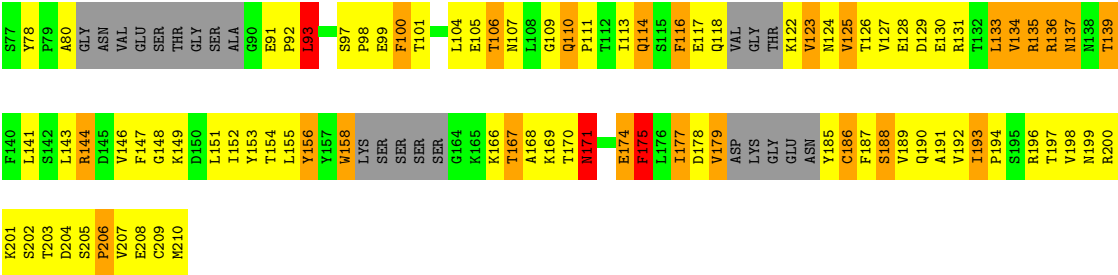


- Molecule 2: PROTEIN (BLOOD COAGULATION FACTOR VIIA)

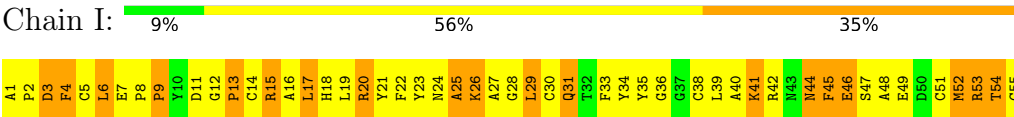


- Molecule 3: PROTEIN (SOLUBLE TISSUE FACTOR)





● Molecule 4: PROTEIN (5L15)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.49Å 190.00Å 175.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 2.10	Depositor
% Data completeness (in resolution range)	80.0 (9.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.237 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5079	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: GLC, FUC, CA

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	1.45	1/844 (0.1%)	2.43	56/1139 (4.9%)
2	H	1.81	27/2004 (1.3%)	2.55	166/2726 (6.1%)
3	T	1.40	4/1527 (0.3%)	2.25	77/2075 (3.7%)
4	I	1.40	3/452 (0.7%)	2.36	28/609 (4.6%)
All	All	1.59	35/4827 (0.7%)	2.42	327/6549 (5.0%)

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	2
4	I	0	1
All	All	0	3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	235	ILE	CA-CB	10.47	1.66	1.54
2	H	43	GLY	N-CA	8.30	1.52	1.44
2	H	128	PHE	C-N	7.50	1.43	1.33
2	H	199	HIS	CA-C	7.05	1.61	1.52
2	H	209	LEU	N-CA	6.89	1.54	1.46
3	T	100	PHE	N-CA	6.67	1.54	1.46
3	T	21	THR	CA-CB	6.57	1.63	1.53
2	H	44	GLY	N-CA	6.45	1.52	1.45
2	H	85	VAL	N-CA	6.36	1.53	1.46
2	H	152	ALA	CA-CB	6.22	1.63	1.53
2	H	94	TYR	CA-CB	6.17	1.61	1.53
2	H	207	TRP	N-CA	6.17	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	103	ILE	CA-CB	6.11	1.61	1.55
4	I	18	HIS	N-CA	6.05	1.54	1.46
2	H	198	PRO	N-CA	5.89	1.53	1.46
2	H	95	VAL	CA-C	5.84	1.57	1.53
2	H	213	VAL	CA-C	5.78	1.59	1.52
2	H	125	GLU	C-O	5.70	1.31	1.23
4	I	15	ARG	CA-CB	5.62	1.60	1.53
2	H	213	VAL	N-CA	5.58	1.53	1.46
2	H	127	THR	N-CA	5.57	1.53	1.46
4	I	12	GLY	N-CA	5.48	1.52	1.44
3	T	66	ASP	C-O	5.46	1.28	1.23
2	H	138	VAL	N-CA	5.43	1.52	1.46
2	H	236	GLU	N-CA	5.41	1.52	1.46
2	H	82	SER	N-CA	5.38	1.52	1.46
1	L	100	GLN	N-CA	5.38	1.52	1.45
2	H	234	TYR	CA-CB	5.33	1.61	1.53
2	H	89	ILE	CA-CB	5.30	1.60	1.54
2	H	160	VAL	CA-CB	5.28	1.60	1.54
2	H	44	GLY	CA-C	5.24	1.57	1.51
3	T	61	ASP	C-N	-5.14	1.26	1.33
2	H	118	VAL	CA-C	5.12	1.59	1.52
2	H	113	VAL	N-CA	5.03	1.52	1.46
2	H	229	THR	CA-C	5.01	1.59	1.52

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	107	ARG	CD-NE-CZ	17.90	149.47	124.40
3	T	76	PHE	CA-CB-CG	12.76	126.56	113.80
4	I	4	PHE	CA-CB-CG	11.72	125.52	113.80
2	H	42	CYS	CA-C-N	-11.51	112.18	122.43
2	H	42	CYS	C-N-CA	-11.51	112.18	122.43
2	H	37	ASN	CA-CB-CG	-10.19	102.41	112.60
1	L	84	HIS	CA-CB-CG	10.05	123.85	113.80
2	H	170(C)	ARG	CD-NE-CZ	9.92	138.29	124.40
3	T	131	ARG	CD-NE-CZ	9.92	138.29	124.40
3	T	204	ASP	CA-CB-CG	9.36	121.96	112.60
2	H	202	HIS	CA-CB-CG	-9.19	104.61	113.80
2	H	198	PRO	CA-C-N	8.95	136.14	123.07
2	H	198	PRO	C-N-CA	8.95	136.14	123.07
2	H	253	ARG	NE-CZ-NH1	8.92	130.42	121.50
1	L	36	ARG	NE-CZ-NH1	-8.87	112.63	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	54	THR	N-CA-C	8.83	120.99	111.36
2	H	126	ARG	CD-NE-CZ	8.81	136.73	124.40
1	L	113	ARG	CA-CB-CG	8.73	131.55	114.10
2	H	49	THR	CA-C-O	-8.65	110.32	120.10
2	H	248	PRO	N-CA-C	8.65	130.28	112.47
2	H	185	SER	CA-CB-OG	8.57	128.24	111.10
2	H	247	ARG	CD-NE-CZ	8.55	136.38	124.40
3	T	144	ARG	CD-NE-CZ	-8.50	112.50	124.40
3	T	129	ASP	CA-C-N	8.48	133.56	120.75
3	T	129	ASP	C-N-CA	8.48	133.56	120.75
1	L	115	HIS	CA-CB-CG	8.42	122.22	113.80
2	H	230	ARG	CA-C-N	8.41	134.41	120.62
2	H	230	ARG	C-N-CA	8.41	134.41	120.62
2	H	17	VAL	CA-C-N	8.40	134.52	120.91
2	H	17	VAL	C-N-CA	8.40	134.52	120.91
1	L	36	ARG	CD-NE-CZ	-8.40	112.64	124.40
3	T	35	THR	CA-CB-OG1	-8.28	97.18	109.60
3	T	21	THR	N-CA-C	8.19	122.36	108.02
3	T	54	ASP	CA-CB-CG	8.18	120.78	112.60
2	H	224	HIS	CA-CB-CG	-8.16	105.64	113.80
2	H	100	ASN	CB-CA-C	8.08	122.81	109.89
2	H	94	TYR	CA-C-N	8.05	128.38	122.59
2	H	94	TYR	C-N-CA	8.05	128.38	122.59
2	H	164	MET	N-CA-C	-8.03	98.59	110.48
2	H	113	VAL	CB-CA-C	7.99	121.71	110.84
2	H	39	ALA	O-C-N	7.98	132.53	123.19
1	L	57	ASN	N-CA-CB	-7.92	100.03	111.84
2	H	37	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	L	81	CYS	CA-C-O	7.88	129.19	120.12
2	H	54	SER	O-C-N	7.87	132.51	122.68
3	T	178	ASP	CA-CB-CG	-7.83	104.77	112.60
1	L	142	GLU	CA-C-N	7.74	135.63	121.70
1	L	142	GLU	C-N-CA	7.74	135.63	121.70
2	H	115	THR	CA-C-N	7.71	131.38	120.28
2	H	115	THR	C-N-CA	7.71	131.38	120.28
3	T	175	PHE	CA-CB-CG	7.66	121.45	113.80
2	H	67	VAL	O-C-N	7.63	131.50	123.26
3	T	193	ILE	O-C-N	7.62	129.78	121.10
3	T	42	SER	N-CA-C	7.56	123.55	113.72
4	I	20	ARG	CD-NE-CZ	7.51	134.91	124.40
4	I	45	PHE	CA-C-N	7.47	131.66	120.31
4	I	45	PHE	C-N-CA	7.47	131.66	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	14	CYS	CB-CA-C	7.44	123.22	109.54
2	H	203	TYR	CA-C-O	7.42	130.27	120.11
2	H	199	HIS	N-CA-C	-7.39	95.09	108.02
1	L	121	LEU	CA-C-N	7.27	131.00	120.38
1	L	121	LEU	C-N-CA	7.27	131.00	120.38
2	H	18	GLY	CA-C-N	7.27	132.05	122.75
2	H	18	GLY	C-N-CA	7.27	132.05	122.75
2	H	134	ARG	NE-CZ-NH1	-7.24	114.26	121.50
2	H	245	GLU	N-CA-C	-7.19	100.15	110.08
1	L	104	ASP	CA-CB-CG	7.18	119.78	112.60
2	H	217	GLN	CB-CA-C	7.17	123.22	112.03
2	H	253	ARG	CD-NE-CZ	7.16	134.43	124.40
3	T	71	TYR	CA-C-N	7.13	134.31	122.33
3	T	71	TYR	C-N-CA	7.13	134.31	122.33
3	T	146	VAL	N-CA-C	7.13	117.92	110.72
1	L	40	PHE	CA-CB-CG	-7.05	106.75	113.80
1	L	99	GLU	O-C-N	7.04	131.39	122.23
3	T	110	GLN	O-C-N	7.02	127.55	121.30
2	H	104	ALA	CA-C-N	7.00	133.29	123.07
2	H	104	ALA	C-N-CA	7.00	133.29	123.07
2	H	50	ILE	CA-CB-CG2	7.00	122.39	110.50
2	H	103	ILE	CA-C-O	-6.98	115.10	120.96
2	H	226	GLY	N-CA-C	-6.94	102.66	112.37
3	T	70	THR	CA-CB-CG2	6.93	122.28	110.50
2	H	65	ILE	O-C-N	6.91	130.64	123.18
2	H	102	ASP	CA-C-N	-6.91	112.70	121.96
2	H	102	ASP	C-N-CA	-6.91	112.70	121.96
2	H	21	VAL	N-CA-C	-6.90	100.68	109.58
4	I	9	PRO	CB-CA-C	6.86	120.01	111.23
1	L	87	ASP	CA-C-O	-6.85	112.68	121.17
2	H	22	CYS	CA-C-O	-6.83	114.26	119.32
1	L	82	GLU	CB-CG-CD	6.76	124.09	112.60
4	I	13	PRO	CB-CA-C	6.72	121.05	110.49
2	H	134	ARG	N-CA-C	6.71	118.29	110.97
1	L	57	ASN	CA-C-O	-6.70	113.77	121.54
1	L	115	HIS	CA-C-N	6.69	130.21	120.71
1	L	115	HIS	C-N-CA	6.69	130.21	120.71
2	H	22	CYS	O-C-N	6.68	127.50	121.35
2	H	96	PRO	CA-C-N	6.66	131.71	120.91
2	H	96	PRO	C-N-CA	6.66	131.71	120.91
2	H	40	GLN	CA-C-O	6.64	128.44	120.81
2	H	129(D)	LEU	N-CA-C	6.64	119.34	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	17	LEU	CA-C-N	-6.63	114.22	122.84
4	I	17	LEU	C-N-CA	-6.63	114.22	122.84
2	H	80	GLU	CA-CB-CG	6.62	127.33	114.10
2	H	60(B)	ILE	N-CA-C	-6.61	100.16	108.89
2	H	199	HIS	CA-CB-CG	6.59	120.39	113.80
3	T	179	VAL	CB-CA-C	6.58	123.90	111.40
2	H	170(C)	ARG	N-CA-C	-6.58	100.55	110.28
2	H	59	PHE	CA-CB-CG	-6.57	107.23	113.80
2	H	42	CYS	O-C-N	6.57	130.02	122.99
2	H	21	VAL	O-C-N	6.57	129.77	122.61
2	H	155	LEU	O-C-N	6.53	131.04	122.95
1	L	129	PRO	O-C-N	-6.51	115.15	123.03
2	H	85	VAL	CA-CB-CG1	6.50	121.46	110.40
2	H	217	GLN	CA-CB-CG	6.48	127.07	114.10
2	H	178	GLU	CB-CG-CD	6.48	123.62	112.60
3	T	197	THR	N-CA-C	-6.48	105.91	113.88
2	H	126	ARG	NE-CZ-NH1	6.46	127.96	121.50
2	H	247	ARG	CA-C-N	6.43	127.88	119.84
2	H	247	ARG	C-N-CA	6.43	127.88	119.84
3	T	171	ASN	N-CA-C	-6.40	104.78	112.59
2	H	247	ARG	NE-CZ-NH1	6.39	127.89	121.50
3	T	58	ASP	O-C-N	6.37	130.50	123.04
2	H	151	THR	CA-CB-CG2	6.36	121.32	110.50
3	T	158	TRP	CA-CB-CG	6.36	125.68	113.60
2	H	234	TYR	N-CA-C	6.34	123.13	113.61
3	T	104	LEU	N-CA-C	6.34	119.17	111.82
3	T	53	THR	N-CA-CB	6.34	119.97	110.53
3	T	109	GLY	CA-C-N	6.33	129.26	120.65
3	T	109	GLY	C-N-CA	6.33	129.26	120.65
2	H	129(F)	PHE	CA-CB-CG	-6.31	107.49	113.80
4	I	51	CYS	N-CA-C	-6.31	103.71	111.40
1	L	36	ARG	NE-CZ-NH2	6.30	124.88	119.20
2	H	243	ARG	CD-NE-CZ	6.29	133.21	124.40
2	H	85	VAL	N-CA-C	-6.29	99.23	108.54
1	L	76	PHE	CA-CB-CG	-6.27	107.53	113.80
2	H	185	SER	N-CA-CB	6.26	119.55	110.47
3	T	51	TYR	CA-C-O	-6.25	115.02	122.27
1	L	102	CYS	O-C-N	6.24	130.61	123.31
1	L	101	TYR	CA-C-N	6.21	132.31	122.74
1	L	101	TYR	C-N-CA	6.21	132.31	122.74
4	I	13	PRO	CA-C-N	6.21	130.69	120.94
4	I	13	PRO	C-N-CA	6.21	130.69	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	125	GLU	OE1-CD-OE2	6.20	137.77	122.90
1	L	129	PRO	CA-C-O	6.19	128.39	121.34
3	T	101	THR	O-C-N	6.19	128.17	121.12
2	H	200	ALA	O-C-N	6.18	130.65	123.30
3	T	29	PRO	N-CA-C	6.12	120.79	111.19
2	H	245	GLU	CB-CA-C	6.10	119.09	109.27
2	H	107	ARG	NE-CZ-NH1	6.08	127.58	121.50
2	H	30	GLN	O-C-N	6.07	130.48	122.95
3	T	186	CYS	CA-C-O	6.06	127.63	120.66
1	L	46	ASP	CA-CB-CG	-6.04	106.56	112.60
1	L	71	PHE	N-CA-C	-6.03	98.91	108.73
3	T	11	ASN	CA-C-O	-6.03	114.50	122.03
3	T	21	THR	CA-CB-OG1	-6.03	100.56	109.60
1	L	99	GLU	CG-CD-OE2	-6.02	104.55	118.40
3	T	36	VAL	CA-C-N	6.01	131.99	122.74
3	T	36	VAL	C-N-CA	6.01	131.99	122.74
1	L	37	THR	CB-CA-C	6.00	122.18	110.67
3	T	107	ASN	CA-C-O	-5.99	114.59	121.47
2	H	181	PHE	N-CA-CB	5.98	121.86	111.39
3	T	73	ALA	N-CA-C	-5.98	100.25	109.52
2	H	121	LEU	N-CA-C	-5.98	99.92	109.96
3	T	40	THR	N-CA-C	-5.96	101.18	110.42
3	T	22	ILE	CB-CG1-CD1	5.95	126.29	113.80
2	H	57	HIS	CA-CB-CG	-5.94	107.86	113.80
1	L	58	GLY	CA-C-O	5.93	125.60	119.01
2	H	92	SER	CA-C-N	5.93	131.52	121.14
2	H	92	SER	C-N-CA	5.93	131.52	121.14
2	H	230	ARG	CA-C-O	5.93	128.22	121.58
2	H	60(D)	ASN	CA-C-N	5.93	132.92	121.18
2	H	60(D)	ASN	C-N-CA	5.93	132.92	121.18
2	H	177	THR	CA-CB-OG1	-5.93	100.71	109.60
2	H	217	GLN	N-CA-CB	-5.92	102.57	110.57
1	L	113	ARG	N-CA-CB	-5.92	102.21	111.56
3	T	197	THR	CB-CA-C	5.91	118.61	109.03
2	H	22	CYS	N-CA-C	-5.91	101.02	109.24
2	H	189	ASP	N-CA-CB	-5.91	101.09	111.49
2	H	201	THR	CA-C-N	5.90	129.94	121.50
2	H	201	THR	C-N-CA	5.90	129.94	121.50
2	H	26	GLU	CB-CG-CD	5.90	122.63	112.60
3	T	117	GLU	CA-CB-CG	5.90	125.90	114.10
1	L	71	PHE	CA-C-N	-5.89	112.56	122.92
1	L	71	PHE	C-N-CA	-5.89	112.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	79	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	L	137	LYS	N-CA-CB	5.85	120.50	110.68
2	H	123	LEU	N-CA-C	-5.84	100.77	109.42
2	H	55	ALA	O-C-N	5.84	130.63	123.21
1	L	71	PHE	CA-C-O	-5.80	114.15	120.36
3	T	74	ARG	O-C-N	5.79	129.99	123.27
2	H	225	PHE	CA-C-N	5.79	126.45	120.60
2	H	225	PHE	C-N-CA	5.79	126.45	120.60
2	H	190	SER	N-CA-CB	5.79	119.43	110.46
2	H	117	HIS	CA-CB-CG	-5.77	108.03	113.80
2	H	103	ILE	O-C-N	5.77	127.99	122.97
2	H	128	PHE	CA-C-N	-5.74	112.79	120.54
2	H	128	PHE	C-N-CA	-5.74	112.79	120.54
2	H	253	ARG	NH1-CZ-NH2	-5.74	111.84	119.30
3	T	106	THR	CA-CB-CG2	5.73	120.24	110.50
2	H	126	ARG	N-CA-C	5.73	117.52	111.28
1	L	99	GLU	CG-CD-OE1	5.71	131.53	118.40
3	T	53	THR	N-CA-C	-5.70	106.37	113.38
4	I	49	GLU	CA-CB-CG	5.70	125.50	114.10
2	H	196	GLY	O-C-N	5.69	129.46	122.46
2	H	183	ALA	O-C-N	5.68	129.95	123.48
2	H	114	LEU	O-C-N	5.65	129.88	122.93
2	H	125	GLU	CB-CA-C	-5.65	99.15	109.54
4	I	15	ARG	CA-C-O	5.64	128.16	121.17
2	H	151	THR	CA-CB-OG1	-5.63	101.16	109.60
2	H	137	LEU	CA-C-N	-5.61	115.79	123.14
2	H	137	LEU	C-N-CA	-5.61	115.79	123.14
3	T	116	PHE	CA-CB-CG	5.60	119.40	113.80
3	T	47	SER	CA-C-O	5.60	127.43	121.05
2	H	243	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	L	76	PHE	O-C-N	5.59	129.76	123.27
2	H	183	ALA	CA-C-O	-5.59	113.83	120.43
2	H	92	SER	CA-C-O	5.57	126.23	119.49
3	T	135	ARG	NE-CZ-NH1	5.57	127.06	121.50
1	L	71	PHE	O-C-N	5.56	129.56	123.22
3	T	136	ARG	O-C-N	5.55	130.39	123.28
2	H	42	CYS	CB-CA-C	-5.55	100.48	111.91
3	T	179	VAL	CA-CB-CG2	5.55	119.83	110.40
2	H	60(D)	ASN	CA-C-O	5.55	127.93	121.11
2	H	65	ILE	CB-CG1-CD1	5.54	125.44	113.80
3	T	98	PRO	N-CA-C	-5.53	102.77	111.34
2	H	122	CYS	CB-CA-C	-5.52	100.84	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	93	LEU	N-CA-C	-5.52	100.24	109.24
2	H	235	ILE	CA-CB-CG2	-5.52	101.12	110.50
3	T	178	ASP	N-CA-C	5.49	117.59	108.20
4	I	15	ARG	N-CA-CB	-5.49	103.23	111.25
3	T	66	ASP	CA-C-O	-5.48	114.88	120.63
3	T	66	ASP	O-C-N	5.48	128.54	123.50
1	L	115	HIS	CA-C-O	5.47	128.23	121.94
2	H	235	ILE	N-CA-C	5.46	116.10	110.36
2	H	48	ASN	N-CA-CB	5.46	119.72	110.49
3	T	143	LEU	CB-CA-C	5.45	119.95	110.68
2	H	184	TYR	N-CA-C	5.44	118.33	109.24
4	I	34	TYR	CA-C-N	-5.44	114.04	122.09
4	I	34	TYR	C-N-CA	-5.44	114.04	122.09
1	L	72	CYS	O-C-N	5.44	130.11	123.10
4	I	11	ASP	CB-CA-C	5.44	120.60	109.67
3	T	101	THR	CB-CA-C	5.42	116.18	110.17
2	H	193	GLY	N-CA-C	-5.40	107.57	114.37
3	T	156	TYR	O-C-N	5.40	129.94	123.36
2	H	162	ARG	CA-CB-CG	5.39	124.87	114.10
2	H	166	GLN	O-C-N	-5.38	116.41	122.12
2	H	54	SER	CA-C-O	-5.37	115.17	120.80
2	H	129(B)	ARG	CA-C-O	5.36	126.19	120.24
3	T	54	ASP	O-C-N	5.36	129.19	122.65
2	H	60(A)	LYS	N-CA-CB	5.36	119.82	111.84
2	H	118	VAL	CA-CB-CG2	5.35	119.49	110.40
3	T	144	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	H	28	PRO	N-CA-C	5.34	120.61	114.03
4	I	44	ASN	CA-CB-CG	5.33	117.93	112.60
4	I	11	ASP	CA-C-O	-5.33	113.36	119.60
3	T	20	LYS	N-CA-C	-5.33	101.76	109.59
4	I	12	GLY	O-C-N	5.33	127.10	121.77
1	L	87	ASP	O-C-N	5.32	129.15	121.97
2	H	87	GLN	N-CA-C	5.32	117.84	108.75
2	H	203	TYR	CB-CA-C	5.32	118.00	110.24
3	T	47	SER	CB-CA-C	5.31	118.51	109.53
2	H	134	ARG	CB-CA-C	5.31	119.14	110.96
3	T	137	ASN	CB-CA-C	5.31	120.98	110.42
2	H	27	CYS	N-CA-CB	-5.30	100.94	110.37
3	T	133	LEU	CA-C-N	5.30	128.97	121.66
3	T	133	LEU	C-N-CA	5.30	128.97	121.66
1	L	45	SER	N-CA-C	5.29	118.75	112.72
2	H	20	LYS	O-C-N	5.27	129.16	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	228	TYR	N-CA-CB	-5.27	102.06	111.08
2	H	60(C)	LYS	N-CA-CB	5.27	118.04	110.40
2	H	138	VAL	CB-CA-C	5.27	118.43	110.63
2	H	190	SER	N-CA-C	-5.27	102.67	110.46
3	T	11	ASN	CA-CB-CG	5.27	117.87	112.60
1	L	84	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	H	175	ASN	CA-C-O	5.25	126.96	120.92
2	H	116	ASP	CA-C-O	5.25	126.03	120.10
1	L	94	GLU	CG-CD-OE2	5.25	130.47	118.40
4	I	11	ASP	O-C-N	5.25	129.81	122.36
1	L	39	LEU	CB-CA-C	5.24	119.76	110.85
3	T	130	GLU	CA-CB-CG	5.24	124.58	114.10
3	T	134	VAL	CA-C-N	5.23	130.78	122.94
3	T	134	VAL	C-N-CA	5.23	130.78	122.94
2	H	145	LEU	O-C-N	5.21	129.19	123.25
1	L	106	THR	CB-CA-C	5.20	118.55	109.65
4	I	25	ALA	N-CA-C	-5.19	105.52	111.07
2	H	53	VAL	O-C-N	5.18	128.43	123.14
1	L	91	CYS	N-CA-C	5.18	117.67	111.71
1	L	98	CYS	O-C-N	5.18	128.81	122.96
1	L	132	GLU	CA-C-O	5.18	126.04	120.55
2	H	247	ARG	CG-CD-NE	5.18	123.39	112.00
4	I	47	SER	O-C-N	5.16	128.94	123.42
3	T	99	GLU	CA-C-N	-5.16	113.67	122.33
3	T	99	GLU	C-N-CA	-5.16	113.67	122.33
1	L	69	ILE	N-CA-CB	5.15	119.89	111.44
1	L	88	GLN	O-C-N	5.14	128.36	121.99
2	H	21	VAL	CA-C-N	-5.13	114.48	121.61
2	H	21	VAL	C-N-CA	-5.13	114.48	121.61
2	H	202	HIS	CB-CA-C	-5.13	101.48	109.84
2	H	27	CYS	CA-C-N	5.12	125.20	119.87
2	H	27	CYS	C-N-CA	5.12	125.20	119.87
2	H	140	GLY	CA-C-O	5.12	127.06	121.83
3	T	25	TRP	CA-C-N	5.12	133.28	123.65
3	T	25	TRP	C-N-CA	5.12	133.28	123.65
4	I	47	SER	CA-C-N	5.12	127.46	120.54
4	I	47	SER	C-N-CA	5.12	127.46	120.54
3	T	101	THR	CA-CB-OG1	-5.12	101.92	109.60
3	T	137	ASN	CA-CB-CG	-5.11	107.49	112.60
2	H	245	GLU	CB-CG-CD	5.10	121.27	112.60
2	H	160	VAL	N-CA-CB	-5.09	104.08	111.21
1	L	73	LEU	N-CA-C	-5.08	103.06	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	102	ASP	CA-CB-CG	5.08	117.68	112.60
2	H	59	PHE	CB-CA-C	5.08	119.60	110.81
2	H	95	VAL	CA-C-N	5.08	126.19	119.84
2	H	95	VAL	C-N-CA	5.08	126.19	119.84
2	H	237	TRP	CA-C-O	5.07	126.14	120.82
2	H	122	CYS	CA-C-N	-5.06	114.11	121.20
2	H	122	CYS	C-N-CA	-5.06	114.11	121.20
2	H	39	ALA	N-CA-CB	5.06	118.87	110.52
3	T	206	PRO	N-CA-C	-5.06	103.16	110.80
3	T	144	ARG	CB-CG-CD	5.06	122.93	111.30
2	H	68	LEU	CB-CA-C	5.05	118.61	109.37
2	H	209	LEU	CA-C-O	-5.05	114.64	120.49
1	L	78	GLY	CA-C-N	5.04	127.28	120.38
1	L	78	GLY	C-N-CA	5.04	127.28	120.38
3	T	58	ASP	CA-C-O	-5.01	114.97	120.69
4	I	15	ARG	CB-CG-CD	5.01	122.83	111.30
2	H	145	LEU	CA-C-O	-5.01	115.92	121.33
2	H	169	LEU	O-C-N	5.00	127.22	122.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	134	ARG	Sidechain
2	H	230	ARG	Sidechain
4	I	53	ARG	Sidechain

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	827	0	755	47	0
2	H	1955	0	1933	92	0
3	T	1495	0	1455	136	0
4	I	439	0	401	55	0
5	L	11	0	10	1	0
6	L	10	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	H	164	0	0	9	0
8	I	23	0	0	2	0
8	L	78	0	0	0	0
8	T	75	0	0	6	0
All	All	5079	0	4564	305	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 33.

All (305) 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)
3:T:158:TRP:CH2	3:T:207:VAL:HG11	1.77	1.20
3:T:155:LEU:HB2	3:T:175:PHE:CE2	1.82	1.15
3:T:185:TYR:O	3:T:209:CYS:HA	1.44	1.14
3:T:186:CYS:HA	3:T:208:GLU:O	1.58	1.04
2:H:46:LEU:HD13	2:H:68:LEU:HD11	1.39	1.03
3:T:7:VAL:HG23	3:T:32:GLN:HE22	1.22	1.03
2:H:68:LEU:HD12	2:H:112:VAL:HG11	1.38	1.01
3:T:158:TRP:HH2	3:T:207:VAL:CG1	1.74	1.01
3:T:158:TRP:HH2	3:T:207:VAL:HG11	1.21	0.99
3:T:155:LEU:CB	3:T:175:PHE:CE2	2.44	0.99
3:T:158:TRP:CH2	3:T:207:VAL:CG1	2.45	0.99
1:L:140:ILE:CD1	2:H:26:GLU:HG2	1.93	0.98
3:T:185:TYR:HB2	3:T:210:MET:SD	2.07	0.95
3:T:155:LEU:HB2	3:T:175:PHE:CD2	2.03	0.94
4:I:7:GLU:OE2	4:I:41:LYS:NZ	2.01	0.93
3:T:136:ARG:O	3:T:139:THR:HG23	1.70	0.91
1:L:140:ILE:HD11	2:H:26:GLU:HG2	1.52	0.90
3:T:155:LEU:CB	3:T:175:PHE:CD2	2.56	0.89
3:T:20:LYS:HB2	3:T:133:LEU:HD13	1.54	0.89
3:T:7:VAL:HG23	3:T:32:GLN:NE2	1.88	0.89
2:H:164:MET:HE3	3:T:91:GLU:HG2	1.56	0.88
3:T:7:VAL:CG2	3:T:32:GLN:NE2	2.38	0.87
3:T:155:LEU:HD11	3:T:187:PHE:HB3	1.57	0.86
2:H:60(D):ASN:HB3	2:H:63:ASN:HD21	1.38	0.86
3:T:185:TYR:O	3:T:209:CYS:CA	2.23	0.85
2:H:187:GLY:HA2	2:H:221(A):ALA:O	1.77	0.84
3:T:192:VAL:HG13	3:T:201:LYS:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:MET:CE	3:T:91:GLU:HB3	2.09	0.82
4:I:27:ALA:HB1	4:I:29:LEU:CD1	2.10	0.82
2:H:60(C):LYS:NZ	4:I:46:GLU:HG2	1.95	0.81
2:H:60(D):ASN:CB	2:H:63:ASN:HD21	1.92	0.81
1:L:138:ILE:HG22	1:L:140:ILE:HG13	1.62	0.81
4:I:27:ALA:CB	4:I:29:LEU:HD12	2.12	0.80
2:H:45:THR:OG1	2:H:198:PRO:HB3	1.82	0.79
3:T:137:ASN:O	3:T:139:THR:HG22	1.82	0.79
4:I:27:ALA:HB3	4:I:29:LEU:HD12	1.64	0.78
4:I:27:ALA:HB1	4:I:29:LEU:HD11	1.65	0.78
3:T:196:ARG:O	3:T:200:ARG:HD2	1.83	0.78
4:I:27:ALA:CB	4:I:29:LEU:CD1	2.61	0.77
1:L:143:LYS:O	1:L:143:LYS:HG3	1.82	0.77
2:H:60(D):ASN:HB3	2:H:63:ASN:ND2	2.00	0.76
2:H:164:MET:HE3	3:T:91:GLU:CG	2.16	0.75
2:H:60(D):ASN:CB	2:H:63:ASN:ND2	2.50	0.75
3:T:136:ARG:HB3	3:T:141:LEU:HD21	1.69	0.74
4:I:24:ASN:OD1	4:I:31:GLN:NE2	2.21	0.74
2:H:165:THR:HG21	8:H:364:HOH:O	1.86	0.74
3:T:155:LEU:HB3	3:T:175:PHE:CD2	2.23	0.73
4:I:35:TYR:CZ	4:I:40:ALA:HB2	2.24	0.73
3:T:155:LEU:N	3:T:175:PHE:HE2	1.87	0.72
2:H:83:ARG:HG2	8:H:383:HOH:O	1.89	0.72
3:T:32:GLN:HA	3:T:78:TYR:O	1.91	0.71
1:L:140:ILE:HG12	8:H:317:HOH:O	1.91	0.71
3:T:196:ARG:O	3:T:200:ARG:CD	2.39	0.71
3:T:185:TYR:O	3:T:210:MET:N	2.25	0.70
1:L:121:LEU:HD21	1:L:128:THR:CG2	2.23	0.69
4:I:24:ASN:O	4:I:28:GLY:N	2.26	0.69
3:T:35:THR:HG21	8:T:230:HOH:O	1.93	0.68
3:T:158:TRP:CZ2	3:T:207:VAL:HG11	2.29	0.68
3:T:186:CYS:CA	3:T:208:GLU:O	2.39	0.67
4:I:25:ALA:O	4:I:28:GLY:N	2.28	0.67
4:I:6:LEU:N	4:I:6:LEU:HD23	2.09	0.66
1:L:110:ARG:HD2	1:L:110:ARG:C	2.20	0.66
3:T:6:THR:HG21	3:T:78:TYR:CA	2.26	0.66
4:I:29:LEU:HA	4:I:52:MET:HE1	1.78	0.66
3:T:196:ARG:HB2	3:T:200:ARG:HG2	1.76	0.66
3:T:179:VAL:HB	3:T:185:TYR:CE2	2.31	0.65
4:I:23:TYR:OH	4:I:28:GLY:HA2	1.95	0.65
2:H:60(C):LYS:HZ3	4:I:46:GLU:HG2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ILE:HD12	2:H:107:ARG:HG3	1.80	0.63
3:T:37:GLN:O	3:T:73:ALA:HA	1.98	0.63
1:L:92:VAL:HG12	2:H:129(B):ARG:HG2	1.81	0.63
3:T:155:LEU:N	3:T:175:PHE:CE2	2.66	0.63
2:H:89:ILE:HG23	2:H:252:LEU:HB3	1.81	0.62
3:T:123:VAL:CG1	3:T:177:ILE:HD11	2.29	0.62
1:L:101:TYR:CE2	2:H:125:GLU:HG3	2.34	0.62
3:T:156:TYR:HA	3:T:166:LYS:O	1.99	0.61
3:T:156:TYR:O	3:T:187:PHE:HA	2.00	0.61
2:H:236:GLU:OE2	2:H:240:LYS:HE3	2.00	0.61
3:T:155:LEU:O	3:T:167:THR:HA	2.01	0.61
3:T:114:GLN:HG3	3:T:128:GLU:HB2	1.83	0.60
4:I:39:LEU:HD12	4:I:39:LEU:N	2.16	0.60
3:T:179:VAL:HB	3:T:185:TYR:HE2	1.66	0.60
3:T:6:THR:HG21	3:T:78:TYR:N	2.16	0.60
3:T:193:ILE:HG21	8:T:241:HOH:O	2.02	0.60
4:I:27:ALA:CB	4:I:29:LEU:HD11	2.29	0.59
2:H:73:LEU:HD12	8:H:321:HOH:O	2.03	0.59
4:I:38:CYS:SG	4:I:39:LEU:HD13	2.42	0.59
3:T:158:TRP:CH2	3:T:207:VAL:HG13	2.37	0.58
3:T:202:SER:OG	3:T:203:THR:O	2.21	0.58
3:T:48:LYS:HG3	3:T:59:LEU:CD2	2.33	0.58
3:T:203:THR:HG22	8:T:220:HOH:O	2.03	0.58
2:H:245:GLU:CD	2:H:246:PRO:HD2	2.28	0.58
3:T:192:VAL:O	3:T:194:PRO:HD3	2.03	0.58
1:L:140:ILE:HD12	2:H:26:GLU:HG2	1.85	0.58
2:H:241:LEU:HG	8:H:382:HOH:O	2.02	0.58
3:T:124:ASN:ND2	8:T:263:HOH:O	2.37	0.58
2:H:59:PHE:HA	2:H:60(B):ILE:HG12	1.86	0.58
2:H:140:GLY:HA3	2:H:194:ASP:OD1	2.04	0.57
3:T:36:VAL:O	3:T:47:SER:HA	2.03	0.57
3:T:185:TYR:HB3	3:T:187:PHE:CZ	2.39	0.57
3:T:7:VAL:HG22	3:T:32:GLN:NE2	2.20	0.57
3:T:114:GLN:HB2	3:T:126:THR:HG22	1.87	0.56
1:L:36:ARG:NH2	3:T:190:GLN:NE2	2.53	0.56
3:T:72:LEU:HD11	3:T:97:SER:O	2.05	0.56
1:L:140:ILE:HD11	2:H:26:GLU:HA	1.88	0.56
3:T:207:VAL:HG12	3:T:208:GLU:N	2.20	0.56
2:H:54:SER:O	2:H:212:ILE:HD13	2.05	0.56
1:L:105:HIS:NE2	1:L:111:SER:OG	2.25	0.56
1:L:121:LEU:HD21	1:L:128:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:ILE:CD1	2:H:26:GLU:CG	2.79	0.56
2:H:143:GLN:HG2	2:H:149:GLY:O	2.05	0.56
3:T:196:ARG:HB2	3:T:200:ARG:CG	2.35	0.56
2:H:216:GLY:HA3	4:I:15:ARG:NH2	2.20	0.56
4:I:27:ALA:HB3	4:I:29:LEU:CD1	2.31	0.56
3:T:187:PHE:O	3:T:207:VAL:HG13	2.06	0.55
3:T:6:THR:HG22	3:T:32:GLN:OE1	2.06	0.55
3:T:155:LEU:CD1	3:T:187:PHE:HB3	2.34	0.55
2:H:126:ARG:O	2:H:129(A):GLU:HG3	2.06	0.55
2:H:164:MET:CE	3:T:91:GLU:CG	2.85	0.55
3:T:6:THR:CG2	3:T:78:TYR:C	2.80	0.55
4:I:7:GLU:HG3	8:I:112:HOH:O	2.06	0.55
2:H:127:THR:O	2:H:129(B):ARG:HB2	2.06	0.54
3:T:144:ARG:CZ	3:T:151:LEU:HD23	2.37	0.54
4:I:38:CYS:SG	4:I:39:LEU:CD1	2.95	0.54
4:I:4:PHE:HZ	4:I:54:THR:HG21	1.71	0.54
3:T:16:SER:HA	3:T:20:LYS:O	2.07	0.54
3:T:76:PHE:HD2	3:T:92:PRO:HB2	1.72	0.54
2:H:27:CYS:N	2:H:28:PRO:CD	2.70	0.54
3:T:76:PHE:CD2	3:T:92:PRO:HB2	2.43	0.54
3:T:153:TYR:O	3:T:169:LYS:HA	2.07	0.54
2:H:164:MET:CE	3:T:91:GLU:CB	2.85	0.54
3:T:34:TYR:HA	3:T:76:PHE:O	2.08	0.53
2:H:46:LEU:HD11	2:H:48:ASN:O	2.08	0.53
4:I:23:TYR:CZ	4:I:28:GLY:HA2	2.42	0.53
2:H:22:CYS:HB2	2:H:157:VAL:HB	1.90	0.53
3:T:147:PHE:O	3:T:148:GLY:C	2.49	0.53
3:T:37:GLN:HA	3:T:46:LYS:O	2.09	0.53
2:H:60(D):ASN:HB2	2:H:63:ASN:ND2	2.22	0.52
3:T:48:LYS:HG3	3:T:59:LEU:HD23	1.90	0.52
4:I:1:ALA:HB2	4:I:55:CYS:HA	1.90	0.52
1:L:110:ARG:HD2	1:L:110:ARG:O	2.08	0.52
3:T:33:VAL:CG2	3:T:78:TYR:HB2	2.39	0.52
2:H:60(D):ASN:HB2	2:H:63:ASN:HD21	1.74	0.52
2:H:50:ILE:HG13	2:H:51:TRP:CD1	2.44	0.52
1:L:141:LEU:HD23	1:L:141:LEU:N	2.24	0.52
4:I:38:CYS:C	4:I:39:LEU:HD12	2.35	0.52
4:I:25:ALA:C	4:I:28:GLY:H	2.18	0.52
1:L:131:VAL:O	1:L:134:PRO:HD3	2.10	0.51
1:L:101:TYR:CD2	2:H:125:GLU:HG3	2.45	0.51
2:H:83:ARG:HD2	2:H:110:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:LYS:O	2:H:156:MET:HA	2.10	0.51
4:I:1:ALA:CB	4:I:55:CYS:HA	2.40	0.51
2:H:135:PHE:HB3	2:H:159:ASN:ND2	2.25	0.51
3:T:71:TYR:O	3:T:100:PHE:N	2.41	0.51
2:H:30:GLN:HG3	2:H:31:VAL:N	2.25	0.51
4:I:48:ALA:O	4:I:52:MET:N	2.36	0.51
4:I:7:GLU:CG	8:I:112:HOH:O	2.60	0.50
3:T:144:ARG:NH1	3:T:151:LEU:HB3	2.26	0.50
4:I:16:ALA:HB3	4:I:36:GLY:O	2.12	0.50
2:H:235:ILE:O	2:H:239:GLN:HG3	2.11	0.50
3:T:72:LEU:CD1	3:T:97:SER:O	2.60	0.50
3:T:114:GLN:HG3	3:T:128:GLU:CB	2.42	0.50
1:L:41:TRP:HA	1:L:41:TRP:CE3	2.47	0.50
2:H:46:LEU:CD1	2:H:48:ASN:O	2.60	0.49
3:T:33:VAL:HG23	3:T:78:TYR:HD2	1.75	0.49
3:T:207:VAL:CG1	3:T:208:GLU:N	2.75	0.49
1:L:85:LYS:HE2	3:T:61:ASP:OD2	2.12	0.49
3:T:155:LEU:HB3	3:T:175:PHE:CE2	2.40	0.49
2:H:60(C):LYS:NZ	4:I:46:GLU:CG	2.70	0.49
2:H:159:ASN:ND2	8:H:326:HOH:O	2.44	0.49
1:L:84:HIS:C	1:L:86:ASP:H	2.20	0.48
2:H:16:ILE:N	2:H:194:ASP:OD2	2.46	0.48
2:H:126:ARG:HG3	2:H:232:SER:O	2.13	0.48
3:T:31:ASN:HA	3:T:80:ALA:HB3	1.95	0.48
1:L:115:HIS:O	1:L:118:TYR:HB2	2.13	0.48
3:T:127:VAL:CG2	3:T:189:VAL:HG11	2.44	0.48
3:T:155:LEU:HB2	3:T:175:PHE:CZ	2.44	0.48
1:L:39:LEU:O	1:L:43:SER:HB2	2.13	0.48
3:T:116:PHE:HA	3:T:124:ASN:O	2.14	0.48
3:T:170:THR:HG21	3:T:174:GLU:O	2.14	0.48
2:H:45:THR:HG21	2:H:121:LEU:HD23	1.96	0.47
3:T:155:LEU:CA	3:T:175:PHE:CE2	2.96	0.47
1:L:85:LYS:CE	3:T:61:ASP:OD2	2.62	0.47
2:H:87:GLN:CD	2:H:252:LEU:HD13	2.39	0.47
2:H:137:LEU:HA	2:H:158:LEU:O	2.14	0.47
2:H:209:LEU:HG	2:H:231:VAL:HG11	1.96	0.47
2:H:60(A):LYS:HE2	8:H:421:HOH:O	2.13	0.47
3:T:170:THR:OG1	3:T:171:ASN:N	2.47	0.47
3:T:192:VAL:C	3:T:194:PRO:HD3	2.38	0.47
4:I:23:TYR:HA	4:I:30:CYS:HA	1.96	0.47
3:T:106:THR:O	3:T:196:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:GLN:HB3	2:H:145:LEU:O	2.15	0.47
3:T:33:VAL:HG22	3:T:78:TYR:HB2	1.97	0.47
3:T:38:ILE:HA	3:T:73:ALA:HA	1.96	0.47
4:I:4:PHE:O	4:I:7:GLU:HB3	2.14	0.47
2:H:135:PHE:HB3	2:H:159:ASN:HD21	1.80	0.47
4:I:30:CYS:H	4:I:52:MET:HE2	1.80	0.47
3:T:118:GLN:NE2	3:T:210:MET:CE	2.78	0.47
2:H:203:TYR:O	2:H:204:ARG:C	2.55	0.46
4:I:24:ASN:HD21	4:I:26:LYS:HB2	1.79	0.46
2:H:87:GLN:NE2	2:H:252:LEU:CD1	2.78	0.46
8:H:390:HOH:O	4:I:46:GLU:HG3	2.16	0.46
4:I:24:ASN:ND2	4:I:26:LYS:HB2	2.30	0.46
1:L:36:ARG:NH2	3:T:190:GLN:HE22	2.13	0.46
2:H:192:LYS:HE3	8:H:419:HOH:O	2.15	0.46
3:T:114:GLN:HE21	3:T:114:GLN:HB3	1.42	0.46
2:H:68:LEU:HD13	2:H:118:VAL:HG13	1.96	0.46
3:T:122:LYS:HA	3:T:177:ILE:O	2.15	0.46
5:L:600:GLC:O6	5:L:600:GLC:O4	2.21	0.46
2:H:68:LEU:HD12	2:H:112:VAL:CG1	2.28	0.46
3:T:205:SER:HB2	3:T:206:PRO:CD	2.45	0.46
2:H:256:PHE:CD1	2:H:257:PRO:HA	2.51	0.46
1:L:110:ARG:C	1:L:110:ARG:CD	2.85	0.46
2:H:47:ILE:HD13	2:H:53:VAL:CG2	2.46	0.46
2:H:192:LYS:HD2	4:I:17:LEU:HD23	1.98	0.46
1:L:61:CYS:SG	1:L:68:TYR:HB2	2.56	0.45
1:L:48:ASP:OD1	1:L:50:CYS:HB2	2.16	0.45
1:L:140:ILE:HD11	2:H:26:GLU:CG	2.35	0.45
1:L:138:ILE:CG2	1:L:140:ILE:HG13	2.39	0.45
4:I:24:ASN:HB3	4:I:27:ALA:HB3	1.97	0.45
3:T:93:LEU:HA	3:T:93:LEU:HD23	1.60	0.45
3:T:154:THR:O	3:T:189:VAL:HA	2.17	0.45
1:L:39:LEU:HD13	1:L:39:LEU:HA	1.78	0.45
1:L:132:GLU:O	1:L:134:PRO:HD2	2.18	0.44
2:H:60(C):LYS:NZ	4:I:46:GLU:OE2	2.50	0.44
2:H:113:VAL:O	2:H:115:THR:HG23	2.17	0.44
2:H:164:MET:HE2	3:T:91:GLU:HB3	1.94	0.44
1:L:55:CYS:SG	1:L:61:CYS:HB2	2.58	0.44
2:H:239:GLN:O	2:H:243:ARG:HG2	2.18	0.44
3:T:123:VAL:HB	3:T:177:ILE:CD1	2.48	0.44
2:H:100:ASN:HD22	2:H:100:ASN:HA	1.52	0.44
3:T:135:ARG:HA	3:T:139:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:88:GLN:HE21	1:L:88:GLN:HB3	1.65	0.44
4:I:20:ARG:HB2	4:I:33:PHE:CE1	2.52	0.44
3:T:34:TYR:O	3:T:51:TYR:HA	2.17	0.44
3:T:125:VAL:O	3:T:174:GLU:HA	2.18	0.44
3:T:110:GLN:HA	3:T:111:PRO:HD3	1.84	0.43
3:T:196:ARG:HD3	3:T:198:VAL:O	2.17	0.43
2:H:51:TRP:CE3	2:H:105:LEU:HG	2.53	0.43
3:T:6:THR:HG21	3:T:78:TYR:C	2.42	0.43
3:T:134:VAL:HG12	3:T:141:LEU:HD12	1.99	0.43
1:L:52:SER:O	1:L:53:SER:C	2.61	0.43
1:L:62:LYS:HB3	1:L:69:ILE:HG13	2.01	0.43
3:T:6:THR:HG23	3:T:78:TYR:C	2.43	0.43
3:T:91:GLU:HA	3:T:92:PRO:HD3	1.88	0.43
3:T:194:PRO:HA	3:T:200:ARG:NH2	2.33	0.43
3:T:10:TYR:HB2	8:T:257:HOH:O	2.17	0.43
3:T:59:LEU:O	3:T:62:GLU:HB2	2.19	0.43
3:T:114:GLN:NE2	8:T:252:HOH:O	2.51	0.43
3:T:111:PRO:HB2	3:T:189:VAL:HG23	2.00	0.43
2:H:87:GLN:O	2:H:106:LEU:HA	2.19	0.42
2:H:95:VAL:HA	2:H:96:PRO:HD2	1.80	0.42
2:H:153:LEU:HD23	2:H:153:LEU:HA	1.71	0.42
1:L:41:TRP:O	1:L:42:ILE:C	2.63	0.42
2:H:29:TRP:HA	2:H:119:VAL:O	2.19	0.42
1:L:105:HIS:HB2	1:L:108:THR:HG23	2.02	0.42
2:H:212:ILE:HB	2:H:229:THR:HB	2.00	0.42
2:H:47:ILE:HD13	2:H:53:VAL:HG23	2.00	0.42
3:T:37:GLN:HG3	3:T:76:PHE:HE1	1.83	0.42
4:I:45:PHE:CD1	4:I:45:PHE:N	2.88	0.42
4:I:3:ASP:O	4:I:6:LEU:HG	2.20	0.42
1:L:84:HIS:C	1:L:86:ASP:N	2.78	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD23	1.87	0.42
2:H:236:GLU:OE2	2:H:240:LYS:CE	2.68	0.42
3:T:191:ALA:HB3	3:T:202:SER:HB3	2.02	0.42
4:I:29:LEU:C	4:I:29:LEU:HD13	2.44	0.42
4:I:6:LEU:N	4:I:6:LEU:CD2	2.80	0.42
2:H:187:GLY:CA	2:H:221(A):ALA:O	2.58	0.41
4:I:7:GLU:HG3	4:I:8:PRO:O	2.20	0.41
2:H:68:LEU:HD13	2:H:118:VAL:CG1	2.51	0.41
2:H:211:GLY:HA2	2:H:229:THR:O	2.20	0.41
3:T:168:ALA:HB3	3:T:175:PHE:HD2	1.85	0.41
3:T:205:SER:HB2	3:T:206:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:4:PHE:CZ	4:I:54:THR:HG21	2.54	0.41
1:L:103:SER:OG	1:L:113:ARG:NE	2.53	0.41
2:H:256:PHE:HA	2:H:257:PRO:C	2.46	0.41
3:T:151:LEU:HD21	3:T:153:TYR:OH	2.21	0.41
4:I:2:PRO:HD2	4:I:5:CYS:SG	2.60	0.41
1:L:73:LEU:HA	1:L:73:LEU:HD23	1.61	0.41
1:L:121:LEU:O	1:L:124:GLY:N	2.45	0.41
3:T:105:GLU:O	3:T:199:ASN:ND2	2.50	0.41
3:T:187:PHE:N	3:T:208:GLU:O	2.48	0.41
4:I:9:PRO:HG3	4:I:22:PHE:CE2	2.56	0.41
2:H:89:ILE:O	2:H:104:ALA:HA	2.20	0.41
3:T:179:VAL:CB	3:T:185:TYR:CE2	3.03	0.41
4:I:9:PRO:HG3	4:I:22:PHE:CZ	2.55	0.41
3:T:114:GLN:N	3:T:126:THR:O	2.38	0.40
3:T:147:PHE:CD1	3:T:193:ILE:HD13	2.55	0.40
3:T:37:GLN:O	3:T:73:ALA:CA	2.67	0.40
4:I:21:TYR:CD1	4:I:21:TYR:N	2.89	0.40
4:I:38:CYS:CB	4:I:39:LEU:HD12	2.50	0.40
1:L:37:THR:HG23	1:L:41:TRP:CD1	2.57	0.40
1:L:53:SER:N	1:L:54:PRO:HD3	2.37	0.40
1:L:139:PRO:HG2	2:H:116:ASP:HA	2.04	0.40
2:H:68:LEU:CD1	2:H:112:VAL:HG21	2.52	0.40
3:T:158:TRP:CE2	3:T:186:CYS:HB2	2.57	0.40
3:T:186:CYS:HA	3:T:209:CYS:HA	2.03	0.40
4:I:23:TYR:CE1	4:I:29:LEU:N	2.89	0.40
3:T:105:GLU:O	3:T:106:THR:C	2.65	0.40
3:T:123:VAL:HB	3:T:177:ILE:HD11	2.04	0.40
3:T:185:TYR:O	3:T:209:CYS:C	2.65	0.40
4:I:39:LEU:N	4:I:39:LEU:CD1	2.85	0.40
1:L:76:PHE:HA	1:L:83:THR:O	2.21	0.40
2:H:66:ALA:O	2:H:82:SER:HA	2.22	0.40
3:T:155:LEU:HA	3:T:188:SER:O	2.21	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	106/152 (70%)	100 (94%)	6 (6%)	0	100	100
2	H	247/254 (97%)	235 (95%)	11 (4%)	1 (0%)	30	28
3	T	173/206 (84%)	163 (94%)	10 (6%)	0	100	100
4	I	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	579/667 (87%)	548 (95%)	30 (5%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	249	GLY

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	95/122 (78%)	82 (86%)	13 (14%)	3	2
2	H	214/216 (99%)	204 (95%)	10 (5%)	23	24
3	T	172/190 (90%)	149 (87%)	23 (13%)	4	2
4	I	45/45 (100%)	32 (71%)	13 (29%)	0	0
All	All	526/573 (92%)	467 (89%)	59 (11%)	6	3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	36	ARG
1	L	37	THR
1	L	39	LEU
1	L	43	SER
1	L	62	LYS

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Mol	Chain	Res	Type
1	L	86	ASP
1	L	88	GLN
1	L	89	LEU
1	L	106	THR
1	L	113	ARG
1	L	119	SER
1	L	140	ILE
1	L	143	LYS
2	H	20	LYS
2	H	34	LEU
2	H	62	ARG
2	H	63	ASN
2	H	89	ILE
2	H	110	GLN
2	H	134	ARG
2	H	159	ASN
2	H	202	HIS
2	H	252	LEU
3	T	6	THR
3	T	13	THR
3	T	27	PRO
3	T	28	LYS
3	T	53	THR
3	T	62	GLU
3	T	68	LYS
3	T	69	GLN
3	T	72	LEU
3	T	93	LEU
3	T	113	ILE
3	T	114	GLN
3	T	123	VAL
3	T	125	VAL
3	T	139	THR
3	T	149	LYS
3	T	152	ILE
3	T	167	THR
3	T	171	ASN
3	T	174	GLU
3	T	175	PHE
3	T	177	ILE
3	T	188	SER
4	I	3	ASP

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Mol	Chain	Res	Type
4	I	6	LEU
4	I	13	PRO
4	I	19	LEU
4	I	26	LYS
4	I	29	LEU
4	I	31	GLN
4	I	41	LYS
4	I	42	ARG
4	I	44	ASN
4	I	46	GLU
4	I	52	MET
4	I	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	80	ASN
1	L	84	HIS
1	L	88	GLN
1	L	115	HIS
2	H	60(D)	ASN
2	H	63	ASN
2	H	100	ASN
2	H	110	GLN
2	H	159	ASN
3	T	107	ASN
3	T	114	GLN
3	T	118	GLN
3	T	137	ASN
3	T	171	ASN
4	I	24	ASN
4	I	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
5	GLC	L	600	1	11,11,12	1.27	1 (9%)	15,15,17	2.34	3 (20%)
6	FUC	L	601	1	10,10,11	1.42	1 (10%)	14,14,16	1.47	2 (14%)

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
5	GLC	L	600	1	1/1/4/5	2/2/19/22	0/1/1/1
6	FUC	L	601	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	601	FUC	C4-C5	2.29	1.57	1.52
5	L	600	GLC	C4-C5	2.12	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	600	GLC	C1-O5-C5	6.72	121.19	112.19
5	L	600	GLC	O5-C1-C2	3.42	118.95	110.79
6	L	601	FUC	C1-O5-C5	3.35	120.86	112.97
5	L	600	GLC	O5-C5-C6	2.84	113.19	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	601	FUC	C2-C3-C4	-2.15	107.09	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	600	GLC	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	600	GLC	C4-C5-C6-O6
5	L	600	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	600	GLC	1	0

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.