



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 PM UTC

PDB ID : 4HTC / pdb_00004htc
Title : THE REFINED STRUCTURE OF THE HIRUDIN-THROMBIN COMPLEX
Authors : Tulinsky, A.; Rydel, T.J.; Bode, W.; Huber, R.
Deposited on : 1993-06-25
Resolution : 2.30 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

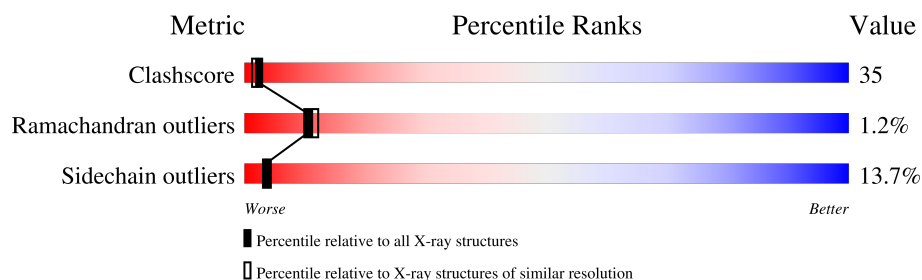
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	36	28% 36% 28% 8%
2	H	259	36% 36% 23% 5%
3	I	65	20% 37% 25% 12% 6%

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
4	NAG	H	400	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3045 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	33	Total	C	N	O	S	0	0	0
			253	158	41	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	1
			2069	1323	366	366	14			

- Molecule 3 is a protein called HIRUDIN VARIANT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	61	Total	C	N	O	S	0	0	0
			447	267	75	99	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	47	LYS	ASN	conflict	UNP P09945

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	18	Total	O	0	0
			18	18		
5	H	199	Total	O	0	0
			199	199		
5	I	45	Total	O	0	0
			45	45		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

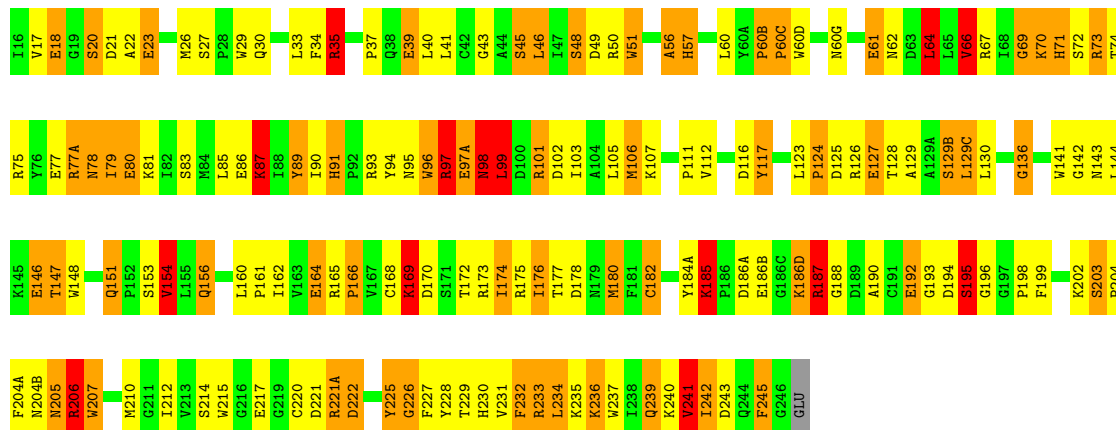
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 28% 36% 28% 8%



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 36% 36% 23% 5%



• Molecule 3: HIRUDIN VARIANT 2

Chain I: 20% 37% 25% 12% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.54Å 90.54Å 132.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3045	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: NAG

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	1.34	0/255	2.54	19/338 (5.6%)
2	H	1.52	11/2124 (0.5%)	2.66	190/2872 (6.6%)
3	I	1.50	0/452	2.79	53/607 (8.7%)
All	All	1.50	11/2831 (0.4%)	2.67	262/3817 (6.9%)

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	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	27	SER	N-CA	7.75	1.55	1.46
2	H	70	LYS	CA-CB	6.91	1.63	1.53
2	H	195	SER	CA-CB	6.73	1.64	1.53
2	H	245	PHE	C-N	-6.47	1.24	1.33
2	H	71	HIS	N-CA	6.18	1.53	1.46
2	H	73	ARG	C-O	6.06	1.31	1.24
2	H	207	TRP	CA-C	5.76	1.59	1.52
2	H	229	THR	CA-C	5.35	1.59	1.52
2	H	78	ASN	N-CA	5.22	1.51	1.46
2	H	74	THR	CA-CB	5.07	1.61	1.54
2	H	233	ARG	NE-CZ	5.05	1.38	1.33

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	ARG	NE-CZ-NH2	-12.81	107.67	119.20
2	H	204(A)	PHE	CA-C-O	-12.35	107.29	120.63
2	H	212	ILE	O-C-N	12.22	136.27	123.07
2	H	35	ARG	NE-CZ-NH1	11.29	132.79	121.50
2	H	73	ARG	NE-CZ-NH1	11.23	132.73	121.50
2	H	175	ARG	NE-CZ-NH1	11.09	132.59	121.50
2	H	205	ASN	OD1-CG-ND2	11.01	133.61	122.60
2	H	175	ARG	CD-NE-CZ	10.38	138.93	124.40
2	H	212	ILE	CA-C-O	-10.24	109.27	120.43
2	H	77(A)	ARG	NE-CZ-NH1	10.23	131.73	121.50
2	H	151	GLN	CA-CB-CG	10.00	134.10	114.10
2	H	233	ARG	CD-NE-CZ	-9.91	110.53	124.40
1	L	1(A)	ASP	CA-CB-CG	9.72	122.32	112.60
2	H	178	ASP	CA-CB-CG	-9.61	102.99	112.60
2	H	206	ARG	NE-CZ-NH1	-9.58	111.92	121.50
2	H	123	LEU	CB-CA-C	9.46	122.21	108.87
3	I	12	ASN	OD1-CG-ND2	-9.40	113.20	122.60
2	H	62	ASN	OD1-CG-ND2	9.35	131.95	122.60
2	H	123	LEU	N-CA-C	-9.05	98.66	110.07
2	H	176	ILE	CB-CA-C	8.91	121.96	110.91
2	H	175	ARG	NE-CZ-NH2	-8.75	111.33	119.20
2	H	221(A)	ARG	CD-NE-CZ	8.72	136.61	124.40
2	H	127	GLU	CB-CG-CD	8.70	127.39	112.60
2	H	168	CYS	CA-C-N	8.70	132.28	120.54
2	H	168	CYS	C-N-CA	8.70	132.28	120.54
2	H	97	ARG	CA-C-O	8.67	132.91	120.51
2	H	98	ASN	CA-CB-CG	-8.57	104.03	112.60
3	I	52	ASN	N-CA-C	8.57	124.16	111.81
2	H	151	GLN	OE1-CD-NE2	8.52	131.12	122.60
2	H	78	ASN	OD1-CG-ND2	8.50	131.10	122.60
2	H	237	TRP	CA-C-O	8.46	129.41	120.70
2	H	99	LEU	N-CA-C	-8.42	102.31	112.58
2	H	101	ARG	CD-NE-CZ	-8.38	112.67	124.40
3	I	58	GLU	CB-CA-C	-8.33	99.56	109.80
2	H	204(A)	PHE	CA-CB-CG	-8.32	105.48	113.80
2	H	116	ASP	CA-C-O	-8.30	111.75	120.55
2	H	69	GLY	CA-C-N	8.21	134.24	122.09
2	H	69	GLY	C-N-CA	8.21	134.24	122.09
2	H	78	ASN	CA-CB-CG	-8.21	104.39	112.60
2	H	60(B)	PRO	CB-CA-C	8.20	120.92	110.92
2	H	77(A)	ARG	CD-NE-CZ	8.14	135.80	124.40
2	H	27	SER	N-CA-CB	-8.07	100.30	110.79
2	H	245	PHE	O-C-N	8.03	135.84	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	65	GLN	CG-CD-NE2	-7.95	104.47	116.40
2	H	221(A)	ARG	NE-CZ-NH2	7.94	126.35	119.20
2	H	195	SER	CA-CB-OG	-7.88	95.34	111.10
2	H	73	ARG	O-C-N	-7.82	113.83	122.12
3	I	56	PHE	CA-CB-CG	-7.80	106.00	113.80
2	H	185	LYS	CA-CB-CG	-7.78	98.54	114.10
3	I	21	VAL	CB-CA-C	-7.75	100.59	111.28
3	I	29	ILE	CA-C-O	-7.66	111.85	120.97
2	H	66	VAL	CA-C-O	7.66	128.44	120.39
2	H	66	VAL	CB-CA-C	7.63	121.92	110.63
2	H	18	GLU	CB-CG-CD	-7.62	99.64	112.60
3	I	26	ASN	N-CA-CB	7.62	123.55	111.43
2	H	87	LYS	O-C-N	7.54	131.48	123.42
2	H	116	ASP	O-C-N	7.53	130.10	122.12
1	L	14(C)	GLU	CB-CA-C	-7.51	98.32	110.79
2	H	206	ARG	NE-CZ-NH2	7.50	125.95	119.20
2	H	35	ARG	CD-NE-CZ	7.48	134.87	124.40
2	H	45	SER	CA-C-N	7.42	132.49	121.72
2	H	45	SER	C-N-CA	7.42	132.49	121.72
3	I	58	GLU	CA-C-O	-7.40	113.92	120.88
3	I	7	THR	CA-CB-OG1	-7.40	98.50	109.60
3	I	7	THR	CA-CB-CG2	7.38	123.06	110.50
2	H	151	GLN	CB-CA-C	7.37	119.93	108.88
2	H	245	PHE	N-CA-CB	7.34	122.98	110.50
2	H	77(A)	ARG	CA-C-N	-7.26	111.66	122.83
2	H	77(A)	ARG	C-N-CA	-7.26	111.66	122.83
2	H	27	SER	O-C-N	7.25	127.10	121.23
3	I	55	ASP	N-CA-CB	-7.23	100.73	111.43
2	H	57	HIS	CA-CB-CG	-7.19	106.61	113.80
2	H	146	GLU	CG-CD-OE2	-7.16	101.94	118.40
3	I	38	GLN	O-C-N	7.16	131.69	123.31
2	H	166	PRO	O-C-N	7.10	130.75	122.23
2	H	226	GLY	N-CA-C	-7.09	101.89	111.54
2	H	196	GLY	O-C-N	7.07	130.64	122.65
1	L	9	LYS	CA-CB-CG	7.06	128.21	114.10
3	I	48	PRO	CA-C-O	7.05	130.27	121.67
2	H	205	ASN	N-CA-CB	-7.01	101.72	113.15
2	H	61	GLU	CA-CB-CG	6.96	128.02	114.10
2	H	194	ASP	CA-CB-CG	6.89	119.49	112.60
3	I	29	ILE	O-C-N	6.88	132.16	122.59
2	H	73	ARG	CG-CD-NE	-6.81	97.01	112.00
1	L	14(D)	ARG	NE-CZ-NH1	6.77	128.27	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	GLU	CA-C-N	6.75	132.50	122.99
2	H	80	GLU	C-N-CA	6.75	132.50	122.99
2	H	180	MET	O-C-N	6.75	131.34	123.17
2	H	207	TRP	CA-C-N	6.66	132.38	122.99
2	H	207	TRP	C-N-CA	6.66	132.38	122.99
1	L	1(A)	ASP	N-CA-CB	-6.66	99.24	110.49
3	I	53	ASN	CA-CB-CG	6.62	119.22	112.60
2	H	117	TYR	N-CA-C	6.59	121.03	112.92
2	H	186(D)	LYS	N-CA-C	-6.58	99.34	109.14
2	H	170	ASP	CA-C-O	-6.56	110.52	119.05
1	L	4	ARG	CD-NE-CZ	6.54	133.56	124.40
2	H	95	ASN	CA-CB-CG	-6.53	106.07	112.60
2	H	34	PHE	CA-CB-CG	6.49	120.29	113.80
3	I	59	ILE	O-C-N	6.49	128.50	121.10
1	L	14	ASP	N-CA-C	-6.49	101.97	110.53
2	H	231	VAL	N-CA-C	6.46	117.14	110.36
2	H	154	VAL	CA-CB-CG1	6.43	121.33	110.40
2	H	222	ASP	CA-C-O	-6.42	113.97	121.16
3	I	57	GLU	CA-C-N	6.42	133.08	121.97
3	I	57	GLU	C-N-CA	6.42	133.08	121.97
1	L	14(H)	GLU	CG-CD-OE2	-6.42	103.64	118.40
2	H	96	TRP	O-C-N	6.38	130.12	122.27
2	H	62	ASN	CA-CB-CG	-6.38	106.22	112.60
2	H	232	PHE	CA-CB-CG	-6.38	107.42	113.80
2	H	125	ASP	CA-C-N	6.37	128.82	120.28
2	H	125	ASP	C-N-CA	6.37	128.82	120.28
3	I	15	LEU	CB-CA-C	6.35	120.33	110.67
2	H	91	HIS	CA-CB-CG	-6.34	107.46	113.80
2	H	204	PRO	N-CA-C	-6.34	104.90	113.40
3	I	57	GLU	N-CA-CB	6.33	119.91	110.29
2	H	205	ASN	CA-CB-CG	-6.32	106.28	112.60
3	I	41	THR	N-CA-C	-6.29	101.80	110.35
2	H	77	GLU	C-N-CA	6.29	137.42	121.70
3	I	62	GLU	CB-CG-CD	6.29	123.29	112.60
3	I	45	THR	O-C-N	6.28	126.98	121.39
2	H	214	SER	CA-C-O	-6.26	112.40	119.98
2	H	98	ASN	N-CA-CB	6.25	121.06	110.49
2	H	117	TYR	CB-CA-C	-6.25	99.99	110.56
2	H	147	THR	CA-CB-CG2	6.23	121.09	110.50
2	H	178	ASP	O-C-N	6.22	129.50	122.22
2	H	98	ASN	O-C-N	6.17	130.79	122.59
3	I	28	CYS	CA-C-O	6.16	127.15	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	GLN	N-CA-CB	6.16	122.19	110.49
3	I	47	LYS	N-CA-C	-6.15	102.52	109.60
2	H	229	THR	N-CA-CB	6.15	119.01	109.85
2	H	225	TYR	CA-C-N	6.14	126.58	120.31
2	H	225	TYR	C-N-CA	6.14	126.58	120.31
3	I	9	SER	CB-CA-C	6.13	120.13	109.65
2	H	78	ASN	CB-CG-OD1	-6.13	108.55	120.80
2	H	129(B)	SER	CB-CA-C	-6.12	101.23	110.90
3	I	11	GLN	O-C-N	6.12	130.14	123.10
1	L	14(I)	SER	N-CA-C	-6.10	103.95	111.33
2	H	186(D)	LYS	N-CA-CB	6.10	121.50	111.62
1	L	12	LEU	CA-C-O	-6.05	114.30	120.71
2	H	195	SER	CB-CA-C	-6.05	99.96	109.70
2	H	239	GLN	CG-CD-NE2	6.05	125.47	116.40
2	H	128	THR	O-C-N	6.04	128.62	122.09
2	H	71	HIS	ND1-CE1-NE2	-6.04	102.36	108.40
2	H	169	LYS	O-C-N	6.04	128.37	122.09
2	H	233	ARG	CG-CD-NE	6.02	125.25	112.00
2	H	190	ALA	N-CA-C	-6.01	102.78	110.53
3	I	8	GLU	O-C-N	5.94	130.55	123.24
2	H	125	ASP	N-CA-C	-5.93	101.21	110.17
2	H	245	PHE	CA-C-O	-5.92	110.73	120.80
3	I	40	VAL	N-CA-C	5.91	118.13	108.97
2	H	129(C)	LEU	CA-C-O	-5.91	113.68	120.24
3	I	53	ASN	CA-C-O	-5.89	112.09	120.51
2	H	185	LYS	CG-CD-CE	-5.89	97.76	111.30
2	H	174	ILE	O-C-N	5.88	129.96	122.61
2	H	60(C)	PRO	CB-CA-C	5.85	121.22	111.56
2	H	227	PHE	CA-CB-CG	-5.83	107.97	113.80
2	H	156	GLN	OE1-CD-NE2	5.82	128.42	122.60
2	H	221	ASP	N-CA-C	5.82	119.68	112.24
3	I	11	GLN	N-CA-CB	5.81	120.10	110.63
2	H	125	ASP	CA-CB-CG	-5.80	106.80	112.60
2	H	34	PHE	CA-C-O	5.79	126.62	120.36
3	I	26	ASN	CA-CB-CG	-5.79	106.81	112.60
1	L	1(C)	GLU	N-CA-C	-5.79	101.27	109.96
2	H	51	TRP	CA-C-N	5.79	130.72	123.14
2	H	51	TRP	C-N-CA	5.79	130.72	123.14
2	H	40	LEU	CB-CA-C	5.78	119.77	110.29
2	H	64	LEU	N-CA-C	5.78	118.47	109.52
2	H	206	ARG	O-C-N	5.78	129.95	123.19
2	H	30	GLN	OE1-CD-NE2	-5.76	116.84	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	40	VAL	CA-C-O	5.72	128.75	121.48
2	H	198	PRO	CA-C-N	5.71	131.22	123.11
2	H	198	PRO	C-N-CA	5.71	131.22	123.11
2	H	240	LYS	CA-C-O	-5.71	114.50	120.55
2	H	127	GLU	CB-CA-C	5.67	121.94	110.38
2	H	43	GLY	N-CA-C	-5.66	103.94	112.60
2	H	169	LYS	CA-C-O	-5.66	114.85	120.90
3	I	38	GLN	OE1-CD-NE2	5.66	128.25	122.60
2	H	39	GLU	O-C-N	5.61	129.51	123.56
2	H	71	HIS	N-CA-C	-5.60	104.46	112.13
3	I	15	LEU	N-CA-CB	-5.60	100.42	109.60
2	H	176	ILE	N-CA-CB	-5.57	104.65	110.72
1	L	12	LEU	N-CA-CB	-5.57	101.73	110.69
2	H	187	ARG	O-C-N	5.56	129.43	122.92
1	L	14(A)	LYS	N-CA-CB	5.54	118.75	110.22
2	H	20	SER	O-C-N	5.54	129.47	123.10
2	H	156	GLN	CB-CG-CD	-5.54	103.18	112.60
2	H	220	CYS	CA-C-O	-5.54	114.17	120.32
2	H	96	TRP	N-CA-C	-5.53	105.40	111.82
2	H	241	VAL	N-CA-CB	5.52	118.86	110.58
2	H	136	GLY	N-CA-C	-5.51	101.99	111.57
3	I	53	ASN	O-C-N	5.50	129.91	122.59
2	H	56	ALA	CA-C-O	-5.50	114.72	120.55
2	H	239	GLN	CA-C-O	5.50	126.78	120.90
2	H	206	ARG	N-CA-C	5.50	118.78	109.76
3	I	22	CYS	CA-C-O	5.49	126.96	120.70
2	H	79	ILE	CA-CB-CG1	-5.49	101.07	110.40
2	H	192	GLU	N-CA-CB	5.49	117.64	109.19
2	H	136	GLY	CA-C-N	5.47	130.70	122.99
2	H	136	GLY	C-N-CA	5.47	130.70	122.99
3	I	61	GLU	CG-CD-OE1	-5.46	105.84	118.40
1	L	13	GLU	CA-CB-CG	5.44	124.99	114.10
2	H	187	ARG	NE-CZ-NH1	-5.43	116.07	121.50
2	H	83	SER	CA-CB-OG	5.43	121.95	111.10
2	H	143	ASN	O-C-N	5.43	129.63	123.12
2	H	77	GLU	CA-C-O	5.42	128.26	120.51
3	I	37	ASN	CA-C-N	-5.41	114.41	122.74
3	I	37	ASN	C-N-CA	-5.41	114.41	122.74
2	H	86	GLU	CG-CD-OE2	5.40	130.83	118.40
2	H	61	GLU	CB-CG-CD	5.38	121.75	112.60
2	H	124	PRO	CB-CA-C	-5.38	103.18	110.60
2	H	142	GLY	CA-C-N	5.37	129.31	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	142	GLY	C-N-CA	5.37	129.31	121.31
3	I	11	GLN	OE1-CD-NE2	5.37	127.97	122.60
2	H	35	ARG	NH1-CZ-NH2	-5.37	112.33	119.30
2	H	180	MET	CB-CA-C	-5.36	98.29	110.07
3	I	61	GLU	CB-CG-CD	-5.35	103.51	112.60
2	H	101	ARG	NH1-CZ-NH2	5.35	126.25	119.30
2	H	172	THR	CA-CB-CG2	5.34	119.58	110.50
1	L	14(D)	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	L	14(F)	LEU	CA-C-O	-5.30	115.24	120.70
2	H	212	ILE	N-CA-C	-5.30	100.43	108.17
2	H	74	THR	CA-C-O	-5.29	113.23	119.05
2	H	77(A)	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
2	H	193	GLY	O-C-N	5.28	128.61	122.65
2	H	226	GLY	O-C-N	5.25	128.25	122.84
2	H	67	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	L	13	GLU	CG-CD-OE2	5.25	130.46	118.40
3	I	46	PRO	O-C-N	5.23	128.96	123.10
1	L	14(F)	LEU	N-CA-CB	5.23	117.65	110.07
2	H	151	GLN	O-C-N	5.22	126.57	121.66
3	I	51	HIS	CA-C-N	5.22	131.94	122.27
3	I	51	HIS	C-N-CA	5.22	131.94	122.27
3	I	5	ASP	N-CA-C	5.21	117.59	110.24
2	H	243	ASP	N-CA-CB	-5.21	104.17	111.62
2	H	48	SER	CA-C-O	-5.19	115.59	121.25
2	H	186(A)	ASP	O-C-N	5.19	131.00	122.70
2	H	236	LYS	CA-C-O	-5.18	114.24	120.10
3	I	45	THR	CA-CB-OG1	-5.18	101.83	109.60
2	H	215	TRP	CA-C-O	5.17	126.76	121.23
3	I	8	GLU	CB-CG-CD	-5.16	103.83	112.60
2	H	89	TYR	O-C-N	5.16	129.88	123.28
2	H	23	GLU	CA-C-O	-5.13	115.57	121.47
3	I	14	CYS	O-C-N	5.13	128.91	123.42
2	H	153	SER	CA-C-N	5.12	130.16	122.58
2	H	153	SER	C-N-CA	5.12	130.16	122.58
2	H	242	ILE	CB-CA-C	5.12	119.29	112.22
2	H	71	HIS	CE1-NE2-CD2	5.12	114.12	109.00
2	H	196	GLY	N-CA-C	-5.11	108.61	114.69
2	H	233	ARG	CA-C-O	-5.10	114.49	120.20
3	I	61	GLU	OE1-CD-OE2	5.09	135.12	122.90
2	H	148	TRP	CA-C-O	5.06	126.87	121.45
2	H	151	GLN	CG-CD-NE2	-5.06	108.81	116.40
2	H	71	HIS	CA-C-N	5.05	128.02	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	71	HIS	C-N-CA	5.05	128.02	120.95
3	I	26	ASN	OD1-CG-ND2	5.05	127.65	122.60
2	H	71	HIS	CA-C-O	5.04	127.68	120.16
3	I	21	VAL	CA-C-O	-5.04	116.39	121.59
1	L	14(C)	GLU	CG-CD-OE1	-5.04	106.81	118.40
2	H	205	ASN	CB-CG-OD1	-5.03	110.74	120.80
2	H	101	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	H	203	SER	CA-C-N	5.01	124.31	118.85
2	H	203	SER	C-N-CA	5.01	124.31	118.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	206	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	253	0	244	19	1
2	H	2069	0	2040	126	1
3	I	447	0	399	62	0
4	H	14	0	13	2	0
5	H	199	0	0	21	0
5	I	45	0	0	14	0
5	L	18	0	0	5	0
All	All	3045	0	2696	193	1

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 35.

All (193) 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)
5:H:452:HOH:O	3:I:53:ASN:HB3	1.26	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.33	1.09
3:I:58:GLU:O	3:I:58:GLU:CG	2.08	1.01
3:I:58:GLU:O	3:I:58:GLU:HG2	1.22	1.01
3:I:40:VAL:HG23	3:I:41:THR:O	1.60	1.00
1:L:14(M):GLY:HA3	5:L:603:HOH:O	1.58	0.99
3:I:13:LEU:HD12	3:I:46:PRO:HB3	1.46	0.97
3:I:55:ASP:N	3:I:55:ASP:OD1	1.98	0.97
3:I:52:ASN:HA	5:I:691:HOH:O	1.71	0.90
5:H:452:HOH:O	3:I:53:ASN:CB	1.93	0.85
2:H:23:GLU:H	2:H:26:MET:HE3	1.43	0.83
3:I:13:LEU:HD11	3:I:24:LYS:HE3	1.60	0.83
2:H:173:ARG:HD3	3:I:20:ASN:OD1	1.78	0.82
2:H:126:ARG:HD2	5:H:738:HOH:O	1.79	0.82
1:L:14(I):SER:HA	1:L:14(M):GLY:C	2.06	0.81
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.16	0.80
2:H:35:ARG:HG3	2:H:35:ARG:HH11	1.48	0.79
2:H:174:ILE:HD11	3:I:21:VAL:HG21	1.66	0.78
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.18	0.77
2:H:165:ARG:NH1	2:H:180:MET:O	2.18	0.77
3:I:27:LYS:HG3	3:I:40:VAL:HG22	1.65	0.77
2:H:35:ARG:HD2	2:H:37:PRO:O	1.85	0.76
2:H:78:ASN:N	5:H:596:HOH:O	1.65	0.76
5:H:663:HOH:O	3:I:53:ASN:HA	1.86	0.76
2:H:78:ASN:HB2	5:H:571:HOH:O	1.87	0.75
5:L:437:HOH:O	2:H:26:MET:HE1	1.86	0.74
3:I:11:GLN:HA	3:I:45:THR:O	1.89	0.73
2:H:96:TRP:HZ3	3:I:24:LYS:HZ1	1.37	0.71
2:H:185:LYS:O	2:H:186(B):GLU:HB2	1.92	0.70
3:I:12:ASN:N	3:I:45:THR:O	2.24	0.70
3:I:29:ILE:HG12	3:I:40:VAL:CG1	2.21	0.70
3:I:58:GLU:HB3	5:I:722:HOH:O	1.90	0.69
2:H:174:ILE:HD11	3:I:21:VAL:CG2	2.21	0.69
2:H:195:SER:HB2	5:H:538:HOH:O	1.92	0.69
2:H:96:TRP:O	2:H:97(A):GLU:N	2.25	0.69
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ2	2.28	0.69
3:I:31:GLY:HA3	3:I:36:GLY:O	1.92	0.68
3:I:12:ASN:O	3:I:46:PRO:HA	1.94	0.67
2:H:185:LYS:CB	2:H:186(B):GLU:HG3	2.19	0.67
3:I:27:LYS:CG	3:I:40:VAL:HG22	2.25	0.67
1:L:1(B):ALA:O	5:L:447:HOH:O	2.12	0.66
3:I:30:LEU:HA	3:I:37:ASN:ND2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:230:HIS:HE1	2:H:232:PHE:HB3	1.61	0.66
2:H:46:LEU:HD22	2:H:48:SER:O	1.96	0.65
2:H:70:LYS:HE3	2:H:72:SER:O	1.97	0.64
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.32	0.64
3:I:30:LEU:HD23	3:I:37:ASN:ND2	2.13	0.64
2:H:164:GLU:HB2	2:H:166:PRO:HD2	1.80	0.62
1:L:1(C):GLU:HB2	5:L:447:HOH:O	2.00	0.62
2:H:35:ARG:HG3	2:H:35:ARG:NH1	2.10	0.62
2:H:17:VAL:O	2:H:18:GLU:HB2	1.99	0.61
3:I:53:ASN:ND2	5:I:574:HOH:O	2.34	0.61
3:I:29:ILE:HG12	3:I:40:VAL:HG11	1.81	0.61
2:H:85:LEU:HD13	2:H:106:MET:HG2	1.82	0.61
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.36	0.61
3:I:62:GLU:HB3	5:I:472:HOH:O	2.02	0.60
3:I:11:GLN:CA	3:I:45:THR:O	2.49	0.60
2:H:96:TRP:CH2	2:H:97:ARG:HG3	2.36	0.59
3:I:7:THR:HG22	3:I:8:GLU:HG3	1.84	0.59
2:H:35:ARG:CB	2:H:39:GLU:HG2	2.32	0.59
2:H:185:LYS:HG3	2:H:225:TYR:OH	2.03	0.58
2:H:124:PRO:O	2:H:235:LYS:HE2	2.04	0.58
2:H:51:TRP:CE2	2:H:242:ILE:HG12	2.39	0.57
2:H:60(D):TRP:CD2	3:I:49:GLU:HB2	2.39	0.57
2:H:87:LYS:HD2	2:H:89:TYR:CZ	2.39	0.57
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.53	0.57
3:I:60:PRO:HG2	3:I:63:TYR:HE2	1.70	0.57
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.40	0.56
2:H:51:TRP:CZ2	2:H:107:LYS:HD2	2.40	0.56
1:L:14(D):ARG:HG3	1:L:14(H):GLU:OE2	2.05	0.56
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.20	0.56
2:H:96:TRP:HZ3	3:I:24:LYS:NZ	2.03	0.56
2:H:77(A):ARG:HD2	5:I:467:HOH:O	2.04	0.56
2:H:94:TYR:HE1	2:H:99:LEU:HD12	1.71	0.55
3:I:65:GLN:HA	5:I:615:HOH:O	2.06	0.55
2:H:165:ARG:NH2	2:H:177:THR:O	2.38	0.55
2:H:17:VAL:O	2:H:188:GLY:HA2	2.06	0.55
2:H:66:VAL:HG21	2:H:106:MET:CE	2.37	0.54
3:I:27:LYS:N	3:I:40:VAL:O	2.39	0.54
2:H:49:ASP:O	2:H:111:PRO:HA	2.07	0.54
2:H:126:ARG:HG2	5:H:575:HOH:O	2.07	0.54
3:I:52:ASN:C	3:I:53:ASN:HD22	2.16	0.54
2:H:217:GLU:OE2	3:I:21:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:GLU:C	2:H:166:PRO:HD2	2.34	0.53
2:H:22:ALA:O	2:H:71:HIS:HE1	1.90	0.53
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.38	0.53
3:I:54:GLY:HA3	5:I:564:HOH:O	2.08	0.52
2:H:70:LYS:CE	2:H:72:SER:O	2.57	0.52
3:I:29:ILE:HG12	3:I:40:VAL:HG13	1.92	0.52
2:H:85:LEU:HD22	2:H:106:MET:HG2	1.93	0.51
3:I:60:PRO:HG2	3:I:63:TYR:CE2	2.44	0.51
2:H:192:GLU:HG3	5:H:414:HOH:O	2.09	0.51
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.74	0.51
2:H:60(G):ASN:HB2	5:H:442:HOH:O	2.10	0.51
1:L:14(D):ARG:O	1:L:14(H):GLU:HG2	2.11	0.51
3:I:16:CYS:HB3	5:I:502:HOH:O	2.10	0.51
2:H:185:LYS:HD3	5:H:421:HOH:O	2.11	0.51
2:H:20:SER:O	2:H:156:GLN:HA	2.11	0.51
2:H:230:HIS:CE1	2:H:232:PHE:HB3	2.44	0.51
2:H:96:TRP:CZ3	2:H:97:ARG:HG3	2.46	0.50
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.41	0.50
2:H:101:ARG:NE	5:H:624:HOH:O	2.17	0.50
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.18	0.50
3:I:26:ASN:HA	3:I:40:VAL:O	2.11	0.50
3:I:3:TYR:HB3	3:I:15:LEU:HD13	1.93	0.50
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.92	0.50
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.95	0.49
2:H:164:GLU:HG3	5:H:694:HOH:O	2.13	0.49
3:I:61:GLU:HB3	5:I:451:HOH:O	2.13	0.48
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	2.13	0.48
2:H:203:SER:HB2	5:H:562:HOH:O	2.13	0.48
2:H:99:LEU:HD12	2:H:99:LEU:HA	1.80	0.48
3:I:61:GLU:HA	3:I:64:LEU:HB2	1.95	0.48
2:H:60:LEU:CD1	4:H:400:NAG:H5	2.44	0.48
1:L:5:PRO:O	1:L:10:LYS:HG3	2.14	0.47
2:H:46:LEU:CD2	2:H:48:SER:O	2.62	0.47
3:I:65:GLN:HG3	5:I:615:HOH:O	2.14	0.47
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.47	0.47
2:H:98:ASN:HD22	2:H:98:ASN:HA	1.35	0.47
2:H:239:GLN:NE2	5:H:689:HOH:O	2.46	0.47
2:H:56:ALA:N	2:H:102:ASP:OD1	2.47	0.47
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.14	0.47
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.96	0.47
2:H:91:HIS:CE1	2:H:101:ARG:CD	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:TYR:CE1	2:H:99:LEU:HD12	2.49	0.47
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.30	0.47
1:L:14:ASP:CG	1:L:14(C):GLU:HG3	2.41	0.46
3:I:52:ASN:C	3:I:53:ASN:ND2	2.73	0.46
1:L:9:LYS:HE2	5:L:614:HOH:O	2.16	0.46
2:H:192:GLU:HG2	3:I:2:THR:HB	1.98	0.46
2:H:60:LEU:HD13	4:H:400:NAG:H5	1.97	0.46
2:H:33:LEU:HD21	2:H:106:MET:CE	2.46	0.46
2:H:99:LEU:O	2:H:102:ASP:HB2	2.16	0.46
2:H:85:LEU:CD1	2:H:106:MET:HG2	2.46	0.45
3:I:59:ILE:HD11	3:I:64:LEU:HD13	1.98	0.45
2:H:79:ILE:HD12	5:H:593:HOH:O	2.16	0.45
2:H:129:ALA:HA	2:H:210:MET:HE1	1.98	0.45
2:H:73:ARG:HB2	2:H:141:TRP:HD1	1.78	0.45
1:L:1(A):ASP:OD1	1:L:3:LEU:HD12	2.17	0.45
2:H:41:LEU:CD1	2:H:64:LEU:HD23	2.48	0.44
2:H:236:LYS:HD3	2:H:236:LYS:HA	1.77	0.44
5:H:713:HOH:O	3:I:24:LYS:HE2	2.16	0.44
2:H:70:LYS:NZ	2:H:75:ARG:O	2.47	0.44
2:H:169:LYS:HE2	2:H:169:LYS:HB3	1.65	0.44
2:H:69:GLY:HA2	2:H:117:TYR:O	2.18	0.44
2:H:78:ASN:C	2:H:79:ILE:HG13	2.42	0.44
2:H:66:VAL:CG2	2:H:106:MET:CE	2.95	0.43
2:H:90:ILE:HG22	2:H:91:HIS:O	2.19	0.43
2:H:136:GLY:O	2:H:160:LEU:N	2.44	0.43
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.93	0.43
2:H:29:TRP:O	2:H:45:SER:HA	2.18	0.43
3:I:27:LYS:O	3:I:40:VAL:N	2.42	0.43
1:L:14(F):LEU:HD12	2:H:207:TRP:CH2	2.53	0.43
2:H:23:GLU:HG3	2:H:26:MET:HE3	2.01	0.43
3:I:3:TYR:CB	3:I:15:LEU:HD13	2.49	0.43
3:I:30:LEU:CD2	3:I:37:ASN:HD21	2.32	0.43
3:I:54:GLY:N	3:I:55:ASP:OD1	2.52	0.43
2:H:80:GLU:O	5:H:583:HOH:O	2.21	0.43
1:L:14(K):ILE:C	1:L:14(L):ASP:CG	2.85	0.42
2:H:41:LEU:HD12	2:H:64:LEU:HD23	2.01	0.42
3:I:7:THR:N	3:I:11:GLN:OE1	2.48	0.42
3:I:52:ASN:N	5:I:574:HOH:O	2.51	0.42
2:H:57:HIS:CD2	3:I:1:ILE:HG12	2.55	0.42
2:H:77(A):ARG:CD	5:I:467:HOH:O	2.64	0.42
2:H:165:ARG:N	2:H:166:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:ASP:OD2	1:L:14(C):GLU:HG3	2.20	0.42
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.85	0.42
2:H:60(C):PRO:HG3	3:I:24:LYS:HZ1	1.85	0.42
2:H:105:LEU:HD13	2:H:241:VAL:HG22	2.01	0.42
3:I:7:THR:CG2	3:I:8:GLU:HG3	2.48	0.42
2:H:50:ARG:HD3	2:H:107:LYS:HE2	2.01	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD23	1.74	0.42
3:I:45:THR:HG23	3:I:46:PRO:HD2	2.01	0.42
1:L:8:GLU:OE2	2:H:202:LYS:NZ	2.46	0.41
3:I:52:ASN:HB3	5:I:569:HOH:O	2.19	0.41
2:H:85:LEU:CD2	2:H:106:MET:HG2	2.51	0.41
2:H:96:TRP:C	2:H:97(A):GLU:N	2.78	0.41
2:H:182:CYS:HA	2:H:226:GLY:O	2.20	0.41
1:L:14(H):GLU:HG2	1:L:14(H):GLU:H	1.39	0.41
2:H:51:TRP:CD2	2:H:242:ILE:HG12	2.55	0.41
1:L:14(D):ARG:CG	1:L:14(H):GLU:OE2	2.68	0.41
1:L:14(F):LEU:HD12	2:H:207:TRP:HH2	1.84	0.41
2:H:228:TYR:CD1	2:H:228:TYR:N	2.89	0.41
3:I:26:ASN:CA	3:I:40:VAL:O	2.69	0.41
2:H:103:ILE:CD1	5:H:529:HOH:O	2.68	0.41
2:H:165:ARG:N	2:H:166:PRO:HD2	2.35	0.41
2:H:60(B):PRO:O	2:H:60(C):PRO:C	2.64	0.41
2:H:184(A):TYR:CZ	2:H:186(D):LYS:HD3	2.56	0.41
2:H:234:LEU:HB2	5:H:529:HOH:O	2.20	0.41
3:I:63:TYR:HE2	5:I:657:HOH:O	2.03	0.41
2:H:187:ARG:HH11	2:H:187:ARG:HD2	1.53	0.41
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.19	0.40
2:H:221(A):ARG:HB2	5:H:580:HOH:O	2.21	0.40

All (1) 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:1(E):SER:O	2:H:146:GLU:O[5_645]	2.13	0.07

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	31/36 (86%)	24 (77%)	7 (23%)	0	100	100
2	H	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	10	12
3	I	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	6	6
All	All	344/360 (96%)	316 (92%)	24 (7%)	4 (1%)	10	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	ARG
2	H	97(A)	GLU
2	H	98	ASN
3	I	53	ASN

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	26/31 (84%)	25 (96%)	1 (4%)	29	44
2	H	222/225 (99%)	193 (87%)	29 (13%)	4	4
3	I	51/55 (93%)	40 (78%)	11 (22%)	1	1
All	All	299/311 (96%)	258 (86%)	41 (14%)	3	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
2	H	35	ARG
2	H	46	LEU
2	H	61	GLU
2	H	64	LEU
2	H	66	VAL
2	H	81	LYS
2	H	87	LYS
2	H	93	ARG
2	H	98	ASN
2	H	99	LEU
2	H	106	MET
2	H	112	VAL
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	147	THR
2	H	151	GLN
2	H	154	VAL
2	H	164	GLU
2	H	169	LYS
2	H	176	ILE
2	H	182	CYS
2	H	185	LYS
2	H	187	ARG
2	H	195	SER
2	H	233	ARG
2	H	234	LEU
2	H	241	VAL
2	H	245	PHE
3	I	7	THR
3	I	21	VAL
3	I	27	LYS
3	I	29	ILE
3	I	38	GLN
3	I	40	VAL
3	I	53	ASN
3	I	55	ASP
3	I	58	GLU
3	I	64	LEU
3	I	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	98	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	230	HIS
2	H	239	GLN
3	I	26	ASN
3	I	37	ASN
3	I	52	ASN
3	I	53	ASN
3	I	65	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	H	400	2	14,14,15	0.44	0	17,19,21	0.77	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	400	2	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	C1-O5-C5	2.05	114.94	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	400	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAG	C8-C7-N2-C2
4	H	400	NAG	O7-C7-N2-C2
4	H	400	NAG	C4-C5-C6-O6
4	H	400	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	400	NAG	2	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.