



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:21 AM UTC

PDB ID : 1HRT / pdb_00001hrt
Title : THE STRUCTURE OF A COMPLEX OF BOVINE ALPHA-THROMBIN
AND RECOMBINANT HIRUDIN AT 2.8 ANGSTROMS RESOLUTION
Authors : Vitali, J.; Edwards, B.F.P.
Deposited on : 1993-02-25
Resolution : 2.80 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
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

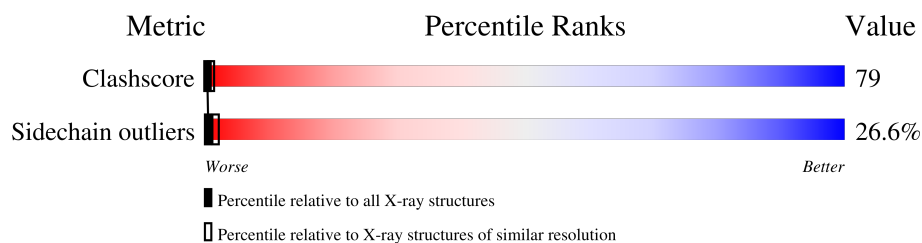
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	49	
2	H	259	
3	I	65	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2996 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 3 is a protein called HIRUDIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	65	Total	C	N	O	S	0	0	0
			483	287	80	110	6			

- Molecule 4 is water.

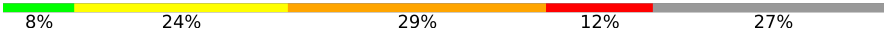
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	25	Total	O	0	0
			25	25		
4	H	79	Total	O	0	0
			79	79		
4	I	25	Total	O	0	0
			25	25		

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.

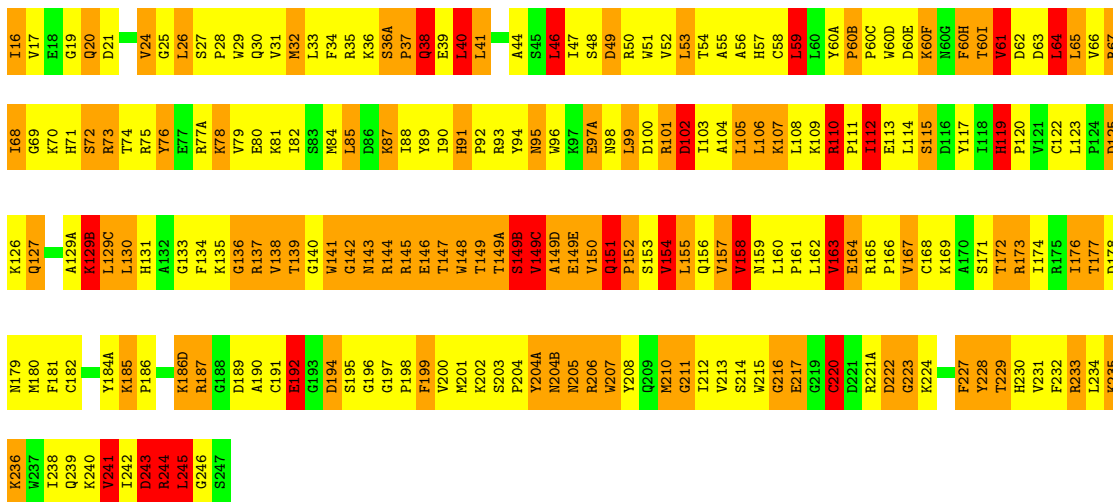
• Molecule 1: THROMBIN (SMALL SUBUNIT)

Chain L: 



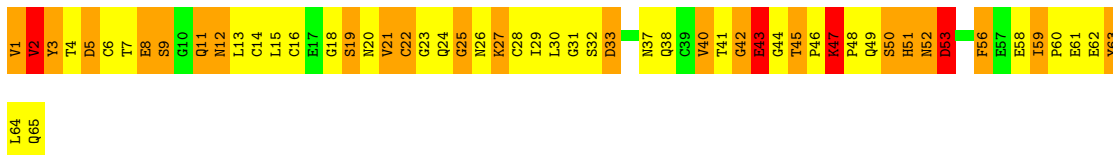
• Molecule 2: THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRUDIN

Chain I: 



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	59.11Å 102.62Å 143.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2996	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.30	1/294 (0.3%)	2.39	20/390 (5.1%)
2	H	1.45	12/2148 (0.6%)	2.55	165/2905 (5.7%)
3	I	1.49	1/489 (0.2%)	2.72	50/659 (7.6%)
All	All	1.44	14/2931 (0.5%)	2.57	235/3954 (5.9%)

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
1	L	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	204(B)	ASN	C-O	7.63	1.32	1.24
2	H	95	ASN	CA-CB	7.50	1.61	1.52
2	H	147	THR	CA-CB	6.04	1.63	1.53
2	H	113	GLU	CA-CB	-5.88	1.45	1.53
2	H	205	ASN	N-CA	5.87	1.53	1.46
2	H	136	GLY	N-CA	5.66	1.49	1.44
2	H	95	ASN	C-O	5.49	1.30	1.23
2	H	24	VAL	N-CA	5.27	1.52	1.46
2	H	182	CYS	CA-CB	-5.22	1.46	1.53
2	H	107	LYS	N-CA	5.19	1.52	1.46
1	L	14(M)	GLY	N-CA	-5.12	1.38	1.45
2	H	46	LEU	N-CA	5.08	1.52	1.46
3	I	22	CYS	CA-CB	-5.08	1.46	1.53
2	H	144	ARG	CD-NE	-5.06	1.39	1.46

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	110	ARG	CD-NE-CZ	17.75	149.26	124.40
2	H	144	ARG	CD-NE-CZ	17.54	148.96	124.40
2	H	113	GLU	CA-CB-CG	14.57	143.23	114.10
2	H	149(B)	SER	N-CA-C	13.97	130.32	108.67
2	H	60(H)	PHE	CA-CB-CG	13.96	127.77	113.80
3	I	62	GLU	CA-C-N	13.71	147.72	121.54
3	I	62	GLU	C-N-CA	13.71	147.72	121.54
2	H	21	ASP	CA-CB-CG	13.43	126.03	112.60
2	H	204(B)	ASN	CA-C-O	-12.55	106.51	121.32
2	H	123	LEU	CB-CA-C	12.43	126.79	110.13
2	H	137	ARG	CD-NE-CZ	11.78	140.89	124.40
2	H	149(B)	SER	CA-C-O	11.37	133.45	120.60
2	H	187	ARG	CD-NE-CZ	11.37	140.32	124.40
2	H	243	ASP	CA-CB-CG	9.85	122.45	112.60
2	H	206	ARG	N-CA-C	9.81	123.79	110.55
1	L	14	ASP	CA-CB-CG	9.69	122.29	112.60
2	H	125	ASP	CA-CB-CG	9.33	121.93	112.60
3	I	3	TYR	CA-CB-CG	9.33	130.70	113.90
3	I	62	GLU	CA-C-O	9.27	130.18	120.54
2	H	244	ARG	CA-C-N	9.15	139.01	121.54
2	H	244	ARG	C-N-CA	9.15	139.01	121.54
2	H	147	THR	N-CA-C	9.12	124.00	113.15
2	H	146	GLU	CA-CB-CG	8.98	132.06	114.10
2	H	95	ASN	N-CA-C	8.89	124.49	110.70
2	H	149(D)	ALA	N-CA-C	-8.81	92.04	110.80
2	H	217	GLU	CA-CB-CG	8.73	131.56	114.10
2	H	102	ASP	CA-CB-CG	8.72	121.32	112.60
1	L	14(K)	ILE	N-CA-CB	-8.60	100.95	112.22
1	L	14(L)	GLU	N-CA-C	-8.56	101.98	114.39
2	H	181	PHE	CA-C-O	-8.40	111.62	121.11
2	H	163	VAL	CA-C-O	-8.37	112.55	121.93
1	L	14(M)	GLY	N-CA-C	8.37	133.01	113.18
2	H	227	PHE	CA-CB-CG	-8.31	105.49	113.80
2	H	94	TYR	CA-C-N	8.20	134.34	122.21
2	H	94	TYR	C-N-CA	8.20	134.34	122.21
2	H	185	LYS	CB-CA-C	8.14	124.09	109.61
1	L	14(L)	GLU	CA-C-O	7.79	127.65	118.69
2	H	194	ASP	CA-C-N	7.79	133.72	121.56
2	H	194	ASP	C-N-CA	7.79	133.72	121.56
2	H	199	PHE	N-CA-CB	7.75	124.14	111.58
2	H	129(B)	LYS	CB-CG-CD	7.71	129.04	111.30
2	H	204(B)	ASN	N-CA-C	-7.62	98.35	108.34
2	H	194	ASP	CA-CB-CG	7.62	120.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	49	ASP	CA-CB-CG	7.52	120.12	112.60
2	H	187	ARG	N-CA-CB	-7.46	99.45	111.24
2	H	149(C)	VAL	N-CA-C	-7.44	99.09	109.21
2	H	158	VAL	O-C-N	7.36	131.21	123.05
2	H	162	LEU	CB-CA-C	7.35	121.66	109.53
3	I	40	VAL	CA-C-O	-7.29	115.92	121.68
1	L	14(F)	LEU	CA-C-O	-7.28	113.11	120.90
1	L	1(G)	PHE	CA-CB-CG	-7.28	106.52	113.80
2	H	49	ASP	N-CA-C	-7.27	103.39	114.16
2	H	129(B)	LYS	CA-CB-CG	7.25	128.59	114.10
2	H	26	LEU	CA-C-N	-7.24	115.64	122.37
2	H	26	LEU	C-N-CA	-7.24	115.64	122.37
3	I	43	GLU	N-CA-C	-7.19	99.84	110.48
2	H	164	GLU	N-CA-C	7.18	120.37	108.96
2	H	97(A)	GLU	CA-CB-CG	7.15	128.40	114.10
2	H	189	ASP	CA-C-O	-7.13	113.65	121.28
3	I	44	GLY	CA-C-N	7.05	131.07	121.20
3	I	44	GLY	C-N-CA	7.05	131.07	121.20
2	H	186(D)	LYS	N-CA-C	-7.02	101.08	110.55
2	H	144	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	H	60(B)	PRO	N-CA-C	6.98	119.22	110.70
3	I	31	GLY	N-CA-C	-6.96	103.17	112.14
2	H	185	LYS	N-CA-C	-6.93	99.96	110.01
2	H	119	HIS	CA-CB-CG	-6.92	106.88	113.80
2	H	49	ASP	CA-C-O	6.91	126.12	118.52
2	H	179	ASN	CA-CB-CG	6.79	119.39	112.60
2	H	194	ASP	N-CA-C	-6.77	104.83	113.23
2	H	229	THR	N-CA-C	-6.75	101.17	110.35
1	L	14(H)	GLU	N-CA-C	-6.69	105.12	113.28
2	H	223	GLY	N-CA-C	-6.68	106.01	115.30
2	H	60(F)	LYS	CA-C-O	6.68	127.44	120.30
3	I	62	GLU	N-CA-CB	6.68	121.39	110.37
2	H	172	THR	N-CA-CB	-6.66	100.42	111.20
2	H	112	ILE	CB-CG1-CD1	6.65	127.77	113.80
2	H	152	PRO	N-CA-C	-6.65	101.47	111.57
2	H	130	LEU	CA-CB-CG	6.63	139.51	116.30
3	I	33	ASP	CA-CB-CG	-6.61	105.99	112.60
2	H	73	ARG	N-CA-C	-6.57	103.39	111.40
3	I	43	GLU	CB-CG-CD	6.54	123.72	112.60
3	I	6	CYS	O-C-N	6.54	131.20	122.96
1	L	14(K)	ILE	N-CA-C	6.52	118.56	111.77
2	H	241	VAL	N-CA-CB	6.51	120.91	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	46	LEU	CB-CA-C	6.46	120.37	110.62
2	H	115	SER	CA-CB-OG	6.46	124.01	111.10
2	H	79	VAL	N-CA-C	6.43	122.72	109.34
2	H	154	VAL	CA-C-O	-6.42	115.27	121.63
2	H	76	TYR	CA-C-O	-6.40	113.30	120.54
3	I	1	VAL	CA-C-O	-6.40	109.92	120.80
2	H	106	LEU	CA-C-O	-6.40	113.59	121.78
2	H	229	THR	N-CA-CB	6.38	119.42	110.04
2	H	76	TYR	N-CA-CB	6.38	120.68	110.16
3	I	51	HIS	CA-C-N	6.37	133.71	121.54
3	I	51	HIS	C-N-CA	6.37	133.71	121.54
2	H	67	ARG	NE-CZ-NH2	6.31	124.88	119.20
2	H	36(A)	SER	CA-CB-OG	6.29	123.68	111.10
2	H	129(B)	LYS	N-CA-CB	6.27	120.00	110.28
3	I	21	VAL	O-C-N	6.26	129.45	122.75
3	I	52	ASN	CA-CB-CG	-6.25	106.35	112.60
2	H	142	GLY	CA-C-N	6.20	130.54	121.31
2	H	142	GLY	C-N-CA	6.20	130.54	121.31
2	H	37	PRO	N-CA-C	6.18	128.16	112.10
2	H	63	ASP	CA-C-O	-6.17	112.11	119.15
2	H	61	VAL	CA-C-O	6.16	127.46	121.05
3	I	22	CYS	N-CA-C	-6.14	97.13	107.99
3	I	23	GLY	O-C-N	6.14	128.91	122.59
2	H	145	ARG	CA-CB-CG	6.08	126.26	114.10
2	H	112	ILE	CB-CA-C	6.07	118.27	111.59
2	H	76	TYR	N-CA-C	-6.06	99.39	109.46
3	I	63	TYR	N-CA-C	-6.05	97.91	110.80
3	I	53	ASP	N-CA-C	6.04	123.66	110.80
2	H	182	CYS	CA-CB-SG	6.02	128.24	114.40
2	H	148	TRP	CA-C-O	6.01	127.85	119.80
3	I	9	SER	CA-C-O	-6.00	114.91	121.87
2	H	146	GLU	CB-CG-CD	5.95	122.72	112.60
3	I	5	ASP	CB-CA-C	5.95	119.59	109.72
2	H	90	ILE	CB-CA-C	5.94	119.45	110.90
3	I	42	GLY	N-CA-C	-5.94	102.22	111.00
2	H	187	ARG	NE-CZ-NH1	5.89	127.39	121.50
2	H	245	LEU	N-CA-C	-5.89	98.26	110.80
3	I	12	ASN	N-CA-C	5.88	123.32	110.80
2	H	151	GLN	CB-CG-CD	5.87	122.59	112.60
2	H	65	LEU	CA-C-O	5.87	126.93	120.71
2	H	149(B)	SER	CA-CB-OG	-5.87	99.37	111.10
2	H	150	VAL	CA-C-O	-5.87	113.45	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	157	VAL	N-CA-C	5.86	116.08	108.35
2	H	38	GLN	OE1-CD-NE2	-5.85	116.75	122.60
3	I	37	ASN	CA-C-O	-5.84	115.36	121.55
2	H	101	ARG	CD-NE-CZ	5.83	132.57	124.40
3	I	28	CYS	N-CA-CB	5.80	119.33	109.87
3	I	25	GLY	N-CA-C	-5.80	107.32	115.32
3	I	43	GLU	CA-CB-CG	5.79	125.67	114.10
2	H	171	SER	CA-CB-OG	5.78	122.67	111.10
1	L	14	ASP	CB-CA-C	5.78	119.78	109.38
2	H	91	HIS	CA-C-O	5.76	123.89	119.46
1	L	7	PHE	CA-CB-CG	-5.73	108.07	113.80
3	I	50	SER	N-CA-C	-5.72	98.61	110.80
2	H	228	TYR	CA-C-O	-5.71	114.09	120.66
2	H	64	LEU	N-CA-C	5.71	118.77	109.06
3	I	20	ASN	CA-CB-CG	5.70	118.30	112.60
1	L	14(H)	GLU	N-CA-CB	5.69	119.40	110.46
2	H	129(C)	LEU	N-CA-C	5.69	120.36	112.90
2	H	34	PHE	N-CA-C	5.69	118.05	107.99
2	H	59	LEU	CA-C-N	5.67	130.66	122.44
2	H	59	LEU	C-N-CA	5.67	130.66	122.44
2	H	204(A)	TYR	CA-C-O	5.64	126.46	119.97
3	I	63	TYR	N-CA-CB	5.62	119.99	110.49
2	H	151	GLN	CG-CD-NE2	5.62	124.83	116.40
2	H	145	ARG	CB-CG-CD	5.61	124.20	111.30
3	I	6	CYS	CA-C-O	-5.60	114.09	120.58
1	L	14(H)	GLU	CA-CB-CG	5.58	125.26	114.10
2	H	182	CYS	CB-CA-C	5.57	120.27	110.36
2	H	40	LEU	CB-CA-C	5.57	119.42	110.29
2	H	204(B)	ASN	CB-CA-C	5.56	126.38	113.19
2	H	158	VAL	N-CA-CB	5.55	120.55	111.45
2	H	78	LYS	CA-C-N	5.53	131.92	121.97
2	H	78	LYS	C-N-CA	5.53	131.92	121.97
2	H	145	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	H	79	VAL	N-CA-CB	-5.52	102.12	111.23
2	H	207	TRP	N-CA-C	-5.50	100.28	109.24
2	H	211	GLY	CA-C-O	5.50	126.47	121.47
2	H	32	MET	CA-C-O	-5.49	114.42	120.24
1	L	14(G)	PHE	N-CA-CB	5.48	119.29	110.42
2	H	97(A)	GLU	CB-CG-CD	5.48	121.91	112.60
2	H	198	PRO	CB-CA-C	-5.48	104.61	111.56
1	L	14(D)	LYS	N-CA-CB	5.44	118.12	110.12
3	I	47	LYS	O-C-N	5.44	127.68	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	241	VAL	N-CA-C	-5.44	108.20	113.53
2	H	194	ASP	CA-C-O	5.43	125.63	119.27
2	H	172	THR	N-CA-C	5.43	118.42	109.85
3	I	5	ASP	CA-C-O	5.41	127.14	121.19
2	H	55	ALA	N-CA-CB	5.41	119.04	110.55
2	H	162	LEU	N-CA-C	-5.36	100.95	109.96
2	H	141	TRP	CA-CB-CG	5.35	123.77	113.60
2	H	102	ASP	O-C-N	5.35	128.59	122.55
2	H	204(B)	ASN	OD1-CG-ND2	5.34	127.94	122.60
3	I	18	GLY	N-CA-C	-5.34	100.53	113.18
3	I	2	VAL	N-CA-CB	5.33	119.39	110.86
2	H	60(E)	ASP	N-CA-C	-5.32	103.89	111.24
2	H	220	CYS	CA-C-N	5.31	131.39	123.05
2	H	220	CYS	C-N-CA	5.31	131.39	123.05
2	H	217	GLU	CA-C-O	5.30	128.09	120.51
2	H	187	ARG	CA-CB-CG	5.28	124.67	114.10
2	H	153	SER	N-CA-C	-5.28	106.86	113.72
2	H	154	VAL	O-C-N	5.28	128.99	123.02
2	H	61	VAL	CA-C-N	5.27	129.04	120.60
2	H	61	VAL	C-N-CA	5.27	129.04	120.60
3	I	6	CYS	CB-CA-C	-5.27	102.36	110.26
3	I	16	CYS	N-CA-C	5.27	120.78	110.56
3	I	56	PHE	CA-CB-CG	-5.27	108.53	113.80
3	I	1	VAL	N-CA-CB	-5.27	102.54	111.50
2	H	244	ARG	N-CA-CB	5.26	119.38	110.49
2	H	80	GLU	CA-C-O	-5.25	115.91	121.94
2	H	101	ARG	CA-C-O	5.25	128.01	120.51
1	L	14(A)	GLN	N-CA-C	5.25	121.97	110.80
2	H	63	ASP	CA-CB-CG	5.24	117.84	112.60
3	I	51	HIS	N-CA-C	5.24	118.34	108.65
2	H	216	GLY	O-C-N	5.22	127.67	123.49
2	H	72	SER	N-CA-C	-5.22	103.25	110.35
2	H	105	LEU	CA-C-O	-5.22	115.18	120.71
2	H	74	THR	CA-C-O	-5.18	113.83	120.31
2	H	143	ASN	CA-CB-CG	-5.18	107.42	112.60
2	H	195	SER	N-CA-C	5.18	117.98	110.42
2	H	84	MET	CB-CA-C	5.17	118.28	109.80
1	L	14(L)	GLU	C-N-CA	5.17	133.16	122.30
2	H	149(E)	GLU	CA-C-N	5.17	131.27	121.97
2	H	149(E)	GLU	C-N-CA	5.17	131.27	121.97
2	H	95	ASN	N-CA-CB	-5.17	102.33	110.49
2	H	206	ARG	CB-CA-C	-5.16	99.50	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYR	O-C-N	5.16	129.45	122.59
2	H	60(I)	THR	CB-CA-C	-5.13	99.71	109.66
2	H	67	ARG	CA-CB-CG	5.13	124.35	114.10
2	H	55	ALA	O-C-N	5.12	129.32	123.27
1	L	14(L)	GLU	CB-CG-CD	5.12	121.31	112.60
3	I	52	ASN	CA-C-O	5.11	127.82	120.51
2	H	133	GLY	CA-C-N	5.11	128.59	121.24
2	H	133	GLY	C-N-CA	5.11	128.59	121.24
2	H	67	ARG	N-CA-C	-5.10	99.67	108.69
2	H	236	LYS	N-CA-C	5.10	116.92	111.36
1	L	1	CYS	CA-C-N	5.09	127.80	120.11
1	L	1	CYS	C-N-CA	5.09	127.80	120.11
3	I	51	HIS	CA-C-O	5.09	129.46	121.98
2	H	149(D)	ALA	O-C-N	5.08	130.84	122.70
3	I	53	ASP	CA-CB-CG	-5.08	107.52	112.60
3	I	9	SER	N-CA-C	-5.07	103.84	110.53
2	H	189	ASP	O-C-N	5.06	128.35	123.29
3	I	11	GLN	OE1-CD-NE2	5.06	127.66	122.60
2	H	41	LEU	N-CA-CB	-5.05	102.74	110.26
2	H	111	PRO	N-CD-CG	-5.04	95.64	103.20
2	H	173	ARG	CA-C-O	5.04	125.17	119.27
2	H	192	GLU	CA-CB-CG	5.02	124.14	114.10
2	H	181	PHE	CA-CB-CG	5.02	118.82	113.80
3	I	7	THR	N-CA-CB	-5.02	103.16	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	4	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	290	0	276	63	0
2	H	2094	0	2097	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	483	0	430	87	0
4	H	79	0	0	42	0
4	I	25	0	0	3	0
4	L	25	0	0	10	0
All	All	2996	0	2803	448	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 79.

All (448) 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:143:ASN:HA	2:H:150:VAL:O	1.53	1.09
3:I:49:GLN:OE1	3:I:49:GLN:HA	1.48	1.09
1:L:1(G):PHE:HB2	2:H:51:TRP:NE1	1.73	1.03
2:H:147:THR:HA	2:H:149(B):SER:OG	1.58	1.03
2:H:204:PRO:HD2	2:H:204(A):TYR:HD1	1.22	1.02
1:L:1(G):PHE:HB2	2:H:51:TRP:HE1	1.21	0.97
2:H:149(C):VAL:HG13	4:H:527:HOH:O	1.67	0.93
2:H:19:GLY:HA2	2:H:158:VAL:HG13	1.52	0.92
2:H:174:ILE:HD11	3:I:21:VAL:CG1	2.00	0.92
1:L:14(D):LYS:HE2	1:L:14(D):LYS:H	1.36	0.90
2:H:60(I):THR:HG22	2:H:62:ASP:H	1.38	0.89
3:I:60:PRO:HB2	3:I:63:TYR:CE2	2.08	0.88
2:H:137:ARG:HD2	2:H:157:VAL:CG2	2.04	0.86
2:H:204:PRO:HD2	2:H:204(A):TYR:CD1	2.11	0.86
2:H:186:PRO:HG3	2:H:223:GLY:HA2	1.59	0.85
1:L:9:LYS:HE3	4:L:522:HOH:O	1.77	0.84
2:H:31:VAL:HG21	4:H:565:HOH:O	1.76	0.84
2:H:176:ILE:HG13	2:H:180:MET:HE2	1.58	0.83
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.14	0.83
3:I:48:PRO:O	3:I:49:GLN:HB2	1.79	0.83
2:H:127:GLN:HE21	2:H:127:GLN:HA	1.44	0.82
2:H:31:VAL:HG13	2:H:66:VAL:HG13	1.61	0.82
2:H:98:ASN:HA	4:H:487:HOH:O	1.77	0.82
2:H:244:ARG:HA	2:H:244:ARG:NE	1.93	0.82
2:H:236:LYS:HD2	2:H:239:GLN:OE1	1.79	0.81
3:I:47:LYS:HD2	3:I:48:PRO:HD2	1.61	0.81
2:H:196:GLY:HA2	2:H:212:ILE:HG22	1.63	0.81
2:H:174:ILE:HD11	3:I:21:VAL:HG12	1.61	0.80
2:H:105:LEU:HD13	2:H:242:ILE:HD11	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:MET:O	2:H:231:VAL:HG23	1.80	0.80
2:H:173:ARG:NH1	4:H:490:HOH:O	2.11	0.79
2:H:165:ARG:NH2	2:H:178:ASP:HA	1.97	0.79
2:H:32:MET:CE	2:H:70:LYS:HD3	2.13	0.79
2:H:122:CYS:SG	2:H:206:ARG:HG2	2.22	0.79
2:H:16:ILE:HG23	2:H:158:VAL:HG22	1.64	0.79
2:H:46:LEU:O	2:H:120:PRO:HA	1.83	0.79
2:H:41:LEU:HD21	2:H:60(H):PHE:CE2	2.17	0.78
2:H:16:ILE:CG2	2:H:158:VAL:HG22	2.14	0.78
2:H:173:ARG:HB2	4:I:554:HOH:O	1.83	0.78
2:H:100:ASP:CG	2:H:177:THR:HG21	2.09	0.77
2:H:149(C):VAL:O	4:H:581:HOH:O	2.01	0.77
2:H:164:GLU:HG2	2:H:167:VAL:HG13	1.66	0.77
1:L:14(D):LYS:H	1:L:14(D):LYS:CE	1.97	0.77
2:H:174:ILE:HD11	3:I:21:VAL:HG11	1.67	0.76
2:H:36:LYS:HG2	2:H:36:LYS:O	1.85	0.76
3:I:12:ASN:HD21	3:I:24:GLN:HA	1.48	0.76
2:H:50:ARG:NH1	4:H:558:HOH:O	2.05	0.75
2:H:16:ILE:N	2:H:194:ASP:OD2	2.19	0.75
1:L:1(G):PHE:CB	2:H:51:TRP:HE1	1.97	0.75
2:H:46:LEU:HD23	2:H:51:TRP:O	1.85	0.75
2:H:131:HIS:HA	4:H:511:HOH:O	1.87	0.74
3:I:27:LYS:HE3	3:I:42:GLY:HA3	1.69	0.74
2:H:149(B):SER:O	4:H:523:HOH:O	2.05	0.74
2:H:57:HIS:HE1	2:H:214:SER:O	1.70	0.74
2:H:148:TRP:CD1	3:I:4:THR:HG21	2.23	0.74
1:L:14(H):GLU:O	1:L:14(L):GLU:HG2	1.89	0.72
2:H:143:ASN:HD22	2:H:192:GLU:HG3	1.53	0.72
1:L:8:GLU:O	1:L:11:GLN:N	2.15	0.72
3:I:11:GLN:HA	3:I:45:THR:O	1.89	0.72
1:L:6:LEU:HA	1:L:10:LYS:HD3	1.72	0.71
2:H:244:ARG:NE	2:H:244:ARG:CA	2.53	0.71
2:H:146:GLU:HA	4:H:507:HOH:O	1.89	0.71
2:H:36:LYS:HD2	3:I:64:LEU:HA	1.73	0.71
2:H:146:GLU:CA	4:H:507:HOH:O	2.37	0.71
1:L:15:ARG:NH1	4:L:583:HOH:O	2.24	0.70
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.21	0.70
3:I:49:GLN:OE1	3:I:49:GLN:CA	2.34	0.70
2:H:30:GLN:HG2	2:H:155:LEU:HD11	1.73	0.70
2:H:137:ARG:HD2	2:H:157:VAL:HG21	1.74	0.70
2:H:146:GLU:HB3	2:H:148:TRP:HE1	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:LEU:O	1:L:10:LYS:HB2	1.91	0.70
2:H:73:ARG:NE	2:H:152:PRO:O	2.24	0.70
2:H:48:SER:HB2	2:H:51:TRP:HD1	1.57	0.69
2:H:29:TRP:CH2	2:H:207:TRP:HB2	2.27	0.69
2:H:46:LEU:C	2:H:46:LEU:HD22	2.17	0.69
2:H:126:LYS:HG3	2:H:232:PHE:HZ	1.57	0.69
2:H:19:GLY:CA	2:H:158:VAL:HG13	2.22	0.69
1:L:1(G):PHE:HB2	2:H:51:TRP:CE2	2.28	0.69
2:H:31:VAL:HG11	4:H:565:HOH:O	1.92	0.69
3:I:60:PRO:HB2	3:I:63:TYR:HE2	1.57	0.69
2:H:192:GLU:OE2	4:H:508:HOH:O	2.09	0.69
2:H:47:ILE:O	2:H:120:PRO:HB3	1.93	0.68
1:L:3:LEU:HB3	4:L:522:HOH:O	1.94	0.68
2:H:146:GLU:HB3	2:H:148:TRP:NE1	2.09	0.68
1:L:1(H):THR:OG1	2:H:245:LEU:HD11	1.94	0.68
2:H:60(I):THR:HG22	2:H:61:VAL:N	2.09	0.68
2:H:136:GLY:N	2:H:160:LEU:O	2.21	0.68
2:H:244:ARG:CA	2:H:244:ARG:HE	2.05	0.68
2:H:138:VAL:HG22	2:H:199:PHE:HD2	1.59	0.67
2:H:69:GLY:N	4:H:512:HOH:O	2.21	0.67
2:H:186:PRO:CG	2:H:223:GLY:HA2	2.24	0.67
3:I:59:ILE:HG12	3:I:60:PRO:HD2	1.76	0.67
2:H:245:LEU:HD12	2:H:246:GLY:N	2.10	0.66
2:H:197:GLY:O	2:H:213:VAL:HG23	1.96	0.66
2:H:204:PRO:O	4:H:586:HOH:O	2.13	0.66
1:L:3:LEU:CB	4:L:522:HOH:O	2.44	0.66
2:H:65:LEU:HD13	2:H:82:ILE:HG21	1.77	0.66
2:H:186(D):LYS:HD2	4:H:533:HOH:O	1.95	0.65
3:I:53:ASP:CB	3:I:56:PHE:HE2	2.08	0.65
3:I:47:LYS:HB3	3:I:48:PRO:HD2	1.77	0.65
2:H:192:GLU:HG3	4:H:508:HOH:O	1.96	0.65
2:H:62:ASP:OD1	4:H:541:HOH:O	2.14	0.65
2:H:240:LYS:HD2	2:H:244:ARG:NH1	2.12	0.65
3:I:49:GLN:HG3	3:I:50:SER:H	1.60	0.65
1:L:14(G):PHE:HA	1:L:14(J):TYR:CD2	2.31	0.65
2:H:141:TRP:HH2	4:H:578:HOH:O	1.79	0.64
1:L:1(G):PHE:CB	2:H:51:TRP:NE1	2.56	0.64
2:H:49:ASP:HB2	4:H:503:HOH:O	1.97	0.64
2:H:147:THR:OG1	2:H:149(B):SER:HB2	1.97	0.64
2:H:163:VAL:HG13	2:H:167:VAL:CG2	2.27	0.64
2:H:163:VAL:HG13	2:H:167:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129(A):ALA:O	4:H:572:HOH:O	2.14	0.64
2:H:60(A):TYR:HB3	2:H:60(F):LYS:HD3	1.79	0.64
2:H:66:VAL:CG2	2:H:85:LEU:HD11	2.27	0.64
2:H:211:GLY:HA2	2:H:231:VAL:HG23	1.80	0.64
1:L:14(D):LYS:HZ3	1:L:14(D):LYS:HB3	1.63	0.63
2:H:127:GLN:HA	2:H:127:GLN:NE2	2.11	0.63
2:H:147:THR:C	2:H:149:THR:H	2.05	0.63
2:H:148:TRP:CD1	2:H:148:TRP:H	2.15	0.63
2:H:137:ARG:HD3	2:H:159:ASN:ND2	2.13	0.63
3:I:29:ILE:HD12	3:I:40:VAL:CG1	2.28	0.63
1:L:4:ARG:NH1	1:L:8:GLU:OE1	2.32	0.62
2:H:125:ASP:O	2:H:127:GLN:N	2.32	0.62
2:H:109:LYS:HB3	2:H:110:ARG:NH1	2.14	0.62
2:H:148:TRP:NE1	3:I:4:THR:CG2	2.62	0.62
2:H:135:LYS:HA	2:H:160:LEU:O	1.98	0.62
2:H:236:LYS:HA	2:H:239:GLN:OE1	1.99	0.62
2:H:243:ASP:O	2:H:244:ARG:C	2.42	0.62
3:I:13:LEU:HD12	3:I:46:PRO:HB3	1.81	0.62
2:H:70:LYS:HB3	4:H:578:HOH:O	1.98	0.62
1:L:14(E):GLU:OE1	4:L:529:HOH:O	2.16	0.62
2:H:148:TRP:CZ3	3:I:5:ASP:HB2	2.34	0.62
3:I:52:ASN:O	3:I:53:ASP:HB2	2.00	0.62
1:L:1(E):ALA:HA	2:H:48:SER:CA	2.30	0.61
2:H:40:LEU:HD13	2:H:40:LEU:O	2.00	0.61
2:H:73:ARG:O	3:I:56:PHE:HE1	1.82	0.61
2:H:82:ILE:HD11	3:I:59:ILE:HD11	1.82	0.61
2:H:82:ILE:CD1	3:I:59:ILE:CD1	2.78	0.61
2:H:109:LYS:C	2:H:110:ARG:HD2	2.26	0.61
3:I:38:GLN:HB2	4:I:486:HOH:O	2.01	0.60
2:H:110:ARG:HD2	2:H:110:ARG:N	2.16	0.60
2:H:59:LEU:N	2:H:59:LEU:HD13	2.16	0.60
1:L:14(K):ILE:C	1:L:14(L):GLU:OE1	2.43	0.60
3:I:22:CYS:SG	3:I:26:ASN:HB3	2.42	0.60
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.83	0.60
3:I:49:GLN:HG3	3:I:50:SER:N	2.17	0.60
2:H:243:ASP:O	2:H:245:LEU:HG	2.01	0.60
1:L:14:ASP:OD2	2:H:26:LEU:HG	2.02	0.60
2:H:126:LYS:HG3	2:H:232:PHE:CZ	2.37	0.60
3:I:12:ASN:HB3	3:I:46:PRO:HA	1.84	0.60
2:H:216:GLY:O	3:I:3:TYR:HD1	1.84	0.59
3:I:53:ASP:HB3	3:I:56:PHE:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:TRP:CE3	3:I:5:ASP:HB2	2.38	0.59
2:H:20:GLN:NE2	2:H:157:VAL:O	2.35	0.59
2:H:87:LYS:HZ2	2:H:87:LYS:HA	1.68	0.59
2:H:122:CYS:SG	2:H:206:ARG:CG	2.90	0.59
1:L:4:ARG:NH1	2:H:207:TRP:HE1	2.01	0.59
2:H:147:THR:CB	2:H:149(B):SER:HB2	2.33	0.59
3:I:60:PRO:CB	3:I:63:TYR:HE2	2.16	0.58
2:H:36:LYS:O	2:H:36(A):SER:OG	2.19	0.58
2:H:190:ALA:O	2:H:220:CYS:HB3	2.02	0.58
2:H:221(A):ARG:HB3	2:H:224:LYS:HG3	1.84	0.58
2:H:41:LEU:HD21	2:H:60(H):PHE:CZ	2.38	0.58
2:H:66:VAL:HG23	2:H:85:LEU:HD11	1.85	0.58
2:H:52:VAL:CG2	4:H:565:HOH:O	2.51	0.58
2:H:233:ARG:NE	4:H:549:HOH:O	2.35	0.58
2:H:243:ASP:OD2	2:H:244:ARG:NH2	2.37	0.58
2:H:151:GLN:HG3	4:H:579:HOH:O	2.04	0.57
2:H:137:ARG:O	2:H:199:PHE:HA	2.03	0.57
2:H:105:LEU:CD1	2:H:242:ILE:HD11	2.32	0.57
3:I:13:LEU:HD11	3:I:24:GLN:HE21	1.69	0.57
1:L:4:ARG:HH22	1:L:14:ASP:CB	2.17	0.57
2:H:60(A):TYR:CB	2:H:60(F):LYS:HD3	2.34	0.57
2:H:82:ILE:HD13	3:I:59:ILE:HD13	1.86	0.57
3:I:60:PRO:HG2	3:I:63:TYR:HE2	1.69	0.57
2:H:240:LYS:HD3	2:H:244:ARG:HH22	1.69	0.57
2:H:125:ASP:C	2:H:127:GLN:N	2.61	0.57
3:I:29:ILE:HD12	3:I:40:VAL:HG11	1.87	0.57
2:H:143:ASN:HD22	2:H:192:GLU:HB2	1.70	0.57
3:I:60:PRO:CG	3:I:63:TYR:HE2	2.18	0.57
2:H:30:GLN:HG2	2:H:155:LEU:CD1	2.34	0.56
2:H:52:VAL:HG22	4:H:565:HOH:O	2.05	0.56
3:I:13:LEU:HA	3:I:22:CYS:O	2.04	0.56
3:I:47:LYS:CD	3:I:48:PRO:HD2	2.31	0.56
2:H:98:ASN:O	2:H:99:LEU:HB2	2.06	0.56
2:H:177:THR:HG23	2:H:180:MET:SD	2.46	0.56
1:L:4:ARG:HH22	1:L:14:ASP:HB3	1.70	0.56
2:H:130:LEU:C	2:H:131:HIS:HD2	2.14	0.56
2:H:141:TRP:NE1	2:H:155:LEU:HB2	2.21	0.56
2:H:77(A):ARG:HD2	4:H:520:HOH:O	2.05	0.56
1:L:4:ARG:NH2	1:L:14:ASP:CB	2.68	0.56
1:L:8:GLU:O	1:L:9:LYS:C	2.48	0.56
2:H:51:TRP:CH2	2:H:107:LYS:HD3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(E):ALA:HA	2:H:48:SER:HA	1.88	0.56
2:H:33:LEU:CD1	2:H:44:ALA:HB2	2.36	0.55
2:H:235:LYS:HE2	2:H:239:GLN:CD	2.31	0.55
2:H:31:VAL:CG1	2:H:32:MET:N	2.68	0.55
2:H:165:ARG:O	2:H:169:LYS:HD2	2.07	0.55
2:H:82:ILE:CD1	3:I:59:ILE:HD11	2.36	0.55
2:H:102:ASP:OD2	2:H:214:SER:OG	2.18	0.55
2:H:109:LYS:HG3	2:H:109:LYS:O	2.06	0.55
2:H:148:TRP:CD1	3:I:4:THR:CG2	2.90	0.55
2:H:204(B):ASN:OD1	2:H:206:ARG:HD3	2.07	0.55
2:H:245:LEU:HD12	2:H:245:LEU:C	2.32	0.55
2:H:91:HIS:O	2:H:93:ARG:N	2.40	0.55
2:H:125:ASP:C	2:H:127:GLN:H	2.15	0.55
1:L:1(H):THR:HG22	4:L:488:HOH:O	2.06	0.55
2:H:221(A):ARG:NH1	3:I:15:LEU:HD12	2.21	0.55
3:I:47:LYS:HD2	3:I:48:PRO:CD	2.35	0.54
2:H:32:MET:HE1	2:H:70:LYS:HD3	1.89	0.54
2:H:144:ARG:N	2:H:150:VAL:O	2.40	0.54
2:H:146:GLU:HB3	4:H:507:HOH:O	2.07	0.54
2:H:108:LEU:C	2:H:110:ARG:H	2.16	0.54
1:L:8:GLU:O	1:L:10:LYS:N	2.40	0.54
2:H:48:SER:HB2	2:H:51:TRP:CD1	2.39	0.54
2:H:49:ASP:O	2:H:112:ILE:HD13	2.07	0.54
2:H:137:ARG:CD	2:H:159:ASN:ND2	2.71	0.54
3:I:12:ASN:O	3:I:22:CYS:O	2.26	0.54
1:L:9:LYS:HB3	4:L:526:HOH:O	2.07	0.54
3:I:25:GLY:HA2	3:I:43:GLU:OE1	2.07	0.54
2:H:140:GLY:HA2	4:H:577:HOH:O	2.08	0.54
2:H:186(D):LYS:CD	4:H:533:HOH:O	2.54	0.54
2:H:200:VAL:HG23	2:H:207:TRP:CE3	2.43	0.54
2:H:105:LEU:HD12	2:H:241:VAL:HG22	1.89	0.53
2:H:163:VAL:HG12	2:H:168:CYS:SG	2.48	0.53
2:H:164:GLU:H	2:H:164:GLU:CD	2.16	0.53
2:H:51:TRP:CE2	2:H:242:ILE:HD12	2.44	0.53
1:L:14(G):PHE:CZ	2:H:202:LYS:HD3	2.44	0.53
1:L:14(D):LYS:HZ3	1:L:14(D):LYS:CB	2.21	0.53
2:H:60(D):TRP:CZ3	3:I:49:GLN:HG2	2.44	0.53
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.43	0.53
2:H:244:ARG:HE	2:H:244:ARG:N	2.06	0.53
2:H:58:CYS:C	2:H:59:LEU:HD13	2.34	0.53
2:H:54:THR:CG2	2:H:59:LEU:HD21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:ILE:CD1	3:I:59:ILE:HD13	2.40	0.52
2:H:109:LYS:O	2:H:110:ARG:HB3	2.09	0.52
2:H:141:TRP:CE2	2:H:155:LEU:HB2	2.44	0.52
2:H:52:VAL:HG13	4:H:565:HOH:O	2.09	0.52
2:H:184(A):TYR:OH	2:H:186(D):LYS:HE3	2.08	0.52
2:H:114:LEU:CD2	4:H:503:HOH:O	2.56	0.52
2:H:138:VAL:HG22	2:H:199:PHE:CD2	2.42	0.52
2:H:204(B):ASN:ND2	2:H:208:TYR:OH	2.42	0.52
2:H:31:VAL:HG12	2:H:32:MET:N	2.24	0.52
2:H:38:GLN:NE2	4:H:569:HOH:O	2.43	0.52
2:H:60(A):TYR:HD2	2:H:60(D):TRP:HB2	1.75	0.52
2:H:36:LYS:O	2:H:36:LYS:CG	2.56	0.52
3:I:59:ILE:HG12	3:I:60:PRO:CD	2.40	0.52
1:L:14(H):GLU:HG3	4:L:591:HOH:O	2.10	0.52
3:I:60:PRO:HB2	3:I:63:TYR:CD2	2.45	0.52
2:H:221(A):ARG:HB3	2:H:224:LYS:HB2	1.92	0.52
2:H:220:CYS:SG	3:I:2:VAL:HG11	2.50	0.51
2:H:224:LYS:HE2	4:H:501:HOH:O	2.11	0.51
2:H:244:ARG:HE	2:H:244:ARG:H	1.57	0.51
1:L:1(F):GLY:C	1:L:1(D):GLY:H	2.18	0.51
2:H:234:LEU:O	2:H:235:LYS:C	2.52	0.51
1:L:14(G):PHE:CE1	2:H:204:PRO:HB3	2.44	0.51
2:H:26:LEU:HD23	2:H:26:LEU:O	2.09	0.51
2:H:36:LYS:CD	3:I:64:LEU:HA	2.40	0.51
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.40	0.51
3:I:47:LYS:HB3	3:I:48:PRO:CD	2.41	0.51
2:H:109:LYS:CB	2:H:110:ARG:NH1	2.74	0.51
2:H:147:THR:N	4:H:507:HOH:O	2.43	0.51
2:H:240:LYS:HD3	2:H:244:ARG:NH2	2.26	0.51
2:H:149:THR:O	2:H:149(A):THR:HG23	2.11	0.51
2:H:52:VAL:CG1	4:H:565:HOH:O	2.59	0.50
2:H:109:LYS:CG	2:H:110:ARG:NH1	2.74	0.50
2:H:200:VAL:HG23	2:H:207:TRP:HE3	1.77	0.50
2:H:165:ARG:HH21	2:H:178:ASP:HA	1.76	0.50
1:L:14(B):THR:OG1	2:H:159:ASN:OD1	2.29	0.50
2:H:60(I):THR:CG2	2:H:61:VAL:N	2.75	0.50
2:H:212:ILE:O	2:H:228:TYR:HA	2.11	0.50
3:I:53:ASP:HB3	3:I:56:PHE:CE2	2.45	0.50
1:L:14(M):GLY:O	1:L:15:ARG:HG2	2.12	0.50
2:H:200:VAL:CG2	2:H:207:TRP:HE3	2.25	0.50
2:H:93:ARG:HB2	2:H:101:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:CB	2:H:166:PRO:CD	2.90	0.50
1:L:1:CYS:O	2:H:206:ARG:HG3	2.12	0.50
2:H:35:ARG:NH2	2:H:39:GLU:OE2	2.45	0.50
2:H:145:ARG:N	2:H:150:VAL:HG12	2.27	0.50
2:H:217:GLU:HB3	4:H:499:HOH:O	2.12	0.50
2:H:50:ARG:HG2	2:H:50:ARG:HH11	1.77	0.50
2:H:60(A):TYR:CZ	3:I:1:VAL:HG21	2.47	0.50
2:H:60(D):TRP:CH2	3:I:49:GLN:HG2	2.47	0.49
3:I:49:GLN:CG	3:I:50:SER:H	2.24	0.49
2:H:60(A):TYR:HB3	2:H:60(F):LYS:CD	2.42	0.49
2:H:56:ALA:O	2:H:59:LEU:HD22	2.13	0.49
2:H:164:GLU:HG2	2:H:167:VAL:CG1	2.39	0.49
2:H:245:LEU:C	2:H:245:LEU:CD1	2.86	0.49
2:H:16:ILE:HD12	2:H:194:ASP:CG	2.37	0.49
1:L:4:ARG:HH11	2:H:207:TRP:HE1	1.60	0.49
2:H:17:VAL:HG23	2:H:191:CYS:HB2	1.95	0.49
2:H:143:ASN:HD22	2:H:192:GLU:CG	2.24	0.49
2:H:127:GLN:O	2:H:129(B):LYS:HG2	2.13	0.49
2:H:148:TRP:NE1	3:I:4:THR:HG21	2.26	0.49
1:L:5:PRO:HA	1:L:9:LYS:CG	2.43	0.49
2:H:66:VAL:HG21	2:H:85:LEU:HD11	1.94	0.49
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.76	0.49
2:H:105:LEU:HD13	2:H:242:ILE:CD1	2.36	0.49
2:H:67:ARG:C	2:H:68:ILE:HG12	2.38	0.48
1:L:1(G):PHE:HB3	2:H:50:ARG:HD2	1.94	0.48
2:H:137:ARG:HD2	2:H:157:VAL:HG23	1.93	0.48
1:L:10:LYS:O	1:L:11:GLN:HB2	2.13	0.48
2:H:108:LEU:HD13	2:H:112:ILE:CG2	2.43	0.48
2:H:143:ASN:CA	2:H:150:VAL:O	2.44	0.48
2:H:87:LYS:HZ1	2:H:88:ILE:H	1.62	0.48
2:H:114:LEU:HG	4:H:503:HOH:O	2.13	0.48
2:H:91:HIS:HA	2:H:92:PRO:HD2	1.68	0.48
2:H:149(D):ALA:O	2:H:150:VAL:N	2.47	0.48
2:H:202:LYS:HE3	2:H:205:ASN:O	2.14	0.48
3:I:47:LYS:CB	3:I:48:PRO:HD2	2.41	0.48
2:H:20:GLN:O	2:H:20:GLN:HG2	2.14	0.48
2:H:60(B):PRO:N	2:H:60(C):PRO:HD3	2.29	0.48
2:H:147:THR:HA	2:H:149(B):SER:CB	2.44	0.48
2:H:165:ARG:N	2:H:166:PRO:HD2	2.28	0.48
2:H:210:MET:O	2:H:231:VAL:CG2	2.58	0.48
1:L:5:PRO:HA	1:L:9:LYS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:LYS:O	2:H:36(A):SER:CB	2.61	0.47
2:H:192:GLU:CG	4:H:508:HOH:O	2.60	0.47
1:L:3:LEU:HG	4:L:522:HOH:O	2.15	0.47
1:L:14(D):LYS:CE	1:L:14(D):LYS:N	2.73	0.47
2:H:164:GLU:C	2:H:166:PRO:HD2	2.39	0.47
3:I:58:GLU:CD	3:I:58:GLU:H	2.22	0.47
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.49	0.47
3:I:48:PRO:O	3:I:49:GLN:CB	2.53	0.47
2:H:16:ILE:HG23	2:H:158:VAL:CG2	2.39	0.47
2:H:180:MET:HE3	2:H:227:PHE:CD2	2.50	0.47
1:L:4:ARG:NH1	2:H:207:TRP:NE1	2.63	0.47
2:H:39:GLU:HB2	3:I:52:ASN:O	2.15	0.47
2:H:46:LEU:HD22	2:H:47:ILE:N	2.30	0.47
2:H:109:LYS:CB	2:H:110:ARG:HH11	2.26	0.47
3:I:14:CYS:O	3:I:22:CYS:N	2.47	0.47
1:L:1(A):ASP:OD1	1:L:3:LEU:HD23	2.15	0.47
1:L:3:LEU:CG	4:L:522:HOH:O	2.62	0.47
2:H:25:GLY:O	2:H:28:PRO:HD3	2.14	0.47
2:H:146:GLU:CB	2:H:148:TRP:HE1	2.24	0.47
2:H:136:GLY:O	2:H:159:ASN:HA	2.15	0.47
2:H:204:PRO:HG2	2:H:204(A):TYR:CE1	2.50	0.47
2:H:50:ARG:NH1	2:H:50:ARG:HG2	2.30	0.46
2:H:57:HIS:O	2:H:60(A):TYR:HB2	2.15	0.46
2:H:215:TRP:HZ3	2:H:217:GLU:HB2	1.80	0.46
2:H:29:TRP:CH2	2:H:207:TRP:CB	2.97	0.46
2:H:200:VAL:CG2	2:H:207:TRP:CE3	2.99	0.46
3:I:12:ASN:HB3	3:I:46:PRO:CA	2.45	0.46
2:H:33:LEU:HD23	2:H:64:LEU:HD13	1.96	0.46
2:H:51:TRP:CZ3	2:H:107:LYS:HB2	2.51	0.46
2:H:97(A):GLU:HB3	2:H:98:ASN:H	1.44	0.46
2:H:50:ARG:HA	2:H:108:LEU:HB2	1.98	0.46
2:H:52:VAL:HB	2:H:106:LEU:HB2	1.98	0.46
2:H:143:ASN:HB3	2:H:150:VAL:HB	1.96	0.46
1:L:1(A):ASP:O	2:H:119:HIS:NE2	2.49	0.46
2:H:137:ARG:CD	2:H:159:ASN:HD21	2.29	0.46
2:H:187:ARG:NH2	2:H:222:ASP:OD2	2.43	0.46
2:H:240:LYS:CD	2:H:244:ARG:NH1	2.79	0.46
2:H:58:CYS:HB2	2:H:59:LEU:HD13	1.98	0.46
2:H:149(A):THR:CG2	4:H:513:HOH:O	2.64	0.46
2:H:176:ILE:HG13	2:H:180:MET:CE	2.37	0.46
2:H:165:ARG:O	2:H:166:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:230:HIS:O	2:H:234:LEU:HD12	2.15	0.45
1:L:14(D):LYS:N	1:L:14(D):LYS:NZ	2.65	0.45
2:H:108:LEU:HD13	2:H:112:ILE:HG23	1.98	0.45
1:L:3:LEU:O	2:H:119:HIS:CD2	2.69	0.45
1:L:3:LEU:O	1:L:5:PRO:HD3	2.16	0.45
3:I:61:GLU:O	3:I:64:LEU:HD12	2.17	0.45
2:H:204:PRO:CD	2:H:204(A):TYR:CD1	2.93	0.45
2:H:234:LEU:C	2:H:236:LYS:N	2.69	0.45
3:I:53:ASP:CB	3:I:56:PHE:CE2	2.95	0.45
1:L:14(G):PHE:CE2	2:H:202:LYS:HD3	2.51	0.45
2:H:51:TRP:C	2:H:52:VAL:HG23	2.42	0.45
2:H:110:ARG:O	2:H:110:ARG:HG2	2.13	0.45
1:L:14(G):PHE:CD1	2:H:204:PRO:HB3	2.52	0.45
2:H:130:LEU:C	2:H:131:HIS:CD2	2.95	0.45
2:H:240:LYS:NZ	2:H:244:ARG:HH12	2.14	0.45
2:H:109:LYS:C	2:H:110:ARG:HH11	2.24	0.44
2:H:200:VAL:HB	2:H:208:TYR:O	2.17	0.44
3:I:15:LEU:HD13	3:I:19:SER:HA	1.99	0.44
2:H:217:GLU:CB	4:H:499:HOH:O	2.65	0.44
3:I:49:GLN:CG	3:I:50:SER:N	2.79	0.44
2:H:16:ILE:HG21	2:H:158:VAL:HG22	1.96	0.44
2:H:148:TRP:NE1	3:I:4:THR:HG22	2.32	0.44
2:H:234:LEU:O	2:H:236:LYS:N	2.51	0.44
3:I:38:GLN:CB	4:I:489:HOH:O	2.65	0.44
2:H:51:TRP:HE3	2:H:106:LEU:O	2.00	0.44
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.99	0.44
2:H:95:ASN:OD1	2:H:97(A):GLU:HB2	2.18	0.44
2:H:17:VAL:HG21	2:H:220:CYS:HB2	1.99	0.43
2:H:73:ARG:HH11	3:I:53:ASP:CG	2.25	0.43
2:H:32:MET:HE3	2:H:70:LYS:HD3	1.95	0.43
2:H:142:GLY:HA3	2:H:192:GLU:O	2.18	0.43
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.82	0.43
3:I:53:ASP:CG	3:I:56:PHE:CE2	2.96	0.43
2:H:235:LYS:HA	2:H:238:ILE:HD12	1.99	0.43
2:H:46:LEU:C	2:H:46:LEU:CD2	2.90	0.43
2:H:60(D):TRP:CZ3	3:I:49:GLN:CG	3.02	0.43
2:H:76:TYR:HE1	4:H:510:HOH:O	1.96	0.43
2:H:149(C):VAL:O	2:H:149(D):ALA:HB3	2.18	0.43
2:H:240:LYS:CD	2:H:244:ARG:HH12	2.32	0.43
2:H:129(A):ALA:O	2:H:131:HIS:NE2	2.45	0.43
2:H:164:GLU:O	2:H:165:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:184(A):TYR:C	2:H:185:LYS:O	2.56	0.43
1:L:14(B):THR:O	1:L:14(E):GLU:HB2	2.18	0.43
2:H:164:GLU:N	2:H:164:GLU:OE1	2.52	0.43
2:H:164:GLU:O	2:H:167:VAL:N	2.52	0.42
2:H:143:ASN:ND2	2:H:192:GLU:HG3	2.28	0.42
1:L:7:PHE:C	1:L:12:VAL:O	2.62	0.42
2:H:137:ARG:HG3	2:H:138:VAL:N	2.34	0.42
3:I:47:LYS:CB	3:I:48:PRO:CD	2.96	0.42
2:H:139:THR:HA	2:H:156:GLN:O	2.19	0.42
2:H:201:MET:SD	2:H:210:MET:HG2	2.59	0.42
2:H:48:SER:HB3	2:H:50:ARG:H	1.84	0.42
3:I:45:THR:HA	3:I:46:PRO:HD3	1.88	0.42
3:I:32:SER:HB3	3:I:33:ASP:H	1.71	0.42
1:L:5:PRO:C	1:L:9:LYS:HB2	2.45	0.42
2:H:60(D):TRP:CH2	3:I:1:VAL:CG1	3.03	0.42
2:H:60(D):TRP:CH2	3:I:1:VAL:HG13	2.55	0.42
3:I:8:GLU:C	3:I:30:LEU:HD23	2.45	0.42
2:H:67:ARG:NH1	2:H:70:LYS:HZ2	2.18	0.42
2:H:109:LYS:CG	2:H:110:ARG:HH11	2.33	0.42
2:H:191:CYS:O	2:H:194:ASP:HB2	2.20	0.41
2:H:197:GLY:H	2:H:213:VAL:HB	1.85	0.41
2:H:235:LYS:HE2	2:H:239:GLN:OE1	2.19	0.41
2:H:89:TYR:O	2:H:104:ALA:HB1	2.20	0.41
2:H:91:HIS:C	2:H:93:ARG:N	2.76	0.41
2:H:140:GLY:HA3	2:H:194:ASP:OD1	2.19	0.41
2:H:146:GLU:O	2:H:149:THR:OG1	2.38	0.41
2:H:221(A):ARG:NH1	3:I:15:LEU:CD1	2.83	0.41
1:L:14(I):SER:OG	2:H:134:PHE:HA	2.20	0.41
2:H:53:LEU:HD21	2:H:103:ILE:HG13	2.02	0.41
2:H:60(D):TRP:CD2	3:I:49:GLN:HB3	2.55	0.41
2:H:163:VAL:CG1	2:H:167:VAL:CG2	2.98	0.41
3:I:29:ILE:HD12	3:I:40:VAL:HG13	2.01	0.41
2:H:87:LYS:HA	2:H:87:LYS:HD2	1.84	0.41
2:H:66:VAL:HG23	2:H:85:LEU:CD1	2.50	0.41
2:H:73:ARG:HD2	3:I:53:ASP:OD1	2.20	0.41
2:H:115:SER:C	2:H:117:TYR:N	2.78	0.41
2:H:177:THR:OG1	2:H:178:ASP:N	2.54	0.41
2:H:36:LYS:HD2	3:I:63:TYR:O	2.21	0.41
2:H:59:LEU:N	2:H:59:LEU:CD1	2.82	0.41
2:H:73:ARG:O	3:I:56:PHE:CE1	2.70	0.41
2:H:196:GLY:HA2	2:H:212:ILE:CG2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:60:PRO:CB	3:I:63:TYR:CE2	2.89	0.41
1:L:1(G):PHE:CD1	1:L:1(G):PHE:N	2.89	0.41
2:H:56:ALA:O	2:H:58:CYS:N	2.53	0.41
2:H:145:ARG:HB2	2:H:150:VAL:CG1	2.50	0.41
2:H:212:ILE:O	2:H:229:THR:N	2.50	0.40
2:H:57:HIS:CE1	2:H:214:SER:O	2.61	0.40
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.56	0.40
2:H:87:LYS:NZ	2:H:88:ILE:H	2.19	0.40
2:H:150:VAL:CG2	4:H:515:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	30/43 (70%)	14 (47%)	16 (53%)	0	0
2	H	226/226 (100%)	172 (76%)	54 (24%)	1	3
3	I	56/56 (100%)	43 (77%)	13 (23%)	1	3
All	All	312/325 (96%)	229 (73%)	83 (27%)	0	2

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	LEU
1	L	8	GLU
1	L	14	ASP

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Mol	Chain	Res	Type
1	L	14(A)	GLN
1	L	14(B)	THR
1	L	14(C)	GLU
1	L	14(D)	LYS
1	L	14(E)	GLU
1	L	14(F)	LEU
1	L	14(G)	PHE
1	L	14(H)	GLU
1	L	14(I)	SER
1	L	14(J)	TYR
1	L	14(K)	ILE
1	L	14(L)	GLU
1	L	15	ARG
2	H	16	ILE
2	H	20	GLN
2	H	24	VAL
2	H	27	SER
2	H	37	PRO
2	H	38	GLN
2	H	40	LEU
2	H	46	LEU
2	H	53	LEU
2	H	59	LEU
2	H	61	VAL
2	H	64	LEU
2	H	68	ILE
2	H	72	SER
2	H	75	ARG
2	H	78	LYS
2	H	81	LYS
2	H	85	LEU
2	H	87	LYS
2	H	99	LEU
2	H	102	ASP
2	H	110	ARG
2	H	112	ILE
2	H	119	HIS
2	H	127	GLN
2	H	129(B)	LYS
2	H	129(C)	LEU
2	H	138	VAL
2	H	139	THR

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Mol	Chain	Res	Type
2	H	149	THR
2	H	149(A)	THR
2	H	149(B)	SER
2	H	149(C)	VAL
2	H	149(E)	GLU
2	H	151	GLN
2	H	154	VAL
2	H	155	LEU
2	H	158	VAL
2	H	163	VAL
2	H	167	VAL
2	H	172	THR
2	H	176	ILE
2	H	177	THR
2	H	192	GLU
2	H	203	SER
2	H	210	MET
2	H	220	CYS
2	H	222	ASP
2	H	233	ARG
2	H	235	LYS
2	H	241	VAL
2	H	243	ASP
2	H	244	ARG
2	H	245	LEU
3	I	2	VAL
3	I	8	GLU
3	I	9	SER
3	I	19	SER
3	I	27	LYS
3	I	41	THR
3	I	43	GLU
3	I	45	THR
3	I	47	LYS
3	I	51	HIS
3	I	53	ASP
3	I	59	ILE
3	I	65	GLN

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	11	GLN
1	L	14(A)	GLN
2	H	20	GLN
2	H	38	GLN
2	H	57	HIS
2	H	60(G)	ASN
2	H	71	HIS
2	H	127	GLN
2	H	143	ASN
2	H	156	GLN
2	H	159	ASN
2	H	230	HIS
3	I	12	ASN
3	I	20	ASN
3	I	24	GLN
3	I	51	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.