



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:42 AM UTC

PDB ID : 1HJR / pdb_00001hjr
Title : ATOMIC STRUCTURE OF THE RUVB RESOLVASE: A HOLLIDAY
JUNCTION-SPECIFIC ENDONUCLEASE FROM E. COLI
Authors : Ariyoshi, M.; Vassylyev, D.G.; Morikawa, K.
Deposited on : 1994-12-02
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

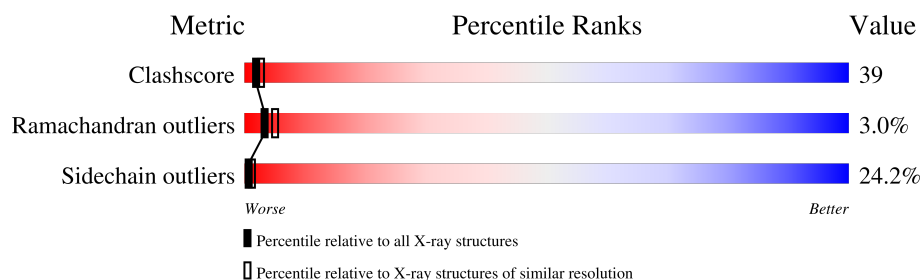
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	158	23% 43% 27% 8%
1	B	158	17% 46% 30% 7%
1	C	158	20% 47% 24% 9%
1	D	158	27% 41% 27% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4966 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 HOLLIDAY JUNCTION RESOLVASE (RUVB).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1192	754	213	220	5			
1	B	158	Total	C	N	O	S	0	0	0
			1192	754	213	220	5			
1	C	158	Total	C	N	O	S	0	0	0
			1192	754	213	220	5			
1	D	158	Total	C	N	O	S	0	0	0
			1192	754	213	220	5			

- Molecule 2 is water.

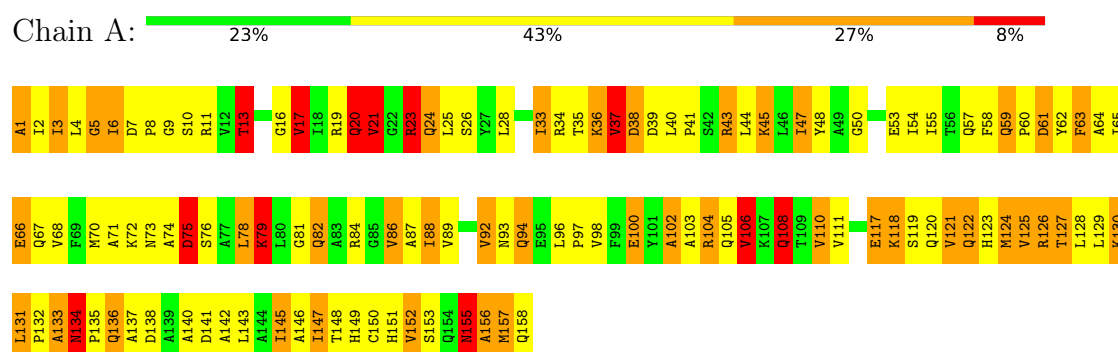
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	47	Total	O	0	0
			47	47		
2	C	40	Total	O	0	0
			40	40		
2	D	53	Total	O	0	0
			53	53		

3 Residue-property plots

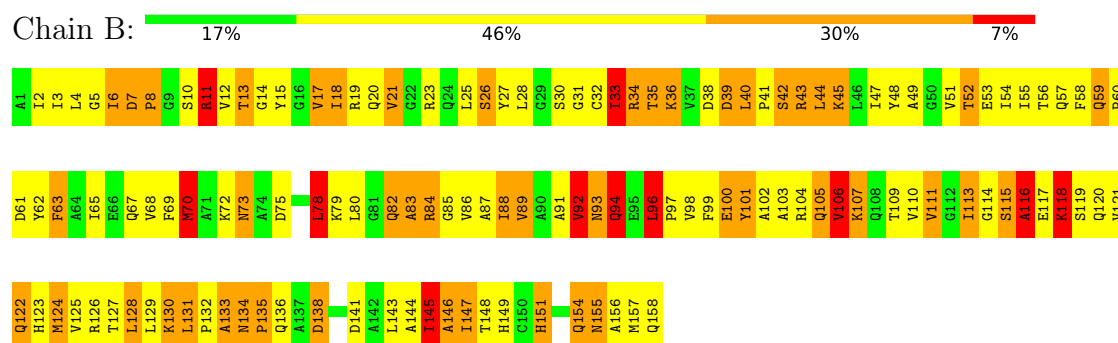
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

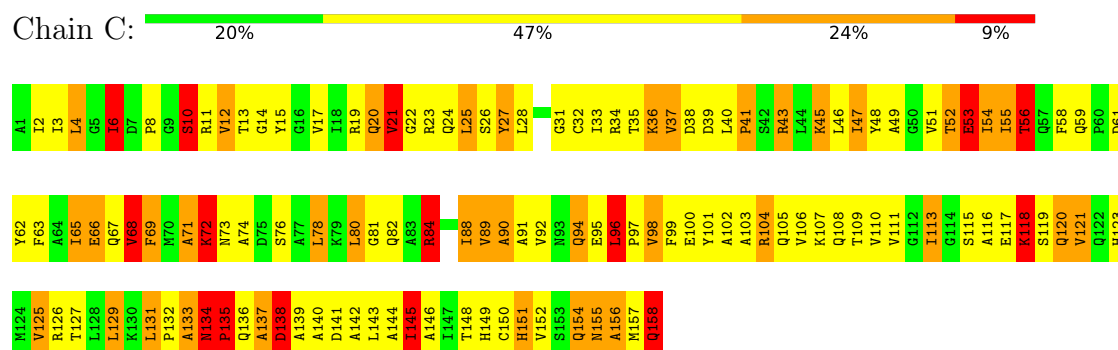
• Molecule 1: HOLLIDAY JUNCTION RESOLVASE (RUVB)



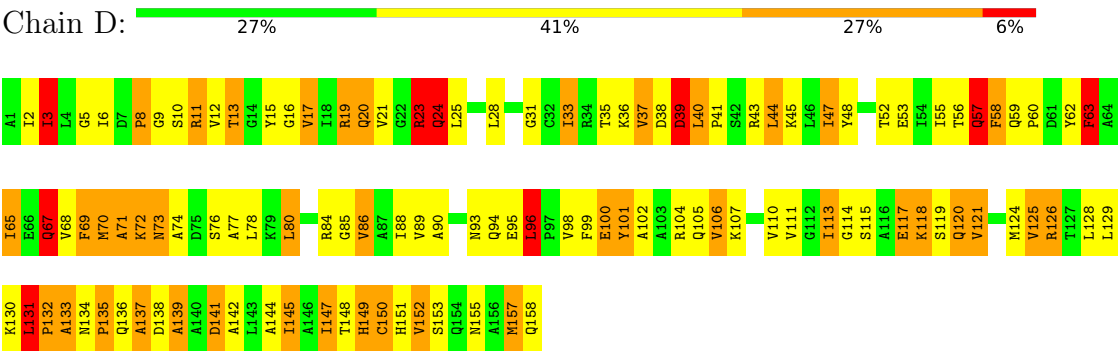
• Molecule 1: HOLLIDAY JUNCTION RESOLVASE (RUVB)



• Molecule 1: HOLLIDAY JUNCTION RESOLVASE (RUVB)



● Molecule 1: HOLLIDAY JUNCTION RESOLVASE (RUVB)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.80 Å 139.60 Å 32.40 Å 90.00° 93.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	1.15	1/1209 (0.1%)	2.71	112/1639 (6.8%)
1	B	1.18	2/1209 (0.2%)	2.92	125/1639 (7.6%)
1	C	1.11	0/1209	2.80	114/1639 (7.0%)
1	D	1.15	1/1209 (0.1%)	2.85	134/1639 (8.2%)
All	All	1.15	4/4836 (0.1%)	2.82	485/6556 (7.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	GLN	CD-OE1	5.59	1.34	1.23
1	B	82	GLN	CD-OE1	5.55	1.34	1.23
1	D	59	GLN	N-CA	5.22	1.52	1.46
1	B	82	GLN	CD-NE2	-5.00	1.22	1.33

All (485) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ASN	CA-CB-CG	26.22	138.82	112.60
1	A	43	ARG	CD-NE-CZ	18.34	150.07	124.40
1	C	133	ALA	CA-C-O	17.48	139.54	120.32
1	C	69	PHE	CA-CB-CG	15.40	129.20	113.80
1	D	80	LEU	CA-C-N	15.17	137.02	120.03
1	D	80	LEU	C-N-CA	15.17	137.02	120.03
1	B	63	PHE	CA-CB-CG	14.53	128.33	113.80
1	A	20	GLN	CA-C-O	-14.33	105.64	120.54
1	C	133	ALA	CA-C-N	14.28	156.64	121.80
1	C	133	ALA	C-N-CA	14.28	156.64	121.80
1	A	53	GLU	CA-CB-CG	13.57	141.23	114.10
1	D	94	GLN	CA-C-O	-13.30	106.12	120.89
1	D	59	GLN	CB-CA-C	13.25	123.84	110.33
1	A	43	ARG	NE-CZ-NH2	13.02	130.92	119.20
1	B	83	ALA	CA-C-O	-12.92	107.40	120.70
1	D	39	ASP	CA-CB-CG	-12.89	99.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	PRO	CB-CA-C	12.48	122.76	111.40
1	D	135	PRO	CA-C-O	11.88	135.34	121.56
1	C	84	ARG	NE-CZ-NH2	-11.70	108.67	119.20
1	A	23	ARG	CD-NE-CZ	11.57	140.60	124.40
1	A	155	ASN	CA-C-O	-11.57	103.97	120.51
1	B	96	LEU	CA-CB-CG	11.43	156.29	116.30
1	B	43	ARG	CA-CB-CG	11.38	136.86	114.10
1	C	73	ASN	CA-CB-CG	11.27	123.87	112.60
1	C	72	LYS	CA-C-O	-11.25	108.48	120.63
1	B	23	ARG	NE-CZ-NH2	-10.95	109.34	119.20
1	B	157	MET	N-CA-C	10.85	124.84	110.53
1	D	76	SER	CA-C-O	-10.78	109.60	120.70
1	C	137	ALA	CA-C-N	10.63	137.45	122.36
1	C	137	ALA	C-N-CA	10.63	137.45	122.36
1	C	84	ARG	CA-C-N	10.62	131.98	119.99
1	C	84	ARG	C-N-CA	10.62	131.98	119.99
1	C	72	LYS	N-CA-C	10.54	124.08	111.33
1	C	134	ASN	CA-CB-CG	10.37	122.97	112.60
1	A	75	ASP	CA-CB-CG	10.33	122.93	112.60
1	D	58	PHE	CA-C-O	-10.33	109.49	121.16
1	B	156	ALA	N-CA-C	10.26	127.64	108.65
1	D	138	ASP	CA-CB-CG	10.18	122.78	112.60
1	C	71	ALA	CA-C-N	10.12	134.25	120.38
1	C	71	ALA	C-N-CA	10.12	134.25	120.38
1	B	138	ASP	CA-C-O	10.07	131.86	120.98
1	A	17	VAL	CB-CA-C	9.94	125.92	110.81
1	B	155	ASN	N-CA-C	-9.93	89.80	108.17
1	B	147	ILE	N-CA-C	-9.82	100.02	110.23
1	D	37	VAL	N-CA-C	-9.71	96.97	108.82
1	D	120	GLN	CB-CG-CD	9.69	129.08	112.60
1	B	67	GLN	CA-C-O	-9.52	109.94	121.36
1	B	43	ARG	CD-NE-CZ	9.46	137.64	124.40
1	C	104	ARG	NE-CZ-NH1	9.35	130.85	121.50
1	B	154	GLN	N-CA-C	-9.28	101.97	113.38
1	D	134	ASN	N-CA-C	-9.27	96.70	110.24
1	C	21	VAL	N-CA-CB	9.15	121.40	111.89
1	C	10	SER	CA-C-N	9.12	132.68	120.65
1	C	10	SER	C-N-CA	9.12	132.68	120.65
1	B	73	ASN	OD1-CG-ND2	9.02	131.62	122.60
1	D	135	PRO	CA-C-N	8.93	141.07	122.41
1	D	135	PRO	C-N-CA	8.93	141.07	122.41
1	B	138	ASP	CA-C-N	8.86	136.76	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ASP	C-N-CA	8.86	136.76	122.67
1	D	38	ASP	N-CA-C	-8.81	103.11	114.04
1	B	43	ARG	N-CA-C	-8.81	101.64	111.07
1	B	145	ILE	N-CA-C	-8.69	101.53	111.00
1	B	63	PHE	CA-C-O	-8.68	111.01	120.30
1	B	92	VAL	N-CA-C	-8.68	101.96	110.72
1	B	125	VAL	N-CA-C	-8.65	101.99	110.72
1	B	80	LEU	CA-C-N	8.53	129.63	119.99
1	B	80	LEU	C-N-CA	8.53	129.63	119.99
1	D	63	PHE	CA-CB-CG	8.51	122.31	113.80
1	C	104	ARG	NE-CZ-NH2	-8.48	111.57	119.20
1	D	121	VAL	CB-CA-C	8.46	121.28	111.55
1	A	153	SER	N-CA-C	-8.46	104.98	114.62
1	A	82	GLN	CA-C-N	8.46	131.96	120.54
1	A	82	GLN	C-N-CA	8.46	131.96	120.54
1	B	121	VAL	N-CA-C	-8.45	102.11	110.30
1	C	27	TYR	CA-C-O	8.40	130.33	120.58
1	B	105	GLN	CA-CB-CG	8.38	130.85	114.10
1	C	43	ARG	NE-CZ-NH2	8.36	126.72	119.20
1	A	75	ASP	N-CA-C	-8.35	101.96	112.90
1	B	38	ASP	CA-C-N	8.35	134.53	121.26
1	B	38	ASP	C-N-CA	8.35	134.53	121.26
1	C	123	HIS	O-C-N	8.33	130.95	122.12
1	C	38	ASP	CA-CB-CG	8.32	120.92	112.60
1	D	96	LEU	O-C-N	8.25	130.81	121.32
1	C	2	ILE	N-CA-CB	8.22	122.32	111.64
1	D	76	SER	O-C-N	8.17	130.91	122.09
1	C	53	GLU	CB-CG-CD	8.14	126.44	112.60
1	C	43	ARG	CB-CA-C	8.13	124.68	110.85
1	B	156	ALA	CA-C-N	8.13	135.76	120.97
1	B	156	ALA	C-N-CA	8.13	135.76	120.97
1	B	131	LEU	N-CA-C	8.12	126.76	108.74
1	C	43	ARG	CA-CB-CG	8.11	130.32	114.10
1	A	117	GLU	CB-CG-CD	8.09	126.36	112.60
1	D	74	ALA	CA-C-N	8.08	131.45	120.54
1	D	74	ALA	C-N-CA	8.08	131.45	120.54
1	A	136	GLN	N-CA-C	-7.99	93.78	110.80
1	B	131	LEU	N-CA-CB	-7.97	97.00	111.03
1	B	133	ALA	CA-C-O	7.93	128.79	120.54
1	C	125	VAL	O-C-N	7.88	129.52	121.87
1	D	37	VAL	N-CA-CB	7.87	121.27	112.45
1	D	132	PRO	CB-CA-C	7.87	124.55	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	ASN	CA-C-N	7.82	130.75	120.28
1	D	73	ASN	C-N-CA	7.82	130.75	120.28
1	A	16	GLY	CA-C-N	-7.78	113.07	123.10
1	A	16	GLY	C-N-CA	-7.78	113.07	123.10
1	C	55	ILE	CA-C-N	7.76	133.69	120.72
1	C	55	ILE	C-N-CA	7.76	133.69	120.72
1	B	40	LEU	O-C-N	7.75	126.50	120.38
1	D	117	GLU	CB-CG-CD	7.74	125.76	112.60
1	B	23	ARG	NE-CZ-NH1	7.72	129.22	121.50
1	B	96	LEU	CB-CA-C	7.69	119.81	109.42
1	A	70	MET	CA-C-N	7.68	136.22	121.54
1	A	70	MET	C-N-CA	7.68	136.22	121.54
1	C	134	ASN	N-CA-C	-7.67	92.85	109.81
1	D	88	ILE	CA-C-O	-7.66	112.30	121.18
1	B	82	GLN	CG-CD-NE2	7.58	127.77	116.40
1	B	93	ASN	CA-CB-CG	7.53	120.13	112.60
1	C	145	ILE	CA-CB-CG2	7.51	123.28	110.50
1	D	56	THR	CB-CA-C	7.50	122.62	110.09
1	A	1	ALA	CB-CA-C	-7.49	99.26	110.50
1	A	137	ALA	N-CA-C	-7.47	94.89	110.80
1	C	61	ASP	CA-C-O	-7.44	112.99	120.80
1	C	43	ARG	N-CA-C	-7.43	103.27	111.36
1	B	51	VAL	CA-C-O	-7.40	113.35	121.05
1	A	138	ASP	CA-CB-CG	-7.40	105.20	112.60
1	B	96	LEU	N-CA-CB	-7.38	97.17	110.23
1	B	101	TYR	CA-C-O	7.35	128.29	120.36
1	C	127	THR	N-CA-CB	7.34	120.63	109.98
1	B	120	GLN	CA-C-O	7.33	129.29	119.47
1	C	127	THR	N-CA-C	-7.33	102.90	111.03
1	B	89	VAL	O-C-N	7.31	130.06	121.80
1	C	25	LEU	CA-C-O	-7.31	113.80	121.55
1	B	155	ASN	N-CA-CB	7.30	120.83	110.46
1	B	61	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	104	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	D	136	GLN	N-CA-C	-7.25	96.05	107.73
1	B	78	LEU	O-C-N	7.25	130.94	122.17
1	D	134	ASN	N-CA-CB	7.24	119.81	110.04
1	D	88	ILE	N-CA-C	-7.22	103.63	110.42
1	A	98	VAL	N-CA-C	7.21	118.51	107.99
1	B	18	ILE	O-C-N	7.19	130.69	123.00
1	A	146	ALA	N-CA-C	-7.17	103.39	111.14
1	D	73	ASN	CA-CB-CG	-7.17	105.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ILE	O-C-N	7.14	129.30	121.94
1	C	132	PRO	N-CA-C	-7.13	99.00	112.33
1	D	88	ILE	N-CA-CB	7.12	118.69	110.65
1	D	67	GLN	N-CA-C	-7.10	98.03	109.96
1	D	58	PHE	N-CA-C	-7.08	98.69	109.95
1	D	93	ASN	CB-CA-C	7.08	125.10	110.31
1	C	62	TYR	N-CA-C	7.05	121.07	110.14
1	C	157	MET	N-CA-C	7.04	120.35	111.69
1	C	132	PRO	CB-CA-C	7.03	122.65	113.09
1	D	138	ASP	CA-C-O	-7.02	113.94	121.45
1	B	135	PRO	CA-C-N	6.97	134.86	121.54
1	B	135	PRO	C-N-CA	6.97	134.86	121.54
1	A	122	GLN	CA-CB-CG	6.97	128.03	114.10
1	D	59	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	A	57	GLN	CA-CB-CG	6.93	127.96	114.10
1	C	120	GLN	N-CA-C	-6.93	103.81	111.36
1	B	34	ARG	CA-C-O	6.92	127.87	120.46
1	C	46	LEU	CA-C-O	-6.91	113.22	120.55
1	D	53	GLU	CB-CG-CD	6.91	124.34	112.60
1	B	155	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	B	94	GLN	N-CA-C	-6.89	104.87	112.72
1	B	63	PHE	O-C-N	6.88	131.26	123.27
1	A	73	ASN	CA-CB-CG	-6.84	105.76	112.60
1	A	71	ALA	CA-C-O	-6.84	110.73	120.51
1	C	98	VAL	CA-C-N	6.83	132.80	123.11
1	C	98	VAL	C-N-CA	6.83	132.80	123.11
1	B	49	ALA	O-C-N	6.81	129.08	122.07
1	B	105	GLN	CB-CG-CD	6.81	124.17	112.60
1	D	94	GLN	CA-C-N	-6.80	111.95	122.49
1	D	94	GLN	C-N-CA	-6.80	111.95	122.49
1	D	71	ALA	CA-C-O	6.79	127.53	120.40
1	A	158	GLN	N-CA-CB	6.79	122.05	110.50
1	C	26	SER	N-CA-C	6.74	119.06	107.93
1	C	4	LEU	N-CA-C	-6.74	98.71	109.76
1	D	94	GLN	O-C-N	-6.72	114.81	122.20
1	A	10	SER	CA-C-O	-6.72	113.71	120.90
1	D	37	VAL	O-C-N	6.71	129.97	122.92
1	B	107	LYS	N-CA-C	-6.70	102.85	111.02
1	D	138	ASP	N-CA-CB	6.69	122.13	111.56
1	C	80	LEU	N-CA-C	-6.68	103.47	111.69
1	A	13	THR	CB-CA-C	-6.66	100.90	110.62
1	A	87	ALA	CA-C-N	6.65	129.86	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ALA	C-N-CA	6.65	129.86	120.42
1	B	79	LYS	N-CA-C	-6.64	103.97	111.14
1	D	100	GLU	CB-CA-C	-6.64	100.94	111.17
1	A	105	GLN	N-CA-CB	6.63	120.52	110.30
1	D	35	THR	CA-C-N	6.63	131.28	122.06
1	D	35	THR	C-N-CA	6.63	131.28	122.06
1	B	48	TYR	O-C-N	6.62	128.89	122.07
1	D	121	VAL	CA-CB-CG1	6.61	121.64	110.40
1	A	86	VAL	N-CA-CB	6.60	120.48	110.58
1	C	145	ILE	N-CA-C	-6.60	103.33	112.50
1	B	39	ASP	N-CA-C	6.58	120.17	110.30
1	B	11	ARG	CA-C-O	-6.57	111.94	118.97
1	D	94	GLN	OE1-CD-NE2	6.56	129.16	122.60
1	B	99	PHE	CA-C-N	-6.56	113.95	123.00
1	B	99	PHE	C-N-CA	-6.56	113.95	123.00
1	D	35	THR	CA-C-O	6.56	129.54	122.13
1	A	35	THR	CA-CB-OG1	-6.54	99.79	109.60
1	A	9	GLY	O-C-N	6.53	131.19	122.70
1	C	142	ALA	CA-C-N	6.50	129.52	120.29
1	C	142	ALA	C-N-CA	6.50	129.52	120.29
1	D	144	ALA	O-C-N	6.49	128.84	122.09
1	D	155	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	21	VAL	CB-CA-C	6.49	119.17	111.32
1	A	93	ASN	CA-CB-CG	-6.48	106.12	112.60
1	D	48	TYR	CA-C-N	6.48	133.92	121.54
1	D	48	TYR	C-N-CA	6.48	133.92	121.54
1	A	132	PRO	N-CA-C	-6.47	99.13	112.47
1	B	48	TYR	CA-C-O	-6.47	114.02	120.82
1	C	53	GLU	N-CA-C	-6.46	102.91	111.24
1	D	88	ILE	O-C-N	6.46	128.85	121.94
1	D	104	ARG	CA-C-O	-6.46	112.80	120.10
1	C	96	LEU	O-C-N	6.40	128.60	121.43
1	B	141	ASP	CB-CA-C	6.38	121.07	110.92
1	C	138	ASP	N-CA-C	6.38	120.19	111.39
1	B	100	GLU	CG-CD-OE2	-6.34	103.81	118.40
1	C	105	GLN	CA-CB-CG	6.33	126.77	114.10
1	B	67	GLN	CA-CB-CG	6.33	126.76	114.10
1	A	33	ILE	CB-CA-C	6.33	119.45	110.84
1	B	83	ALA	O-C-N	6.32	128.92	122.09
1	A	43	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	1	ALA	N-CA-CB	6.29	119.84	110.40
1	C	156	ALA	N-CA-C	6.29	124.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	A	33	ILE	N-CA-C	-6.24	99.44	108.36
1	C	6	ILE	CB-CA-C	6.24	119.44	110.33
1	C	55	ILE	N-CA-C	6.23	116.40	110.42
1	D	147	ILE	N-CA-C	-6.23	104.26	110.30
1	A	62	TYR	O-C-N	6.23	131.46	123.11
1	C	129	LEU	O-C-N	6.23	131.25	122.41
1	A	1	ALA	O-C-N	6.22	132.96	123.00
1	D	52	THR	O-C-N	6.21	129.23	122.15
1	D	121	VAL	N-CA-C	-6.19	106.49	111.81
1	D	39	ASP	OD1-CG-OD2	6.18	137.73	122.90
1	D	80	LEU	N-CA-C	-6.18	104.47	111.14
1	D	67	GLN	N-CA-CB	6.17	120.22	110.23
1	D	117	GLU	N-CA-CB	6.15	119.35	110.06
1	A	108	GLN	N-CA-CB	6.15	119.69	110.22
1	D	147	ILE	N-CA-CB	6.15	117.32	110.62
1	C	55	ILE	CA-C-O	6.14	127.68	121.17
1	C	94	GLN	N-CA-CB	6.14	119.89	110.61
1	B	8	PRO	O-C-N	6.13	130.79	123.06
1	C	129	LEU	N-CA-C	-6.13	105.80	113.28
1	D	47	ILE	N-CA-C	-6.13	104.77	110.53
1	D	12	VAL	O-C-N	6.10	130.19	122.57
1	C	96	LEU	CA-C-N	6.09	127.01	120.13
1	C	96	LEU	C-N-CA	6.09	127.01	120.13
1	C	151	HIS	CA-CB-CG	6.08	119.88	113.80
1	B	122	GLN	CA-C-N	6.08	130.32	120.60
1	B	122	GLN	C-N-CA	6.08	130.32	120.60
1	D	33	ILE	CB-CA-C	6.08	118.97	111.25
1	D	141	ASP	CA-C-N	6.07	128.91	120.29
1	D	141	ASP	C-N-CA	6.07	128.91	120.29
1	C	89	VAL	CA-CB-CG1	6.07	120.72	110.40
1	B	19	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	A	105	GLN	N-CA-C	-6.07	104.59	112.23
1	B	116	ALA	N-CA-C	6.06	123.71	110.80
1	C	47	ILE	O-C-N	6.04	127.98	121.94
1	C	68	VAL	N-CA-C	6.04	116.88	107.28
1	D	40	LEU	O-C-N	6.03	128.26	121.32
1	C	53	GLU	CA-CB-CG	6.03	126.16	114.10
1	A	148	THR	N-CA-CB	6.03	118.71	109.91
1	A	1	ALA	CA-C-O	-6.01	110.57	120.80
1	D	150	CYS	O-C-N	6.01	128.28	122.03
1	B	106	VAL	N-CA-C	-6.00	105.86	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	PHE	CA-C-O	-6.00	112.80	119.40
1	B	132	PRO	N-CA-C	-6.00	101.11	112.33
1	A	147	ILE	O-C-N	5.99	127.68	121.87
1	C	123	HIS	CA-C-O	-5.98	114.21	120.55
1	A	53	GLU	CA-C-O	-5.98	113.09	119.97
1	B	67	GLN	N-CA-C	-5.98	100.82	110.32
1	B	52	THR	N-CA-CB	5.97	118.90	110.12
1	B	121	VAL	CA-C-N	5.96	132.93	121.54
1	B	121	VAL	C-N-CA	5.96	132.93	121.54
1	A	132	PRO	CB-CA-C	5.96	121.39	111.56
1	B	70	MET	CA-C-O	5.95	128.86	122.13
1	C	65	ILE	N-CA-CB	5.95	121.12	111.36
1	D	149	HIS	CA-CB-CG	-5.95	107.85	113.80
1	D	38	ASP	CB-CA-C	5.94	119.73	109.15
1	B	143	LEU	CA-C-N	5.94	131.54	121.14
1	B	143	LEU	C-N-CA	5.94	131.54	121.14
1	B	12	VAL	CA-C-O	-5.92	114.30	120.64
1	B	34	ARG	CA-C-N	5.90	131.34	123.20
1	B	34	ARG	C-N-CA	5.90	131.34	123.20
1	C	25	LEU	CB-CA-C	5.90	120.18	109.62
1	C	34	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	C	69	PHE	N-CA-C	-5.88	105.77	113.12
1	C	104	ARG	CD-NE-CZ	5.88	132.63	124.40
1	D	23	ARG	CD-NE-CZ	5.88	132.63	124.40
1	A	20	GLN	CA-C-N	-5.87	115.11	123.10
1	A	20	GLN	C-N-CA	-5.87	115.11	123.10
1	C	36	LYS	CA-C-O	-5.87	114.20	120.42
1	B	8	PRO	CB-CA-C	-5.86	102.58	110.85
1	A	105	GLN	CA-CB-CG	5.86	125.83	114.10
1	A	5	GLY	CA-C-O	-5.86	114.90	120.64
1	A	73	ASN	CA-C-O	-5.86	114.31	120.58
1	D	98	VAL	CA-C-N	5.85	132.16	122.33
1	D	98	VAL	C-N-CA	5.85	132.16	122.33
1	C	6	ILE	CA-C-N	5.82	133.08	123.08
1	C	6	ILE	C-N-CA	5.82	133.08	123.08
1	C	19	ARG	N-CA-CB	5.81	119.80	110.85
1	C	133	ALA	O-C-N	-5.81	116.41	123.27
1	B	83	ALA	N-CA-CB	5.81	118.49	110.07
1	A	68	VAL	CA-C-O	-5.79	114.36	120.39
1	D	119	SER	O-C-N	5.79	128.11	122.09
1	D	141	ASP	N-CA-C	-5.78	104.94	112.23
1	A	62	TYR	CA-C-O	-5.78	114.70	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ILE	CB-CA-C	5.76	119.08	111.70
1	D	85	GLY	CA-C-N	5.76	127.82	120.56
1	D	85	GLY	C-N-CA	5.76	127.82	120.56
1	B	7	ASP	N-CA-CB	-5.76	103.94	111.09
1	B	121	VAL	CB-CA-C	5.76	119.01	111.81
1	A	66	GLU	CA-C-O	-5.74	114.05	120.54
1	D	17	VAL	CA-C-N	5.74	130.84	123.03
1	D	17	VAL	C-N-CA	5.74	130.84	123.03
1	D	19	ARG	CA-C-O	-5.74	114.41	121.06
1	B	117	GLU	CA-C-N	5.73	132.49	121.54
1	B	117	GLU	C-N-CA	5.73	132.49	121.54
1	A	92	VAL	N-CA-C	-5.72	104.93	110.42
1	D	57	GLN	CA-C-O	5.71	127.45	120.31
1	B	53	GLU	CB-CG-CD	5.70	122.30	112.60
1	D	94	GLN	N-CA-C	-5.70	101.13	109.63
1	D	120	GLN	CA-CB-CG	5.70	125.50	114.10
1	B	39	ASP	N-CA-CB	-5.70	99.94	109.28
1	B	107	LYS	N-CA-CB	5.70	118.48	109.82
1	B	158	GLN	CB-CG-CD	5.69	122.27	112.60
1	D	58	PHE	CA-C-N	-5.69	112.11	122.35
1	D	58	PHE	C-N-CA	-5.69	112.11	122.35
1	A	123	HIS	N-CA-C	-5.68	105.00	111.14
1	B	143	LEU	N-CA-C	5.68	118.25	111.71
1	C	118	LYS	CA-C-O	-5.68	114.50	120.63
1	C	158	GLN	CB-CG-CD	5.68	122.25	112.60
1	A	7	ASP	CA-C-N	5.68	126.00	119.93
1	A	7	ASP	C-N-CA	5.68	126.00	119.93
1	D	8	PRO	N-CA-C	5.68	119.93	111.41
1	D	11	ARG	CD-NE-CZ	5.67	132.33	124.40
1	A	11	ARG	CA-C-O	-5.65	113.11	120.00
1	C	90	ALA	N-CA-C	-5.65	105.27	111.82
1	D	47	ILE	O-C-N	5.65	127.77	121.90
1	A	11	ARG	CD-NE-CZ	5.64	132.29	124.40
1	A	133	ALA	CA-C-N	5.63	135.54	121.80
1	A	133	ALA	C-N-CA	5.63	135.54	121.80
1	C	152	VAL	CB-CA-C	5.63	120.53	111.29
1	D	133	ALA	N-CA-C	5.63	119.01	107.69
1	A	156	ALA	N-CA-C	5.63	120.67	113.18
1	D	16	GLY	CA-C-N	5.63	130.44	123.12
1	D	16	GLY	C-N-CA	5.63	130.44	123.12
1	B	39	ASP	CA-C-O	-5.62	114.73	120.80
1	A	123	HIS	N-CA-CB	5.62	118.22	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	HIS	CA-CB-CG	5.62	119.42	113.80
1	D	126	ARG	O-C-N	5.62	128.60	122.20
1	D	72	LYS	N-CA-C	-5.61	100.60	108.96
1	D	3	ILE	O-C-N	5.61	129.26	123.20
1	A	134	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	61	ASP	CA-C-O	5.58	126.53	119.78
1	D	74	ALA	N-CA-CB	-5.58	101.92	110.12
1	C	37	VAL	CA-C-N	5.58	127.69	120.44
1	C	37	VAL	C-N-CA	5.58	127.69	120.44
1	D	67	GLN	CA-C-O	-5.58	114.51	120.92
1	A	71	ALA	CA-C-N	-5.57	113.22	122.08
1	A	71	ALA	C-N-CA	-5.57	113.22	122.08
1	C	84	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	D	84	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	B	146	ALA	CA-C-O	5.57	126.67	120.82
1	C	3	ILE	CA-C-O	-5.57	114.54	120.39
1	C	131	LEU	O-C-N	5.56	126.35	121.18
1	B	42	SER	N-CA-C	5.54	117.13	111.14
1	C	76	SER	N-CA-C	-5.54	105.65	112.90
1	A	102	ALA	CA-C-O	-5.53	114.96	121.16
1	A	37	VAL	N-CA-CB	5.51	118.63	111.19
1	B	10	SER	O-C-N	5.51	128.05	122.09
1	C	66	GLU	CA-CB-CG	5.51	125.12	114.10
1	A	93	ASN	N-CA-C	5.50	119.61	113.01
1	B	21	VAL	CA-C-O	-5.50	114.36	120.74
1	D	99	PHE	CA-C-N	5.50	130.87	122.95
1	D	99	PHE	C-N-CA	5.50	130.87	122.95
1	D	90	ALA	CA-C-N	5.49	128.18	120.28
1	D	90	ALA	C-N-CA	5.49	128.18	120.28
1	A	158	GLN	CA-C-O	-5.48	111.49	120.80
1	A	47	ILE	N-CA-C	-5.47	105.38	110.53
1	B	26	SER	N-CA-CB	5.47	119.82	110.57
1	D	44	LEU	O-C-N	5.47	127.72	122.03
1	D	145	ILE	O-C-N	5.47	127.25	121.89
1	B	4	LEU	O-C-N	5.46	129.72	123.27
1	A	43	ARG	CA-C-N	5.46	129.86	121.19
1	A	43	ARG	C-N-CA	5.46	129.86	121.19
1	D	139	ALA	N-CA-CB	-5.45	101.27	110.49
1	A	155	ASN	N-CA-C	5.44	122.39	110.80
1	B	134	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	157	MET	N-CA-CB	-5.42	102.61	110.36
1	C	127	THR	O-C-N	5.42	127.88	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	MET	N-CA-CB	-5.41	101.41	110.39
1	A	133	ALA	N-CA-C	5.41	118.04	109.50
1	C	94	GLN	CB-CG-CD	5.41	121.79	112.60
1	B	5	GLY	CA-C-N	-5.40	114.59	122.58
1	B	5	GLY	C-N-CA	-5.40	114.59	122.58
1	D	39	ASP	CB-CG-OD1	-5.40	105.99	118.40
1	C	141	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	35	THR	CB-CA-C	5.39	120.25	112.05
1	B	115	SER	CA-C-N	5.38	131.82	121.54
1	B	115	SER	C-N-CA	5.38	131.82	121.54
1	C	21	VAL	N-CA-C	-5.38	97.66	106.32
1	A	37	VAL	CA-C-O	5.38	126.01	120.96
1	D	138	ASP	N-CA-C	-5.37	100.97	108.96
1	D	10	SER	CA-C-O	-5.36	114.85	120.63
1	D	63	PHE	CB-CA-C	5.36	118.44	110.62
1	B	154	GLN	N-CA-CB	5.35	118.50	110.53
1	D	137	ALA	CA-C-N	5.35	130.65	121.87
1	D	137	ALA	C-N-CA	5.35	130.65	121.87
1	A	148	THR	O-C-N	5.35	127.59	122.03
1	C	88	ILE	CA-C-N	5.34	127.78	120.46
1	C	88	ILE	C-N-CA	5.34	127.78	120.46
1	C	135	PRO	N-CD-CG	-5.34	95.18	103.20
1	D	131	LEU	O-C-N	5.34	127.46	121.32
1	C	104	ARG	N-CA-C	-5.33	105.36	111.07
1	A	38	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	106	VAL	CB-CA-C	5.32	118.78	111.97
1	D	147	ILE	CA-C-O	-5.31	115.61	121.29
1	A	79	LYS	CB-CG-CD	5.30	123.50	111.30
1	A	47	ILE	CA-C-N	5.30	127.64	120.38
1	A	47	ILE	C-N-CA	5.30	127.64	120.38
1	C	134	ASN	O-C-N	5.30	127.42	121.32
1	A	126	ARG	CD-NE-CZ	5.30	131.81	124.40
1	D	24	GLN	CB-CG-CD	5.30	121.60	112.60
1	A	61	ASP	N-CA-C	-5.29	106.50	113.12
1	C	123	HIS	N-CA-CB	5.29	117.89	110.12
1	C	2	ILE	CA-C-O	-5.26	114.92	120.39
1	C	96	LEU	CA-C-O	-5.26	114.57	120.25
1	A	50	GLY	O-C-N	5.25	129.53	122.70
1	D	119	SER	CA-C-O	-5.25	115.28	120.90
1	A	59	GLN	CA-C-N	5.24	125.71	120.52
1	A	59	GLN	C-N-CA	5.24	125.71	120.52
1	D	84	ARG	N-CA-CB	-5.24	102.48	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ILE	CA-C-N	5.23	127.84	120.42
1	A	88	ILE	C-N-CA	5.23	127.84	120.42
1	B	88	ILE	N-CA-C	5.22	115.99	110.72
1	C	150	CYS	CB-CA-C	-5.22	102.46	110.81
1	D	104	ARG	N-CA-CB	5.22	118.25	110.22
1	D	58	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	78	LEU	CA-CB-CG	5.21	134.53	116.30
1	D	20	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	B	70	MET	CB-CA-C	5.20	119.95	112.05
1	B	128	LEU	CB-CA-C	5.19	119.69	109.72
1	C	78	LEU	CA-C-N	5.19	128.21	120.31
1	C	78	LEU	C-N-CA	5.19	128.21	120.31
1	D	21	VAL	N-CA-C	-5.19	98.99	106.88
1	C	56	THR	CA-C-O	5.18	125.76	119.38
1	A	63	PHE	CA-C-O	-5.17	114.58	120.32
1	B	147	ILE	O-C-N	5.17	127.55	121.96
1	D	21	VAL	O-C-N	5.16	129.76	122.59
1	C	43	ARG	CA-C-O	-5.16	114.95	120.42
1	D	53	GLU	CG-CD-OE1	5.16	130.27	118.40
1	B	7	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	36	LYS	N-CA-C	5.15	119.25	112.25
1	D	93	ASN	N-CA-C	-5.14	106.27	112.54
1	C	72	LYS	N-CA-CB	-5.14	102.35	110.06
1	D	67	GLN	CA-CB-CG	5.13	124.36	114.10
1	A	100	GLU	O-C-N	-5.12	117.48	123.27
1	B	35	THR	N-CA-CB	-5.12	101.39	110.60
1	A	138	ASP	O-C-N	5.11	129.39	122.59
1	B	87	ALA	CA-C-N	5.10	127.66	120.42
1	B	87	ALA	C-N-CA	5.10	127.66	120.42
1	A	149	HIS	CA-C-O	-5.09	115.22	120.92
1	D	125	VAL	CA-CB-CG2	5.09	119.05	110.40
1	A	117	GLU	N-CA-CB	5.08	118.68	110.85
1	A	26	SER	CA-C-N	5.07	129.07	121.72
1	A	26	SER	C-N-CA	5.07	129.07	121.72
1	B	20	GLN	CB-CA-C	-5.06	102.72	111.23
1	C	98	VAL	CA-C-O	5.06	126.11	120.59
1	B	33	ILE	CA-CB-CG1	5.05	118.99	110.40
1	A	94	GLN	N-CA-C	-5.05	106.53	113.30
1	B	124	MET	N-CA-C	-5.05	106.96	113.23
1	C	39	ASP	CA-C-O	-5.05	115.63	121.19
1	A	35	THR	OG1-CB-CG2	5.05	119.40	109.30
1	A	53	GLU	N-CA-C	-5.05	105.96	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	GLN	CB-CA-C	5.05	118.14	109.51
1	C	6	ILE	N-CA-CB	-5.04	104.16	111.52
1	C	43	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
1	D	57	GLN	CB-CG-CD	-5.01	104.09	112.60
1	A	108	GLN	CA-C-O	-5.00	114.44	120.10
1	D	53	GLU	O-C-N	5.00	127.44	122.08
1	D	132	PRO	N-CA-C	-5.00	102.17	112.47

There are no chirality outliers.

There are no planarity outliers.

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	A	1192	0	1232	93	3
1	B	1192	0	1232	119	3
1	C	1192	0	1231	109	1
1	D	1192	0	1232	72	4
2	A	58	0	0	3	6
2	B	47	0	0	13	1
2	C	40	0	0	8	0
2	D	53	0	0	6	5
All	All	4966	0	4927	376	12

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 39.

All (376) 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)
1:A:130:LYS:HB2	1:B:155:ASN:HD22	1.18	1.02
1:B:102:ALA:HB3	1:B:105:GLN:HG3	1.39	1.02
1:C:55:ILE:HG21	1:C:94:GLN:HG3	1.37	1.01
1:A:8:PRO:HA	1:A:13:THR:HG23	1.46	0.97
1:C:4:LEU:HD11	1:C:6:ILE:HD12	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:HB2	1:B:145:ILE:HD11	1.49	0.93
1:B:94:GLN:HA	1:B:94:GLN:HE21	1.34	0.91
1:B:13:THR:HG22	2:B:256:HOH:O	1.72	0.89
1:B:113:ILE:HD12	1:B:114:GLY:H	1.37	0.89
1:B:124:MET:HA	1:B:127:THR:HG22	1.52	0.89
1:B:40:LEU:HB3	1:B:41:PRO:HD3	1.52	0.88
1:C:27:TYR:HB2	1:C:129:LEU:HD22	1.55	0.87
1:A:4:LEU:HD22	1:A:60:PRO:HG2	1.55	0.86
1:B:13:THR:HG23	1:B:33:ILE:HG13	1.56	0.86
1:C:52:THR:HA	1:C:55:ILE:HD12	1.59	0.84
1:C:151:HIS:O	1:C:155:ASN:HB2	1.79	0.83
1:D:40:LEU:HB3	1:D:41:PRO:HD3	1.59	0.83
1:A:103:ALA:O	1:A:106:VAL:HG13	1.80	0.81
1:D:20:GLN:HE21	1:D:23:ARG:HA	1.47	0.79
1:C:12:VAL:HB	1:C:33:ILE:O	1.82	0.78
1:B:105:GLN:HB2	2:B:322:HOH:O	1.83	0.78
1:D:8:PRO:HA	1:D:13:THR:HB	1.66	0.77
1:A:126:ARG:HA	1:A:131:LEU:HD23	1.65	0.77
1:C:109:THR:HG21	1:C:148:THR:HA	1.66	0.76
1:D:11:ARG:HB3	1:D:36:LYS:NZ	2.01	0.75
1:C:52:THR:HG22	1:C:90:ALA:HB1	1.68	0.75
1:B:130:LYS:HE2	1:B:130:LYS:HA	1.66	0.75
1:D:11:ARG:HB3	1:D:36:LYS:HZ3	1.51	0.75
1:D:135:PRO:HD2	2:D:217:HOH:O	1.85	0.75
1:B:118:LYS:H	1:B:118:LYS:HD2	1.51	0.74
1:B:124:MET:O	1:B:128:LEU:HB2	1.86	0.74
1:B:101:TYR:HB3	2:B:322:HOH:O	1.87	0.74
1:D:20:GLN:NE2	1:D:23:ARG:HA	2.03	0.74
1:B:28:LEU:HD13	2:B:314:HOH:O	1.89	0.73
1:C:47:ILE:O	1:C:51:VAL:HG23	1.89	0.72
1:D:113:ILE:HD12	1:D:114:GLY:N	2.04	0.72
1:A:65:ILE:O	1:A:100:GLU:HA	1.90	0.72
1:C:14:GLY:HA2	1:C:32:CYS:HA	1.71	0.71
1:B:107:LYS:HG3	1:B:114:GLY:O	1.91	0.71
1:B:111:VAL:HG21	1:B:116:ALA:HB2	1.72	0.71
1:B:89:VAL:HA	1:B:92:VAL:HG22	1.72	0.71
1:D:106:VAL:HG12	2:D:390:HOH:O	1.91	0.71
1:A:45:LYS:HG3	1:C:92:VAL:HG11	1.74	0.70
1:D:117:GLU:OE2	1:D:118:LYS:HD3	1.91	0.70
1:C:94:GLN:NE2	2:C:435:HOH:O	2.24	0.70
1:A:130:LYS:CB	1:B:155:ASN:HD22	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HH22	1:B:135:PRO:HG3	1.57	0.69
1:A:78:LEU:O	1:A:82:GLN:HG3	1.93	0.69
1:B:63:PHE:HB2	1:B:96:LEU:CD1	2.23	0.69
1:C:33:ILE:HG22	1:C:35:THR:HG23	1.75	0.69
1:A:6:ILE:HG22	1:A:65:ILE:HG12	1.74	0.68
1:B:18:ILE:HD12	1:B:25:LEU:HD22	1.75	0.68
1:D:58:PHE:O	1:D:60:PRO:HD3	1.94	0.68
1:D:118:LYS:H	1:D:118:LYS:HD2	1.58	0.68
1:A:6:ILE:HG23	1:A:8:PRO:HD3	1.75	0.68
1:A:25:LEU:HD23	1:A:129:LEU:HD23	1.75	0.68
1:C:13:THR:HG23	1:C:33:ILE:HB	1.74	0.68
1:B:11:ARG:NH2	1:B:36:LYS:HE3	2.09	0.67
1:A:131:LEU:HG	1:A:131:LEU:O	1.93	0.67
1:A:2:ILE:HD11	1:A:19:ARG:HH12	1.58	0.67
1:B:93:ASN:ND2	1:D:45:LYS:NZ	2.43	0.67
1:A:17:VAL:HG22	1:A:28:LEU:HD12	1.77	0.67
1:B:107:LYS:HB2	1:B:114:GLY:HA2	1.77	0.67
1:B:52:THR:O	1:B:56:THR:HG23	1.94	0.67
1:B:78:LEU:HD23	1:D:77:ALA:HB1	1.78	0.67
1:C:48:TYR:O	1:C:52:THR:HG23	1.94	0.67
1:B:101:TYR:HB2	1:B:145:ILE:CD1	2.25	0.66
1:C:15:TYR:N	1:C:31:GLY:O	2.28	0.66
1:B:39:ASP:HB3	1:B:42:SER:HB2	1.78	0.65
1:B:113:ILE:HG13	1:B:115:SER:OG	1.96	0.65
1:C:40:LEU:HB3	1:C:41:PRO:HD3	1.79	0.65
1:D:110:VAL:HG23	1:D:111:VAL:HG13	1.77	0.65
1:A:45:LYS:HG3	1:C:92:VAL:CG1	2.27	0.64
1:B:43:ARG:O	1:B:47:ILE:HG12	1.97	0.64
1:B:6:ILE:HG21	1:B:63:PHE:CZ	2.32	0.64
1:A:5:GLY:HA2	1:A:64:ALA:O	1.97	0.64
1:C:113:ILE:HD11	1:C:115:SER:HB2	1.78	0.63
1:B:57:GLN:HB2	2:B:324:HOH:O	1.98	0.63
1:C:126:ARG:HG3	1:C:131:LEU:HB2	1.81	0.63
1:B:104:ARG:HG2	1:B:104:ARG:HH11	1.63	0.63
1:B:113:ILE:HD12	1:B:114:GLY:N	2.12	0.62
1:C:21:VAL:O	1:C:23:ARG:N	2.31	0.62
1:C:6:ILE:HG22	1:C:65:ILE:HG22	1.81	0.62
1:A:8:PRO:CA	1:A:13:THR:HG23	2.26	0.62
1:C:65:ILE:HD12	1:C:84:ARG:NH2	2.14	0.62
1:B:118:LYS:O	1:B:122:GLN:HG3	2.00	0.62
1:D:25:LEU:HD23	1:D:25:LEU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:131:LEU:HB3	1.99	0.62
1:D:67:GLN:HA	1:D:67:GLN:HE21	1.65	0.61
1:A:118:LYS:O	1:A:119:SER:C	2.41	0.61
1:A:130:LYS:HB2	1:B:155:ASN:ND2	2.02	0.61
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.04	0.61
1:D:113:ILE:HG13	1:D:115:SER:H	1.64	0.61
1:C:69:PHE:CE2	1:C:104:ARG:HB2	2.36	0.61
1:D:57:GLN:HE21	1:D:57:GLN:HA	1.65	0.61
1:C:84:ARG:O	1:C:88:ILE:HG13	2.01	0.61
1:B:40:LEU:O	1:B:44:LEU:HB2	2.01	0.61
1:C:25:LEU:HD13	2:C:428:HOH:O	2.01	0.60
1:C:158:GLN:C	1:C:158:GLN:HE21	2.09	0.60
1:B:124:MET:HA	1:B:127:THR:CG2	2.30	0.60
1:D:141:ASP:O	1:D:145:ILE:HG12	2.02	0.60
1:B:34:ARG:HG2	2:B:421:HOH:O	2.01	0.60
1:C:41:PRO:HD2	2:C:413:HOH:O	2.01	0.60
1:C:63:PHE:HD2	1:C:98:VAL:HG13	1.66	0.60
1:B:60:PRO:HG2	1:B:96:LEU:HD21	1.83	0.59
1:A:48:TYR:HE2	1:A:89:VAL:HG13	1.66	0.59
1:A:63:PHE:HE1	1:A:65:ILE:HD11	1.66	0.59
1:D:118:LYS:H	1:D:118:LYS:CD	2.13	0.59
1:B:17:VAL:HG11	1:B:58:PHE:CD1	2.38	0.59
1:D:111:VAL:HG12	1:D:124:MET:HG3	1.85	0.59
1:D:125:VAL:HG22	1:D:147:ILE:HD12	1.85	0.58
1:D:110:VAL:HG21	1:D:121:VAL:HG13	1.84	0.58
1:C:20:GLN:NE2	1:C:154:GLN:OE1	2.37	0.58
1:D:15:TYR:CZ	1:D:31:GLY:HA3	2.38	0.58
1:D:128:LEU:HD13	1:D:147:ILE:HD13	1.85	0.58
1:A:124:MET:HA	1:A:127:THR:HG23	1.86	0.58
1:B:104:ARG:HG2	1:B:104:ARG:NH1	2.16	0.58
1:B:69:PHE:CD2	1:B:70:MET:HB3	2.38	0.58
1:D:40:LEU:CB	1:D:41:PRO:HD3	2.32	0.57
1:B:8:PRO:HA	1:B:13:THR:HB	1.85	0.57
1:A:104:ARG:HD3	2:A:278:HOH:O	2.03	0.57
1:B:69:PHE:CD1	1:B:69:PHE:N	2.71	0.57
1:A:128:LEU:HD12	1:A:147:ILE:HD13	1.85	0.57
1:B:13:THR:O	1:B:32:CYS:HA	2.04	0.57
1:A:134:ASN:H	1:A:134:ASN:ND2	2.00	0.57
1:B:40:LEU:HB3	1:B:41:PRO:CD	2.32	0.57
1:C:55:ILE:HD13	1:C:94:GLN:HG2	1.87	0.57
1:D:131:LEU:C	1:D:133:ALA:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:VAL:CG2	1:D:121:VAL:HG13	2.35	0.57
1:C:125:VAL:HG21	1:C:144:ALA:HB2	1.87	0.56
1:D:65:ILE:O	1:D:100:GLU:HA	2.05	0.56
1:B:124:MET:CA	1:B:127:THR:HG22	2.31	0.56
1:B:3:ILE:HD12	1:B:62:TYR:HB2	1.88	0.56
1:A:141:ASP:O	1:A:145:ILE:HG22	2.06	0.56
1:C:56:THR:HG23	2:C:423:HOH:O	2.06	0.56
1:B:63:PHE:HB2	1:B:96:LEU:HD11	1.87	0.55
1:D:131:LEU:C	1:D:133:ALA:N	2.65	0.55
1:C:97:PRO:HB2	1:C:99:PHE:HE1	1.71	0.55
1:D:157:MET:HG2	2:D:380:HOH:O	2.07	0.55
1:A:65:ILE:HD12	1:A:88:ILE:HG12	1.88	0.55
1:A:129:LEU:O	1:A:131:LEU:N	2.40	0.55
1:B:93:ASN:ND2	1:D:45:LYS:HZ3	2.04	0.55
1:C:116:ALA:HA	1:C:120:GLN:OE1	2.07	0.55
1:A:3:ILE:HD12	1:A:3:ILE:H	1.71	0.55
1:A:3:ILE:HD12	1:A:3:ILE:N	2.22	0.55
1:A:40:LEU:HA	1:A:43:ARG:HH11	1.71	0.55
1:C:52:THR:CG2	1:C:90:ALA:HB1	2.36	0.55
1:C:97:PRO:HB2	1:C:99:PHE:CE1	2.42	0.54
1:C:136:GLN:HG3	1:C:137:ALA:N	2.23	0.54
1:B:17:VAL:HG11	1:B:58:PHE:CE1	2.42	0.54
1:C:72:LYS:H	1:C:72:LYS:HD2	1.73	0.54
1:B:15:TYR:CZ	1:B:31:GLY:HA3	2.42	0.54
1:A:23:ARG:NH2	2:A:259:HOH:O	2.40	0.54
1:B:118:LYS:H	1:B:118:LYS:CD	2.20	0.54
1:C:53:GLU:HG2	1:C:54:ILE:N	2.22	0.54
1:A:122:GLN:HG2	1:A:140:ALA:HB3	1.89	0.54
1:C:136:GLN:HG3	1:C:137:ALA:H	1.73	0.54
1:D:15:TYR:CE2	1:D:31:GLY:HA3	2.43	0.54
1:C:140:ALA:HA	1:C:143:LEU:HB2	1.90	0.54
1:A:40:LEU:HB3	1:A:41:PRO:HD3	1.89	0.53
1:C:126:ARG:HH22	1:C:135:PRO:HB3	1.71	0.53
1:D:113:ILE:HD12	1:D:114:GLY:H	1.70	0.53
1:A:117:GLU:H	1:A:120:GLN:HE21	1.56	0.53
1:B:126:ARG:HA	1:B:131:LEU:HD23	1.90	0.53
1:B:83:ALA:HA	2:B:327:HOH:O	2.07	0.53
1:C:11:ARG:HG2	1:C:11:ARG:HH11	1.74	0.53
1:B:93:ASN:ND2	1:D:45:LYS:HZ2	2.07	0.53
1:C:65:ILE:O	1:C:100:GLU:HA	2.09	0.53
1:C:80:LEU:O	1:C:84:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:130:LYS:C	2.51	0.53
1:C:139:ALA:C	1:C:143:LEU:HD12	2.34	0.53
1:D:107:LYS:O	1:D:111:VAL:HG22	2.07	0.53
1:B:35:THR:HG21	1:B:47:ILE:CD1	2.38	0.52
1:B:92:VAL:HG12	2:B:312:HOH:O	2.09	0.52
1:B:126:ARG:NH2	1:B:133:ALA:O	2.42	0.52
1:C:6:ILE:HG22	1:C:65:ILE:CG2	2.38	0.52
1:B:35:THR:HG21	2:B:256:HOH:O	2.09	0.52
1:C:17:VAL:HG11	1:C:58:PHE:CG	2.44	0.52
1:A:127:THR:O	1:A:128:LEU:C	2.52	0.52
1:B:6:ILE:HD12	1:B:7:ASP:H	1.74	0.52
1:B:45:LYS:O	1:B:45:LYS:HD2	2.09	0.52
1:C:40:LEU:O	1:C:41:PRO:C	2.52	0.52
1:A:4:LEU:HD23	1:A:63:PHE:CD2	2.45	0.52
1:B:68:VAL:HG23	1:B:84:ARG:HH11	1.75	0.52
1:C:54:ILE:HG23	1:C:58:PHE:HD2	1.74	0.52
1:A:143:LEU:O	1:A:147:ILE:HG13	2.10	0.52
1:C:72:LYS:HE3	1:C:72:LYS:HA	1.92	0.52
1:B:72:LYS:HG3	1:B:73:ASN:OD1	2.10	0.51
1:C:107:LYS:O	1:C:108:GLN:C	2.53	0.51
1:A:40:LEU:HB2	1:A:43:ARG:NH1	2.24	0.51
1:B:113:ILE:HG23	1:B:116:ALA:H	1.75	0.51
1:B:93:ASN:HD22	1:D:45:LYS:HZ3	1.58	0.51
1:A:34:ARG:HB3	1:A:36:LYS:HD3	1.93	0.51
1:C:17:VAL:HG11	1:C:58:PHE:HB3	1.93	0.51
1:D:47:ILE:HB	1:D:86:VAL:HG11	1.92	0.51
1:D:111:VAL:HG12	1:D:124:MET:CG	2.41	0.51
1:A:88:ILE:O	1:A:92:VAL:HG23	2.11	0.50
1:C:136:GLN:C	1:C:138:ASP:H	2.19	0.50
1:B:103:ALA:O	1:B:106:VAL:HG13	2.12	0.50
1:C:103:ALA:O	1:C:106:VAL:HG22	2.12	0.50
1:B:130:LYS:HA	1:B:130:LYS:CE	2.37	0.50
1:C:52:THR:O	1:C:56:THR:HB	2.12	0.50
1:A:156:ALA:O	1:A:157:MET:C	2.54	0.50
1:D:24:GLN:HE21	1:D:24:GLN:C	2.20	0.50
1:D:67:GLN:HB2	1:D:69:PHE:CE2	2.47	0.49
1:A:48:TYR:CE2	1:A:89:VAL:HG13	2.46	0.49
1:A:75:ASP:O	1:A:79:LYS:HG3	2.12	0.49
1:C:17:VAL:HG11	1:C:58:PHE:CB	2.43	0.49
1:B:89:VAL:HA	1:B:92:VAL:CG2	2.41	0.49
1:D:130:LYS:O	1:D:132:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:THR:O	1:C:149:HIS:C	2.55	0.49
1:A:86:VAL:O	1:A:89:VAL:HG12	2.13	0.49
1:C:66:GLU:HA	1:C:101:TYR:O	2.13	0.49
1:C:84:ARG:NH2	1:C:100:GLU:OE2	2.46	0.49
1:C:107:LYS:HE2	1:C:116:ALA:O	2.13	0.49
1:D:69:PHE:O	1:D:71:ALA:N	2.45	0.49
1:B:40:LEU:HB3	2:D:325:HOH:O	2.12	0.48
1:C:55:ILE:CG2	1:C:94:GLN:HG3	2.27	0.48
1:D:20:GLN:HE21	1:D:23:ARG:CA	2.24	0.48
1:A:4:LEU:HD23	1:A:63:PHE:HD2	1.78	0.48
1:D:157:MET:O	1:D:158:GLN:C	2.55	0.48
1:D:23:ARG:HH11	1:D:23:ARG:HG3	1.78	0.48
1:B:122:GLN:O	1:B:126:ARG:HG3	2.13	0.48
1:C:53:GLU:O	1:C:54:ILE:C	2.57	0.48
1:B:21:VAL:HA	2:B:414:HOH:O	2.14	0.48
1:C:55:ILE:HG21	1:C:94:GLN:CG	2.26	0.48
1:A:117:GLU:H	1:A:120:GLN:NE2	2.11	0.48
1:A:81:GLY:O	1:C:82:GLN:HA	2.14	0.48
1:C:69:PHE:HE2	1:C:104:ARG:HB2	1.75	0.47
1:C:136:GLN:CG	1:C:137:ALA:H	2.26	0.47
1:D:102:ALA:O	1:D:105:GLN:N	2.43	0.47
1:A:1:ALA:HB3	1:A:61:ASP:OD2	2.14	0.47
1:B:2:ILE:HG23	1:B:17:VAL:HG23	1.96	0.47
1:B:44:LEU:HG	1:B:86:VAL:HG21	1.96	0.47
1:B:104:ARG:HH11	1:B:104:ARG:CG	2.26	0.47
1:B:96:LEU:HA	1:B:97:PRO:HD3	1.72	0.47
1:C:4:LEU:HD13	1:C:54:ILE:HG21	1.96	0.47
1:C:131:LEU:C	1:C:133:ALA:N	2.72	0.47
1:D:20:GLN:OE1	1:D:150:CYS:HB3	2.15	0.47
1:A:122:GLN:O	1:A:126:ARG:HG2	2.15	0.47
1:C:4:LEU:CD1	1:C:6:ILE:HD12	2.30	0.47
1:D:148:THR:O	1:D:149:HIS:C	2.57	0.47
1:A:102:ALA:O	1:A:103:ALA:C	2.57	0.47
1:C:69:PHE:CZ	1:C:104:ARG:HD3	2.50	0.47
1:A:21:VAL:N	1:A:24:GLN:O	2.40	0.47
1:B:2:ILE:O	1:B:3:ILE:HD13	2.14	0.47
1:D:9:GLY:H	1:D:13:THR:HG22	1.78	0.46
1:D:137:ALA:HB1	2:D:372:HOH:O	2.14	0.46
1:D:157:MET:SD	1:D:157:MET:N	2.88	0.46
1:D:106:VAL:HG22	1:D:107:LYS:N	2.29	0.46
1:B:33:ILE:HG23	2:B:255:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PRO:HD3	2:D:325:HOH:O	2.16	0.46
1:B:91:ALA:HB1	1:B:96:LEU:HD12	1.97	0.46
1:D:101:TYR:CD2	1:D:152:VAL:HG11	2.50	0.46
1:B:69:PHE:CG	1:B:70:MET:N	2.84	0.46
1:B:151:HIS:HD2	1:B:155:ASN:OD1	1.98	0.46
1:A:92:VAL:HG11	1:C:45:LYS:HB2	1.96	0.46
1:C:67:GLN:CG	1:C:100:GLU:HB3	2.45	0.46
1:A:3:ILE:HG12	1:A:150:CYS:SG	2.56	0.45
1:A:17:VAL:CG2	1:A:28:LEU:HD12	2.44	0.45
1:B:27:TYR:HE1	1:B:30:SER:HB2	1.81	0.45
1:B:75:ASP:HB3	2:B:335:HOH:O	2.16	0.45
1:D:69:PHE:O	1:D:70:MET:C	2.57	0.45
1:D:139:ALA:O	1:D:142:ALA:HB3	2.15	0.45
1:B:3:ILE:HD11	1:B:62:TYR:HD2	1.80	0.45
1:B:111:VAL:HG21	1:B:116:ALA:CB	2.45	0.45
1:C:71:ALA:C	2:C:354:HOH:O	2.59	0.45
1:A:74:ALA:HB2	1:C:74:ALA:HA	1.99	0.45
1:A:125:VAL:HG22	1:A:147:ILE:HD12	1.98	0.45
1:B:40:LEU:CB	1:B:41:PRO:HD3	2.33	0.45
1:B:111:VAL:CG2	1:B:116:ALA:HB2	2.46	0.45
1:D:6:ILE:HG13	1:D:63:PHE:CE2	2.52	0.45
1:A:54:ILE:O	1:A:58:PHE:HB2	2.15	0.45
1:A:110:VAL:O	1:A:124:MET:HG2	2.16	0.45
1:A:20:GLN:HE21	1:A:20:GLN:HB3	1.49	0.45
1:A:78:LEU:HD11	1:C:68:VAL:HG21	1.97	0.45
1:A:127:THR:O	1:A:130:LYS:HE2	2.16	0.45
1:B:14:GLY:HA2	1:B:32:CYS:HA	1.98	0.45
1:A:24:GLN:HE21	1:A:24:GLN:HA	1.82	0.45
1:D:40:LEU:O	1:D:43:ARG:HB3	2.17	0.45
1:B:154:GLN:NE2	2:B:418:HOH:O	2.50	0.44
1:D:3:ILE:HG23	1:D:62:TYR:HB2	1.99	0.44
1:C:131:LEU:O	1:C:133:ALA:N	2.47	0.44
1:B:84:ARG:O	1:B:88:ILE:HG13	2.18	0.44
1:C:49:ALA:O	1:C:53:GLU:HB3	2.17	0.44
1:A:40:LEU:C	1:A:40:LEU:HD12	2.41	0.44
1:B:40:LEU:CD1	1:B:43:ARG:HH21	2.30	0.44
1:B:65:ILE:O	1:B:100:GLU:HA	2.18	0.44
1:B:88:ILE:HG23	1:B:98:VAL:HG11	1.99	0.44
1:C:20:GLN:HG3	2:C:428:HOH:O	2.17	0.44
1:C:66:GLU:OE2	1:C:103:ALA:HA	2.16	0.44
1:A:155:ASN:HD22	1:A:155:ASN:HA	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLU:O	1:C:120:GLN:HG3	2.17	0.44
1:C:126:ARG:HG2	1:C:133:ALA:HB3	1.99	0.44
1:A:133:ALA:O	1:A:135:PRO:HD3	2.18	0.43
1:C:113:ILE:CD1	1:C:115:SER:HB2	2.45	0.43
1:B:17:VAL:HG22	1:B:28:LEU:HB2	2.00	0.43
1:B:146:ALA:O	1:B:147:ILE:C	2.61	0.43
1:D:25:LEU:H	1:D:25:LEU:CD2	2.29	0.43
1:A:108:GLN:HE21	1:A:108:GLN:HB2	1.53	0.43
1:A:126:ARG:HA	1:A:131:LEU:CD2	2.42	0.43
1:B:3:ILE:O	1:B:17:VAL:HA	2.18	0.43
1:B:59:GLN:N	1:B:60:PRO:CD	2.81	0.43
1:B:82:GLN:O	1:B:86:VAL:HG23	2.19	0.43
1:B:134:ASN:N	1:B:134:ASN:HD22	2.17	0.43
1:C:13:THR:O	1:C:33:ILE:N	2.44	0.43
1:B:6:ILE:HD12	1:B:7:ASP:N	2.33	0.43
1:C:140:ALA:HA	1:C:143:LEU:HD12	2.01	0.43
1:A:36:LYS:H	1:A:36:LYS:HG2	1.49	0.43
1:C:106:VAL:O	1:C:110:VAL:HG23	2.19	0.43
1:A:40:LEU:HD12	1:A:40:LEU:O	2.18	0.43
1:B:3:ILE:CD1	1:B:62:TYR:HD2	2.30	0.43
1:B:129:LEU:O	1:B:130:LYS:C	2.62	0.43
1:C:101:TYR:HB2	1:C:145:ILE:CD1	2.49	0.43
1:D:47:ILE:HB	1:D:86:VAL:CG1	2.48	0.43
1:A:104:ARG:HB2	2:A:278:HOH:O	2.19	0.42
1:C:102:ALA:C	1:C:104:ARG:N	2.77	0.42
1:D:9:GLY:O	1:D:13:THR:HG22	2.19	0.42
1:A:34:ARG:HB3	1:A:36:LYS:CD	2.49	0.42
1:B:39:ASP:OD2	1:B:42:SER:OG	2.25	0.42
1:C:136:GLN:O	2:C:350:HOH:O	2.21	0.42
1:D:39:ASP:O	1:D:40:LEU:C	2.61	0.42
1:C:72:LYS:HD2	1:C:72:LYS:N	2.32	0.42
1:C:134:ASN:N	1:C:135:PRO:CD	2.81	0.42
1:D:55:ILE:HG12	1:D:96:LEU:HD11	2.01	0.42
1:C:88:ILE:O	1:C:91:ALA:HB3	2.19	0.42
1:C:96:LEU:HA	1:C:97:PRO:HD3	1.81	0.42
1:A:2:ILE:CG2	1:A:60:PRO:HA	2.49	0.42
1:A:152:VAL:HG12	1:A:152:VAL:O	2.20	0.42
1:B:110:VAL:HG21	1:B:144:ALA:HB1	2.00	0.42
1:A:84:ARG:NH1	1:C:82:GLN:OE1	2.52	0.42
1:C:111:VAL:HG21	1:C:116:ALA:CB	2.49	0.42
1:C:125:VAL:CG2	1:C:144:ALA:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD12	1:A:44:LEU:HG	2.02	0.42
1:A:3:ILE:CD1	1:A:150:CYS:SG	3.08	0.41
1:C:143:LEU:O	1:C:146:ALA:HB3	2.20	0.41
1:A:142:ALA:HA	1:A:145:ILE:CG2	2.50	0.41
1:A:142:ALA:O	1:A:145:ILE:HG23	2.20	0.41
1:A:118:LYS:HA	1:A:121:VAL:HB	2.02	0.41
1:A:2:ILE:HG22	1:A:60:PRO:HA	2.02	0.41
1:B:2:ILE:C	1:B:3:ILE:HD13	2.45	0.41
1:C:129:LEU:CB	1:C:131:LEU:HG	2.50	0.41
1:B:54:ILE:HG23	1:B:58:PHE:CE2	2.56	0.41
1:C:101:TYR:HB2	1:C:145:ILE:HD11	2.03	0.41
1:D:43:ARG:O	1:D:47:ILE:HG13	2.20	0.41
1:A:48:TYR:HD2	1:A:86:VAL:HG13	1.85	0.41
1:B:55:ILE:HG21	1:B:94:GLN:HG3	2.03	0.41
1:D:5:GLY:HA3	1:D:142:ALA:O	2.20	0.41
1:D:131:LEU:HB3	1:D:133:ALA:HB3	2.03	0.41
1:A:37:VAL:O	1:A:43:ARG:HG3	2.21	0.41
1:A:55:ILE:HG21	1:A:94:GLN:HG3	2.03	0.41
1:A:81:GLY:O	1:C:82:GLN:HG2	2.21	0.41
1:B:11:ARG:NH2	1:B:36:LYS:HG2	2.36	0.41
1:C:111:VAL:CG1	1:C:121:VAL:HA	2.51	0.41
1:D:19:ARG:HD2	1:D:28:LEU:HD11	2.01	0.41
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.85	0.41
1:A:126:ARG:HB3	1:A:131:LEU:O	2.21	0.41
1:C:78:LEU:O	1:C:82:GLN:HG3	2.21	0.41
1:A:6:ILE:C	1:A:8:PRO:HD3	2.46	0.40
1:B:106:VAL:O	1:B:107:LYS:C	2.64	0.40
1:B:148:THR:O	1:B:149:HIS:C	2.63	0.40
1:C:33:ILE:HG22	1:C:35:THR:CG2	2.48	0.40
1:A:67:GLN:HG3	1:A:100:GLU:HB3	2.02	0.40
1:A:82:GLN:HG2	1:C:81:GLY:O	2.22	0.40
1:B:11:ARG:HH21	1:B:36:LYS:HE3	1.82	0.40
1:B:84:ARG:O	1:B:85:GLY:C	2.65	0.40
1:C:117:GLU:HG2	1:C:118:LYS:N	2.35	0.40
1:D:101:TYR:CE2	1:D:152:VAL:HG11	2.56	0.40
1:B:65:ILE:HD13	1:B:88:ILE:HD11	2.04	0.40
1:B:68:VAL:HG23	1:B:84:ARG:NH1	2.35	0.40
1:C:52:THR:HG21	2:C:435:HOH:O	2.22	0.40
1:A:36:LYS:HZ3	1:A:36:LYS:HG3	1.78	0.40
1:C:129:LEU:HB2	1:C:131:LEU:HG	2.04	0.40
1:D:11:ARG:HB3	1:D:36:LYS:HZ2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:HG23	1:B:151:HIS:ND1	2.37	0.40
1:C:52:THR:CA	1:C:55:ILE:HD12	2.40	0.40

All (12) 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:D:95:GLU:CD	2:D:371:HOH:O[1_556]	1.61	0.59
1:A:23:ARG:CD	2:B:235:HOH:O[1_554]	1.65	0.55
1:B:130:LYS:CB	2:A:291:HOH:O[1_556]	1.72	0.48
1:A:72:LYS:CE	2:A:268:HOH:O[1_554]	1.77	0.43
1:D:95:GLU:CG	2:D:371:HOH:O[1_556]	2.05	0.15
1:D:95:GLU:OE2	2:D:371:HOH:O[1_556]	2.07	0.13
1:A:72:LYS:NZ	2:A:268:HOH:O[1_554]	2.11	0.09
1:B:130:LYS:O	2:A:291:HOH:O[1_556]	2.12	0.08
2:A:273:HOH:O	2:D:214:HOH:O[2_656]	2.13	0.07
1:D:95:GLU:OE1	2:D:371:HOH:O[1_556]	2.15	0.05
1:C:115:SER:OG	1:C:158:GLN:O[1_554]	2.18	0.02
1:B:133:ALA:N	2:A:284:HOH:O[1_556]	2.19	0.01

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	A	156/158 (99%)	125 (80%)	24 (15%)	7 (4%)	2	2
1	B	156/158 (99%)	139 (89%)	15 (10%)	2 (1%)	9	18
1	C	156/158 (99%)	131 (84%)	20 (13%)	5 (3%)	3	4
1	D	156/158 (99%)	129 (83%)	22 (14%)	5 (3%)	3	4
All	All	624/632 (99%)	524 (84%)	81 (13%)	19 (3%)	3	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	LYS
1	A	157	MET
1	B	116	ALA
1	B	118	LYS
1	C	22	GLY
1	C	135	PRO
1	A	38	ASP
1	A	136	GLN
1	C	156	ALA
1	D	39	ASP
1	D	151	HIS
1	D	152	VAL
1	D	70	MET
1	D	73	ASN
1	A	134	ASN
1	A	23	ARG
1	C	10	SER
1	A	152	VAL
1	C	37	VAL

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	A	125/125 (100%)	91 (73%)	34 (27%)	0	1
1	B	125/125 (100%)	100 (80%)	25 (20%)	1	2
1	C	125/125 (100%)	92 (74%)	33 (26%)	0	1
1	D	125/125 (100%)	96 (77%)	29 (23%)	1	1
All	All	500/500 (100%)	379 (76%)	121 (24%)	1	1

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	6	ILE
1	A	13	THR

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Mol	Chain	Res	Type
1	A	17	VAL
1	A	20	GLN
1	A	21	VAL
1	A	23	ARG
1	A	24	GLN
1	A	33	ILE
1	A	36	LYS
1	A	37	VAL
1	A	39	ASP
1	A	45	LYS
1	A	47	ILE
1	A	59	GLN
1	A	66	GLU
1	A	75	ASP
1	A	76	SER
1	A	78	LEU
1	A	79	LYS
1	A	96	LEU
1	A	106	VAL
1	A	108	GLN
1	A	110	VAL
1	A	111	VAL
1	A	118	LYS
1	A	121	VAL
1	A	125	VAL
1	A	127	THR
1	A	131	LEU
1	A	134	ASN
1	A	145	ILE
1	A	151	HIS
1	A	155	ASN
1	B	6	ILE
1	B	11	ARG
1	B	13	THR
1	B	17	VAL
1	B	26	SER
1	B	33	ILE
1	B	44	LEU
1	B	45	LYS
1	B	59	GLN
1	B	70	MET
1	B	78	LEU

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	92	VAL
1	B	94	GLN
1	B	96	LEU
1	B	106	VAL
1	B	111	VAL
1	B	113	ILE
1	B	118	LYS
1	B	119	SER
1	B	123	HIS
1	B	130	LYS
1	B	136	GLN
1	B	138	ASP
1	B	145	ILE
1	C	6	ILE
1	C	8	PRO
1	C	10	SER
1	C	12	VAL
1	C	20	GLN
1	C	21	VAL
1	C	24	GLN
1	C	28	LEU
1	C	36	LYS
1	C	41	PRO
1	C	43	ARG
1	C	45	LYS
1	C	52	THR
1	C	53	GLU
1	C	54	ILE
1	C	56	THR
1	C	59	GLN
1	C	68	VAL
1	C	72	LYS
1	C	84	ARG
1	C	89	VAL
1	C	95	GLU
1	C	96	LEU
1	C	113	ILE
1	C	118	LYS
1	C	119	SER
1	C	121	VAL
1	C	134	ASN

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Mol	Chain	Res	Type
1	C	138	ASP
1	C	145	ILE
1	C	154	GLN
1	C	155	ASN
1	C	158	GLN
1	D	2	ILE
1	D	3	ILE
1	D	13	THR
1	D	17	VAL
1	D	23	ARG
1	D	24	GLN
1	D	33	ILE
1	D	37	VAL
1	D	57	GLN
1	D	63	PHE
1	D	65	ILE
1	D	67	GLN
1	D	68	VAL
1	D	72	LYS
1	D	78	LEU
1	D	80	LEU
1	D	86	VAL
1	D	89	VAL
1	D	96	LEU
1	D	101	TYR
1	D	106	VAL
1	D	113	ILE
1	D	118	LYS
1	D	120	GLN
1	D	126	ARG
1	D	129	LEU
1	D	131	LEU
1	D	153	SER
1	D	157	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	GLN
1	A	59	GLN
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	108	GLN
1	A	120	GLN
1	A	134	ASN
1	A	155	ASN
1	B	24	GLN
1	B	59	GLN
1	B	93	ASN
1	B	105	GLN
1	B	123	HIS
1	B	134	ASN
1	B	151	HIS
1	B	155	ASN
1	B	158	GLN
1	C	20	GLN
1	C	24	GLN
1	C	59	GLN
1	C	67	GLN
1	C	73	ASN
1	C	93	ASN
1	C	122	GLN
1	C	123	HIS
1	C	151	HIS
1	C	158	GLN
1	D	20	GLN
1	D	24	GLN
1	D	57	GLN
1	D	67	GLN
1	D	73	ASN
1	D	82	GLN
1	D	108	GLN
1	D	155	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.