



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:52 pm GMT

PDB ID : 1HJR  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

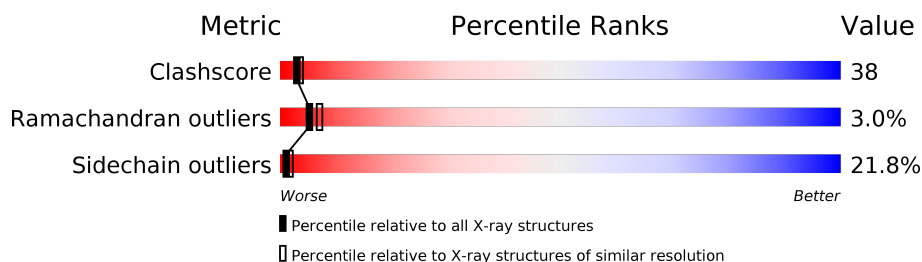
# 1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	
1	C	158	
1	D	158	

## 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.

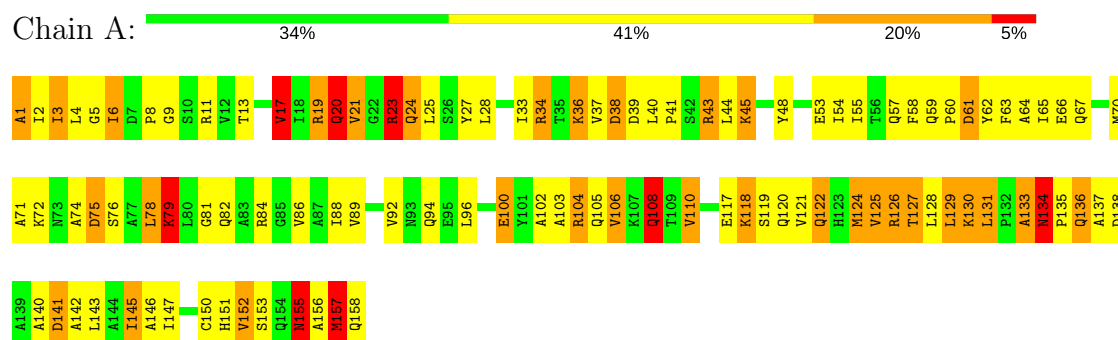
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	47	Total	O	0	0
			47	47		
2	C	40	Total	O	0	0
			40	40		
2	D	53	Total	O	0	0
			53	53		

### 3 Residue-property plots

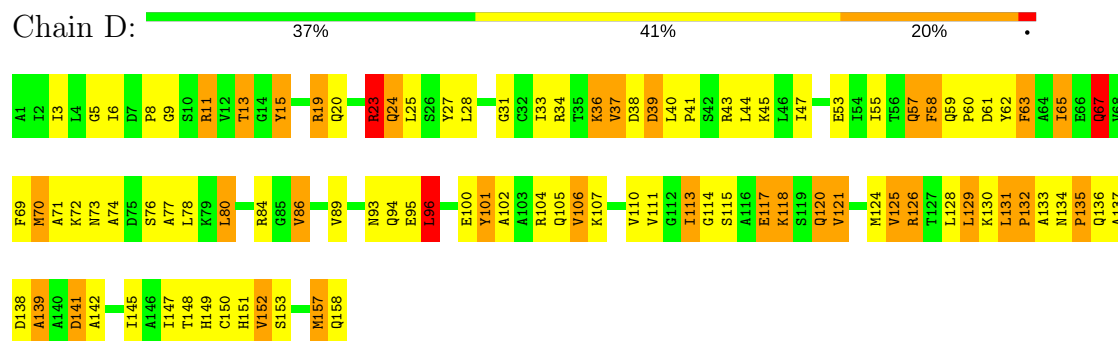
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	27.0	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	A	0.88	0/1209	2.23	46/1639 (2.8%)
1	B	0.89	0/1209	2.26	43/1639 (2.6%)
1	C	0.82	0/1209	2.22	42/1639 (2.6%)
1	D	0.85	0/1209	2.16	53/1639 (3.2%)
All	All	0.86	0/4836	2.22	184/6556 (2.8%)

There are no bond length outliers.

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ARG	NE-CZ-NH2	-23.27	108.67	120.30
1	B	23	ARG	NE-CZ-NH2	-21.91	109.34	120.30
1	A	43	ARG	NE-CZ-NH2	21.24	130.92	120.30
1	C	104	ARG	NE-CZ-NH1	21.10	130.85	120.30
1	A	43	ARG	CD-NE-CZ	18.91	150.07	123.60
1	B	23	ARG	NE-CZ-NH1	17.84	129.22	120.30
1	B	96	LEU	CA-CB-CG	17.82	156.29	115.30
1	C	104	ARG	NE-CZ-NH2	-17.46	111.57	120.30
1	A	104	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	B	19	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	C	133	ALA	C-N-CA	13.98	156.64	121.70
1	D	39	ASP	CB-CG-OD1	-13.68	105.99	118.30
1	C	84	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	C	43	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	C	34	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	A	53	GLU	CA-CB-CG	12.65	141.23	113.40
1	A	23	ARG	CD-NE-CZ	12.14	140.60	123.60
1	D	138	ASP	CB-CG-OD1	11.94	129.05	118.30
1	A	11	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	B	155	ASN	CA-CB-CG	11.55	138.82	113.40
1	A	104	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	C	61	ASP	CB-CG-OD1	11.14	128.32	118.30
1	D	126	ARG	NE-CZ-NH1	11.03	125.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	B	43	ARG	CA-CB-CG	10.66	136.86	113.40
1	A	43	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	B	43	ARG	CD-NE-CZ	10.03	137.64	123.60
1	A	11	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	D	94	GLN	CA-C-N	9.94	139.07	117.20
1	B	19	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	B	100	GLU	OE1-CD-OE2	9.59	134.80	123.30
1	C	133	ALA	CA-C-O	9.26	139.54	120.10
1	D	19	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	43	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	C	38	ASP	CB-CG-OD1	8.73	126.16	118.30
1	A	27	TYR	CB-CG-CD1	8.65	126.19	121.00
1	D	11	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	B	78	LEU	CA-CB-CG	8.36	134.53	115.30
1	B	66	GLU	OE1-CD-OE2	7.98	132.88	123.30
1	B	105	GLN	CA-CB-CG	7.93	130.85	113.40
1	D	117	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	B	155	ASN	N-CA-C	-7.85	89.80	111.00
1	D	135	PRO	C-N-CA	7.75	141.07	121.70
1	C	43	ARG	CA-CB-CG	7.69	130.32	113.40
1	A	155	ASN	CA-C-O	-7.68	103.97	120.10
1	A	17	VAL	CB-CA-C	7.64	125.92	111.40
1	C	34	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	39	ASP	OD1-CG-OD2	7.59	137.73	123.30
1	D	96	LEU	CA-CB-CG	7.49	132.53	115.30
1	A	62	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	D	93	ASN	CB-CA-C	7.35	125.10	110.40
1	D	78	LEU	CA-CB-CG	7.30	132.08	115.30
1	B	100	GLU	CG-CD-OE2	-7.25	103.81	118.30
1	A	1	ALA	CB-CA-C	-7.23	99.26	110.10
1	D	121	VAL	CA-CB-CG1	7.16	121.64	110.90
1	B	156	ALA	N-CA-CB	-7.15	100.09	110.10
1	C	43	ARG	CB-CA-C	7.14	124.68	110.40
1	D	80	LEU	C-N-CA	7.01	137.02	122.30
1	A	1	ALA	N-CA-CB	6.96	119.84	110.10
1	D	38	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	20	GLN	CA-C-O	-6.89	105.64	120.10
1	B	11	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	34	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	141	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	131	LEU	CA-CB-CG	6.73	130.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	GLN	CB-CA-C	6.72	123.84	110.40
1	D	120	GLN	CB-CG-CD	6.72	129.08	111.60
1	C	134	ASN	N-CA-C	-6.72	92.85	111.00
1	A	19	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	131	LEU	N-CA-CB	-6.70	97.00	110.40
1	D	94	GLN	CA-C-O	-6.66	106.12	120.10
1	A	122	GLN	CA-CB-CG	6.65	128.03	113.40
1	A	57	GLN	CA-CB-CG	6.62	127.96	113.40
1	B	96	LEU	N-CA-CB	-6.62	97.17	110.40
1	B	126	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	75	ASP	CB-CG-OD1	6.59	124.24	118.30
1	D	61	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	126	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	89	VAL	CA-CB-CG1	6.55	120.72	110.90
1	A	155	ASN	CA-C-N	6.54	131.59	117.20
1	C	19	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	141	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	C	104	ARG	CD-NE-CZ	6.45	132.63	123.60
1	D	23	ARG	CD-NE-CZ	6.45	132.63	123.60
1	C	4	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	1	ALA	O-C-N	6.41	132.96	122.70
1	D	138	ASP	N-CA-CB	6.40	122.13	110.60
1	A	136	GLN	N-CA-C	-6.38	93.78	111.00
1	C	69	PHE	CA-CB-CG	6.37	129.20	113.90
1	A	158	GLN	N-CA-CB	6.36	122.05	110.60
1	D	84	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	135	PRO	CA-C-O	6.31	135.34	120.20
1	D	139	ALA	N-CA-CB	-6.30	101.27	110.10
1	C	137	ALA	C-N-CA	6.30	137.45	121.70
1	D	58	PHE	CA-C-N	6.29	131.03	117.20
1	A	27	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	D	11	ARG	CD-NE-CZ	6.24	132.33	123.60
1	D	39	ASP	CA-CB-CG	-6.22	99.71	113.40
1	B	26	SER	N-CA-CB	6.21	119.82	110.50
1	A	11	ARG	CD-NE-CZ	6.21	132.29	123.60
1	C	145	ILE	CA-CB-CG2	6.19	123.28	110.90
1	B	156	ALA	N-CA-C	6.16	127.64	111.00
1	C	105	GLN	CA-CB-CG	6.08	126.77	113.40
1	B	67	GLN	CA-CB-CG	6.07	126.76	113.40
1	B	83	ALA	CA-C-O	-6.05	107.40	120.10
1	B	104	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A	138	ASP	CB-CG-OD2	-6.04	112.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ALA	CA-C-N	-6.03	103.92	117.20
1	B	138	ASP	C-N-CA	6.02	136.76	121.70
1	C	43	ARG	NH1-CZ-NH2	-6.02	112.78	119.40
1	B	63	PHE	CA-CB-CG	6.01	128.33	113.90
1	B	83	ALA	N-CA-CB	5.99	118.49	110.10
1	D	53	GLU	CG-CD-OE1	5.98	130.27	118.30
1	A	137	ALA	N-CA-C	-5.97	94.89	111.00
1	C	145	ILE	CB-CA-C	5.95	123.50	111.60
1	B	39	ASP	N-CA-CB	-5.92	99.94	110.60
1	A	126	ARG	CD-NE-CZ	5.87	131.81	123.60
1	D	74	ALA	N-CA-CB	-5.84	101.92	110.10
1	B	131	LEU	N-CA-C	5.84	126.76	111.00
1	A	70	MET	C-N-CA	5.81	136.22	121.70
1	C	53	GLU	CA-CB-CG	5.80	126.16	113.40
1	C	61	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	128	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	A	79	LYS	CD-CE-NZ	5.73	124.88	111.70
1	B	155	ASN	N-CA-CB	5.68	120.83	110.60
1	A	146	ALA	CB-CA-C	5.66	118.59	110.10
1	A	105	GLN	CA-CB-CG	5.65	125.83	113.40
1	B	156	ALA	C-N-CA	5.62	135.76	121.70
1	B	138	ASP	CA-C-O	5.60	131.86	120.10
1	D	34	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	129	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	133	ALA	C-N-CA	5.54	135.54	121.70
1	C	72	LYS	CA-C-O	-5.54	108.48	120.10
1	D	136	GLN	N-CA-C	-5.54	96.05	111.00
1	A	105	GLN	N-CA-CB	5.51	120.52	110.60
1	D	120	GLN	CA-CB-CG	5.50	125.50	113.40
1	A	62	TYR	O-C-N	5.47	131.46	122.70
1	C	127	THR	N-CA-CB	5.44	120.63	110.30
1	D	125	VAL	CA-CB-CG2	5.43	119.05	110.90
1	D	138	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	141	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	63	PHE	O-C-N	5.35	131.26	122.70
1	D	67	GLN	N-CA-CB	5.35	120.22	110.60
1	C	129	LEU	O-C-N	5.34	131.25	122.70
1	C	135	PRO	N-CD-CG	-5.34	95.18	103.20
1	A	71	ALA	N-CA-CB	5.34	117.58	110.10
1	D	104	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	141	ASP	CB-CA-C	5.34	121.07	110.40
1	C	66	GLU	CA-CB-CG	5.33	125.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	GLY	O-C-N	5.31	131.19	122.70
1	D	134	ASN	N-CA-C	-5.30	96.70	111.00
1	C	72	LYS	CA-C-N	5.28	128.82	117.20
1	B	135	PRO	C-N-CA	5.26	134.86	121.70
1	C	25	LEU	CB-CA-C	5.25	120.18	110.20
1	D	27	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	D	121	VAL	CB-CA-C	5.20	121.28	111.40
1	D	37	VAL	N-CA-C	-5.19	96.97	111.00
1	B	34	ARG	CG-CD-NE	5.18	122.67	111.80
1	C	94	GLN	N-CA-CB	5.16	119.89	110.60
1	D	19	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	123	HIS	O-C-N	5.16	130.95	122.70
1	B	78	LEU	O-C-N	5.15	130.94	122.70
1	B	38	ASP	C-N-CA	5.13	134.53	121.70
1	D	76	SER	O-C-N	5.13	130.91	122.70
1	B	157	MET	N-CA-C	5.13	124.84	111.00
1	D	134	ASN	N-CA-CB	5.12	119.81	110.60
1	C	19	ARG	N-CA-CB	5.11	119.80	110.60
1	D	96	LEU	O-C-N	5.11	130.81	121.10
1	A	124	MET	N-CA-CB	-5.10	101.41	110.60
1	A	38	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	15	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	96	LEU	CB-CA-C	5.05	119.81	110.20
1	D	58	PHE	CA-C-O	-5.05	109.49	120.10
1	A	129	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	108	GLN	N-CA-CB	5.05	119.69	110.60
1	C	132	PRO	N-CA-C	-5.04	99.00	112.10
1	A	43	ARG	NH1-CZ-NH2	-5.03	113.86	119.40
1	A	61	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	71	ALA	C-N-CA	5.02	134.25	121.70
1	D	132	PRO	CB-CA-C	5.02	124.55	112.00
1	A	100	GLU	CG-CD-OE2	5.01	128.32	118.30
1	C	2	ILE	N-CA-CB	5.01	122.32	110.80
1	D	76	SER	CA-C-O	-5.00	109.60	120.10
1	D	84	ARG	CD-NE-CZ	-5.00	116.60	123.60

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	91	3
1	B	1192	0	1232	113	3
1	C	1192	0	1231	108	1
1	D	1192	0	1231	71	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	4926	366	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 38.

All (366) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:GLN:HA	1:B:94:GLN:NE2	2.04	0.73
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:B:126:ARG:HH22	1:B:135:PRO:HG3	1.57	0.69
1:A:130:LYS:CB	1:B:155:ASN:HD22	2.00	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:118:LYS:H	1:D:118:LYS:HD2	1.58	0.68
1:D:58:PHE:O	1:D:60:PRO:HD3	1.94	0.68
1:A:25:LEU:HD23	1:A:129:LEU:HD23	1.75	0.68
1:A:6:ILE:HG23	1:A:8:PRO:HD3	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:O	1:A:131:LEU:HG	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:129:LEU:O	1:A:131:LEU:HB3	1.99	0.62
1:D:67:GLN:HE21	1:D:67:GLN:HA	1.65	0.61
1:A:130:LYS:HB2	1:B:155:ASN:ND2	2.02	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:HA	1:D:57:GLN:HE21	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:B:93:ASN:ND2	1:D:45:LYS:HZ3	1.98	0.61
1:C:25:LEU:HD13	2:C:428:HOH:O	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD	1:D:118:LYS:H	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:128:LEU:HD13	1:D:147:ILE:HD13	1.85	0.58
1:D:15:TYR:CZ	1:D:31:GLY:HA3	2.38	0.58
1:A:134:ASN:ND2	1:A:134:ASN:H	2.00	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:N	1:B:69:PHE:CD1	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: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:A:118:LYS:O	1:A:119:SER:C	2.41	0.57
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:B:93:ASN:HD22	1:D:45:LYS:HZ3	1.52	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:C:158:GLN:HE21	1:C:158:GLN:C	2.09	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: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:129:LEU:O	1:A:131:LEU:N	2.40	0.55
1:A:65:ILE:HD12	1:A:88:ILE:HG12	1.88	0.55
1:C:116:ALA:HA	1:C:120:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:H	1:A:3:ILE:HD12	1.71	0.55
1:A:3:ILE:N	1:A:3:ILE:HD12	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:136:GLN:HG3	1:C:137:ALA:N	2.23	0.54
1:C:97:PRO:HB2	1:C:99:PHE:CE1	2.42	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:CD	1:B:118:LYS:H	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: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
1:D:107:LYS:O	1:D:111:VAL:HG22	2.07	0.53
1:B:126:ARG:NH2	1:B:133:ALA:O	2.42	0.52
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: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:B:45:LYS:O	1:B:45:LYS:HD2	2.09	0.52
1:B:6:ILE:HD12	1:B:7:ASP:H	1.74	0.52
1:D:131:LEU:C	1:D:133:ALA:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:111:VAL:HG12	1:D:124:MET:CG	2.41	0.51
1:D:47:ILE:HB	1:D:86:VAL:HG11	1.92	0.51
1:A:88:ILE:O	1:A:92:VAL:HG23	2.11	0.50
1:B:103:ALA:O	1:B:106:VAL:HG13	2.12	0.50
1:D:131:LEU:C	1:D:133:ALA:N	2.65	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: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
1:A:86:VAL:O	1:A:89:VAL:HG12	2.13	0.49
1:C:84:ARG:NH2	1:C:100:GLU:OE2	2.46	0.49
1:C:66:GLU:HA	1:C:101:TYR:O	2.13	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:23:ARG:HG3	1:D:23:ARG:HH11	1.78	0.48
1:B:122:GLN:O	1:B:126:ARG:HG3	2.13	0.48
1:A:129:LEU:O	1:A:130:LYS:C	2.51	0.48
1:C:139:ALA:C	1:C:143:LEU:HD12	2.34	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:127:THR:O	1:A:128:LEU:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HG	1:B:86:VAL:HG21	1.96	0.47
1:C:40:LEU:O	1:C:41:PRO:C	2.52	0.47
1:B:104:ARG:CG	1:B:104:ARG:HH11	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: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:107:LYS:O	1:C:108:GLN:C	2.53	0.47
1:C:4:LEU:CD1	1:C:6:ILE:HD12	2.30	0.47
1:C:69:PHE:CZ	1:C:104:ARG:HD3	2.50	0.47
1:D:106:VAL:HG22	1:D:107:LYS:N	2.29	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:N	1:D:157:MET:SD	2.88	0.46
1:B:33:ILE:HG23	2:B:255:HOH:O	2.15	0.46
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:B:93:ASN:ND2	1:D:45:LYS:HZ2	2.13	0.46
1:C:67:GLN:CG	1:C:100:GLU:HB3	2.45	0.46
1:C:136:GLN:C	1:C:138:ASP:H	2.19	0.46
1:A:92:VAL:HG11	1:C:45:LYS:HB2	1.96	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:139:ALA:O	1:D:142:ALA:HB3	2.15	0.45
1:B:111:VAL:HG21	1:B:116:ALA:CB	2.45	0.45
1:B:3:ILE:HD11	1:B:62:TYR:HD2	1.80	0.45
1:A:125:VAL:HG22	1:A:147:ILE:HD12	1.98	0.45
1:B:111:VAL:CG2	1:B:116:ALA:HB2	2.46	0.45
1:B:40:LEU:CB	1:B:41:PRO:HD3	2.33	0.45
1:A:74:ALA:HB2	1:C:74:ALA:HA	1.99	0.45
1:A:156:ALA:O	1:A:157:MET:C	2.54	0.45
1:D:24:GLN:HE21	1:D:24:GLN:C	2.20	0.45
1:D:6:ILE:HG13	1:D:63:PHE:CE2	2.52	0.45
1:A:110:VAL:O	1:A:124:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:O	1:A:58:PHE:HB2	2.15	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:HA	1:A:24:GLN:HE21	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:C:148:THR:O	1:C:149:HIS:C	2.55	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:B:65:ILE:O	1:B:100:GLU:HA	2.18	0.44
1:B:40:LEU:CD1	1:B:43:ARG:HH21	2.30	0.44
1:B:88:ILE:HG23	1:B:98:VAL:HG11	1.99	0.44
1:C:66:GLU:OE2	1:C:103:ALA:HA	2.16	0.44
1:C:20:GLN:HG3	2:C:428:HOH:O	2.17	0.44
1:A:155:ASN:HA	1:A:155:ASN:HD22	1.60	0.44
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:D:157:MET:O	1:D:158:GLN:C	2.55	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:C:53:GLU:O	1:C:54:ILE:C	2.57	0.43
1:D:25:LEU:CD2	1:D:25:LEU:H	2.29	0.43
1:A:108:GLN:HB2	1:A:108:GLN:HE21	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:HD22	1:B:134:ASN:N	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:O	1:A:40:LEU:HD12	2.18	0.43
1:B:3:ILE:CD1	1:B:62:TYR:HD2	2.30	0.43
1:C:101:TYR:HB2	1:C:145:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:134:ASN:N	1:C:135:PRO:CD	2.81	0.42
1:C:72:LYS:HD2	1:C:72:LYS:N	2.32	0.42
1:D:55:ILE:HG12	1:D:96:LEU:HD11	2.01	0.42
1:C:131:LEU:C	1:C:133:ALA:N	2.72	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:D:148:THR:O	1:D:149:HIS:C	2.57	0.42
1:A:102:ALA:O	1:A:103:ALA:C	2.57	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
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:C:117:GLU:HG2	1:C:118:LYS:N	2.35	0.41
1:A:2:ILE:HG22	1:A:60:PRO:HA	2.02	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:131:LEU:HB3	1:D:133:ALA:HB3	2.03	0.41
1:D:5:GLY:HA3	1:D:142:ALA:O	2.20	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: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:HA	1:D:44:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:O	1:A:43:ARG:HG3	2.21	0.41
1:B:11:ARG:NH2	1:B:36:LYS:HG2	2.36	0.41
1:D:69:PHE:O	1:D:70:MET:C	2.57	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:C:33:ILE:HG22	1:C:35:THR:CG2	2.48	0.40
1:C:71:ALA:C	2:C:354:HOH:O	2.59	0.40
1:A:67:GLN:HG3	1:A:100:GLU:HB3	2.02	0.40
1:B:11:ARG:HH21	1:B:36:LYS:HE3	1.82	0.40
1:A:82:GLN:HG2	1:C:81:GLY:O	2.22	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
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

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/158 (99%)	125 (80%)	24 (15%)	7 (4%)	3	3
1	B	156/158 (99%)	139 (89%)	15 (10%)	2 (1%)	14	25
1	C	156/158 (99%)	131 (84%)	20 (13%)	5 (3%)	5	6
1	D	156/158 (99%)	129 (83%)	22 (14%)	5 (3%)	5	6
All	All	624/632 (99%)	524 (84%)	81 (13%)	19 (3%)	5	7

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%)	94 (75%)	31 (25%)	1	1
1	B	125/125 (100%)	104 (83%)	21 (17%)	2	4
1	C	125/125 (100%)	93 (74%)	32 (26%)	0	1
1	D	125/125 (100%)	100 (80%)	25 (20%)	1	2
All	All	500/500 (100%)	391 (78%)	109 (22%)	1	2

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	6	ILE
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	39	ASP
1	A	45	LYS
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	118	LYS
1	A	125	VAL
1	A	127	THR

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Mol	Chain	Res	Type
1	A	131	LEU
1	A	134	ASN
1	A	145	ILE
1	A	151	HIS
1	A	153	SER
1	A	155	ASN
1	A	157	MET
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	45	LYS
1	B	70	MET
1	B	78	LEU
1	B	84	ARG
1	B	92	VAL
1	B	94	GLN
1	B	96	LEU
1	B	106	VAL
1	B	113	ILE
1	B	118	LYS
1	B	119	SER
1	B	134	ASN
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	19	ARG
1	C	20	GLN
1	C	21	VAL
1	C	24	GLN
1	C	28	LEU
1	C	34	ARG
1	C	41	PRO
1	C	43	ARG
1	C	45	LYS
1	C	52	THR

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Mol	Chain	Res	Type
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	119	SER
1	C	126	ARG
1	C	134	ASN
1	C	138	ASP
1	C	154	GLN
1	C	155	ASN
1	C	158	GLN
1	D	13	THR
1	D	23	ARG
1	D	24	GLN
1	D	33	ILE
1	D	36	LYS
1	D	37	VAL
1	D	57	GLN
1	D	63	PHE
1	D	65	ILE
1	D	67	GLN
1	D	72	LYS
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

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Mol	Chain	Res	Type
1	D	157	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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
1	A	108	GLN
1	A	120	GLN
1	A	134	ASN
1	A	155	ASN
1	B	24	GLN
1	B	57	GLN
1	B	93	ASN
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	67	GLN
1	C	73	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

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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.