



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:14 PM GMT

PDB ID : 1SRD  
Title : Three-dimensional structure of CU,ZN-superoxide dismutase from spinach at 2.0 Angstroms resolution  
Authors : Kitagawa, Y.; Katsube, Y.  
Deposited on : 1993-04-15  
Resolution : 2.00 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

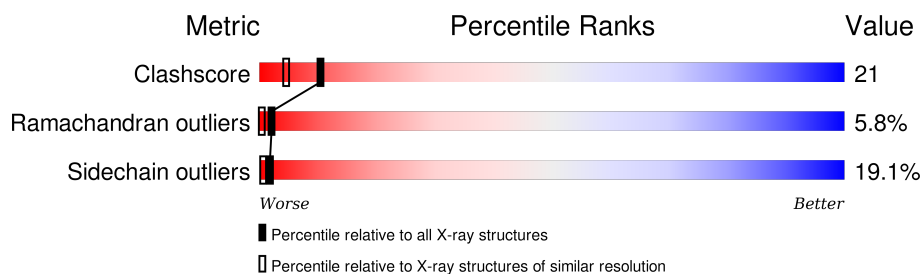
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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	154	<div> <div>46%</div> <div>29%</div> <div>19%</div> <div>6%</div> </div>
1	B	154	<div> <div>49%</div> <div>29%</div> <div>19%</div> <div>.</div> </div>
1	C	154	<div> <div>40%</div> <div>34%</div> <div>17%</div> <div>8%</div> </div>
1	D	154	<div> <div>47%</div> <div>25%</div> <div>19%</div> <div>8%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4524 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 COPPER,ZINC SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1103	675	200	225	3			
1	B	154	Total	C	N	O	S	0	0	0
			1103	675	200	225	3			
1	C	154	Total	C	N	O	S	0	0	0
			1103	675	200	225	3			
1	D	154	Total	C	N	O	S	0	0	0
			1103	675	200	225	3			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

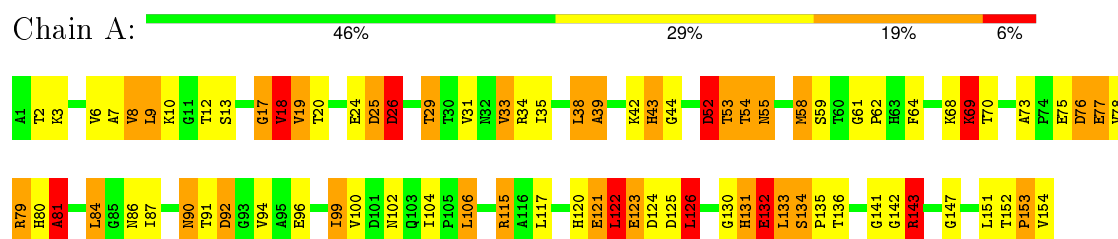
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	26	Total 26	O 26	0	0
4	C	26	Total 26	O 26	0	0
4	D	26	Total 26	O 26	0	0

### 3 Residue-property plots

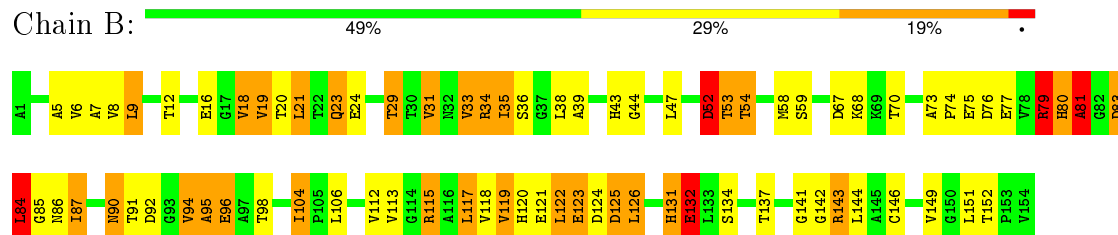
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

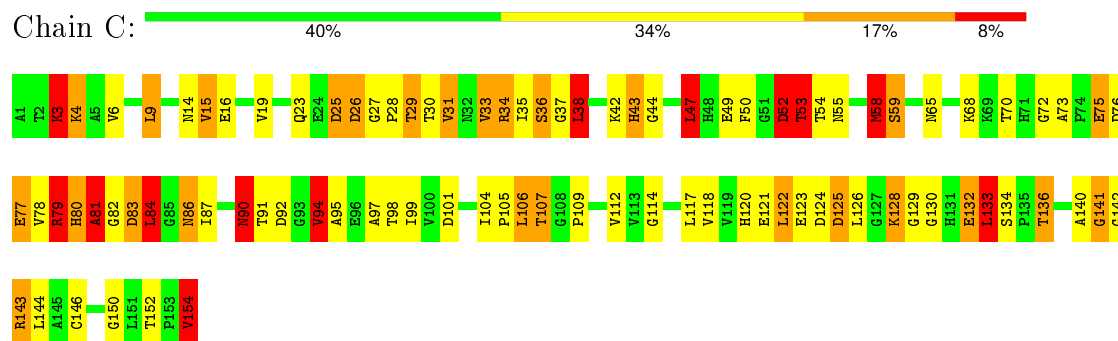
#### • Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



#### • Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

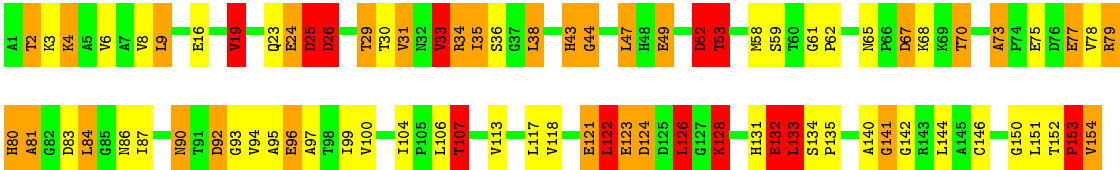


#### • Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



#### • Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.27Å 45.97Å 85.68Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.249 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU

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	1.46	4/1122 (0.4%)	2.56	60/1528 (3.9%)
1	B	1.39	3/1122 (0.3%)	2.14	51/1528 (3.3%)
1	C	1.41	5/1122 (0.4%)	2.18	63/1528 (4.1%)
1	D	1.46	3/1122 (0.3%)	2.32	62/1528 (4.1%)
All	All	1.43	15/4488 (0.3%)	2.31	236/6112 (3.9%)

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	A	0	1
1	D	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	GLY	N-CA	6.77	1.56	1.46
1	A	115	ARG	NE-CZ	-6.76	1.24	1.33
1	D	132	GLU	CD-OE1	-6.19	1.18	1.25
1	C	141	GLY	N-CA	-6.05	1.36	1.46
1	D	141	GLY	N-CA	-5.72	1.37	1.46
1	C	36	SER	CA-CB	5.66	1.61	1.52
1	B	24	GLU	CG-CD	-5.55	1.43	1.51
1	C	43	HIS	C-N	-5.55	1.23	1.33
1	A	13	SER	CA-CB	5.46	1.61	1.52
1	A	130	GLY	N-CA	5.36	1.54	1.46
1	C	16	GLU	CD-OE2	-5.31	1.19	1.25
1	B	96	GLU	CG-CD	-5.15	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	ARG	CD-NE	-5.12	1.37	1.46
1	A	61	GLY	N-CA	5.08	1.53	1.46
1	D	131	HIS	C-N	-5.03	1.22	1.34

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	CD-NE-CZ	31.36	167.51	123.60
1	A	133	LEU	CA-CB-CG	20.27	161.92	115.30
1	A	79	ARG	NE-CZ-NH2	-17.94	111.33	120.30
1	B	143	ARG	CD-NE-CZ	17.30	147.82	123.60
1	A	99	ILE	CB-CG1-CD1	17.25	162.19	113.90
1	D	133	LEU	CA-CB-CG	16.19	152.53	115.30
1	B	115	ARG	CD-NE-CZ	15.43	145.20	123.60
1	D	128	LYS	CA-CB-CG	14.18	144.59	113.40
1	A	115	ARG	NE-CZ-NH1	13.63	127.11	120.30
1	A	115	ARG	NE-CZ-NH2	12.87	126.73	120.30
1	C	133	LEU	CA-CB-CG	12.73	144.57	115.30
1	B	115	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	115	ARG	NH1-CZ-NH2	-12.05	106.14	119.40
1	A	143	ARG	NE-CZ-NH2	11.70	126.15	120.30
1	A	102	ASN	CA-CB-CG	11.02	137.65	113.40
1	A	76	ASP	CB-CG-OD2	10.43	127.68	118.30
1	D	90	ASN	CA-CB-CG	10.41	136.30	113.40
1	D	77	GLU	CB-CG-CD	9.94	141.04	114.20
1	D	133	LEU	CB-CA-C	9.89	129.00	110.20
1	D	38	LEU	CA-CB-CG	9.59	137.36	115.30
1	D	124	ASP	CB-CG-OD1	9.58	126.92	118.30
1	D	52	ASP	CB-CG-OD2	9.47	126.83	118.30
1	C	133	LEU	CB-CA-C	9.45	128.15	110.20
1	B	115	ARG	NH1-CZ-NH2	-9.39	109.07	119.40
1	C	79	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	79	ARG	N-CA-CB	-9.36	93.75	110.60
1	D	83	ASP	CB-CG-OD2	9.36	126.72	118.30
1	C	52	ASP	CB-CG-OD1	9.27	126.64	118.30
1	A	26	ASP	CA-CB-CG	9.16	133.55	113.40
1	D	132	GLU	CA-CB-CG	8.94	133.08	113.40
1	A	143	ARG	CA-CB-CG	8.84	132.85	113.40
1	C	34	ARG	CD-NE-CZ	8.81	135.93	123.60
1	A	76	ASP	CA-CB-CG	8.74	132.63	113.40
1	B	134	SER	N-CA-CB	8.72	123.57	110.50
1	A	55	ASN	CB-CA-C	8.67	127.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	LEU	CA-CB-CG	8.65	135.19	115.30
1	B	81	ALA	N-CA-CB	8.52	122.02	110.10
1	C	125	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	79	ARG	N-CA-CB	-8.35	95.58	110.60
1	C	92	ASP	CB-CG-OD1	-8.31	110.82	118.30
1	D	84	LEU	CA-CB-CG	8.29	134.37	115.30
1	D	79	ARG	CB-CG-CD	8.11	132.67	111.60
1	B	80	HIS	N-CA-CB	8.10	125.18	110.60
1	A	52	ASP	CB-CG-OD1	8.10	125.59	118.30
1	A	134	SER	N-CA-CB	8.10	122.64	110.50
1	B	115	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	34	ARG	CD-NE-CZ	8.04	134.86	123.60
1	C	90	ASN	CA-CB-CG	8.03	131.06	113.40
1	B	87	ILE	CB-CG1-CD1	8.01	136.31	113.90
1	A	106	LEU	CA-CB-CG	7.97	133.64	115.30
1	D	70	THR	CA-CB-CG2	7.85	123.39	112.40
1	A	81	ALA	N-CA-CB	7.83	121.06	110.10
1	C	53	THR	CA-CB-CG2	7.68	123.15	112.40
1	B	52	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	79	ARG	N-CA-CB	-7.61	96.90	110.60
1	A	143	ARG	NH1-CZ-NH2	-7.53	111.12	119.40
1	D	132	GLU	N-CA-CB	7.47	124.04	110.60
1	C	35	ILE	C-N-CA	7.44	140.29	121.70
1	A	69	LYS	CB-CG-CD	7.38	130.78	111.60
1	C	143	ARG	CD-NE-CZ	7.36	133.90	123.60
1	B	94	VAL	CA-CB-CG2	7.31	121.87	110.90
1	C	36	SER	N-CA-CB	-7.23	99.65	110.50
1	D	126	LEU	CA-CB-CG	7.21	131.88	115.30
1	A	125	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	47	LEU	CA-CB-CG	7.10	131.64	115.30
1	B	34	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	C	92	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	121	GLU	CB-CG-CD	6.93	132.91	114.20
1	C	77	GLU	CA-CB-CG	6.92	128.62	113.40
1	B	47	LEU	CA-CB-CG	6.90	131.18	115.30
1	D	84	LEU	CB-CA-C	6.90	123.31	110.20
1	D	107	THR	CA-CB-CG2	6.86	122.00	112.40
1	A	79	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	34	ARG	N-CA-CB	6.85	122.93	110.60
1	C	142	GLY	N-CA-C	-6.84	95.99	113.10
1	D	128	LYS	N-CA-CB	6.83	122.89	110.60
1	D	53	THR	CA-CB-CG2	6.81	121.94	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	CB-CA-C	6.78	123.09	110.20
1	C	34	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	35	ILE	C-N-CA	6.76	138.61	121.70
1	D	19	VAL	CA-CB-CG1	6.70	120.95	110.90
1	B	9	LEU	CB-CG-CD1	6.67	122.34	111.00
1	C	141	GLY	N-CA-C	6.65	129.71	113.10
1	C	125	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	101	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	121	GLU	CA-CB-CG	6.59	127.91	113.40
1	A	13	SER	N-CA-CB	-6.57	100.65	110.50
1	A	102	ASN	CB-CA-C	6.56	123.52	110.40
1	A	38	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	43	HIS	C-N-CA	6.52	136.00	122.30
1	A	43	HIS	CA-CB-CG	-6.52	102.51	113.60
1	D	9	LEU	CB-CG-CD1	6.52	122.09	111.00
1	B	18	VAL	CA-CB-CG1	6.50	120.64	110.90
1	A	92	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	31	VAL	CA-CB-CG2	6.49	120.63	110.90
1	A	131	HIS	C-N-CA	6.45	137.82	121.70
1	C	14	ASN	CA-CB-CG	6.45	127.58	113.40
1	D	122	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	69	LYS	CA-CB-CG	6.41	127.50	113.40
1	D	79	ARG	CD-NE-CZ	6.39	132.55	123.60
1	C	140	ALA	C-N-CA	6.39	135.72	122.30
1	B	84	LEU	CB-CA-C	6.35	122.27	110.20
1	C	52	ASP	OD1-CG-OD2	-6.35	111.24	123.30
1	D	123	GLU	CA-CB-CG	6.33	127.33	113.40
1	A	77	GLU	CA-CB-CG	6.30	127.25	113.40
1	A	126	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	7	ALA	CB-CA-C	6.26	119.48	110.10
1	A	96	GLU	CB-CG-CD	6.24	131.04	114.20
1	D	65	ASN	N-CA-CB	-6.24	99.37	110.60
1	B	119	VAL	CA-CB-CG2	6.24	120.25	110.90
1	C	76	ASP	CA-CB-CG	6.22	127.08	113.40
1	B	76	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	65	ASN	N-CA-CB	-6.19	99.45	110.60
1	D	73	ALA	CB-CA-C	6.18	119.37	110.10
1	D	131	HIS	C-N-CA	6.17	137.12	121.70
1	C	52	ASP	C-N-CA	6.15	137.07	121.70
1	D	25	ASP	CB-CA-C	6.14	122.68	110.40
1	C	86	ASN	N-CA-CB	6.11	121.59	110.60
1	D	131	HIS	O-C-N	-6.11	112.93	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	98	THR	CA-CB-CG2	6.08	120.91	112.40
1	C	44	GLY	N-CA-C	-6.07	97.92	113.10
1	D	77	GLU	CA-CB-CG	6.07	126.74	113.40
1	A	17	GLY	N-CA-C	6.06	128.24	113.10
1	D	35	ILE	C-N-CA	6.04	136.80	121.70
1	D	92	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	67	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	43	HIS	O-C-N	-6.01	112.98	123.20
1	D	25	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	67	ASP	CB-CA-C	5.99	122.39	110.40
1	B	94	VAL	CB-CA-C	5.95	122.71	111.40
1	D	131	HIS	CA-C-N	5.95	130.29	117.20
1	D	44	GLY	N-CA-C	-5.95	98.23	113.10
1	D	52	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	D	77	GLU	CG-CD-OE2	5.93	130.17	118.30
1	D	80	HIS	C-N-CA	5.93	136.53	121.70
1	C	128	LYS	CA-CB-CG	5.90	126.38	113.40
1	B	12	THR	CA-CB-CG2	5.89	120.65	112.40
1	B	5	ALA	CB-CA-C	5.89	118.94	110.10
1	D	83	ASP	OD1-CG-OD2	-5.89	112.11	123.30
1	A	90	ASN	C-N-CA	5.88	136.41	121.70
1	B	96	GLU	CB-CG-CD	5.86	130.03	114.20
1	C	59	SER	CB-CA-C	5.86	121.22	110.10
1	B	90	ASN	CA-CB-CG	5.84	126.24	113.40
1	A	143	ARG	CB-CA-C	5.83	122.06	110.40
1	D	70	THR	CA-CB-OG1	-5.82	96.77	109.00
1	D	79	ARG	N-CA-CB	-5.79	100.17	110.60
1	C	4	LYS	CA-CB-CG	5.79	126.14	113.40
1	C	76	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	26	ASP	CA-CB-CG	5.76	126.08	113.40
1	C	33	VAL	CA-CB-CG2	5.74	119.52	110.90
1	D	34	ARG	CA-CB-CG	5.69	125.92	113.40
1	A	131	HIS	O-C-N	-5.69	113.60	122.70
1	C	122	LEU	CA-CB-CG	5.68	128.38	115.30
1	D	141	GLY	N-CA-C	5.68	127.31	113.10
1	B	54	THR	CA-CB-CG2	5.67	120.34	112.40
1	B	80	HIS	C-N-CA	5.67	135.88	121.70
1	C	95	ALA	N-CA-CB	5.65	118.01	110.10
1	A	132	GLU	N-CA-CB	5.64	120.76	110.60
1	B	31	VAL	CB-CA-C	5.62	122.08	111.40
1	C	83	ASP	CB-CG-OD1	5.62	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ALA	N-CA-CB	-5.61	102.25	110.10
1	C	55	ASN	N-CA-C	-5.59	95.89	111.00
1	C	75	GLU	CG-CD-OE1	5.54	129.38	118.30
1	C	143	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	84	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	53	THR	CA-CB-CG2	5.52	120.13	112.40
1	C	94	VAL	CA-CB-CG1	5.50	119.15	110.90
1	A	44	GLY	N-CA-C	-5.49	99.36	113.10
1	B	34	ARG	N-CA-CB	5.49	120.49	110.60
1	A	52	ASP	CA-CB-CG	5.48	125.46	113.40
1	B	19	VAL	O-C-N	5.48	131.47	122.70
1	C	128	LYS	N-CA-CB	5.48	120.47	110.60
1	C	3	LYS	N-CA-CB	5.48	120.47	110.60
1	A	117	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	81	ALA	N-CA-CB	5.47	117.75	110.10
1	C	29	THR	CA-CB-CG2	5.45	120.03	112.40
1	B	79	ARG	N-CA-C	5.45	125.72	111.00
1	D	153	PRO	CA-C-N	5.45	129.19	117.20
1	A	122	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	44	GLY	N-CA-C	-5.45	99.48	113.10
1	A	18	VAL	CA-CB-CG1	5.39	118.99	110.90
1	C	55	ASN	CB-CA-C	5.39	121.18	110.40
1	D	140	ALA	C-N-CA	5.39	133.62	122.30
1	B	92	ASP	CB-CA-C	5.38	121.16	110.40
1	B	117	LEU	CB-CA-C	5.37	120.41	110.20
1	D	92	ASP	CA-CB-CG	5.37	125.22	113.40
1	B	122	LEU	O-C-N	5.36	131.28	122.70
1	A	121	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	D	33	VAL	CA-CB-CG2	5.34	118.91	110.90
1	B	76	ASP	N-CA-CB	5.33	120.19	110.60
1	D	43	HIS	CA-C-N	5.32	126.84	116.20
1	A	131	HIS	CB-CA-C	5.31	121.03	110.40
1	C	34	ARG	N-CA-CB	5.31	120.16	110.60
1	A	64	PHE	CA-CB-CG	5.30	126.63	113.90
1	C	58	MET	CB-CA-C	5.30	121.00	110.40
1	D	121	GLU	CB-CG-CD	5.28	128.45	114.20
1	C	78	VAL	CA-CB-CG1	5.27	118.81	110.90
1	B	131	HIS	C-N-CA	5.25	134.83	121.70
1	C	134	SER	N-CA-CB	5.25	118.37	110.50
1	D	24	GLU	CG-CD-OE1	-5.24	107.82	118.30
1	C	47	LEU	CB-CA-C	5.23	120.14	110.20
1	B	38	LEU	CB-CA-C	5.22	120.13	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	132	GLU	N-CA-CB	5.21	119.98	110.60
1	B	85	GLY	C-N-CA	5.19	134.67	121.70
1	D	144	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	15	VAL	CA-CB-CG2	5.18	118.67	110.90
1	C	101	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	C	30	THR	CA-CB-CG2	5.17	119.65	112.40
1	A	8	VAL	CA-CB-CG2	5.17	118.66	110.90
1	D	38	LEU	N-CA-CB	-5.17	100.06	110.40
1	D	43	HIS	CA-CB-CG	-5.16	104.84	113.60
1	C	154	VAL	CA-CB-CG1	5.14	118.62	110.90
1	B	95	ALA	N-CA-CB	5.13	117.28	110.10
1	D	134	SER	N-CA-CB	5.13	118.19	110.50
1	A	54	THR	N-CA-CB	5.12	120.03	110.30
1	A	10	LYS	N-CA-CB	5.12	119.81	110.60
1	B	59	SER	CB-CA-C	5.12	119.83	110.10
1	A	58	MET	CA-CB-CG	5.11	121.98	113.30
1	C	38	LEU	N-CA-CB	-5.10	100.19	110.40
1	C	140	ALA	N-CA-CB	-5.10	102.96	110.10
1	B	113	VAL	CB-CA-C	5.10	121.08	111.40
1	C	16	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	B	31	VAL	CA-CB-CG1	5.09	118.53	110.90
1	A	39	ALA	N-CA-CB	-5.08	102.98	110.10
1	D	49	GLU	N-CA-CB	5.07	119.72	110.60
1	D	4	LYS	CA-CB-CG	5.07	124.54	113.40
1	A	76	ASP	OD1-CG-OD2	-5.06	113.68	123.30
1	A	100	VAL	CB-CA-C	5.06	121.01	111.40
1	B	125	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	19	VAL	CA-CB-CG1	5.05	118.47	110.90
1	B	33	VAL	CA-CB-CG2	5.03	118.44	110.90
1	C	49	GLU	N-CA-C	5.01	124.53	111.00
1	A	122	LEU	CB-CA-C	5.01	119.72	110.20
1	D	96	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
1	D	133	LEU	Mainchain

## 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	1103	0	1072	38	5
1	B	1103	0	1074	48	1
1	C	1103	0	1073	64	5
1	D	1103	0	1074	56	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	0	7	0
4	B	26	0	0	13	0
4	C	26	0	0	15	4
4	D	26	0	0	7	1
All	All	4524	0	4293	187	10

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 21.

All (187) 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:C:150:GLY:HA3	4:C:180:HOH:O	1.16	1.26
1:C:50:PHE:CE2	1:D:153:PRO:HG3	1.84	1.12
1:B:118:VAL:HG12	4:B:178:HOH:O	1.51	1.08
1:C:150:GLY:CA	4:C:180:HOH:O	1.86	0.91
1:B:54:THR:HG23	4:B:174:HOH:O	1.74	0.87
1:A:94:VAL:HG13	4:A:158:HOH:O	1.75	0.86
1:C:86:ASN:HD21	1:C:124:ASP:H	1.22	0.86
1:C:52:ASP:OD1	1:D:152:THR:OG1	1.94	0.86
1:D:86:ASN:HD21	1:D:124:ASP:H	1.23	0.85
1:B:121:GLU:HG2	1:B:142:GLY:HA3	1.59	0.82
1:C:54:THR:HG22	1:D:8:VAL:CG2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ASN:ND2	1:C:124:ASP:H	1.81	0.78
4:C:170:HOH:O	1:D:150:GLY:HA3	1.84	0.78
1:C:23:GLN:HB2	1:C:106:LEU:HD23	1.66	0.77
1:B:112:VAL:HA	1:B:115:ARG:HD2	1.66	0.76
1:B:121:GLU:HG3	1:B:122:LEU:HD22	1.70	0.74
1:B:23:GLN:HG3	1:B:29:THR:HG22	1.71	0.72
1:B:118:VAL:CG1	4:B:178:HOH:O	2.21	0.72
1:C:73:ALA:HB2	1:C:126:LEU:HG	1.72	0.72
1:C:87:ILE:HG12	4:C:160:HOH:O	1.90	0.71
1:D:153:PRO:O	1:D:154:VAL:HB	1.88	0.71
1:D:118:VAL:HG22	1:D:146:CYS:HB3	1.72	0.71
1:B:86:ASN:HD21	1:B:124:ASP:H	1.39	0.70
1:C:50:PHE:CD2	1:D:153:PRO:HG3	2.26	0.70
1:A:33:VAL:HG21	1:A:87:ILE:HG21	1.74	0.68
1:C:31:VAL:HG13	1:C:99:ILE:HB	1.75	0.68
1:A:8:VAL:HB	4:A:182:HOH:O	1.92	0.68
1:D:3:LYS:HD2	1:D:106:LEU:HB3	1.76	0.68
1:C:84:LEU:HD11	1:C:104:ILE:HD13	1.75	0.67
1:B:104:ILE:HG22	1:B:112:VAL:HG11	1.75	0.67
1:A:9:LEU:HD21	1:A:19:VAL:HG12	1.75	0.67
1:C:42:LYS:HB3	1:C:123:GLU:HG3	1.79	0.65
1:D:23:GLN:HG3	1:D:29:THR:HG22	1.78	0.65
1:B:6:VAL:HG23	1:B:152:THR:HG21	1.79	0.65
1:D:121:GLU:HG3	1:D:122:LEU:HD13	1.78	0.65
1:C:97:ALA:HB1	1:C:99:ILE:HD11	1.77	0.65
1:D:86:ASN:ND2	1:D:124:ASP:H	1.95	0.64
1:D:30:THR:HG23	1:D:100:VAL:HG22	1.79	0.64
1:C:47:LEU:HD22	1:C:117:LEU:HG	1.80	0.63
1:A:115:ARG:HH11	1:B:151:LEU:HD13	1.64	0.63
1:D:86:ASN:HD21	1:D:124:ASP:N	1.96	0.63
1:A:153:PRO:O	1:A:154:VAL:HB	1.99	0.63
1:C:125:ASP:O	1:C:126:LEU:HB2	1.98	0.62
1:B:8:VAL:HB	4:B:158:HOH:O	1.99	0.62
1:C:50:PHE:HB3	1:D:151:LEU:O	1.99	0.62
1:B:86:ASN:ND2	1:B:124:ASP:H	1.96	0.62
1:C:79:ARG:HG2	4:C:159:HOH:O	2.00	0.62
1:C:118:VAL:HG22	1:C:146:CYS:HB3	1.81	0.61
1:B:33:VAL:HG23	1:B:35:ILE:HD12	1.82	0.61
1:C:52:ASP:HB3	1:C:59:SER:HB2	1.81	0.60
1:D:2:THR:HB	1:D:24:GLU:HG2	1.83	0.60
1:C:118:VAL:HG11	1:C:143:ARG:HG2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HG3	1:C:29:THR:HG22	1.83	0.59
1:B:73:ALA:HB2	1:B:126:LEU:HG	1.84	0.59
1:B:84:LEU:HD11	1:B:104:ILE:HD13	1.85	0.59
1:C:50:PHE:CE2	1:D:153:PRO:CG	2.75	0.58
1:C:53:THR:N	4:C:157:HOH:O	2.37	0.58
1:B:81:ALA:N	4:B:161:HOH:O	2.38	0.57
1:B:19:VAL:HG21	1:B:117:LEU:HD13	1.87	0.56
1:B:21:LEU:HD21	1:B:117:LEU:HD11	1.86	0.56
1:C:143:ARG:HG3	4:C:175:HOH:O	2.06	0.56
1:A:43:HIS:O	1:A:123:GLU:HA	2.06	0.56
1:B:121:GLU:HB3	1:B:144:LEU:HG	1.87	0.55
1:D:35:ILE:HG22	1:D:38:LEU:HD22	1.87	0.55
1:C:81:ALA:N	4:C:159:HOH:O	2.38	0.55
1:D:70:THR:HB	1:D:78:VAL:HG12	1.87	0.55
1:C:54:THR:HG22	1:D:8:VAL:HG22	1.87	0.55
1:D:43:HIS:O	1:D:123:GLU:HA	2.06	0.55
1:C:25:ASP:O	1:C:26:ASP:HB2	2.07	0.55
1:D:135:PRO:HD3	4:D:179:HOH:O	2.05	0.54
1:B:6:VAL:HG22	1:B:20:THR:HG22	1.90	0.54
1:A:121:GLU:HG3	1:A:122:LEU:HD22	1.88	0.54
1:C:31:VAL:HG22	1:C:33:VAL:HG12	1.89	0.54
1:A:8:VAL:HG13	1:A:18:VAL:HG23	1.90	0.54
1:D:87:ILE:HG12	4:D:163:HOH:O	2.08	0.54
1:C:33:VAL:HG22	1:C:97:ALA:HB3	1.89	0.53
1:B:52:ASP:O	1:B:53:THR:HB	2.07	0.53
1:B:36:SER:N	4:B:166:HOH:O	2.41	0.53
1:C:36:SER:N	4:C:164:HOH:O	2.41	0.53
1:A:6:VAL:HG23	1:A:20:THR:HG22	1.90	0.53
1:D:29:THR:HG21	1:D:104:ILE:O	2.10	0.52
1:A:52:ASP:O	1:A:53:THR:HB	2.10	0.52
1:C:152:THR:OG1	1:D:52:ASP:OD2	2.26	0.52
1:A:58:MET:SD	1:A:143:ARG:HG3	2.50	0.51
1:A:121:GLU:HG2	1:A:142:GLY:HA3	1.91	0.51
1:A:143:ARG:HG2	4:A:176:HOH:O	2.11	0.51
1:C:50:PHE:HE2	1:D:153:PRO:HG3	1.59	0.51
1:D:4:LYS:HD2	1:D:154:VAL:HA	1.92	0.51
1:A:42:LYS:HB2	1:A:123:GLU:HB2	1.93	0.51
1:A:86:ASN:HD21	1:A:124:ASP:H	1.57	0.50
4:C:170:HOH:O	1:D:150:GLY:CA	2.51	0.50
1:C:94:VAL:HG13	4:C:158:HOH:O	2.10	0.50
1:D:52:ASP:O	1:D:53:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG22	1:B:8:VAL:HG22	1.93	0.50
1:B:132:GLU:N	4:B:179:HOH:O	2.45	0.50
1:A:151:LEU:HD13	1:B:115:ARG:HH11	1.75	0.50
1:D:135:PRO:CD	4:D:179:HOH:O	2.60	0.50
1:B:53:THR:N	4:B:159:HOH:O	2.40	0.49
1:A:7:ALA:HB3	1:A:19:VAL:HG13	1.94	0.49
1:A:25:ASP:O	1:A:26:ASP:HB3	2.14	0.48
1:A:81:ALA:N	4:A:159:HOH:O	2.46	0.48
1:D:44:GLY:N	4:D:163:HOH:O	2.43	0.48
1:A:8:VAL:HG22	1:B:54:THR:HG22	1.96	0.48
1:B:43:HIS:O	1:B:86:ASN:ND2	2.47	0.48
1:D:23:GLN:NE2	1:D:26:ASP:HA	2.29	0.48
1:B:125:ASP:O	1:B:126:LEU:HB2	2.14	0.47
1:B:94:VAL:HG22	4:B:160:HOH:O	2.14	0.47
1:A:17:GLY:N	4:A:164:HOH:O	2.46	0.47
1:B:31:VAL:O	1:B:98:THR:HA	2.14	0.47
1:C:43:HIS:HB3	1:C:120:HIS:O	2.13	0.47
1:B:86:ASN:HD21	1:B:124:ASP:N	2.11	0.46
1:D:81:ALA:N	4:D:162:HOH:O	2.49	0.46
1:D:25:ASP:O	1:D:26:ASP:HB3	2.15	0.46
1:B:35:ILE:HG23	4:B:166:HOH:O	2.15	0.46
1:C:121:GLU:HB3	1:C:144:LEU:HD21	1.97	0.46
1:C:86:ASN:HD21	1:C:124:ASP:N	2.01	0.46
1:A:6:VAL:HA	1:A:19:VAL:O	2.15	0.46
1:C:54:THR:HG22	1:D:8:VAL:HG21	1.94	0.46
1:D:73:ALA:HB2	1:D:126:LEU:HG	1.97	0.46
1:C:132:GLU:HG3	1:C:133:LEU:HD23	1.97	0.46
1:A:35:ILE:CG2	1:A:38:LEU:HD22	2.46	0.46
1:A:31:VAL:HG22	1:A:99:ILE:HB	1.98	0.46
1:C:150:GLY:N	4:C:180:HOH:O	2.30	0.45
1:C:6:VAL:HG12	1:C:152:THR:HB	1.98	0.45
1:B:23:GLN:HB2	1:B:106:LEU:HD23	1.99	0.45
1:A:134:SER:N	1:A:135:PRO:HD2	2.31	0.45
1:B:43:HIS:O	1:B:123:GLU:HA	2.16	0.45
1:B:34:ARG:HA	1:B:95:ALA:O	2.16	0.45
1:C:15:VAL:HG22	1:C:37:GLY:O	2.17	0.45
1:C:43:HIS:O	1:C:123:GLU:HA	2.16	0.45
1:A:69:LYS:HB3	1:A:78:VAL:O	2.17	0.45
1:A:86:ASN:ND2	1:A:124:ASP:H	2.14	0.45
1:D:33:VAL:O	1:D:96:GLU:HA	2.17	0.45
1:A:86:ASN:HD21	1:A:124:ASP:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:HIS:HB3	1:B:120:HIS:O	2.17	0.44
1:B:117:LEU:HD12	1:B:149:VAL:HG22	1.99	0.44
1:B:87:ILE:HD11	1:B:119:VAL:HG23	1.99	0.44
1:C:6:VAL:CG1	1:D:52:ASP:HA	2.48	0.44
1:C:3:LYS:NZ	1:C:107:THR:HG22	2.33	0.44
1:C:58:MET:HE3	1:C:143:ARG:H	1.83	0.44
1:C:123:GLU:HG2	1:C:124:ASP:N	2.33	0.43
1:B:33:VAL:O	1:B:96:GLU:HA	2.18	0.43
1:C:15:VAL:HG11	1:C:38:LEU:HD13	1.99	0.43
1:D:121:GLU:OE2	1:D:142:GLY:HA3	2.17	0.43
1:A:76:ASP:HB3	4:A:180:HOH:O	2.18	0.43
1:D:3:LYS:CE	1:D:107:THR:HG23	2.48	0.43
1:A:73:ALA:HB2	1:A:126:LEU:HG	2.01	0.43
1:C:79:ARG:N	4:C:179:HOH:O	2.50	0.43
1:A:35:ILE:HG21	1:A:38:LEU:HD22	2.00	0.43
1:D:3:LYS:HE2	1:D:107:THR:HG23	2.01	0.43
1:D:67:ASP:O	1:D:68:LYS:HB2	2.18	0.43
1:A:152:THR:OG1	1:A:153:PRO:HD2	2.18	0.43
1:C:80:HIS:HB2	1:C:83:ASP:OD1	2.18	0.43
1:B:79:ARG:HG2	4:B:161:HOH:O	2.18	0.42
1:C:114:GLY:HA3	1:D:113:VAL:CG1	2.49	0.42
1:C:58:MET:CE	1:C:143:ARG:HD2	2.49	0.42
1:B:74:PRO:O	1:B:79:ARG:HD2	2.18	0.42
1:C:105:PRO:O	1:C:112:VAL:HG22	2.19	0.42
1:B:80:HIS:HB2	1:B:83:ASP:OD1	2.19	0.42
1:D:132:GLU:N	4:D:179:HOH:O	2.52	0.42
4:C:163:HOH:O	1:D:6:VAL:HG11	2.19	0.42
1:D:34:ARG:HA	1:D:95:ALA:O	2.20	0.42
1:A:9:LEU:HD12	1:A:147:GLY:N	2.34	0.42
1:C:58:MET:HE3	1:C:143:ARG:HB2	2.00	0.42
1:A:29:THR:HG21	1:A:104:ILE:O	2.20	0.42
1:A:132:GLU:N	4:A:177:HOH:O	2.52	0.41
1:C:132:GLU:N	4:C:176:HOH:O	2.52	0.41
1:B:16:GLU:N	4:B:166:HOH:O	2.51	0.41
1:B:143:ARG:HA	4:B:178:HOH:O	2.19	0.41
1:D:33:VAL:HG22	1:D:97:ALA:HB3	2.03	0.41
1:B:118:VAL:HG22	1:B:146:CYS:HB3	2.03	0.41
1:C:52:ASP:CG	1:D:152:THR:OG1	2.58	0.41
1:C:72:GLY:HA2	1:C:126:LEU:O	2.21	0.41
1:D:126:LEU:HB2	1:D:128:LYS:HD2	2.03	0.41
1:A:73:ALA:O	1:A:76:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:THR:CG2	1:D:8:VAL:CG2	2.91	0.40
1:C:4:LYS:HG3	1:C:154:VAL:HG23	2.02	0.40
1:C:50:PHE:CD2	1:D:153:PRO:HD3	2.56	0.40
1:D:36:SER:HA	1:D:93:GLY:O	2.21	0.40
1:C:27:GLY:HA3	1:C:28:PRO:HD2	1.72	0.40
1:D:117:LEU:O	1:D:146:CYS:HA	2.21	0.40
1:B:19:VAL:CG2	1:B:117:LEU:HD13	2.50	0.40
1:C:47:LEU:HB3	1:C:82:GLY:HA2	2.01	0.40
1:D:92:ASP:HB2	4:D:161:HOH:O	2.21	0.40
1:D:19:VAL:HG23	1:D:31:VAL:HG23	2.02	0.40
1:C:133:LEU:HA	1:C:136:THR:HG1	1.85	0.40
1:D:61:GLY:HA3	1:D:62:PRO:HD2	1.90	0.40

All (10) 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:97:ALA:O	4:C:172:HOH:O[4_547]	1.00	1.20
1:D:97:ALA:C	4:C:172:HOH:O[4_547]	1.14	1.06
1:A:24:GLU:OE1	1:C:130:GLY:CA[4_547]	1.65	0.55
1:D:97:ALA:CA	4:C:172:HOH:O[4_547]	1.68	0.52
1:A:39:ALA:CB	1:C:132:GLU:OE2[4_557]	1.83	0.37
1:D:97:ALA:N	4:C:172:HOH:O[4_547]	1.83	0.37
1:A:2:THR:CG2	1:C:128:LYS:O[4_547]	1.84	0.36
1:A:91:THR:CG2	4:D:177:HOH:O[1_565]	1.86	0.34
1:B:121:GLU:OE1	1:C:34:ARG:NH1[3_555]	1.91	0.29
1:A:24:GLU:OE1	1:C:129:GLY:O[4_547]	2.04	0.16

## 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	152/154 (99%)	128 (84%)	15 (10%)	9 (6%)	2	0
1	B	152/154 (99%)	124 (82%)	21 (14%)	7 (5%)	3	1
1	C	152/154 (99%)	125 (82%)	17 (11%)	10 (7%)	1	0
1	D	152/154 (99%)	126 (83%)	17 (11%)	9 (6%)	2	0
All	All	608/616 (99%)	503 (83%)	70 (12%)	35 (6%)	2	0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	80	HIS
1	A	153	PRO
1	B	52	ASP
1	B	132	GLU
1	C	26	ASP
1	C	52	ASP
1	C	80	HIS
1	D	26	ASP
1	D	52	ASP
1	D	81	ALA
1	D	153	PRO
1	A	81	ALA
1	A	132	GLU
1	A	141	GLY
1	B	81	ALA
1	B	131	HIS
1	B	141	GLY
1	C	25	ASP
1	C	81	ALA
1	C	132	GLU
1	C	141	GLY
1	D	132	GLU
1	D	141	GLY
1	A	68	LYS
1	A	131	HIS
1	B	68	LYS
1	C	68	LYS
1	C	79	ARG
1	C	90	ASN
1	D	49	GLU
1	B	83	ASP
1	D	25	ASP

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Mol	Chain	Res	Type
1	D	80	HIS
1	A	62	PRO

### 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	119/119 (100%)	92 (77%)	27 (23%)	1	0
1	B	119/119 (100%)	101 (85%)	18 (15%)	3	1
1	C	119/119 (100%)	97 (82%)	22 (18%)	2	1
1	D	119/119 (100%)	95 (80%)	24 (20%)	1	0
All	All	476/476 (100%)	385 (81%)	91 (19%)	2	0

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	9	LEU
1	A	12	THR
1	A	18	VAL
1	A	19	VAL
1	A	25	ASP
1	A	26	ASP
1	A	29	THR
1	A	33	VAL
1	A	52	ASP
1	A	55	ASN
1	A	59	SER
1	A	69	LYS
1	A	70	THR
1	A	75	GLU
1	A	77	GLU
1	A	84	LEU
1	A	90	ASN
1	A	92	ASP

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	120	HIS
1	A	122	LEU
1	A	123	GLU
1	A	126	LEU
1	A	133	LEU
1	A	136	THR
1	A	143	ARG
1	B	9	LEU
1	B	18	VAL
1	B	21	LEU
1	B	23	GLN
1	B	29	THR
1	B	53	THR
1	B	58	MET
1	B	70	THR
1	B	75	GLU
1	B	77	GLU
1	B	79	ARG
1	B	84	LEU
1	B	90	ASN
1	B	91	THR
1	B	104	ILE
1	B	123	GLU
1	B	126	LEU
1	B	137	THR
1	C	3	LYS
1	C	9	LEU
1	C	19	VAL
1	C	31	VAL
1	C	38	LEU
1	C	47	LEU
1	C	52	ASP
1	C	53	THR
1	C	58	MET
1	C	70	THR
1	C	75	GLU
1	C	77	GLU
1	C	84	LEU
1	C	90	ASN
1	C	91	THR
1	C	94	VAL

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Mol	Chain	Res	Type
1	C	107	THR
1	C	109	PRO
1	C	122	LEU
1	C	133	LEU
1	C	136	THR
1	C	154	VAL
1	D	2	THR
1	D	9	LEU
1	D	16	GLU
1	D	19	VAL
1	D	29	THR
1	D	31	VAL
1	D	33	VAL
1	D	47	LEU
1	D	53	THR
1	D	58	MET
1	D	59	SER
1	D	75	GLU
1	D	77	GLU
1	D	79	ARG
1	D	84	LEU
1	D	90	ASN
1	D	94	VAL
1	D	99	ILE
1	D	107	THR
1	D	122	LEU
1	D	126	LEU
1	D	128	LYS
1	D	133	LEU
1	D	154	VAL

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

Mol	Chain	Res	Type
1	A	86	ASN
1	A	103	GLN
1	A	120	HIS
1	A	131	HIS
1	B	32	ASN
1	B	86	ASN
1	B	103	GLN
1	C	32	ASN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	102	ASN
1	C	103	GLN
1	C	110	ASN
1	C	120	HIS
1	D	55	ASN
1	D	86	ASN
1	D	103	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.