



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:44 PM GMT

PDB ID : 1UXM  
Title : A4V MUTANT OF HUMAN SOD1  
Authors : Hough, M.A.; Grossmann, J.G.; Antonyuk, S.V.; Strange, R.W.; Doucette, P.A.; Rodriguez, J.A.; Whitson, L.J.; Hart, P.J.; Hayward, L.J.; Valentine, J.S.; Hasnain, S.S.  
Deposited on : 2004-02-26  
Resolution : 1.90 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

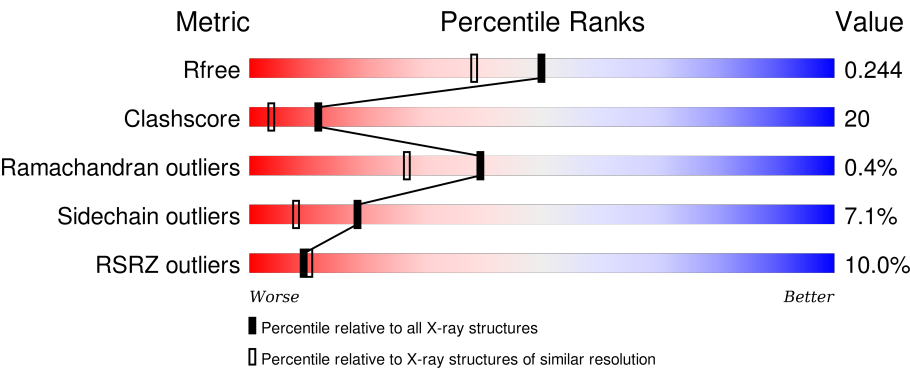
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
R <sub>free</sub>	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	153	<div><div>%</div><div>78%15%5%.</div></div>
1	B	153	<div><div>%</div><div>77%20%..</div></div>
1	C	153	<div><div>%</div><div>84%13%..</div></div>
1	D	153	<div><div>%</div><div>90%9%.</div></div>
1	E	153	<div><div>2%</div><div>84%12%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	153	<div><div>%</div><div><div></div><div>78%</div><div>19%</div><div>• •</div></div></div>
1	G	153	<div><div>30%</div><div><div></div><div>60%</div><div>33%</div><div>7%</div></div></div>
1	H	153	<div><div>44%</div><div><div></div><div>54%</div><div>39%</div><div>7%</div></div></div>
1	I	153	<div><div>8%</div><div><div></div><div>75%</div><div>24%</div><div>•</div></div></div>
1	J	153	<div><div>%</div><div><div></div><div>75%</div><div>22%</div><div>• •</div></div></div>
1	K	153	<div><div>19%</div><div><div></div><div>63%</div><div>34%</div><div>•</div></div></div>
1	L	153	<div><div>10%</div><div><div></div><div>62%</div><div>34%</div><div>•</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14464 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 SUPEROXIDE DISMUTASE [CU-ZN].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	8	0	0
			1112	681	203	224	4			
1	B	153	Total	C	N	O	S	1	0	0
			1112	681	203	224	4			
1	C	153	Total	C	N	O	S	4	0	0
			1112	681	203	224	4			
1	D	153	Total	C	N	O	S	0	0	0
			1112	681	203	224	4			
1	E	153	Total	C	N	O	S	9	0	0
			1112	681	203	224	4			
1	F	153	Total	C	N	O	S	15	0	0
			1112	681	203	224	4			
1	G	153	Total	C	N	O	S	21	0	0
			1112	681	203	224	4			
1	H	153	Total	C	N	O	S	60	0	0
			1112	681	203	224	4			
1	I	153	Total	C	N	O	S	29	0	0
			1112	681	203	224	4			
1	J	153	Total	C	N	O	S	22	0	0
			1112	681	203	224	4			
1	K	153	Total	C	N	O	S	67	0	0
			1112	681	203	224	4			
1	L	153	Total	C	N	O	S	14	0	0
			1112	681	203	224	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
B	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
C	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
D	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
E	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
G	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
H	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
I	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
J	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
K	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441
L	4	VAL	ALA	ENGINEERED MUTATION	UNP P00441

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	131	Total 131	O 131	0	0
4	C	135	Total 135	O 135	0	0
4	D	127	Total 127	O 127	0	0
4	E	78	Total 78	O 78	0	0
4	F	68	Total 68	O 68	0	0
4	G	79	Total 79	O 79	0	0
4	H	82	Total 82	O 82	0	0
4	I	45	Total 45	O 45	0	0

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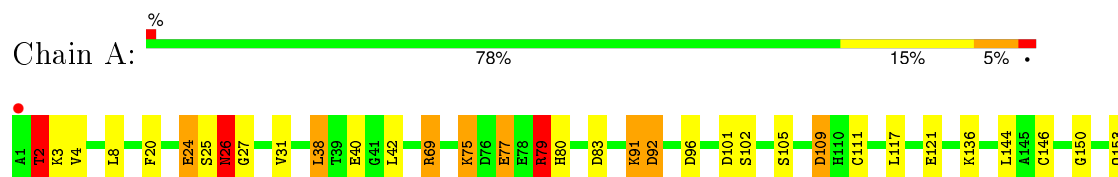
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	73	Total 73	O 73	0	0
4	K	72	Total 72	O 72	0	0
4	L	71	Total 71	O 71	0	0

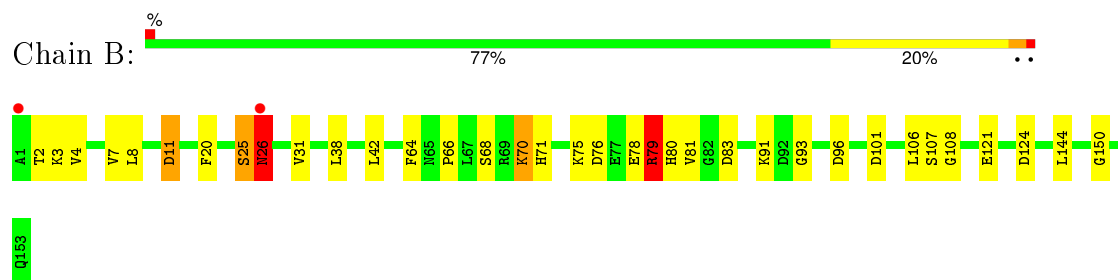
### 3 Residue-property plots [i](#)

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.

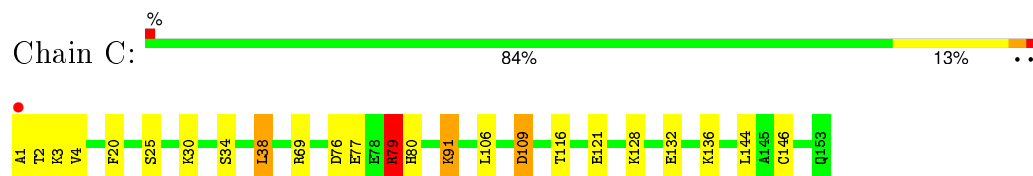
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



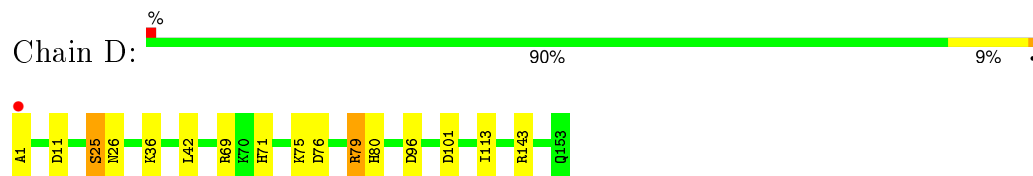
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



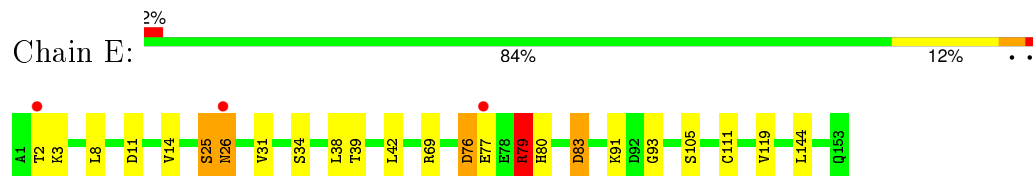
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



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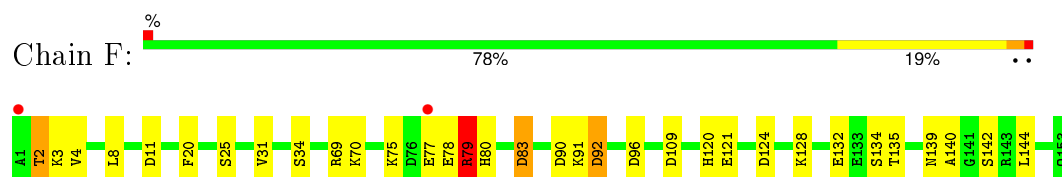


- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

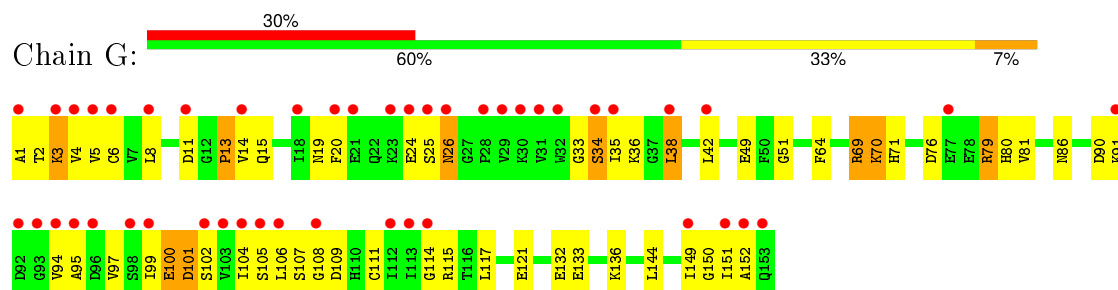




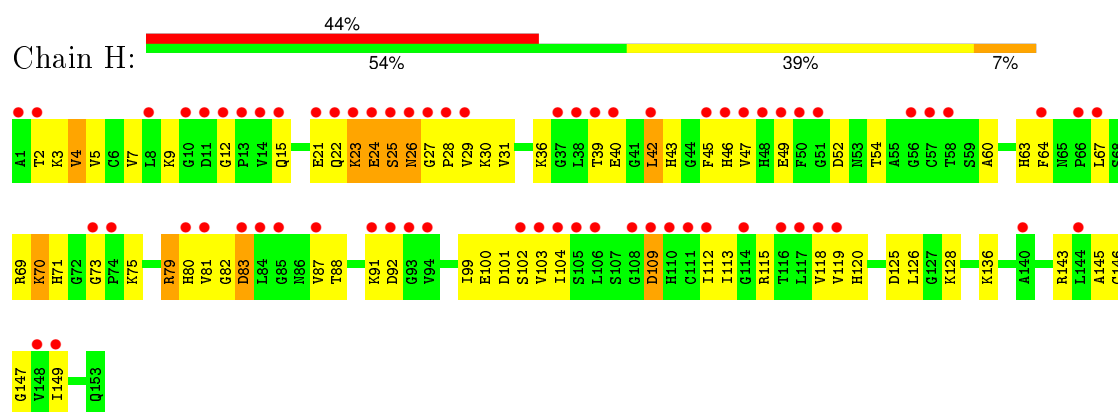
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



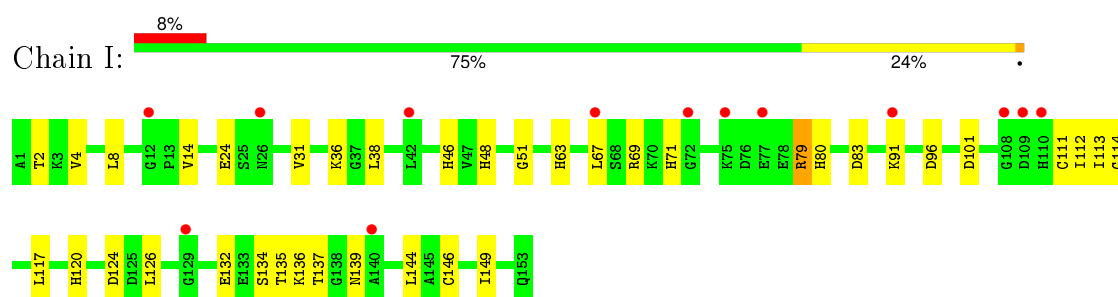
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



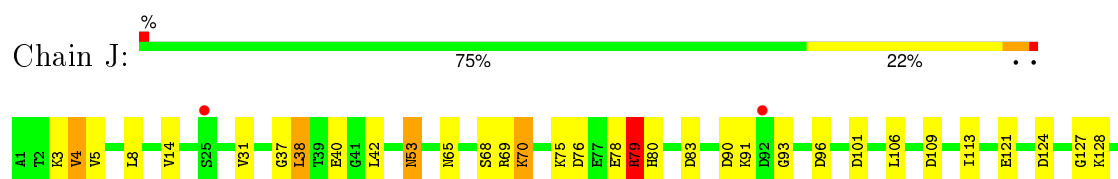
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



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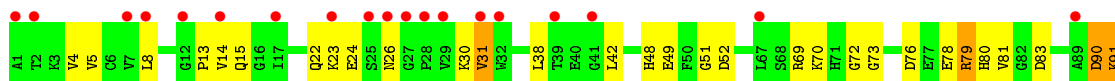


- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

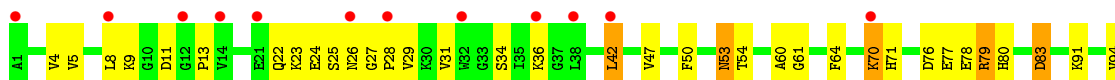




• Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



• Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.37Å 145.58Å 112.50Å 90.00° 120.05° 90.00°	Depositor
Resolution (Å)	27.00 – 1.90 9.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (27.00-1.90) 97.0 (9.99-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.228 , 0.250 0.243 , 0.244	Depositor DCC
$R_{free}$ test set	2364 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.9	EDS
Estimated twinning fraction	0.074 for -h-l,k,h 0.074 for l,k,-h-l 0.085 for l,-k,h 0.074 for h,-k,-h-l 0.260 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 237355 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.91	1/1130 (0.1%)	1.24	12/1523 (0.8%)
1	B	0.87	2/1130 (0.2%)	1.12	6/1523 (0.4%)
1	C	0.87	0/1130	1.11	5/1523 (0.3%)
1	D	0.85	0/1130	1.01	4/1523 (0.3%)
1	E	0.63	0/1130	0.95	5/1523 (0.3%)
1	F	0.74	0/1130	1.03	7/1523 (0.5%)
1	G	0.66	0/1130	0.98	2/1523 (0.1%)
1	H	0.69	0/1130	0.99	5/1523 (0.3%)
1	I	0.57	0/1130	0.90	3/1523 (0.2%)
1	J	0.68	1/1130 (0.1%)	0.99	9/1523 (0.6%)
1	K	0.63	0/1130	0.92	3/1523 (0.2%)
1	L	0.66	0/1130	0.96	4/1523 (0.3%)
All	All	0.74	4/13560 (0.0%)	1.02	65/18276 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	53	ASN	CB-CG	6.12	1.65	1.51
1	A	79	ARG	CG-CD	5.59	1.66	1.51
1	B	7	VAL	CB-CG1	5.46	1.64	1.52
1	B	26	ASN	CB-CG	5.07	1.62	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	C	79	ARG	NE-CZ-NH2	-15.31	112.64	120.30
1	B	79	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	A	79	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	C	79	ARG	NE-CZ-NH1	10.76	125.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	B	79	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	E	79	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	D	96	ASP	CB-CG-OD2	7.97	125.47	118.30
1	J	83	ASP	CB-CG-OD1	7.77	125.29	118.30
1	B	11	ASP	CB-CG-OD2	6.85	124.47	118.30
1	I	124	ASP	CB-CG-OD2	6.73	124.36	118.30
1	G	101	ASP	CB-CG-OD2	6.71	124.34	118.30
1	H	87	VAL	N-CA-C	-6.59	93.20	111.00
1	D	143	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	E	79	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	I	101	ASP	CB-CG-OD2	6.48	124.14	118.30
1	F	79	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	K	90	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	2	THR	N-CA-C	-6.36	93.84	111.00
1	A	26	ASN	C-N-CA	6.30	135.54	122.30
1	B	101	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	79	ARG	CD-NE-CZ	6.19	132.27	123.60
1	L	101	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	101	ASP	CB-CG-OD2	6.10	123.79	118.30
1	L	11	ASP	CB-CG-OD2	6.04	123.73	118.30
1	K	92	ASP	CB-CG-OD2	5.94	123.64	118.30
1	D	101	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	124	ASP	CB-CG-OD2	5.87	123.58	118.30
1	L	83	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	109	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	11	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	27	GLY	N-CA-C	-5.71	98.83	113.10
1	E	76	ASP	CB-CG-OD2	5.70	123.43	118.30
1	H	83	ASP	CB-CG-OD2	5.66	123.39	118.30
1	J	124	ASP	CB-CG-OD2	5.61	123.35	118.30
1	F	109	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	109	ASP	CB-CG-OD2	5.58	123.33	118.30
1	J	96	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	38	LEU	CA-CB-CG	5.51	127.98	115.30
1	J	38	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	76	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	92	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	69	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	F	92	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	38	LEU	CB-CG-CD1	5.42	120.22	111.00
1	L	109	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	109	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	31	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	F	124	ASP	CB-CG-OD2	5.36	123.12	118.30
1	H	125	ASP	CB-CG-OD2	5.36	123.12	118.30
1	I	96	ASP	CB-CG-OD2	5.30	123.07	118.30
1	J	76	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	76	ASP	CB-CG-OD2	5.27	123.04	118.30
1	F	96	ASP	CB-CG-OD2	5.25	123.02	118.30
1	J	101	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	83	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	92	ASP	CB-CG-OD2	5.17	122.96	118.30
1	G	11	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	11	ASP	CB-CG-OD2	5.16	122.94	118.30
1	H	109	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	83	ASP	CB-CG-OD1	5.13	122.92	118.30
1	K	101	ASP	CB-CG-OD2	5.13	122.92	118.30
1	J	79	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	J	53	ASN	CB-CA-C	5.08	120.57	110.40

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	1112	0	1081	29	1
1	B	1112	0	1080	36	0
1	C	1112	0	1080	18	1
1	D	1112	0	1081	13	2
1	E	1112	0	1080	18	0
1	F	1112	0	1081	32	0
1	G	1112	0	1081	70	0
1	H	1112	0	1080	107	1
1	I	1112	0	1080	30	0
1	J	1112	0	1080	36	2
1	K	1112	0	1080	65	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1112	0	1080	75	0
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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	135	0	0	14	0
4	B	131	0	0	3	0
4	C	135	0	0	8	0
4	D	127	0	0	4	0
4	E	78	0	0	3	0
4	F	68	0	0	11	0
4	G	79	0	0	27	0
4	H	82	0	0	58	0
4	I	45	0	0	2	0
4	J	73	0	0	12	0
4	K	72	0	0	30	0
4	L	71	0	0	34	0
All	All	14464	0	12964	517	4

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 20.

All (517) 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:I:132:GLU:O	1:I:135:THR:HG22	1.16	1.30
1:H:70:LYS:HB2	4:H:2031:HOH:O	1.31	1.28
1:K:49:GLU:HB2	4:K:2020:HOH:O	1.31	1.25
1:H:79:ARG:HD3	1:H:80:HIS:O	1.34	1.24
1:G:70:LYS:HB3	1:G:70:LYS:NZ	1.30	1.22
1:J:69:ARG:HD3	1:J:78:GLU:OE2	1.40	1.21
1:H:79:ARG:CD	1:H:80:HIS:O	1.87	1.21
1:L:70:LYS:HB3	1:L:70:LYS:NZ	1.47	1.19
1:B:26:ASN:HA	4:B:2025:HOH:O	1.40	1.19
1:H:73:GLY:HA3	4:H:2033:HOH:O	1.40	1.15
1:G:70:LYS:CB	1:G:70:LYS:NZ	2.09	1.15
1:G:101:ASP:HA	4:G:2046:HOH:O	1.44	1.13
1:L:149:ILE:HD11	4:L:2050:HOH:O	1.48	1.11
1:K:79:ARG:HD3	1:K:80:HIS:O	1.47	1.11
1:B:107:SER:HB2	1:F:77:GLU:OE2	1.49	1.10
1:K:92:ASP:HB3	4:K:2044:HOH:O	1.51	1.09
1:H:119:VAL:HA	4:H:2063:HOH:O	1.52	1.08
1:D:25:SER:O	1:D:26:ASN:HB3	1.52	1.07
1:G:6:CYS:SG	4:G:2076:HOH:O	2.10	1.07
1:A:25:SER:O	1:A:26:ASN:C	1.95	1.05
1:L:104:ILE:HD12	4:L:2045:HOH:O	1.54	1.04
1:C:4:VAL:HG22	1:C:20:PHE:HB2	1.39	1.04
1:I:132:GLU:O	1:I:135:THR:CG2	2.06	1.04
1:H:103:VAL:HG23	4:H:2052:HOH:O	1.57	1.04
1:L:42:LEU:HD11	4:L:2018:HOH:O	1.57	1.04
1:K:107:SER:HB3	4:K:2049:HOH:O	1.55	1.04
4:K:2017:HOH:O	1:L:152:ALA:HA	1.56	1.02
1:L:26:ASN:HA	4:L:2011:HOH:O	1.59	1.01
1:K:72:GLY:HA3	4:K:2035:HOH:O	1.61	1.00
1:G:70:LYS:HB3	1:G:70:LYS:HZ2	1.23	0.98
1:G:151:ILE:HB	4:H:2061:HOH:O	1.63	0.97
1:J:53:ASN:HB3	4:J:2028:HOH:O	1.64	0.96
1:H:80:HIS:HB2	1:H:83:ASP:CG	1.86	0.96
1:L:29:VAL:HG23	4:L:2015:HOH:O	1.66	0.96
1:K:4:VAL:HG21	1:K:113:ILE:CD1	1.97	0.95
1:K:52:ASP:HB2	4:K:2017:HOH:O	1.66	0.95
1:K:70:LYS:HE2	4:K:2028:HOH:O	1.64	0.95
1:K:97:VAL:HG12	4:K:2011:HOH:O	1.65	0.95
1:K:26:ASN:HA	4:K:2006:HOH:O	1.65	0.95
1:A:25:SER:O	1:A:26:ASN:O	1.84	0.94
1:A:79:ARG:CD	1:A:80:HIS:O	2.15	0.94
1:L:70:LYS:CB	1:L:70:LYS:NZ	2.22	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:LYS:HB3	1:L:70:LYS:HZ3	1.27	0.94
1:K:4:VAL:HG21	1:K:113:ILE:HD11	1.46	0.93
1:K:107:SER:HA	4:K:2048:HOH:O	1.70	0.92
1:H:63:HIS:CD2	4:H:2029:HOH:O	2.22	0.92
1:I:120:HIS:CE1	4:I:2031:HOH:O	2.22	0.92
1:L:70:LYS:HB3	1:L:70:LYS:HZ2	1.13	0.91
1:A:79:ARG:HD3	1:A:80:HIS:O	1.71	0.91
1:F:25:SER:HA	4:F:2050:HOH:O	1.71	0.91
1:H:79:ARG:HD2	1:H:80:HIS:O	1.69	0.90
1:H:42:LEU:CD1	1:H:88:THR:HG23	2.03	0.89
1:K:79:ARG:CD	1:K:80:HIS:O	2.20	0.88
1:H:63:HIS:CG	4:H:2029:HOH:O	2.25	0.88
1:G:149:ILE:HG12	4:G:2076:HOH:O	1.72	0.88
1:K:90:ASP:OD1	1:K:92:ASP:N	2.07	0.88
1:L:105:SER:HB2	4:L:2043:HOH:O	1.74	0.87
1:G:69:ARG:HG3	4:G:2037:HOH:O	1.72	0.87
1:G:70:LYS:CB	1:G:70:LYS:HZ2	1.75	0.87
1:F:79:ARG:HD2	1:F:80:HIS:O	1.74	0.87
1:K:23:LYS:HA	4:K:2005:HOH:O	1.75	0.87
1:H:40:GLU:HG3	4:H:2018:HOH:O	1.76	0.86
1:G:1:ALA:HB1	4:G:2002:HOH:O	1.74	0.86
1:H:103:VAL:HG12	4:H:2058:HOH:O	1.76	0.85
1:J:69:ARG:HD3	1:J:78:GLU:CD	1.96	0.85
1:C:128:LYS:HE3	4:C:2119:HOH:O	1.76	0.85
1:H:46:HIS:HB3	4:H:2029:HOH:O	1.75	0.84
1:B:4:VAL:HG22	1:B:20:PHE:HB2	1.59	0.84
1:H:120:HIS:CD2	4:H:2064:HOH:O	2.31	0.83
1:I:4:VAL:HG21	1:I:113:ILE:CD1	2.08	0.83
1:I:4:VAL:HG21	1:I:113:ILE:HD11	1.60	0.83
1:J:106:LEU:HD13	4:J:2001:HOH:O	1.78	0.83
1:L:70:LYS:CB	1:L:70:LYS:HZ2	1.85	0.83
1:G:70:LYS:HB3	1:G:70:LYS:HZ3	0.93	0.82
1:F:79:ARG:CD	1:F:80:HIS:O	2.27	0.82
1:B:25:SER:OG	1:B:25:SER:O	1.91	0.81
1:K:69:ARG:NE	4:K:2026:HOH:O	2.11	0.81
1:K:103:VAL:HG13	4:K:2052:HOH:O	1.79	0.81
1:B:70:LYS:HZ2	1:B:70:LYS:HB3	1.46	0.80
1:G:151:ILE:HD11	4:H:2060:HOH:O	1.80	0.80
1:H:64:PHE:HB3	4:H:2045:HOH:O	1.81	0.80
1:L:113:ILE:HA	4:L:2070:HOH:O	1.81	0.79
1:A:2:THR:CG2	4:A:2001:HOH:O	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG22	1:A:20:PHE:HB2	1.64	0.79
1:B:96:ASP:OD1	4:B:2089:HOH:O	2.01	0.78
1:H:103:VAL:CG1	4:H:2058:HOH:O	2.31	0.78
1:G:4:VAL:HG11	1:G:149:ILE:HG22	1.65	0.78
1:H:80:HIS:HB2	1:H:83:ASP:OD1	1.83	0.78
1:E:25:SER:O	1:E:26:ASN:HB3	1.81	0.78
1:K:118:VAL:HG11	1:K:143:ARG:HG2	1.66	0.78
1:H:28:PRO:HB3	4:H:2051:HOH:O	1.85	0.77
1:A:79:ARG:HD2	1:A:80:HIS:O	1.83	0.77
1:H:69:ARG:HD2	4:H:2043:HOH:O	1.84	0.77
1:L:77:GLU:CG	4:L:2029:HOH:O	2.32	0.77
1:J:4:VAL:HG21	1:J:113:ILE:HD13	1.66	0.77
1:H:120:HIS:HD2	4:H:2064:HOH:O	1.65	0.76
1:H:36:LYS:HB2	4:H:2017:HOH:O	1.85	0.76
1:E:3:LYS:HE2	4:E:2011:HOH:O	1.83	0.76
1:I:79:ARG:HD3	1:I:83:ASP:HB2	1.67	0.75
1:D:26:ASN:O	1:D:26:ASN:ND2	2.20	0.75
1:B:75:LYS:HE3	1:B:75:LYS:HA	1.68	0.74
1:H:21:GLU:HG2	4:H:2009:HOH:O	1.87	0.74
1:J:70:LYS:HG3	1:J:78:GLU:CG	2.17	0.73
1:B:70:LYS:CB	1:B:70:LYS:HZ2	1.97	0.73
1:L:42:LEU:HD12	1:L:42:LEU:N	2.04	0.73
1:H:25:SER:C	1:H:27:GLY:H	1.92	0.73
1:F:128:LYS:NZ	4:F:2059:HOH:O	2.22	0.73
1:G:19:ASN:HB3	4:G:2004:HOH:O	1.88	0.73
1:G:42:LEU:HD12	1:G:42:LEU:N	2.04	0.73
1:A:2:THR:HG23	4:A:2001:HOH:O	1.86	0.73
1:H:46:HIS:CB	4:H:2029:HOH:O	2.35	0.72
1:H:79:ARG:NH1	1:H:81:VAL:O	2.22	0.72
1:E:25:SER:O	1:E:26:ASN:CB	2.37	0.72
1:H:64:PHE:HD2	4:H:2045:HOH:O	1.72	0.72
1:H:29:VAL:HG21	1:H:104:ILE:HG13	1.70	0.72
1:J:69:ARG:CD	1:J:78:GLU:OE2	2.31	0.72
1:G:6:CYS:HB2	4:G:2076:HOH:O	1.89	0.72
1:C:79:ARG:CD	1:C:80:HIS:O	2.36	0.72
1:H:64:PHE:CD2	4:H:2045:HOH:O	2.41	0.72
1:E:76:ASP:CG	4:E:2038:HOH:O	2.27	0.72
1:E:25:SER:O	1:E:25:SER:OG	2.05	0.71
1:F:4:VAL:HG22	1:F:20:PHE:HB2	1.71	0.71
1:H:145:ALA:N	4:H:2081:HOH:O	2.22	0.71
1:L:111:CYS:N	4:L:2048:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:LEU:HD12	1:H:88:THR:HG23	1.70	0.70
1:B:107:SER:CB	1:F:77:GLU:OE2	2.34	0.69
1:B:79:ARG:HD2	1:B:80:HIS:O	1.92	0.69
1:H:60:ALA:N	4:H:2026:HOH:O	2.23	0.69
1:H:2:THR:HG23	4:H:2011:HOH:O	1.91	0.69
1:L:9:LYS:NZ	4:L:2003:HOH:O	2.23	0.68
1:H:79:ARG:NH2	1:H:101:ASP:OD1	2.24	0.68
1:H:12:GLY:N	4:H:2007:HOH:O	2.26	0.68
1:K:31:VAL:HG22	4:K:2011:HOH:O	1.94	0.68
1:L:110:HIS:HB2	4:L:2043:HOH:O	1.93	0.68
1:C:79:ARG:HD3	1:C:80:HIS:O	1.94	0.68
1:G:104:ILE:HA	4:G:2038:HOH:O	1.92	0.67
1:B:66:PRO:HD2	1:B:81:VAL:HG12	1.75	0.67
1:G:104:ILE:CG2	4:G:2038:HOH:O	2.42	0.67
1:K:97:VAL:CG1	4:K:2011:HOH:O	2.34	0.67
1:B:25:SER:O	1:B:26:ASN:CG	2.33	0.67
1:L:53:ASN:ND2	4:L:2022:HOH:O	2.27	0.66
1:D:25:SER:O	1:D:26:ASN:CB	2.31	0.66
1:K:4:VAL:CG1	1:K:5:VAL:N	2.58	0.66
1:H:22:GLN:N	4:H:2009:HOH:O	2.28	0.66
1:H:99:ILE:HG22	1:H:100:GLU:N	2.09	0.66
1:H:79:ARG:HD3	1:H:83:ASP:HB2	1.77	0.66
1:B:66:PRO:HD2	1:B:81:VAL:CG1	2.26	0.66
1:J:69:ARG:HD2	4:J:2039:HOH:O	1.96	0.66
1:J:70:LYS:HG3	1:J:78:GLU:HG2	1.78	0.66
1:B:79:ARG:CD	1:B:80:HIS:O	2.45	0.65
1:G:86:ASN:O	4:G:2039:HOH:O	2.13	0.65
1:G:111:CYS:O	4:G:2054:HOH:O	2.14	0.65
1:I:80:HIS:HB2	1:I:83:ASP:OD1	1.95	0.65
1:L:4:VAL:HG21	1:L:113:ILE:HD11	1.77	0.65
1:J:79:ARG:CD	1:J:80:HIS:O	2.45	0.64
1:L:112:ILE:HD11	4:L:2045:HOH:O	1.96	0.64
1:G:4:VAL:HG11	1:G:149:ILE:CG2	2.27	0.64
1:H:67:LEU:HD13	1:H:69:ARG:HH21	1.62	0.64
1:B:68:SER:O	1:G:26:ASN:HB2	1.97	0.64
1:H:49:GLU:O	1:H:115:ARG:NH1	2.31	0.64
1:L:77:GLU:C	4:L:2029:HOH:O	2.35	0.64
1:K:103:VAL:CG1	4:K:2052:HOH:O	2.40	0.64
1:C:79:ARG:HD2	1:C:80:HIS:O	1.98	0.64
1:K:90:ASP:OD1	1:K:92:ASP:HB2	1.98	0.63
1:A:2:THR:HG21	4:A:2001:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:LYS:NZ	4:F:2026:HOH:O	2.32	0.63
1:H:81:VAL:HG22	4:H:2058:HOH:O	1.99	0.63
1:G:70:LYS:CB	1:G:70:LYS:HZ3	1.86	0.63
1:H:23:LYS:N	4:H:2009:HOH:O	2.31	0.63
1:H:128:LYS:HE2	4:H:2068:HOH:O	1.97	0.63
1:K:4:VAL:HG21	1:K:113:ILE:HD12	1.78	0.62
1:F:128:LYS:CE	4:F:2060:HOH:O	2.45	0.62
1:A:96:ASP:OD1	4:A:2083:HOH:O	2.16	0.62
1:K:106:LEU:HD22	1:K:113:ILE:HD11	1.80	0.62
1:K:81:VAL:HG22	4:K:2052:HOH:O	1.97	0.62
1:H:149:ILE:HD12	4:H:2062:HOH:O	1.99	0.62
1:L:117:LEU:HB2	4:L:2050:HOH:O	1.99	0.62
1:H:30:LYS:N	4:H:2016:HOH:O	2.31	0.62
1:H:136:LYS:CE	4:H:2075:HOH:O	2.47	0.62
1:G:6:CYS:CB	4:G:2076:HOH:O	2.35	0.61
1:H:81:VAL:HG12	1:H:104:ILE:HG22	1.83	0.61
1:J:3:LYS:C	4:J:2001:HOH:O	2.39	0.61
1:L:4:VAL:HG21	1:L:113:ILE:CD1	2.30	0.61
1:H:47:VAL:CG1	4:H:2045:HOH:O	2.48	0.61
1:F:70:LYS:CG	1:F:78:GLU:HG2	2.30	0.61
1:C:132:GLU:HG3	4:C:2121:HOH:O	2.00	0.61
1:F:79:ARG:HD3	1:F:83:ASP:HB2	1.82	0.60
1:H:103:VAL:CG2	4:H:2014:HOH:O	2.49	0.60
1:H:60:ALA:HB2	4:H:2026:HOH:O	2.01	0.60
1:F:70:LYS:HG3	1:F:78:GLU:HG2	1.83	0.60
1:L:42:LEU:CD1	1:L:42:LEU:N	2.65	0.60
4:K:2017:HOH:O	1:L:152:ALA:CB	2.49	0.60
1:G:42:LEU:CD1	1:G:42:LEU:N	2.65	0.60
1:J:4:VAL:HG21	1:J:113:ILE:CD1	2.30	0.60
1:J:79:ARG:HD2	1:J:80:HIS:O	2.02	0.60
1:J:128:LYS:NZ	4:J:2059:HOH:O	2.33	0.60
1:A:92:ASP:HA	4:A:2081:HOH:O	2.02	0.60
1:G:70:LYS:HB2	1:G:70:LYS:HZ2	1.62	0.59
1:K:110:HIS:CE1	4:K:2052:HOH:O	2.54	0.59
1:G:132:GLU:HB2	4:G:2067:HOH:O	2.01	0.59
1:G:104:ILE:CA	4:G:2038:HOH:O	2.49	0.59
1:G:20:PHE:HZ	1:G:117:LEU:HD22	1.67	0.59
1:K:99:ILE:HG22	1:K:100:GLU:N	2.18	0.59
1:G:81:VAL:HG13	4:G:2038:HOH:O	2.01	0.59
1:L:23:LYS:CG	4:L:2010:HOH:O	2.50	0.59
1:L:77:GLU:HG3	4:L:2029:HOH:O	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:ASP:OD1	1:K:92:ASP:CA	2.50	0.59
1:G:20:PHE:CZ	1:G:117:LEU:HD22	2.37	0.59
1:E:39:THR:CG2	1:K:13:PRO:HG3	2.33	0.59
1:K:73:GLY:N	1:K:76:ASP:OD2	2.30	0.59
1:F:75:LYS:CE	4:F:2026:HOH:O	2.50	0.59
1:G:108:GLY:CA	4:G:2052:HOH:O	2.51	0.58
1:F:69:ARG:NH2	4:F:2023:HOH:O	2.37	0.58
1:H:42:LEU:HD13	1:H:88:THR:HG23	1.81	0.58
1:F:79:ARG:HD3	1:F:80:HIS:O	2.02	0.58
1:G:1:ALA:HB3	1:G:106:LEU:O	2.03	0.58
1:L:100:GLU:HG2	4:L:2037:HOH:O	2.02	0.58
1:G:33:GLY:C	1:G:34:SER:OG	2.41	0.58
1:G:95:ALA:HB1	4:G:2042:HOH:O	2.04	0.58
1:E:14:VAL:HG21	1:E:144:LEU:HB3	1.86	0.58
1:F:11:ASP:HB3	1:L:13:PRO:HG3	1.86	0.58
1:G:4:VAL:HG12	1:G:5:VAL:N	2.18	0.57
1:H:67:LEU:CD2	4:H:2012:HOH:O	2.52	0.57
1:C:128:LYS:CE	4:C:2119:HOH:O	2.44	0.57
1:L:136:LYS:CE	4:L:2061:HOH:O	2.52	0.57
1:H:103:VAL:HG21	4:H:2014:HOH:O	2.05	0.57
1:J:40:GLU:CD	4:J:2020:HOH:O	2.43	0.57
1:H:71:HIS:HB2	1:H:80:HIS:CE1	2.40	0.57
1:G:33:GLY:O	1:G:34:SER:OG	2.21	0.57
1:F:70:LYS:HG2	1:F:78:GLU:OE2	2.04	0.57
1:H:101:ASP:HB3	1:H:104:ILE:HG12	1.86	0.57
1:B:70:LYS:HG3	1:B:78:GLU:OE2	2.05	0.57
1:H:9:LYS:N	1:H:146:CYS:O	2.28	0.57
1:G:108:GLY:HA3	4:G:2052:HOH:O	2.04	0.56
1:L:71:HIS:HB2	1:L:80:HIS:CE1	2.39	0.56
1:H:3:LYS:O	1:H:4:VAL:HG23	2.05	0.56
1:K:69:ARG:CD	4:K:2026:HOH:O	2.52	0.56
1:E:25:SER:HA	4:E:2056:HOH:O	2.05	0.56
1:G:49:GLU:O	1:G:115:ARG:NH1	2.34	0.56
1:J:53:ASN:ND2	4:J:2027:HOH:O	2.31	0.56
1:D:1:ALA:CB	1:D:113:ILE:HD11	2.35	0.56
1:H:45:PHE:HA	4:H:2063:HOH:O	2.06	0.56
1:C:4:VAL:HG13	1:C:106:LEU:HD13	1.87	0.56
1:B:68:SER:O	1:G:26:ASN:CB	2.54	0.56
1:G:51:GLY:HA3	1:G:114:GLY:O	2.04	0.56
1:I:132:GLU:C	1:I:135:THR:HG22	2.16	0.56
1:G:97:VAL:CG2	4:G:2042:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:GLN:HG2	4:H:2017:HOH:O	2.05	0.56
1:H:99:ILE:CG2	1:H:100:GLU:N	2.68	0.56
1:C:1:ALA:HA	4:C:2004:HOH:O	2.06	0.56
1:F:92:ASP:C	4:F:2040:HOH:O	2.43	0.56
1:L:4:VAL:HG11	1:L:149:ILE:CG2	2.36	0.56
1:L:64:PHE:HZ	4:L:2048:HOH:O	1.90	0.55
1:H:67:LEU:HD22	4:H:2012:HOH:O	2.05	0.55
1:G:104:ILE:HG22	4:G:2038:HOH:O	2.06	0.55
1:D:36:LYS:CD	4:D:2018:HOH:O	2.54	0.55
1:L:23:LYS:HG3	4:L:2010:HOH:O	2.05	0.55
1:L:4:VAL:HG13	1:L:150:GLY:O	2.06	0.55
1:H:67:LEU:HD13	1:H:69:ARG:NH2	2.21	0.55
1:J:79:ARG:HD3	1:J:80:HIS:O	2.06	0.55
1:K:153:GLN:HB2	1:L:50:PHE:CE1	2.41	0.55
1:A:24:GLU:O	1:A:25:SER:C	2.45	0.55
1:L:22:GLN:OE1	1:L:106:LEU:HB2	2.07	0.55
1:E:39:THR:HG22	1:K:13:PRO:HG3	1.89	0.55
1:C:1:ALA:N	4:C:2001:HOH:O	2.39	0.55
1:H:80:HIS:O	1:H:83:ASP:HB2	2.07	0.55
1:K:4:VAL:HG12	1:K:5:VAL:N	2.20	0.54
1:B:71:HIS:HB2	1:B:80:HIS:CE1	2.43	0.54
1:L:76:ASP:O	1:L:79:ARG:HG2	2.06	0.54
1:F:132:GLU:O	1:F:135:THR:OG1	2.19	0.54
1:I:4:VAL:HG21	1:I:113:ILE:HD12	1.87	0.54
1:B:70:LYS:HD2	4:B:2075:HOH:O	2.07	0.54
1:J:75:LYS:HG2	4:J:2036:HOH:O	2.08	0.54
1:K:22:GLN:OE1	1:K:106:LEU:HB2	2.08	0.54
1:H:118:VAL:HG11	1:H:143:ARG:HG2	1.90	0.54
1:H:4:VAL:CG1	1:H:5:VAL:N	2.71	0.54
1:K:102:SER:HB3	4:K:2008:HOH:O	2.08	0.54
1:H:23:LYS:HG3	4:H:2013:HOH:O	2.08	0.54
1:L:70:LYS:CB	1:L:70:LYS:HZ3	1.98	0.53
1:H:22:GLN:C	4:H:2009:HOH:O	2.45	0.53
1:B:66:PRO:CD	1:B:81:VAL:CG1	2.86	0.53
1:B:2:THR:HG22	1:B:3:LYS:HG3	1.90	0.53
1:J:69:ARG:CD	1:J:78:GLU:CD	2.72	0.53
1:J:70:LYS:HG3	1:J:78:GLU:HG3	1.88	0.53
1:H:46:HIS:CE1	1:H:120:HIS:CD2	2.97	0.53
1:I:48:HIS:CE1	1:I:63:HIS:HD2	2.26	0.53
1:G:4:VAL:HG13	1:G:150:GLY:O	2.08	0.53
1:H:112:ILE:HD12	1:H:149:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:HB3	4:A:2100:HOH:O	2.08	0.53
1:H:47:VAL:HG12	4:H:2045:HOH:O	2.08	0.53
1:F:121:GLU:HA	1:F:144:LEU:HD11	1.90	0.53
1:J:4:VAL:CG2	1:J:113:ILE:HD13	2.37	0.53
1:H:81:VAL:HG13	1:H:103:VAL:HG12	1.89	0.53
1:L:28:PRO:C	4:L:2015:HOH:O	2.48	0.53
1:H:79:ARG:HH22	1:H:101:ASP:CG	2.13	0.52
1:L:113:ILE:HG23	4:L:2070:HOH:O	2.09	0.52
1:B:66:PRO:CD	1:B:81:VAL:HG11	2.39	0.52
1:J:121:GLU:HB2	1:J:142:SER:HB2	1.91	0.52
1:D:71:HIS:HB2	1:D:80:HIS:CE1	2.44	0.52
1:G:4:VAL:CG1	1:G:149:ILE:HG22	2.36	0.52
1:G:4:VAL:CG1	1:G:5:VAL:N	2.72	0.52
1:F:92:ASP:HA	4:F:2040:HOH:O	2.08	0.52
1:B:91:LYS:HD2	4:D:2098:HOH:O	2.07	0.52
1:G:111:CYS:N	4:G:2054:HOH:O	2.43	0.52
1:F:2:THR:HG22	1:F:3:LYS:HG3	1.92	0.52
1:F:121:GLU:HB2	1:F:142:SER:HB3	1.92	0.52
1:L:29:VAL:N	4:L:2015:HOH:O	2.42	0.52
1:I:134:SER:HB2	1:I:139:ASN:ND2	2.24	0.52
1:K:48:HIS:N	1:K:116:THR:O	2.33	0.52
1:K:80:HIS:HB2	1:K:83:ASP:CG	2.29	0.52
1:A:40:GLU:HG2	4:A:2080:HOH:O	2.09	0.52
1:A:153:GLN:O	4:A:2135:HOH:O	2.19	0.52
1:B:75:LYS:HE3	1:B:75:LYS:CA	2.34	0.51
1:B:79:ARG:HD3	1:B:83:ASP:HB2	1.92	0.51
1:I:79:ARG:HD2	1:I:80:HIS:O	2.10	0.51
1:C:132:GLU:HG2	1:C:136:LYS:HE2	1.93	0.51
1:H:7:VAL:O	1:H:147:GLY:HA3	2.09	0.51
1:G:105:SER:OG	1:G:107:SER:O	2.15	0.51
1:J:65:ASN:HD21	1:J:69:ARG:N	2.08	0.51
1:F:75:LYS:HE3	4:F:2026:HOH:O	2.08	0.51
1:G:109:ASP:OD1	1:G:109:ASP:C	2.49	0.51
1:L:80:HIS:HB2	1:L:83:ASP:CG	2.31	0.50
1:E:38:LEU:O	1:E:93:GLY:HA2	2.11	0.50
1:J:4:VAL:HG23	4:J:2001:HOH:O	2.10	0.50
1:I:63:HIS:CE1	1:I:137:THR:HA	2.47	0.50
1:G:71:HIS:HB2	1:G:80:HIS:CE1	2.47	0.50
1:K:99:ILE:HG13	4:K:2011:HOH:O	2.10	0.50
1:L:42:LEU:HB2	1:L:123:ALA:HB2	1.94	0.50
1:K:90:ASP:OD1	1:K:92:ASP:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:LEU:HD12	4:I:2022:HOH:O	2.11	0.49
1:H:81:VAL:HA	1:H:103:VAL:HG12	1.94	0.49
1:E:80:HIS:HB2	1:E:83:ASP:OD1	2.12	0.49
1:L:71:HIS:HB2	1:L:80:HIS:HE1	1.77	0.49
1:I:135:THR:HG23	1:I:136:LYS:HG3	1.95	0.49
4:K:2017:HOH:O	1:L:152:ALA:CA	2.29	0.49
1:I:46:HIS:CE1	1:I:120:HIS:CD2	3.01	0.49
1:L:22:GLN:NE2	1:L:25:SER:O	2.45	0.49
1:H:113:ILE:HA	1:H:149:ILE:HG22	1.93	0.49
1:B:64:PHE:CD2	1:B:81:VAL:HG11	2.47	0.49
1:K:99:ILE:CG2	1:K:100:GLU:N	2.75	0.48
1:H:47:VAL:HG11	1:H:112:ILE:HG22	1.94	0.48
1:H:47:VAL:HG11	4:H:2045:HOH:O	2.12	0.48
1:H:64:PHE:CB	4:H:2045:HOH:O	2.48	0.48
1:C:30:LYS:HD2	4:C:2026:HOH:O	2.13	0.48
1:I:51:GLY:HA3	1:I:114:GLY:O	2.13	0.48
1:L:8:LEU:HD11	1:L:117:LEU:HD23	1.94	0.48
1:G:97:VAL:HG22	4:G:2042:HOH:O	2.13	0.48
1:A:79:ARG:HD3	1:A:83:ASP:HB2	1.95	0.48
1:I:111:CYS:SG	1:I:113:ILE:HG12	2.54	0.48
1:I:48:HIS:CE1	1:I:63:HIS:CD2	3.01	0.48
1:E:80:HIS:HB2	1:E:83:ASP:CG	2.34	0.48
1:G:64:PHE:HZ	4:G:2054:HOH:O	1.97	0.48
1:K:111:CYS:SG	1:K:113:ILE:HG12	2.54	0.48
1:E:79:ARG:HD2	1:E:80:HIS:O	2.14	0.48
1:K:4:VAL:HG13	1:K:150:GLY:O	2.14	0.48
1:H:67:LEU:HD21	4:H:2019:HOH:O	2.13	0.48
1:C:3:LYS:HB2	1:C:3:LYS:HE3	1.28	0.48
1:K:42:LEU:CD1	1:K:42:LEU:N	2.77	0.47
1:G:1:ALA:C	4:G:2002:HOH:O	2.53	0.47
1:L:100:GLU:O	4:L:2038:HOH:O	2.19	0.47
1:G:34:SER:HA	1:G:95:ALA:O	2.14	0.47
1:K:30:LYS:HG3	4:K:2009:HOH:O	2.14	0.47
1:A:92:ASP:CA	4:A:2081:HOH:O	2.61	0.47
1:G:97:VAL:HG23	4:G:2042:HOH:O	2.13	0.47
1:K:153:GLN:HB2	1:L:50:PHE:CZ	2.48	0.47
1:G:14:VAL:HG13	1:G:35:ILE:HG22	1.96	0.47
1:H:101:ASP:N	4:H:2051:HOH:O	2.48	0.47
1:G:14:VAL:HA	1:G:36:LYS:O	2.14	0.47
1:L:70:LYS:HG3	1:L:78:GLU:CG	2.44	0.47
1:B:108:GLY:N	1:F:77:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB1	4:G:2077:HOH:O	2.14	0.47
1:I:71:HIS:HB2	1:I:80:HIS:CE1	2.49	0.47
1:G:42:LEU:H	1:G:42:LEU:CD1	2.27	0.47
1:K:42:LEU:N	1:K:42:LEU:HD12	2.30	0.47
1:A:136:LYS:NZ	4:A:2119:HOH:O	2.46	0.47
1:K:51:GLY:HA2	1:K:116:THR:OG1	2.15	0.47
1:I:4:VAL:HG11	1:I:149:ILE:CG2	2.45	0.47
1:L:80:HIS:HB2	1:L:83:ASP:OD1	2.14	0.47
1:J:4:VAL:N	4:J:2001:HOH:O	2.46	0.46
1:J:90:ASP:O	1:J:93:GLY:N	2.39	0.46
1:J:70:LYS:CG	1:J:78:GLU:HG2	2.45	0.46
1:L:47:VAL:HG22	4:L:2050:HOH:O	2.15	0.46
1:K:69:ARG:HD2	4:K:2026:HOH:O	2.14	0.46
1:H:136:LYS:HE3	4:H:2075:HOH:O	2.10	0.46
1:H:25:SER:C	1:H:27:GLY:N	2.60	0.46
1:K:72:GLY:CA	4:K:2035:HOH:O	2.37	0.46
1:G:121:GLU:HA	1:G:144:LEU:HD11	1.97	0.46
1:G:5:VAL:HG22	1:G:6:CYS:N	2.31	0.46
1:G:2:THR:N	4:G:2002:HOH:O	2.49	0.46
1:B:79:ARG:HD3	1:B:80:HIS:O	2.15	0.46
1:A:75:LYS:HE3	4:A:2070:HOH:O	2.15	0.46
1:L:4:VAL:HG11	1:L:149:ILE:HG22	1.97	0.46
1:L:120:HIS:HB3	1:L:140:ALA:O	2.15	0.46
1:G:3:LYS:HB2	1:G:3:LYS:HE3	1.54	0.46
1:H:40:GLU:CG	4:H:2018:HOH:O	2.49	0.46
1:L:23:LYS:HB2	1:L:24:GLU:OE1	2.16	0.46
1:G:99:ILE:CG2	1:G:100:GLU:N	2.79	0.46
1:A:4:VAL:HB	1:A:150:GLY:O	2.16	0.46
1:K:14:VAL:HG21	1:K:144:LEU:HB3	1.97	0.46
1:A:121:GLU:HA	1:A:144:LEU:HD11	1.97	0.46
1:A:4:VAL:CG2	1:A:20:PHE:HB2	2.41	0.46
1:K:4:VAL:HG13	1:K:5:VAL:H	1.80	0.45
1:H:49:GLU:HG2	4:H:2022:HOH:O	2.15	0.45
1:G:133:GLU:HA	1:G:136:LYS:HE2	1.97	0.45
1:I:4:VAL:CG1	1:I:149:ILE:CG2	2.94	0.45
1:J:90:ASP:OD1	1:J:90:ASP:C	2.54	0.45
1:C:77:GLU:HG2	4:C:2078:HOH:O	2.15	0.45
1:H:4:VAL:HG13	1:H:5:VAL:N	2.31	0.45
1:D:1:ALA:HB2	1:D:113:ILE:HD11	1.97	0.45
1:H:103:VAL:HG22	4:H:2014:HOH:O	2.13	0.45
1:J:14:VAL:HG21	1:J:144:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LYS:HE3	4:K:2027:HOH:O	2.17	0.45
1:I:46:HIS:ND1	1:I:120:HIS:HD2	2.15	0.45
1:H:23:LYS:HA	4:H:2011:HOH:O	2.17	0.45
1:G:14:VAL:HG21	1:G:38:LEU:HD13	2.00	0.45
1:K:49:GLU:O	1:K:115:ARG:NH1	2.46	0.44
1:B:70:LYS:HZ3	1:B:70:LYS:HG2	1.50	0.44
1:E:105:SER:O	1:E:111:CYS:HA	2.18	0.44
1:D:26:ASN:C	1:D:26:ASN:ND2	2.71	0.44
1:L:36:LYS:HG2	1:L:94:VAL:HG22	1.98	0.44
1:K:80:HIS:HB2	1:K:83:ASP:OD1	2.17	0.44
1:H:81:VAL:HG13	4:H:2058:HOH:O	2.18	0.44
1:F:70:LYS:CG	1:F:78:GLU:CG	2.95	0.44
1:F:92:ASP:CA	4:F:2040:HOH:O	2.63	0.44
1:H:52:ASP:OD1	1:H:54:THR:HG23	2.18	0.44
1:L:70:LYS:HG2	1:L:78:GLU:OE2	2.17	0.44
1:K:107:SER:CB	4:K:2049:HOH:O	2.37	0.44
1:L:28:PRO:HA	4:L:2015:HOH:O	2.17	0.44
1:H:47:VAL:HB	1:H:82:GLY:HA2	2.00	0.43
1:A:92:ASP:C	4:A:2081:HOH:O	2.56	0.43
1:D:79:ARG:HD3	1:D:80:HIS:O	2.17	0.43
1:H:81:VAL:N	4:H:2044:HOH:O	2.51	0.43
1:E:39:THR:HG23	1:K:13:PRO:HG3	1.99	0.43
1:C:121:GLU:HA	1:C:144:LEU:HD11	1.98	0.43
1:F:120:HIS:HB3	1:F:140:ALA:O	2.18	0.43
1:I:46:HIS:CE1	1:I:120:HIS:HD2	2.35	0.43
1:E:79:ARG:CD	1:E:80:HIS:O	2.66	0.43
1:J:132:GLU:O	1:J:135:THR:OG1	2.29	0.43
1:L:109:ASP:OD2	1:L:110:HIS:HD2	2.02	0.43
1:G:8:LEU:O	1:G:15:GLN:HA	2.19	0.43
1:L:128:LYS:NZ	4:L:2027:HOH:O	2.50	0.43
1:A:3:LYS:HB2	1:A:3:LYS:HE3	1.44	0.43
1:H:79:ARG:HD2	1:H:80:HIS:C	2.35	0.43
1:E:25:SER:O	1:E:26:ASN:OD1	2.37	0.43
1:L:111:CYS:SG	1:L:113:ILE:HG12	2.59	0.43
1:H:22:GLN:O	1:H:24:GLU:N	2.52	0.43
1:D:76:ASP:O	1:D:79:ARG:HG2	2.18	0.43
1:H:80:HIS:HB2	1:H:83:ASP:OD2	2.17	0.43
1:F:70:LYS:HG3	1:F:78:GLU:CG	2.48	0.43
1:A:40:GLU:OE1	4:A:2040:HOH:O	2.22	0.43
1:F:134:SER:HB2	1:F:139:ASN:ND2	2.34	0.43
1:L:78:GLU:N	4:L:2029:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:GLY:HA2	1:J:134:SER:OG	2.19	0.42
1:L:77:GLU:HG2	4:L:2029:HOH:O	2.07	0.42
1:D:75:LYS:HD3	1:D:75:LYS:HA	1.62	0.42
1:I:117:LEU:O	1:I:146:CYS:HA	2.18	0.42
1:K:120:HIS:HE1	4:K:2064:HOH:O	2.02	0.42
1:J:68:SER:C	4:J:2033:HOH:O	2.58	0.42
1:C:128:LYS:CD	4:C:2119:HOH:O	2.67	0.42
1:B:64:PHE:O	1:B:81:VAL:CG1	2.68	0.42
1:B:66:PRO:HD3	1:B:81:VAL:HG11	2.00	0.42
1:L:4:VAL:HG12	1:L:5:VAL:N	2.33	0.42
1:H:67:LEU:HA	1:H:67:LEU:HD23	1.78	0.42
1:K:30:LYS:CG	4:K:2009:HOH:O	2.67	0.42
1:I:14:VAL:HG21	1:I:144:LEU:HD13	2.00	0.42
1:C:116:THR:CG2	1:C:146:CYS:HB2	2.50	0.42
1:J:4:VAL:CG1	1:J:5:VAL:N	2.81	0.42
1:K:121:GLU:HB2	1:K:142:SER:HB2	2.01	0.42
1:B:38:LEU:O	1:B:93:GLY:HA2	2.19	0.42
1:H:27:GLY:HA2	1:H:28:PRO:HD3	1.90	0.42
1:H:81:VAL:HA	1:H:103:VAL:CG1	2.49	0.42
1:I:112:ILE:HD12	1:I:149:ILE:HD13	2.02	0.42
1:K:69:ARG:HD2	1:K:78:GLU:OE1	2.19	0.42
1:A:91:LYS:HG3	1:A:91:LYS:H	1.62	0.42
1:L:26:ASN:N	4:L:2013:HOH:O	2.46	0.41
1:F:128:LYS:HE3	4:F:2060:HOH:O	2.16	0.41
1:H:143:ARG:C	4:H:2081:HOH:O	2.58	0.41
1:A:105:SER:O	1:A:111:CYS:HA	2.20	0.41
1:G:13:PRO:HG3	1:J:37:GLY:HA2	2.02	0.41
1:H:118:VAL:HG22	1:H:146:CYS:HB3	2.01	0.41
1:B:4:VAL:HG13	1:B:106:LEU:HD13	2.02	0.41
1:H:126:LEU:HB2	1:H:128:LYS:HE3	2.02	0.41
1:D:69:ARG:NH2	4:D:2071:HOH:O	2.54	0.41
1:K:90:ASP:OD1	1:K:93:GLY:N	2.53	0.41
1:E:119:VAL:HG13	1:E:119:VAL:O	2.20	0.41
1:H:112:ILE:HA	1:H:115:ARG:HD2	2.02	0.41
1:D:36:LYS:HG2	4:D:2018:HOH:O	2.21	0.41
1:L:60:ALA:HB2	4:L:2021:HOH:O	2.20	0.41
1:H:79:ARG:HD2	1:H:103:VAL:HG11	2.02	0.41
1:H:80:HIS:N	1:H:83:ASP:OD2	2.45	0.41
1:G:76:ASP:O	1:G:79:ARG:HG2	2.21	0.41
1:H:80:HIS:H	1:H:83:ASP:CG	2.22	0.41
1:L:4:VAL:CG1	1:L:149:ILE:CG2	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:LEU:H	1:L:42:LEU:CD1	2.34	0.41
1:J:4:VAL:HB	4:J:2001:HOH:O	2.20	0.41
1:B:64:PHE:CD2	1:B:81:VAL:CG1	3.03	0.41
1:H:39:THR:OG1	1:H:43:HIS:CE1	2.73	0.41
1:C:91:LYS:HG3	1:C:91:LYS:H	1.67	0.41
1:A:117:LEU:O	1:A:146:CYS:HA	2.21	0.41
1:H:126:LEU:HB3	4:H:2068:HOH:O	2.21	0.41
1:K:133:GLU:HA	1:K:136:LYS:HE3	2.03	0.41
1:J:65:ASN:HD21	1:J:69:ARG:H	1.67	0.40
1:L:4:VAL:CG1	1:L:5:VAL:N	2.84	0.40
1:F:90:ASP:OD1	1:F:92:ASP:HB2	2.20	0.40
1:G:90:ASP:OD2	1:G:94:VAL:HB	2.21	0.40
1:L:64:PHE:CE1	1:L:115:ARG:CZ	3.05	0.40
1:L:112:ILE:CD1	4:L:2045:HOH:O	2.64	0.40
1:K:105:SER:O	1:K:111:CYS:HA	2.21	0.40
1:B:4:VAL:HB	1:B:150:GLY:O	2.21	0.40
1:B:121:GLU:HA	1:B:144:LEU:HD11	2.02	0.40
1:A:40:GLU:CG	4:A:2080:HOH:O	2.66	0.40
1:I:4:VAL:CG2	1:I:113:ILE:HD12	2.52	0.40
1:H:60:ALA:CB	4:H:2026:HOH:O	2.65	0.40
1:L:128:LYS:CE	4:L:2027:HOH:O	2.70	0.40
1:I:14:VAL:HA	1:I:36:LYS:O	2.21	0.40
1:L:61:GLY:O	1:L:143:ARG:NH1	2.54	0.40
1:I:126:LEU:HD23	1:I:126:LEU:N	2.37	0.40

All (4) 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:26:ASN:ND2	1:J:69:ARG:NH2[1_545]	1.95	0.25
1:D:26:ASN:CG	1:J:69:ARG:NE[1_545]	2.03	0.17
1:A:77:GLU:OE2	1:C:109:ASP:N[2_555]	2.04	0.16
1:H:40:GLU:OE1	1:K:91:LYS:NZ[1_554]	2.10	0.10

## 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	151/153 (99%)	145 (96%)	5 (3%)	1 (1%)	26	14
1	B	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	26	14
1	C	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	D	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	E	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	26	14
1	F	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	G	151/153 (99%)	141 (93%)	9 (6%)	1 (1%)	26	14
1	H	151/153 (99%)	139 (92%)	9 (6%)	3 (2%)	9	2
1	I	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	J	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	K	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
1	L	151/153 (99%)	142 (94%)	8 (5%)	1 (1%)	26	14
All	All	1812/1836 (99%)	1737 (96%)	67 (4%)	8 (0%)	39	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	H	23	LYS
1	H	26	ASN
1	B	26	ASN
1	E	26	ASN
1	H	25	SER
1	L	27	GLY
1	G	13	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%)	108 (91%)	11 (9%)	11	4
1	B	119/119 (100%)	112 (94%)	7 (6%)	24	12
1	C	119/119 (100%)	112 (94%)	7 (6%)	24	12
1	D	119/119 (100%)	116 (98%)	3 (2%)	55	47
1	E	119/119 (100%)	109 (92%)	10 (8%)	14	5
1	F	119/119 (100%)	113 (95%)	6 (5%)	30	18
1	G	119/119 (100%)	107 (90%)	12 (10%)	9	3
1	H	119/119 (100%)	108 (91%)	11 (9%)	11	4
1	I	119/119 (100%)	111 (93%)	8 (7%)	20	9
1	J	119/119 (100%)	111 (93%)	8 (7%)	20	9
1	K	119/119 (100%)	111 (93%)	8 (7%)	20	9
1	L	119/119 (100%)	109 (92%)	10 (8%)	14	5
All	All	1428/1428 (100%)	1327 (93%)	101 (7%)	18	8

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	LEU
1	A	24	GLU
1	A	38	LEU
1	A	42	LEU
1	A	69	ARG
1	A	75	LYS
1	A	77	GLU
1	A	79	ARG
1	A	91	LYS
1	A	102	SER
1	B	8	LEU
1	B	11	ASP
1	B	25	SER
1	B	31	VAL
1	B	42	LEU
1	B	70	LYS
1	B	79	ARG
1	C	2	THR
1	C	25	SER
1	C	34	SER
1	C	38	LEU

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Mol	Chain	Res	Type
1	C	69	ARG
1	C	79	ARG
1	C	91	LYS
1	D	25	SER
1	D	42	LEU
1	D	79	ARG
1	E	2	THR
1	E	8	LEU
1	E	25	SER
1	E	31	VAL
1	E	34	SER
1	E	42	LEU
1	E	69	ARG
1	E	77	GLU
1	E	79	ARG
1	E	91	LYS
1	F	2	THR
1	F	8	LEU
1	F	31	VAL
1	F	34	SER
1	F	79	ARG
1	F	91	LYS
1	G	3	LYS
1	G	24	GLU
1	G	25	SER
1	G	26	ASN
1	G	34	SER
1	G	38	LEU
1	G	69	ARG
1	G	70	LYS
1	G	79	ARG
1	G	91	LYS
1	G	100	GLU
1	G	102	SER
1	H	4	VAL
1	H	24	GLU
1	H	26	ASN
1	H	31	VAL
1	H	42	LEU
1	H	70	LYS
1	H	75	LYS
1	H	79	ARG

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Mol	Chain	Res	Type
1	H	91	LYS
1	H	102	SER
1	H	109	ASP
1	I	2	THR
1	I	8	LEU
1	I	24	GLU
1	I	31	VAL
1	I	38	LEU
1	I	69	ARG
1	I	79	ARG
1	I	91	LYS
1	J	4	VAL
1	J	8	LEU
1	J	31	VAL
1	J	38	LEU
1	J	42	LEU
1	J	70	LYS
1	J	79	ARG
1	J	91	LYS
1	K	8	LEU
1	K	15	GLN
1	K	24	GLU
1	K	31	VAL
1	K	38	LEU
1	K	79	ARG
1	K	91	LYS
1	K	109	ASP
1	L	31	VAL
1	L	34	SER
1	L	42	LEU
1	L	53	ASN
1	L	54	THR
1	L	70	LYS
1	L	79	ARG
1	L	91	LYS
1	L	107	SER
1	L	142	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	ASN

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Mol	Chain	Res	Type
1	D	26	ASN
1	E	15	GLN
1	I	19	ASN
1	L	110	HIS

### 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 24 ligands modelled in this entry, 24 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	153/153 (100%)	0.02	1 (0%) 89 90	6, 11, 19, 28	4 (2%)
1	B	153/153 (100%)	0.11	2 (1%) 79 82	6, 11, 20, 30	1 (0%)
1	C	153/153 (100%)	0.01	1 (0%) 89 90	7, 11, 20, 28	2 (1%)
1	D	153/153 (100%)	0.01	1 (0%) 89 90	7, 11, 20, 28	0
1	E	153/153 (100%)	0.08	3 (1%) 68 71	8, 15, 25, 30	3 (1%)
1	F	153/153 (100%)	0.20	2 (1%) 79 82	7, 14, 22, 29	6 (3%)
1	G	153/153 (100%)	1.29	46 (30%) 1 0	6, 19, 29, 34	7 (4%)
1	H	153/153 (100%)	2.06	67 (43%) 0 0	12, 23, 34, 38	19 (12%)
1	I	153/153 (100%)	0.66	13 (8%) 13 15	10, 19, 28, 32	11 (7%)
1	J	153/153 (100%)	0.17	2 (1%) 79 82	9, 16, 24, 31	7 (4%)
1	K	152/153 (99%)	1.32	29 (19%) 2 2	11, 20, 30, 37	20 (13%)
1	L	153/153 (100%)	0.75	16 (10%) 8 9	10, 18, 28, 33	6 (3%)
All	All	1835/1836 (99%)	0.56	183 (9%) 9 10	6, 16, 28, 38	86 (4%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	ALA	15.9
1	K	1	ALA	14.3
1	K	26	ASN	12.8
1	G	1	ALA	9.2
1	B	1	ALA	9.1
1	I	26	ASN	9.0
1	D	1	ALA	6.2
1	G	26	ASN	6.2
1	G	93	GLY	6.1
1	K	92	ASP	5.7
1	K	27	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	H	29	VAL	5.3
1	H	38	LEU	5.2
1	L	26	ASN	5.2
1	C	1	ALA	5.2
1	G	153	GLN	5.0
1	K	108	GLY	5.0
1	K	2	THR	5.0
1	G	28	PRO	4.9
1	H	106	LEU	4.8
1	G	113	ILE	4.7
1	H	73	GLY	4.7
1	G	114	GLY	4.5
1	K	29	VAL	4.5
1	H	111	CYS	4.5
1	H	27	GLY	4.4
1	G	25	SER	4.3
1	H	39	THR	4.3
1	H	108	GLY	4.3
1	H	109	ASP	4.2
1	H	11	ASP	4.1
1	H	66	PRO	4.0
1	H	26	ASN	4.0
1	H	81	VAL	4.0
1	H	67	LEU	4.0
1	H	119	VAL	3.9
1	H	112	ILE	3.9
1	H	24	GLU	3.9
1	H	105	SER	3.9
1	K	28	PRO	3.9
1	G	23	LYS	3.9
1	H	64	PHE	3.7
1	H	85	GLY	3.7
1	G	92	ASP	3.7
1	H	84	LEU	3.7
1	K	94	VAL	3.7
1	H	28	PRO	3.6
1	L	109	ASP	3.6
1	G	95	ALA	3.6
1	H	15	GLN	3.5
1	H	92	ASP	3.5
1	J	25	SER	3.5
1	L	108	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	8	LEU	3.5
1	K	25	SER	3.5
1	G	151	ILE	3.5
1	H	74	PRO	3.5
1	I	77	GLU	3.4
1	A	1	ALA	3.4
1	H	42	LEU	3.4
1	H	50	PHE	3.4
1	G	6	CYS	3.4
1	H	117	LEU	3.4
1	H	12	GLY	3.4
1	K	89	ALA	3.3
1	G	31	VAL	3.3
1	H	47	VAL	3.3
1	B	26	ASN	3.3
1	I	67	LEU	3.3
1	G	29	VAL	3.3
1	H	83	ASP	3.3
1	H	91	LYS	3.2
1	I	91	LYS	3.2
1	I	72	GLY	3.2
1	G	11	ASP	3.2
1	H	23	LYS	3.2
1	G	96	ASP	3.1
1	H	140	ALA	3.1
1	H	10	GLY	3.1
1	G	91	LYS	3.0
1	K	93	GLY	3.0
1	H	25	SER	3.0
1	K	67	LEU	3.0
1	G	30	LYS	3.0
1	G	14	VAL	3.0
1	H	40	GLU	3.0
1	H	49	GLU	3.0
1	I	140	ALA	2.9
1	G	21	GLU	2.9
1	K	8	LEU	2.9
1	G	5	VAL	2.9
1	H	14	VAL	2.9
1	I	110	HIS	2.9
1	H	144	LEU	2.9
1	H	149	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	32	TRP	2.9
1	H	37	GLY	2.9
1	K	109	ASP	2.8
1	G	4	VAL	2.8
1	H	13	PRO	2.8
1	K	23	LYS	2.8
1	K	7	VAL	2.8
1	H	8	LEU	2.8
1	G	24	GLU	2.8
1	H	57	CYS	2.8
1	H	87	VAL	2.8
1	H	93	GLY	2.8
1	H	102	SER	2.8
1	G	3	LYS	2.7
1	G	35	ILE	2.7
1	H	80	HIS	2.7
1	K	32	TRP	2.6
1	K	151	ILE	2.6
1	H	56	GLY	2.6
1	G	103	VAL	2.6
1	K	14	VAL	2.6
1	I	42	LEU	2.5
1	L	70	LYS	2.5
1	H	104	ILE	2.5
1	H	22	GLN	2.5
1	E	26	ASN	2.5
1	K	105	SER	2.5
1	L	8	LEU	2.5
1	K	12	GLY	2.5
1	G	94	VAL	2.5
1	K	106	LEU	2.5
1	L	42	LEU	2.5
1	H	45	PHE	2.4
1	H	48	HIS	2.4
1	L	14	VAL	2.4
1	G	105	SER	2.4
1	G	18	ILE	2.4
1	F	1	ALA	2.4
1	H	51	GLY	2.4
1	H	2	THR	2.4
1	I	12	GLY	2.4
1	G	104	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	28	PRO	2.3
1	F	77	GLU	2.3
1	I	129	GLY	2.3
1	G	98	SER	2.3
1	K	97	VAL	2.3
1	I	108	GLY	2.3
1	K	39	THR	2.3
1	G	108	GLY	2.2
1	G	20	PHE	2.2
1	G	99	ILE	2.2
1	H	46	HIS	2.2
1	E	2	THR	2.2
1	G	34	SER	2.2
1	K	113	ILE	2.2
1	L	32	TRP	2.2
1	H	21	GLU	2.2
1	G	42	LEU	2.2
1	G	106	LEU	2.2
1	H	148	VAL	2.2
1	L	1	ALA	2.1
1	E	77	GLU	2.1
1	L	21	GLU	2.1
1	G	112	ILE	2.1
1	H	116	THR	2.1
1	G	38	LEU	2.1
1	J	92	ASP	2.1
1	G	152	ALA	2.1
1	H	118	VAL	2.1
1	G	149	ILE	2.1
1	L	96	ASP	2.1
1	L	36	LYS	2.1
1	H	94	VAL	2.1
1	H	103	VAL	2.1
1	H	58	THR	2.1
1	L	12	GLY	2.1
1	G	77	GLU	2.1
1	L	38	LEU	2.1
1	K	31	VAL	2.1
1	K	17	ILE	2.0
1	G	102	SER	2.0
1	L	107	SER	2.0
1	H	110	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	41	GLY	2.0
1	I	75	LYS	2.0
1	H	114	GLY	2.0
1	I	109	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	I	155	1/1	1.00	0.14	-0.71	18,18,18,18	0
3	ZN	H	155	1/1	0.98	0.17	-1.38	21,21,21,21	0
3	ZN	J	155	1/1	0.98	0.05	-2.16	16,16,16,16	0
3	ZN	K	155	1/1	0.99	0.04	-2.68	18,18,18,18	0
3	ZN	G	155	1/1	1.00	0.03	-3.49	12,12,12,12	0
2	CU	K	154	1/1	0.98	0.04	-3.83	21,21,21,21	0
3	ZN	F	155	1/1	0.99	0.03	-4.11	13,13,13,13	0
3	ZN	E	155	1/1	1.00	0.02	-4.25	14,14,14,14	0
3	ZN	B	155	1/1	1.00	0.03	-4.38	12,12,12,12	0
3	ZN	C	155	1/1	0.99	0.04	-4.41	11,11,11,11	0
3	ZN	L	155	1/1	0.99	0.04	-4.50	17,17,17,17	0
3	ZN	D	155	1/1	0.99	0.05	-4.66	11,11,11,11	0
3	ZN	A	155	1/1	0.99	0.06	-5.06	10,10,10,10	0
2	CU	H	154	1/1	0.99	0.09	-	25,25,25,25	0
2	CU	D	154	1/1	0.99	0.06	-	18,18,18,18	0
2	CU	J	154	1/1	0.99	0.03	-	21,21,21,21	0
2	CU	C	154	1/1	0.98	0.07	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	G	154	1/1	0.99	0.03	-	17,17,17,17	0
2	CU	I	154	1/1	0.96	0.11	-	27,27,27,27	0
2	CU	L	154	1/1	0.99	0.07	-	24,24,24,24	0
2	CU	E	154	1/1	0.99	0.03	-	21,21,21,21	0
2	CU	B	154	1/1	0.99	0.03	-	18,18,18,18	0
2	CU	A	154	1/1	0.98	0.04	-	17,17,17,17	0
2	CU	F	154	1/1	0.98	0.03	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.