



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2017 – 12:20 PM EST

PDB ID : 5LZL  
Title : Pyrobaculum calidifontis 5-aminolaevulinic acid dehydratase  
Authors : Azim, N.; Erskine, P.T.; Guo, J.; Cooper, J.B.  
Deposited on : 2016-09-30  
Resolution : 3.47 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

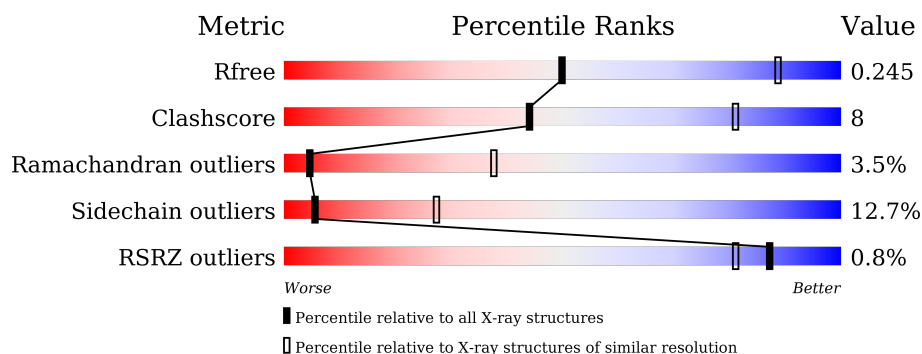
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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))
$R_{free}$	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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	338	<div> <div>66%</div> <div>27%</div> <div>5% ..</div> </div>
1	B	338	<div> <div>65%</div> <div>28%</div> <div>6% ..</div> </div>
1	C	338	<div> <div>71%</div> <div>24%</div> <div>..</div> </div>
1	D	338	<div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	E	338	<div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	F	338	<div> <div>73%</div> <div>24%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	338	 2% 67% 28% 3%
1	H	338	 70% 22% 7%
1	I	338	 73% 20% 5%
1	J	338	 1% 75% 21% 3%
1	K	338	 3% 74% 21% 2%
1	L	338	 2% 73% 22% 3%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31739 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 Delta-aminolevulinic acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	B	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	C	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	D	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	E	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	F	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	G	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	H	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	I	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	J	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	K	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			
1	L	336	Total	C	N	O	S	0	0	0
			2640	1696	453	480	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	6	Total 6	O 6	0	0
3	C	3	Total 3	O 3	0	0
3	D	2	Total 2	O 2	0	0
3	E	4	Total 4	O 4	0	0
3	F	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0
3	I	3	Total 3	O 3	0	0

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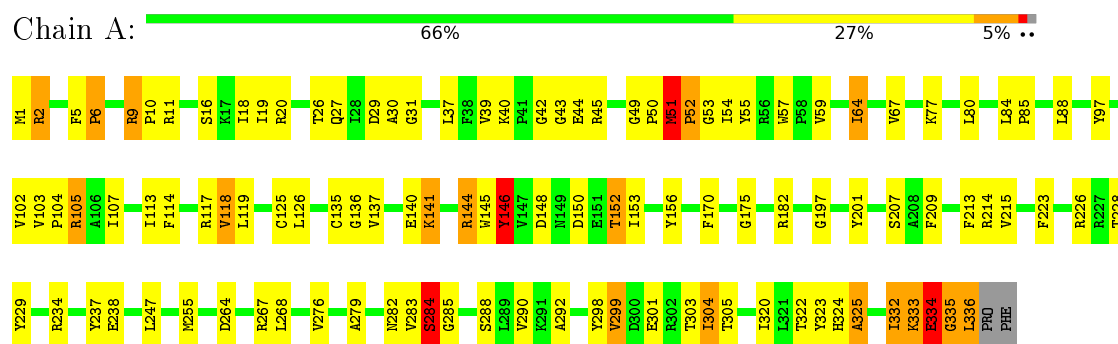
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	3	Total	O	0	0
			3	3		

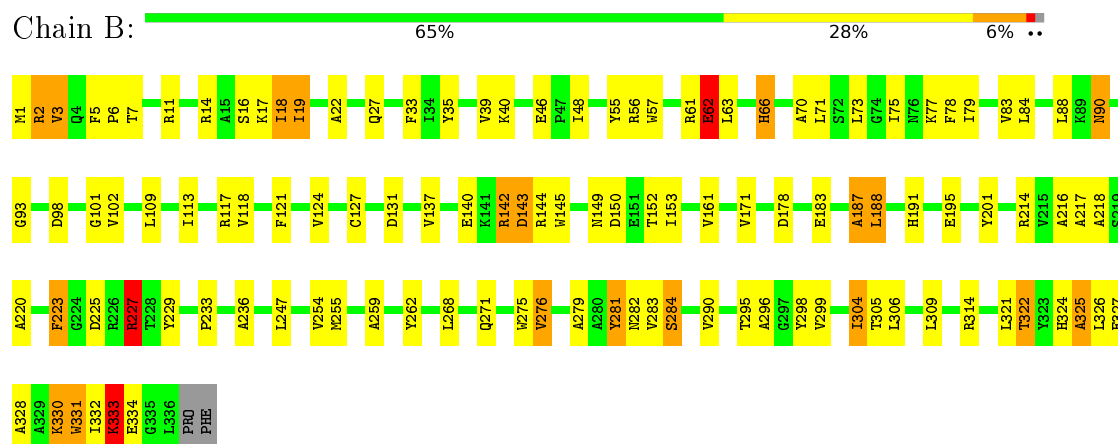
### 3 Residue-property plots

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.

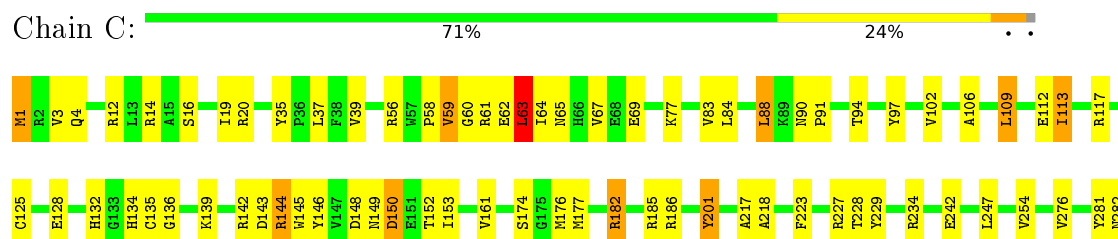
- Molecule 1: Delta-aminolevulinic acid dehydratase

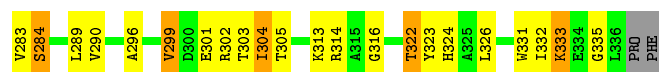


- Molecule 1: Delta-aminolevulinic acid dehydratase



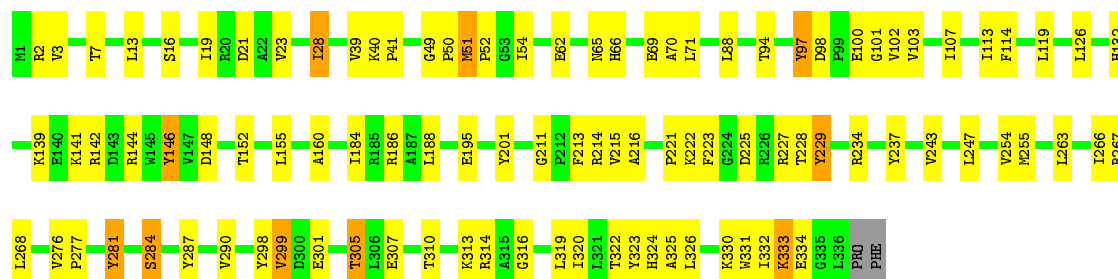
- Molecule 1: Delta-aminolevulinic acid dehydratase





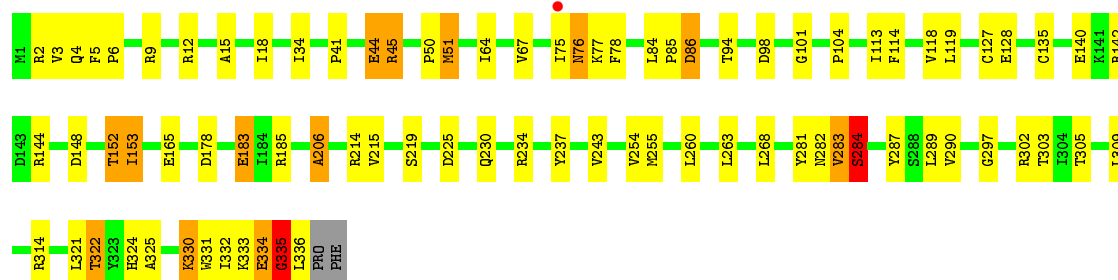
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain D: 70% 27% ..



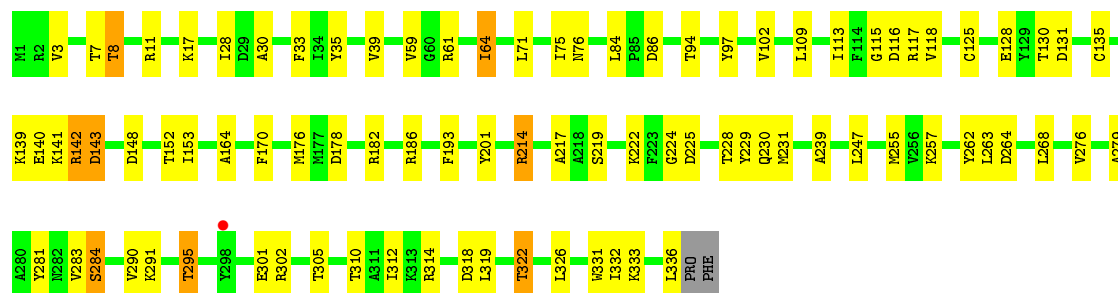
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain E: 75% 20% ..



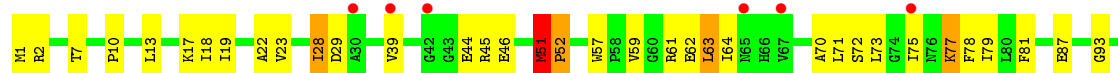
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain F: 73% 24% ..

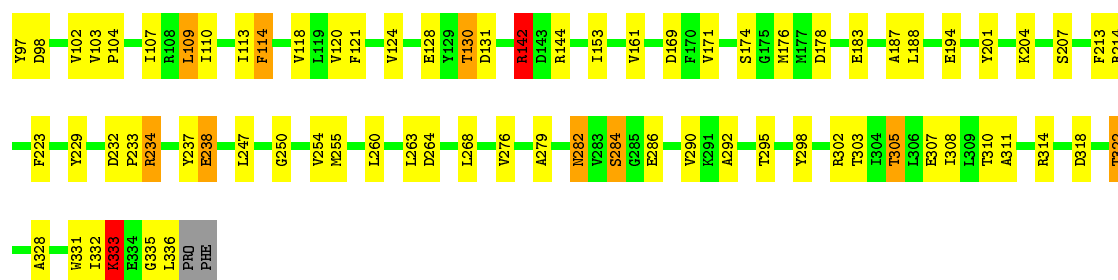


• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain G: 2% 67% 28% ..

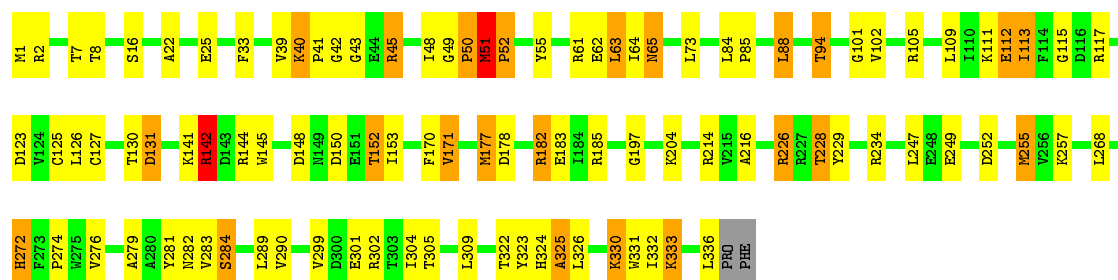






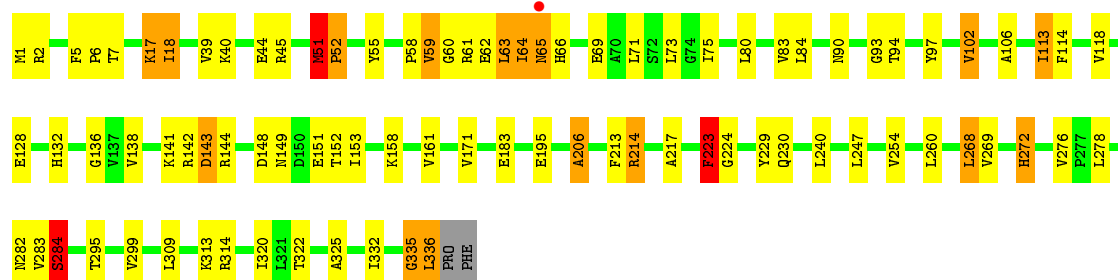
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain H: 70% 22% 7% ..



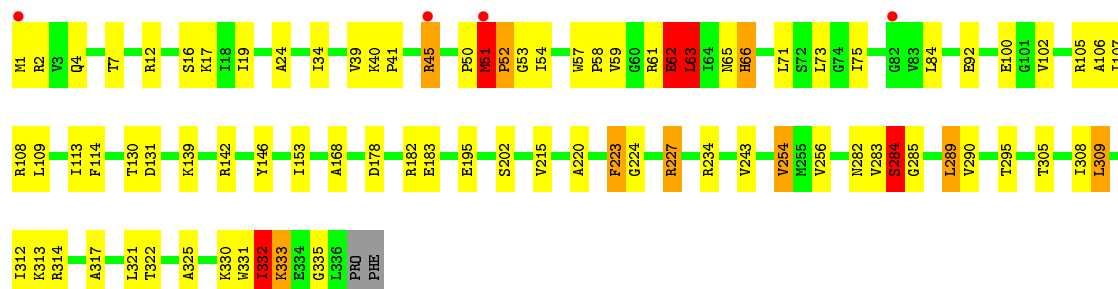
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain I: 73% 20% 5% ..

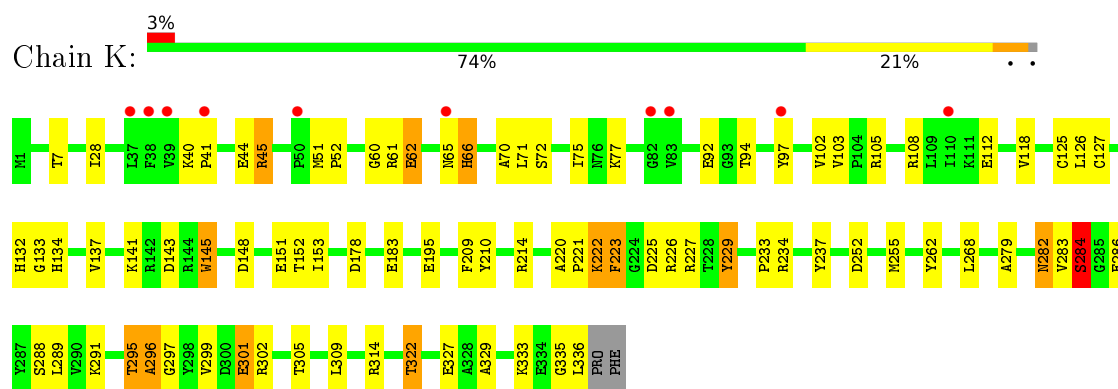


- Molecule 1: Delta-aminolevulinic acid dehydratase

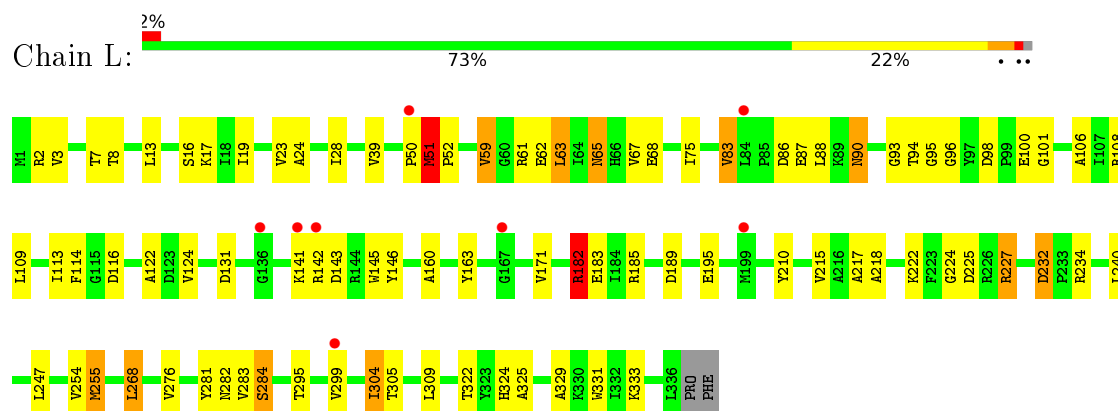
Chain J: 75% 21% ..



- Molecule 1: Delta-aminolevulinic acid dehydratase



• Molecule 1: Delta-aminolevulinic acid dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.56Å 205.56Å 199.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	178.02 – 3.47 91.34 – 3.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (178.02-3.47) 100.0 (91.34-3.47)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.71 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.148 , 0.250 0.151 , 0.245	Depositor DCC
$R_{free}$ test set	3154 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.65	0/2702	0.95	5/3664 (0.1%)
1	B	0.70	1/2702 (0.0%)	0.97	5/3664 (0.1%)
1	C	0.73	1/2702 (0.0%)	0.98	6/3664 (0.2%)
1	D	0.65	1/2702 (0.0%)	0.93	3/3664 (0.1%)
1	E	0.72	0/2702	0.97	2/3664 (0.1%)
1	F	0.69	1/2702 (0.0%)	0.94	5/3664 (0.1%)
1	G	0.71	0/2702	0.99	3/3664 (0.1%)
1	H	0.79	1/2702 (0.0%)	1.04	7/3664 (0.2%)
1	I	0.67	0/2702	0.98	4/3664 (0.1%)
1	J	0.64	1/2702 (0.0%)	0.94	7/3664 (0.2%)
1	K	0.62	0/2702	0.90	4/3664 (0.1%)
1	L	0.60	1/2702 (0.0%)	0.88	1/3664 (0.0%)
All	All	0.68	7/32424 (0.0%)	0.96	52/43968 (0.1%)

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	5
1	B	0	4
1	C	0	5
1	D	0	2
1	E	0	1
1	F	0	2
1	G	0	4
1	H	0	6
1	I	0	3
1	J	0	6
1	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
All	All	0	42

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	331	TRP	CB-CG	6.83	1.62	1.50
1	H	331	TRP	CB-CG	6.16	1.61	1.50
1	J	331	TRP	CB-CG	5.39	1.59	1.50
1	L	331	TRP	CB-CG	5.31	1.59	1.50
1	D	331	TRP	CB-CG	5.10	1.59	1.50
1	B	331	TRP	CB-CG	5.08	1.59	1.50
1	F	331	TRP	CB-CG	5.01	1.59	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	314	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	214	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	227	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	C	88	LEU	CA-CB-CG	7.40	132.32	115.30
1	J	314	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	G	214	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	I	214	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	J	108	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	K	314	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	227	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	J	105	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	2	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	214	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	L	182	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	214	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	I	314	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	1	MET	CG-SD-CE	6.05	109.88	100.20
1	F	314	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	117	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	G	51	MET	CB-CA-C	5.79	121.97	110.40
1	H	185	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	20	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	F	336	LEU	CB-CG-CD2	5.67	120.63	111.00
1	B	314	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	105	ARG	NE-CZ-NH2	-5.61	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	281	TYR	CA-CB-CG	5.58	124.01	113.40
1	H	123	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	51	MET	CB-CG-SD	5.55	129.04	112.40
1	J	12	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	H	171	VAL	N-CA-C	-5.51	96.12	111.00
1	C	322	THR	CB-CA-C	-5.51	96.73	111.60
1	D	214	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	E	314	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	314	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	H	331	TRP	CB-CA-C	5.43	121.27	110.40
1	F	322	THR	CA-CB-CG2	5.35	119.89	112.40
1	J	224	GLY	N-CA-C	5.34	126.44	113.10
1	H	88	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	63	LEU	CA-CB-CG	5.31	127.51	115.30
1	E	214	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	J	333	LYS	N-CA-C	5.20	125.04	111.00
1	I	102	VAL	CB-CA-C	-5.19	101.53	111.40
1	K	314	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	142	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	K	214	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	331	TRP	CB-CA-C	5.09	120.59	110.40
1	F	336	LEU	CA-CB-CG	5.09	127.01	115.30
1	K	45	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	331	TRP	CB-CA-C	5.03	120.45	110.40
1	J	234	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	302	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	GLY	Peptide
1	A	144	ARG	Peptide
1	A	282	ASN	Peptide
1	A	332	ILE	Peptide
1	A	335	GLY	Peptide
1	B	2	ARG	Peptide
1	B	223	PHE	Peptide
1	B	296	ALA	Peptide
1	B	62	GLU	Peptide
1	C	282	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	C	335	GLY	Peptide
1	C	62	GLU	Peptide
1	C	65	ASN	Peptide
1	C	84	LEU	Peptide
1	D	3	VAL	Peptide
1	D	62	GLU	Peptide
1	E	335	GLY	Peptide
1	F	130	THR	Peptide
1	F	224	GLY	Peptide
1	G	130	THR	Peptide
1	G	282	ASN	Peptide
1	G	335	GLY	Peptide
1	G	62	GLU	Peptide
1	H	112	GLU	Peptide
1	H	130	THR	Peptide
1	H	51	MET	Peptide
1	H	61	ARG	Peptide
1	H	64	ILE	Peptide
1	H	65	ASN	Peptide
1	I	223	PHE	Peptide
1	I	335	GLY	Peptide
1	I	62	GLU	Peptide
1	J	130	THR	Peptide
1	J	223	PHE	Peptide
1	J	332	ILE	Peptide
1	J	335	GLY	Peptide
1	J	51	MET	Peptide
1	J	61	ARG	Peptide
1	K	282	ASN	Peptide
1	K	296	ALA	Peptide
1	K	335	GLY	Peptide
1	L	116	ASP	Peptide

## 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	2640	0	2638	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2640	0	2640	63	0
1	C	2640	0	2638	50	0
1	D	2640	0	2638	39	0
1	E	2640	0	2638	45	0
1	F	2640	0	2639	35	0
1	G	2640	0	2638	47	0
1	H	2640	0	2639	55	0
1	I	2640	0	2638	42	0
1	J	2640	0	2639	28	0
1	K	2640	0	2636	39	0
1	L	2640	0	2638	37	0
2	A	2	0	0	0	0
2	B	2	0	0	1	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	1	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
All	All	31739	0	31659	506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (506) 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:E:330:LYS:O	1:E:332:ILE:CD1	1.73	1.32
1:E:330:LYS:O	1:E:332:ILE:HD12	1.32	1.22
1:H:322:THR:HG22	1:H:324:HIS:H	1.04	1.13
1:E:330:LYS:O	1:E:332:ILE:HD13	1.57	1.04
1:C:322:THR:HG22	1:C:324:HIS:H	1.16	1.04
1:E:302:ARG:NH2	1:E:333:LYS:O	1.89	1.03
1:J:63:LEU:HD21	1:J:113:ILE:HG21	1.39	1.03
1:H:322:THR:HG22	1:H:324:HIS:N	1.76	0.99
1:B:127:CYS:HG	2:B:401:ZN:ZN	0.71	0.95
1:C:322:THR:HG22	1:C:324:HIS:N	1.81	0.95
1:E:148:ASP:O	1:E:152:THR:HG22	1.70	0.91
1:B:75:ILE:HD13	1:B:326:LEU:HD12	1.56	0.88
1:K:226:ARG:HG2	1:K:229:TYR:OH	1.74	0.87
1:E:330:LYS:C	1:E:332:ILE:HD12	1.96	0.84
1:J:52:PRO:O	1:J:54:ILE:N	2.10	0.84
1:H:322:THR:CG2	1:H:324:HIS:H	1.89	0.81
1:K:302:ARG:NH2	1:K:333:LYS:O	2.14	0.81
1:K:134:HIS:CD2	1:K:223:PHE:HE1	2.00	0.80
1:A:64:ILE:HG13	1:A:113:ILE:HG21	1.64	0.80
1:C:322:THR:CG2	1:C:324:HIS:H	1.93	0.79
1:K:134:HIS:HD2	1:K:223:PHE:HE1	1.30	0.78
1:A:299:VAL:HG11	1:A:304:ILE:HD12	1.67	0.76
1:C:332:ILE:O	1:C:332:ILE:HG22	1.86	0.75
1:G:290:VAL:HG11	1:G:305:THR:HG22	1.66	0.74
1:H:148:ASP:O	1:H:152:THR:CG2	2.36	0.74
1:K:133:GLY:O	1:K:226:ARG:NH2	2.21	0.74
1:E:206:ALA:HB2	1:E:230:GLN:HB2	1.71	0.72
1:A:207:SER:OG	1:G:307:GLU:OE1	2.06	0.72
1:L:282:ASN:HB3	1:L:322:THR:HG22	1.72	0.71
1:I:141:LYS:O	1:I:143:ASP:N	2.25	0.69
1:K:255:MET:HB3	1:K:279:ALA:HB3	1.74	0.69
1:C:63:LEU:HG	1:C:64:ILE:HG23	1.75	0.68
1:G:124:VAL:HG21	1:G:171:VAL:HG13	1.76	0.68
1:C:332:ILE:C	1:C:333:LYS:HD3	2.13	0.67
1:K:127:CYS:HB2	1:K:226:ARG:HH22	1.58	0.67
1:K:134:HIS:CD2	1:K:223:PHE:CE1	2.83	0.67
1:H:322:THR:HG22	1:H:323:TYR:N	2.08	0.67
1:F:247:LEU:HD11	1:F:276:VAL:HG21	1.75	0.67
1:F:128:GLU:HG2	1:F:217:ALA:HB1	1.75	0.66
1:C:58:PRO:O	1:C:60:GLY:N	2.28	0.66
1:E:332:ILE:HD12	1:E:332:ILE:N	2.11	0.66
1:J:332:ILE:O	1:J:332:ILE:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:285:GLY:O	1:J:289:LEU:HB2	1.96	0.65
1:C:322:THR:HG21	1:C:324:HIS:HB2	1.76	0.65
1:A:301:GLU:O	1:A:305:THR:HG23	1.97	0.64
1:F:148:ASP:O	1:F:152:THR:HG22	1.97	0.64
1:B:70:ALA:HB2	1:B:326:LEU:HD11	1.80	0.64
1:K:62:GLU:HA	1:K:65:ASN:HB2	1.82	0.62
1:J:39:VAL:HG12	1:J:102:VAL:HG12	1.80	0.62
1:I:282:ASN:HB3	1:I:322:THR:HG22	1.81	0.62
1:B:22:ALA:HB1	1:F:319:LEU:HD21	1.80	0.62
1:E:75:ILE:HD12	1:E:325:ALA:HB1	1.82	0.62
1:B:124:VAL:HG21	1:B:171:VAL:HG13	1.82	0.62
1:F:141:LYS:O	1:F:143:ASP:N	2.33	0.61
1:C:322:THR:HG22	1:C:323:TYR:N	2.15	0.61
1:G:63:LEU:HD11	1:G:113:ILE:HG23	1.81	0.61
1:G:255:MET:HB3	1:G:279:ALA:HB3	1.81	0.61
1:C:63:LEU:HG	1:C:64:ILE:N	2.16	0.61
1:B:247:LEU:HD21	1:B:276:VAL:HG21	1.82	0.60
1:L:247:LEU:HD11	1:L:276:VAL:HG11	1.83	0.60
1:E:334:GLU:OE1	1:E:334:GLU:HA	2.00	0.60
1:K:134:HIS:HD2	1:K:223:PHE:CE1	2.14	0.60
1:D:324:HIS:O	1:D:326:LEU:N	2.35	0.60
1:B:40:LYS:HD2	1:B:46:GLU:OE2	2.03	0.59
1:K:309:LEU:HD21	1:K:322:THR:HG21	1.84	0.59
1:G:28:ILE:HD11	1:G:310:THR:OG1	2.03	0.58
1:H:48:ILE:HG21	1:H:216:ALA:HB2	1.85	0.58
1:I:45:ARG:HD3	1:I:55:TYR:CD2	2.38	0.58
1:I:75:ILE:HD13	1:I:325:ALA:HB1	1.84	0.58
1:J:312:ILE:HG22	1:J:317:ALA:HB3	1.85	0.58
1:H:101:GLY:O	1:H:105:ARG:HG3	2.03	0.58
1:H:226:ARG:NH1	1:H:229:TYR:OH	2.36	0.58
1:A:209:PHE:O	1:A:285:GLY:HA3	2.04	0.58
1:A:85:PRO:HD2	1:A:88:LEU:HD12	1.85	0.58
1:H:301:GLU:O	1:H:305:THR:HG23	2.02	0.58
1:K:132:HIS:O	1:K:222:LYS:HG2	2.03	0.58
1:E:76:ASN:ND2	1:E:76:ASN:O	2.37	0.58
1:K:223:PHE:O	1:K:223:PHE:HD1	1.86	0.58
1:E:330:LYS:O	1:E:332:ILE:N	2.36	0.58
1:H:142:ARG:HD2	1:H:142:ARG:N	2.19	0.58
1:H:150:ASP:HA	1:H:153:ILE:HD12	1.86	0.57
1:K:226:ARG:HG2	1:K:229:TYR:CZ	2.39	0.57
1:E:283:VAL:HG12	1:E:284:SER:OG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:ASN:OD1	1:H:322:THR:HG23	2.03	0.57
1:A:213:PHE:HB2	1:A:284:SER:HB3	1.87	0.57
1:B:233:PRO:HG2	1:H:336:LEU:HD22	1.86	0.57
1:G:333:LYS:O	1:G:333:LYS:HG2	2.05	0.57
1:H:322:THR:CG2	1:H:323:TYR:N	2.68	0.57
1:A:64:ILE:CG1	1:A:113:ILE:HG21	2.34	0.57
1:A:125:CYS:SG	1:A:126:LEU:N	2.78	0.57
1:L:63:LEU:HD13	1:L:109:LEU:CD2	2.35	0.57
1:C:182:ARG:HG2	1:C:186:ARG:HD3	1.85	0.56
1:B:56:ARG:HD3	1:B:83:VAL:HG11	1.86	0.56
1:A:51:MET:HB3	1:A:52:PRO:O	2.06	0.56
1:B:55:TYR:HB2	1:B:57:TRP:CZ2	2.40	0.56
1:G:39:VAL:HG12	1:G:102:VAL:HG12	1.87	0.56
1:I:206:ALA:HA	1:I:230:GLN:HE21	1.69	0.56
1:B:11:ARG:NH1	1:H:177:MET:CE	2.69	0.56
1:I:90:ASN:ND2	1:I:94:THR:OG1	2.39	0.56
1:D:332:ILE:O	1:D:332:ILE:HG22	2.06	0.56
1:G:302:ARG:NH2	1:G:333:LYS:O	2.35	0.56
1:L:160:ALA:HB1	1:L:171:VAL:HG21	1.88	0.56
1:I:63:LEU:HD23	1:I:64:ILE:N	2.20	0.56
1:I:51:MET:CB	1:I:52:PRO:HA	2.35	0.56
1:J:153:ILE:HD11	1:J:178:ASP:O	2.06	0.56
1:B:225:ASP:OD1	1:B:227:ARG:HG3	2.06	0.56
1:F:39:VAL:HG12	1:F:102:VAL:HG12	1.88	0.55
1:B:33:PHE:CE1	1:B:309:LEU:HD13	2.42	0.55
1:I:240:LEU:HD21	1:I:268:LEU:HD22	1.89	0.55
1:B:84:LEU:HD21	1:B:102:VAL:HG21	1.88	0.55
1:E:335:GLY:HA3	1:E:336:LEU:HG	1.89	0.55
1:H:330:LYS:O	1:H:332:ILE:HG22	2.06	0.55
1:H:204:LYS:HA	1:H:257:LYS:O	2.07	0.54
1:C:174:SER:HB3	1:C:201:TYR:CE1	2.42	0.54
1:A:320:ILE:HG22	1:A:322:THR:HG23	1.89	0.54
1:E:86:ASP:OD1	1:E:86:ASP:N	2.37	0.54
1:K:127:CYS:CB	1:K:226:ARG:HH22	2.21	0.54
1:D:201:TYR:HA	1:D:255:MET:HG3	1.89	0.54
1:I:17:LYS:O	1:I:18:ILE:C	2.44	0.54
1:L:63:LEU:HD11	1:L:113:ILE:CG2	2.38	0.54
1:H:111:LYS:O	1:H:115:GLY:HA2	2.09	0.53
1:A:201:TYR:HA	1:A:255:MET:HG3	1.89	0.53
1:B:84:LEU:CD2	1:B:102:VAL:HG21	2.38	0.53
1:H:332:ILE:HG23	1:H:332:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:MET:HB2	1:H:279:ALA:HB3	1.90	0.53
1:E:290:VAL:HG11	1:E:305:THR:CG2	2.39	0.53
1:H:322:THR:HG21	1:H:324:HIS:HB2	1.91	0.53
1:I:128:GLU:HG2	1:I:217:ALA:HB1	1.91	0.53
1:I:158:LYS:O	1:I:161:VAL:HG12	2.08	0.53
1:H:148:ASP:O	1:H:152:THR:HG23	2.09	0.53
1:H:63:LEU:HD11	1:H:113:ILE:HG12	1.89	0.52
1:C:35:TYR:CE2	1:C:326:LEU:HD13	2.44	0.52
1:E:332:ILE:N	1:E:332:ILE:CD1	2.72	0.52
1:A:267:ARG:NH1	1:G:264:ASP:OD2	2.43	0.52
1:B:281:TYR:HA	1:B:321:LEU:HB2	1.90	0.52
1:D:290:VAL:HG11	1:D:305:THR:HG23	1.91	0.52
1:A:150:ASP:HA	1:A:153:ILE:HD12	1.91	0.52
1:C:136:GLY:HA2	1:C:152:THR:OG1	2.09	0.52
1:G:213:PHE:HB2	1:G:284:SER:HB3	1.90	0.52
1:K:233:PRO:HB3	1:K:262:TYR:OH	2.09	0.52
1:B:63:LEU:HD11	1:B:113:ILE:HD11	1.91	0.52
1:A:213:PHE:HB2	1:A:284:SER:CB	2.40	0.52
1:C:289:LEU:HD22	1:E:289:LEU:HB3	1.92	0.52
1:A:298:TYR:CE2	1:G:292:ALA:HB2	2.45	0.52
1:G:282:ASN:HB3	1:G:322:THR:HG23	1.92	0.51
1:L:282:ASN:CB	1:L:322:THR:HG22	2.38	0.51
1:B:149:ASN:O	1:B:152:THR:HG22	2.10	0.51
1:C:132:HIS:CD2	1:C:134:HIS:HB2	2.46	0.51
1:H:153:ILE:HD11	1:H:178:ASP:O	2.11	0.51
1:C:77:LYS:HE2	1:H:22:ALA:HB2	1.92	0.51
1:D:301:GLU:O	1:D:305:THR:OG1	2.24	0.51
1:F:64:ILE:HG13	1:F:113:ILE:HG21	1.92	0.51
1:A:59:VAL:O	1:A:59:VAL:HG23	2.10	0.51
1:B:39:VAL:HG12	1:B:102:VAL:HG12	1.93	0.51
1:I:113:ILE:HG22	1:I:114:PHE:CD1	2.45	0.51
1:G:63:LEU:HD23	1:G:64:ILE:N	2.25	0.51
1:L:299:VAL:HG11	1:L:304:ILE:HD13	1.92	0.51
1:C:332:ILE:CG2	1:C:332:ILE:O	2.58	0.51
1:G:104:PRO:HA	1:G:107:ILE:HG12	1.92	0.51
1:I:39:VAL:HG21	1:I:80:LEU:HD22	1.92	0.51
1:J:290:VAL:HG11	1:J:305:THR:CG2	2.40	0.51
1:L:39:VAL:HG11	1:L:106:ALA:HB2	1.92	0.51
1:J:113:ILE:HG23	1:J:114:PHE:CD2	2.46	0.51
1:I:313:LYS:HG2	1:I:320:ILE:HD11	1.92	0.50
1:B:282:ASN:OD1	1:B:322:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:CG2	1:A:114:PHE:CE2	2.94	0.50
1:F:61:ARG:HA	1:F:64:ILE:HG22	1.94	0.50
1:K:125:CYS:SG	1:K:126:LEU:N	2.84	0.50
1:K:94:THR:HA	1:K:97:TYR:CZ	2.47	0.50
1:B:306:LEU:HD11	1:B:331:TRP:HB3	1.94	0.50
1:C:12:ARG:HD2	1:H:252:ASP:OD1	2.12	0.50
1:A:145:TRP:O	1:A:146:TYR:HB3	2.12	0.50
1:D:113:ILE:HG23	1:D:114:PHE:CD1	2.46	0.50
1:D:28:ILE:HD11	1:D:310:THR:HB	1.94	0.50
1:D:319:LEU:HD21	1:G:22:ALA:HB1	1.92	0.50
1:L:240:LEU:HD21	1:L:268:LEU:HD22	1.94	0.50
1:B:233:PRO:CG	1:H:336:LEU:HD22	2.42	0.50
1:I:213:PHE:HB2	1:I:284:SER:OG	2.11	0.50
1:F:3:VAL:HG13	1:F:8:THR:HG21	1.93	0.49
1:I:132:HIS:HE1	1:I:136:GLY:O	1.94	0.49
1:A:290:VAL:HG11	1:A:305:THR:HG22	1.94	0.49
1:G:63:LEU:HD11	1:G:113:ILE:CG2	2.42	0.49
1:C:94:THR:O	1:C:94:THR:HG22	2.12	0.49
1:I:269:VAL:HG12	1:I:278:LEU:HD22	1.94	0.49
1:B:332:ILE:CG2	1:B:332:ILE:O	2.60	0.49
1:C:14:ARG:O	1:C:20:ARG:NH1	2.45	0.49
1:C:182:ARG:HA	1:C:185:ARG:HB3	1.95	0.49
1:B:19:ILE:HD11	1:F:170:PHE:CE1	2.48	0.49
1:F:201:TYR:HA	1:F:255:MET:HG3	1.94	0.49
1:K:148:ASP:O	1:K:152:THR:HG22	2.13	0.49
1:D:16:SER:OG	1:D:19:ILE:HG22	2.13	0.49
1:H:290:VAL:HG11	1:H:305:THR:HG22	1.93	0.49
1:K:210:TYR:HD1	1:K:283:VAL:HG11	1.78	0.49
1:G:290:VAL:CG1	1:G:305:THR:HG22	2.38	0.49
1:K:282:ASN:ND2	1:K:286:GLU:OE1	2.46	0.49
1:C:63:LEU:HD13	1:C:109:LEU:HD22	1.95	0.49
1:E:282:ASN:HB3	1:E:322:THR:HG23	1.94	0.49
1:A:148:ASP:O	1:A:152:THR:CG2	2.61	0.48
1:B:16:SER:HB2	1:B:18:ILE:HD12	1.94	0.48
1:J:57:TRP:CZ2	1:J:66:HIS:CD2	3.00	0.48
1:K:283:VAL:HG12	1:K:284:SER:N	2.28	0.48
1:E:206:ALA:HA	1:E:230:GLN:NE2	2.28	0.48
1:I:149:ASN:O	1:I:152:THR:HG22	2.14	0.48
1:I:5:PHE:CG	1:I:6:PRO:HA	2.48	0.48
1:J:202:SER:OG	1:J:254:VAL:HG22	2.12	0.48
1:F:263:LEU:HD21	1:F:312:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ASP:O	1:E:152:THR:CG2	2.52	0.48
1:I:5:PHE:CD2	1:I:6:PRO:HA	2.48	0.48
1:F:214:ARG:NH1	3:F:501:HOH:O	2.46	0.48
1:H:204:LYS:HD2	1:H:257:LYS:HD3	1.94	0.48
1:B:201:TYR:HA	1:B:255:MET:HG3	1.96	0.48
1:C:148:ASP:O	1:C:152:THR:HG22	2.14	0.48
1:B:217:ALA:O	1:B:218:ALA:HB3	2.13	0.48
1:D:103:VAL:O	1:D:107:ILE:HG13	2.14	0.48
1:L:283:VAL:HG12	1:L:284:SER:H	1.77	0.48
1:A:45:ARG:NH2	1:A:55:TYR:CE2	2.82	0.48
1:C:324:HIS:O	1:C:326:LEU:N	2.46	0.48
1:H:302:ARG:NH2	1:H:333:LYS:O	2.47	0.48
1:I:282:ASN:CB	1:I:322:THR:HG22	2.44	0.48
1:J:57:TRP:CH2	1:J:66:HIS:CD2	3.02	0.48
1:D:139:LYS:HG3	1:D:148:ASP:HB2	1.95	0.48
1:D:97:TYR:CZ	1:D:155:LEU:HD22	2.49	0.48
1:B:90:ASN:OD1	1:B:90:ASN:N	2.46	0.48
1:C:247:LEU:HD11	1:C:276:VAL:HG21	1.96	0.48
1:F:290:VAL:HG11	1:F:305:THR:HG22	1.95	0.48
1:H:247:LEU:HD21	1:H:276:VAL:HG11	1.95	0.48
1:K:71:LEU:HD12	1:K:118:VAL:CG1	2.44	0.48
1:A:144:ARG:NE	1:A:144:ARG:HA	2.28	0.47
1:A:49:GLY:N	1:A:50:PRO:CD	2.76	0.47
1:F:153:ILE:HD11	1:F:178:ASP:O	2.14	0.47
1:C:322:THR:CG2	1:C:323:TYR:N	2.76	0.47
1:H:226:ARG:C	1:H:228:THR:H	2.18	0.47
1:A:324:HIS:O	1:A:325:ALA:C	2.52	0.47
1:E:332:ILE:CD1	1:E:332:ILE:H	2.27	0.47
1:F:231:MET:HE1	1:F:239:ALA:HB2	1.96	0.47
1:L:3:VAL:HG13	1:L:8:THR:HB	1.94	0.47
1:I:213:PHE:HB2	1:I:284:SER:CB	2.45	0.47
1:K:66:HIS:O	1:K:70:ALA:N	2.43	0.47
1:C:150:ASP:O	1:C:153:ILE:HG22	2.15	0.47
1:L:75:ILE:HD11	1:L:329:ALA:HB2	1.97	0.47
1:B:259:ALA:O	1:B:262:TYR:N	2.38	0.47
1:F:64:ILE:CG1	1:F:113:ILE:HG21	2.44	0.47
1:D:39:VAL:HG12	1:D:102:VAL:HG12	1.96	0.47
1:A:18:ILE:HG21	1:E:119:LEU:HB2	1.97	0.47
1:G:59:VAL:HG23	1:G:109:LEU:HD12	1.97	0.47
1:B:5:PHE:CD1	1:B:6:PRO:HA	2.49	0.47
1:I:51:MET:HB3	1:I:52:PRO:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:MET:HB3	1:B:279:ALA:HB3	1.96	0.47
1:C:128:GLU:HG2	1:C:217:ALA:HB1	1.95	0.47
1:D:148:ASP:O	1:D:152:THR:HG22	2.14	0.47
1:G:107:ILE:HG23	1:G:120:VAL:HG11	1.96	0.47
1:A:135:CYS:SG	1:A:226:ARG:NH1	2.88	0.47
1:B:327:GLU:HA	1:B:330:LYS:HE3	1.96	0.47
1:C:37:LEU:HD11	1:C:67:VAL:HG22	1.97	0.47
1:G:110:ILE:O	1:G:114:PHE:HB2	2.15	0.47
1:J:283:VAL:HG12	1:J:284:SER:N	2.30	0.47
1:A:39:VAL:HA	1:A:57:TRP:O	2.15	0.46
1:B:70:ALA:CB	1:B:326:LEU:HD11	2.43	0.46
1:A:237:TYR:O	1:A:238:GLU:C	2.54	0.46
1:F:39:VAL:HG12	1:F:102:VAL:CG1	2.45	0.46
1:L:185:ARG:NE	1:L:189:ASP:OD1	2.49	0.46
1:E:260:LEU:O	1:E:263:LEU:HG	2.15	0.46
1:H:255:MET:CB	1:H:279:ALA:HB3	2.45	0.46
1:L:75:ILE:HD11	1:L:329:ALA:CB	2.46	0.46
1:I:71:LEU:HD11	1:I:118:VAL:CG1	2.46	0.46
1:E:153:ILE:HG23	1:E:183:GLU:HG2	1.98	0.46
1:F:64:ILE:HD11	1:F:113:ILE:HG21	1.98	0.46
1:L:63:LEU:HD11	1:L:113:ILE:HG23	1.97	0.46
1:B:63:LEU:HD11	1:B:113:ILE:CD1	2.46	0.46
1:J:243:VAL:HG13	1:J:254:VAL:HG11	1.98	0.46
1:A:255:MET:HB3	1:A:279:ALA:HB3	1.98	0.46
1:G:153:ILE:HD11	1:G:178:ASP:O	2.16	0.46
1:J:75:ILE:HD13	1:J:325:ALA:HB1	1.97	0.46
1:H:324:HIS:O	1:H:326:LEU:N	2.49	0.46
1:I:94:THR:O	1:I:97:TYR:N	2.49	0.46
1:J:305:THR:O	1:J:309:LEU:HG	2.16	0.46
1:L:67:VAL:HG23	1:L:114:PHE:CE2	2.51	0.45
1:A:9:ARG:O	1:A:11:ARG:N	2.49	0.45
1:B:63:LEU:HD11	1:B:113:ILE:HG12	1.98	0.45
1:D:247:LEU:HD21	1:D:276:VAL:HG11	1.97	0.45
1:G:282:ASN:ND2	1:G:286:GLU:OE1	2.50	0.45
1:L:98:ASP:O	1:L:101:GLY:N	2.49	0.45
1:L:124:VAL:HG21	1:L:171:VAL:HG13	1.97	0.45
1:B:153:ILE:CG2	1:B:183:GLU:HB3	2.47	0.45
1:C:217:ALA:O	1:C:218:ALA:HB3	2.16	0.45
1:K:105:ARG:HA	1:K:108:ARG:HD2	1.97	0.45
1:B:332:ILE:C	1:B:333:LYS:CG	2.85	0.45
1:D:263:LEU:HA	1:D:266:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD12	1:A:80:LEU:HD21	1.99	0.45
1:D:287:TYR:CD2	1:D:324:HIS:CE1	3.05	0.45
1:G:332:ILE:HG23	1:G:332:ILE:O	2.16	0.45
1:L:305:THR:HG22	1:L:324:HIS:CE1	2.52	0.45
1:F:291:LYS:O	1:F:295:THR:HB	2.16	0.45
1:H:49:GLY:O	1:H:51:MET:N	2.50	0.45
1:J:40:LYS:HG3	1:J:58:PRO:HA	1.99	0.45
1:D:243:VAL:HG13	1:D:254:VAL:HG21	1.98	0.45
1:H:41:PRO:O	1:H:43:GLY:N	2.50	0.45
1:I:58:PRO:O	1:I:60:GLY:N	2.50	0.45
1:J:282:ASN:HB3	1:J:322:THR:HG22	1.99	0.45
1:D:119:LEU:HB2	1:G:18:ILE:HG21	1.97	0.45
1:J:153:ILE:HG22	1:J:183:GLU:HG2	1.98	0.45
1:E:287:TYR:CD2	1:E:324:HIS:CE1	3.05	0.45
1:L:51:MET:HB3	1:L:52:PRO:CA	2.47	0.45
1:L:59:VAL:HG13	1:L:59:VAL:O	2.17	0.45
1:A:333:LYS:O	1:A:334:GLU:HG2	2.17	0.44
1:B:143:ASP:N	1:B:143:ASP:OD1	2.49	0.44
1:C:59:VAL:HG13	1:C:59:VAL:O	2.16	0.44
1:F:71:LEU:HA	1:F:75:ILE:O	2.17	0.44
1:A:336:LEU:HD22	1:G:233:PRO:HG2	1.99	0.44
1:E:127:CYS:HB3	1:E:135:CYS:SG	2.56	0.44
1:K:62:GLU:HA	1:K:65:ASN:CB	2.46	0.44
1:A:283:VAL:HG12	1:A:284:SER:N	2.32	0.44
1:B:187:ALA:O	1:B:188:LEU:C	2.55	0.44
1:G:328:ALA:HA	1:G:331:TRP:CE3	2.51	0.44
1:B:14:ARG:O	1:H:228:THR:HA	2.17	0.44
1:H:33:PHE:CE1	1:H:309:LEU:HD13	2.53	0.44
1:B:299:VAL:CG1	1:B:304:ILE:HG21	2.48	0.44
1:E:34:ILE:HG12	1:E:77:LYS:HG3	1.99	0.44
1:I:148:ASP:OD2	1:I:151:GLU:HB2	2.17	0.44
1:I:59:VAL:HG13	1:I:59:VAL:O	2.18	0.44
1:B:324:HIS:O	1:B:325:ALA:C	2.55	0.44
1:C:125:CYS:SG	1:C:135:CYS:HB3	2.56	0.44
1:E:243:VAL:HG13	1:E:254:VAL:HG11	2.00	0.44
1:E:50:PRO:CG	1:E:215:VAL:HG11	2.48	0.44
1:I:39:VAL:HG11	1:I:106:ALA:HB2	1.99	0.44
1:G:44:GLU:O	1:G:46:GLU:N	2.51	0.44
1:G:51:MET:HB3	1:G:52:PRO:O	2.18	0.44
1:G:71:LEU:HA	1:G:75:ILE:O	2.18	0.44
1:A:84:LEU:HD11	1:A:102:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LYS:HB2	1:D:146:TYR:CE1	2.52	0.44
1:G:70:ALA:HA	1:G:73:LEU:HD12	1.98	0.44
1:K:225:ASP:HB2	1:K:227:ARG:HG2	2.00	0.44
1:K:75:ILE:HD11	1:K:329:ALA:HB2	1.99	0.44
1:A:50:PRO:CB	1:A:215:VAL:HG11	2.48	0.44
1:B:161:VAL:HG11	1:B:191:HIS:CD2	2.53	0.44
1:B:35:TYR:O	1:B:78:PHE:HA	2.18	0.44
1:I:132:HIS:CE1	1:I:138:VAL:HG23	2.53	0.44
1:I:223:PHE:N	1:I:223:PHE:CD1	2.85	0.44
1:D:229:TYR:HB3	1:F:11:ARG:HE	1.83	0.44
1:D:320:ILE:HG22	1:D:322:THR:HG23	1.99	0.44
1:B:298:TYR:CE1	1:H:50:PRO:HA	2.53	0.44
1:B:153:ILE:HD11	1:B:178:ASP:O	2.17	0.43
1:C:125:CYS:SG	1:C:135:CYS:CB	3.06	0.43
1:F:164:ALA:HB1	1:F:193:PHE:CD2	2.53	0.43
1:H:170:PHE:CE2	1:H:197:GLY:HA3	2.53	0.43
1:H:148:ASP:O	1:H:152:THR:HG22	2.16	0.43
1:J:39:VAL:HG11	1:J:106:ALA:HB2	2.00	0.43
1:C:63:LEU:CG	1:C:64:ILE:HG23	2.45	0.43
1:D:307:GLU:OE1	1:F:262:TYR:OH	2.32	0.43
1:E:67:VAL:HG23	1:E:78:PHE:CZ	2.53	0.43
1:F:97:TYR:CD1	1:F:97:TYR:N	2.86	0.43
1:I:64:ILE:CG2	1:I:65:ASN:N	2.80	0.43
1:L:225:ASP:OD1	1:L:227:ARG:HG3	2.19	0.43
1:L:232:ASP:OD1	1:L:232:ASP:C	2.57	0.43
1:L:62:GLU:HA	1:L:65:ASN:HB3	2.00	0.43
1:F:176:MET:HG3	1:F:230:GLN:HA	2.01	0.43
1:D:298:TYR:O	1:D:299:VAL:HG13	2.18	0.43
1:E:330:LYS:C	1:E:332:ILE:CD1	2.65	0.43
1:H:63:LEU:HD13	1:H:109:LEU:CD2	2.47	0.43
1:A:141:LYS:O	1:A:144:ARG:N	2.52	0.43
1:D:277:PRO:HG3	1:G:23:VAL:HG13	2.01	0.43
1:D:69:GLU:O	1:D:70:ALA:C	2.57	0.43
1:A:119:LEU:HB2	1:E:18:ILE:HG21	2.01	0.43
1:L:83:VAL:HG12	1:L:217:ALA:HA	2.00	0.43
1:C:132:HIS:HB2	1:C:223:PHE:CE1	2.54	0.43
1:K:295:THR:O	1:K:297:GLY:N	2.51	0.43
1:A:42:GLY:O	1:A:44:GLU:N	2.52	0.43
1:B:324:HIS:O	1:B:326:LEU:N	2.52	0.43
1:B:63:LEU:C	1:B:63:LEU:HD23	2.39	0.43
1:G:247:LEU:HD11	1:G:276:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:ARG:HD3	1:H:55:TYR:HB3	2.01	0.43
1:H:51:MET:CB	1:H:52:PRO:HA	2.49	0.43
1:B:247:LEU:HD21	1:B:276:VAL:CG2	2.48	0.43
1:E:321:LEU:HD12	1:E:321:LEU:N	2.34	0.43
1:I:213:PHE:HB2	1:I:284:SER:HB3	2.01	0.43
1:A:5:PHE:CD1	1:A:6:PRO:HA	2.53	0.43
1:B:98:ASP:O	1:B:101:GLY:N	2.52	0.43
1:G:237:TYR:O	1:G:238:GLU:C	2.56	0.43
1:B:290:VAL:HG11	1:B:305:THR:CG2	2.49	0.42
1:C:63:LEU:HD11	1:C:113:ILE:HG21	2.00	0.42
1:H:125:CYS:SG	1:H:126:LEU:N	2.92	0.42
1:C:149:ASN:O	1:C:153:ILE:HB	2.20	0.42
1:A:264:ASP:HB3	1:G:263:LEU:HB3	2.00	0.42
1:K:60:GLY:C	1:K:62:GLU:H	2.22	0.42
1:A:292:ALA:HB2	1:G:298:TYR:CE2	2.54	0.42
1:C:90:ASN:HB2	1:C:91:PRO:HD2	2.00	0.42
1:L:309:LEU:HD21	1:L:322:THR:HG21	2.00	0.42
1:I:69:GLU:O	1:I:73:LEU:HD12	2.18	0.42
1:J:107:ILE:HD13	1:J:168:ALA:HB2	2.01	0.42
1:E:333:LYS:CE	1:J:65:ASN:HD21	2.32	0.42
1:A:156:TYR:OH	1:A:175:GLY:HA3	2.19	0.42
1:B:236:ALA:N	1:H:25:GLU:OE2	2.51	0.42
1:B:48:ILE:HG21	1:B:216:ALA:HB2	2.02	0.42
1:D:160:ALA:HB1	1:D:188:LEU:HD11	2.01	0.42
1:C:77:LYS:HE2	1:H:22:ALA:CB	2.50	0.42
1:H:51:MET:HB3	1:H:52:PRO:HA	2.02	0.42
1:J:41:PRO:HG3	1:J:102:VAL:HG22	2.01	0.42
1:D:333:LYS:HD3	1:D:333:LYS:N	2.35	0.42
1:B:18:ILE:HG23	1:F:76:ASN:ND2	2.35	0.42
1:G:232:ASP:OD1	1:G:234:ARG:HB2	2.20	0.42
1:G:260:LEU:HD13	1:G:308:ILE:HG23	2.02	0.42
1:H:182:ARG:HB2	1:H:249:GLU:HG2	2.01	0.42
1:K:282:ASN:HB3	1:K:322:THR:HG23	2.01	0.42
1:L:90:ASN:OD1	1:L:90:ASN:N	2.52	0.42
1:C:289:LEU:HD21	1:E:290:VAL:HA	2.00	0.42
1:C:39:VAL:HG12	1:C:102:VAL:HG12	2.01	0.42
1:E:335:GLY:HA3	1:E:336:LEU:CB	2.50	0.42
1:K:153:ILE:HD11	1:K:178:ASP:O	2.20	0.42
1:K:210:TYR:CD1	1:K:283:VAL:HG11	2.55	0.42
1:L:247:LEU:HD11	1:L:276:VAL:CG1	2.48	0.42
1:A:170:PHE:CE1	1:A:197:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:309:LEU:HD21	1:I:322:THR:HG21	2.01	0.42
1:L:100:GLU:OE2	1:L:108:ARG:NH2	2.53	0.42
1:A:29:ASP:O	1:A:31:GLY:N	2.53	0.42
1:B:57:TRP:CZ2	1:B:66:HIS:CD2	3.08	0.42
1:E:9:ARG:HD2	1:E:12:ARG:NH2	2.35	0.42
1:E:324:HIS:O	1:E:325:ALA:C	2.58	0.42
1:I:18:ILE:HD12	1:I:18:ILE:H	1.84	0.42
1:K:153:ILE:HG23	1:K:183:GLU:HG2	2.02	0.42
1:A:50:PRO:HG2	1:A:215:VAL:HG11	2.02	0.41
1:B:63:LEU:HD11	1:B:113:ILE:CG1	2.49	0.41
1:B:79:ILE:HA	1:B:121:PHE:O	2.20	0.41
1:D:213:PHE:HA	1:D:216:ALA:HB3	2.02	0.41
1:F:255:MET:CE	1:F:257:LYS:HB2	2.50	0.41
1:A:117:ARG:O	1:A:118:VAL:HG23	2.19	0.41
1:B:275:TRP:HA	1:D:237:TYR:HB3	2.02	0.41
1:D:19:ILE:O	1:D:23:VAL:HG22	2.21	0.41
1:H:40:LYS:HA	1:H:102:VAL:HG11	2.02	0.41
1:H:109:LEU:O	1:H:113:ILE:HG22	2.20	0.41
1:J:57:TRP:CD1	1:J:62:GLU:HB2	2.55	0.41
1:A:148:ASP:O	1:A:152:THR:HG22	2.19	0.41
1:D:49:GLY:N	1:D:50:PRO:HD2	2.34	0.41
1:G:13:LEU:HD22	1:G:23:VAL:HG21	2.03	0.41
1:G:201:TYR:HA	1:G:255:MET:HG3	2.02	0.41
1:K:291:LYS:NZ	1:K:327:GLU:OE2	2.52	0.41
1:A:247:LEU:HD21	1:A:276:VAL:HG11	2.02	0.41
1:D:281:TYR:OH	1:D:323:TYR:OH	2.31	0.41
1:I:83:VAL:HG13	1:I:217:ALA:HA	2.00	0.41
1:D:184:ILE:O	1:D:188:LEU:HD13	2.20	0.41
1:G:79:ILE:HA	1:G:121:PHE:O	2.19	0.41
1:K:301:GLU:O	1:K:305:THR:HG23	2.19	0.41
1:A:80:LEU:HD12	1:A:107:ILE:CD1	2.51	0.41
1:B:328:ALA:HA	1:B:331:TRP:CE3	2.56	0.41
1:D:320:ILE:HG22	1:D:322:THR:CG2	2.50	0.41
1:F:30:ALA:HA	1:F:33:PHE:CD2	2.55	0.41
1:H:324:HIS:O	1:H:325:ALA:C	2.59	0.41
1:B:63:LEU:HD21	1:B:113:ILE:HD11	2.03	0.41
1:C:56:ARG:HD3	1:C:83:VAL:HG11	2.02	0.41
1:G:79:ILE:HG23	1:G:81:PHE:HE1	1.85	0.41
1:H:299:VAL:HG11	1:H:304:ILE:HG21	2.02	0.41
1:I:247:LEU:HD21	1:I:276:VAL:HG11	2.03	0.41
1:C:63:LEU:HG	1:C:64:ILE:CG2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:NH1	1:F:264:ASP:HB2	2.36	0.41
1:D:287:TYR:CD2	1:D:323:TYR:HB2	2.56	0.41
1:E:101:GLY:C	1:E:104:PRO:HD2	2.41	0.41
1:F:125:CYS:SG	1:F:135:CYS:HB3	2.60	0.41
1:F:35:TYR:CE2	1:F:326:LEU:HD11	2.56	0.41
1:G:311:ALA:HA	1:G:314:ARG:NH1	2.36	0.41
1:L:13:LEU:HD22	1:L:23:VAL:HG21	2.02	0.41
1:B:62:GLU:N	1:B:62:GLU:CD	2.74	0.41
1:C:299:VAL:HG11	1:C:304:ILE:HD13	2.02	0.41
1:D:98:ASP:O	1:D:101:GLY:N	2.51	0.41
1:E:237:TYR:CD2	1:H:274:PRO:HB2	2.55	0.41
1:L:182:ARG:NH1	1:L:182:ARG:HB3	2.35	0.41
1:L:51:MET:HB3	1:L:52:PRO:HA	2.03	0.41
1:A:284:SER:N	1:A:323:TYR:HE2	2.19	0.41
1:C:144:ARG:N	1:C:144:ARG:HD3	2.35	0.41
1:F:76:ASN:OD1	1:F:76:ASN:N	2.53	0.41
1:L:50:PRO:CD	1:L:215:VAL:HG11	2.51	0.41
1:C:39:VAL:HG11	1:C:106:ALA:HB2	2.03	0.41
1:H:85:PRO:O	1:H:88:LEU:HD23	2.21	0.41
1:I:335:GLY:HA2	1:I:336:LEU:C	2.42	0.41
1:J:34:ILE:HD12	1:J:321:LEU:HD11	2.03	0.41
1:L:124:VAL:CG2	1:L:171:VAL:HG13	2.51	0.41
1:L:255:MET:HE3	1:L:255:MET:HB2	1.94	0.41
1:A:26:THR:HG22	1:A:27:GLN:N	2.35	0.40
1:A:5:PHE:CG	1:A:6:PRO:HA	2.56	0.40
1:C:149:ASN:HA	1:C:177:MET:HE2	2.03	0.40
1:E:153:ILE:CD1	1:E:178:ASP:O	2.69	0.40
1:E:84:LEU:HB2	1:E:85:PRO:CD	2.51	0.40
1:F:301:GLU:O	1:F:305:THR:HG23	2.20	0.40
1:G:103:VAL:CG1	1:G:104:PRO:HD3	2.51	0.40
1:G:77:LYS:C	1:G:78:PHE:CD1	2.94	0.40
1:L:122:ALA:HB1	1:L:163:TYR:CD2	2.56	0.40
1:A:59:VAL:HG21	1:A:105:ARG:CZ	2.50	0.40
1:G:187:ALA:O	1:G:188:LEU:C	2.59	0.40
1:I:153:ILE:HG22	1:I:183:GLU:HG2	2.02	0.40
1:K:220:ALA:HB1	1:K:221:PRO:HD2	2.03	0.40
1:D:126:LEU:HD11	1:D:155:LEU:HD12	2.04	0.40
1:J:50:PRO:HG3	1:J:215:VAL:HG11	2.04	0.40
1:J:54:ILE:HD13	1:J:54:ILE:N	2.37	0.40
1:K:237:TYR:CD1	1:K:268:LEU:HD21	2.55	0.40
1:A:103:VAL:HG22	1:A:104:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:MET:CG	1:G:204:LYS:HB3	2.51	0.40
1:I:64:ILE:HG22	1:I:65:ASN:H	1.87	0.40
1:J:332:ILE:HD13	1:J:332:ILE:HG21	1.93	0.40
1:A:209:PHE:O	1:A:285:GLY:CA	2.69	0.40
1:B:40:LYS:CD	1:B:46:GLU:OE2	2.68	0.40
1:B:83:VAL:HG13	1:B:217:ALA:C	2.42	0.40
1:C:290:VAL:HG11	1:C:305:THR:HG22	2.02	0.40
1:C:313:LYS:O	1:C:316:GLY:N	2.54	0.40
1:E:309:LEU:HD21	1:E:322:THR:HG21	2.03	0.40
1:E:5:PHE:CG	1:E:6:PRO:HA	2.56	0.40
1:F:255:MET:HB3	1:F:279:ALA:HB3	2.03	0.40
1:K:102:VAL:HG23	1:K:103:VAL:N	2.37	0.40
1:L:94:THR:O	1:L:96:GLY:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/338 (99%)	286 (86%)	36 (11%)	12 (4%)	4	37
1	B	334/338 (99%)	284 (85%)	38 (11%)	12 (4%)	4	37
1	C	334/338 (99%)	289 (86%)	38 (11%)	7 (2%)	9	49
1	D	334/338 (99%)	287 (86%)	36 (11%)	11 (3%)	5	39
1	E	334/338 (99%)	286 (86%)	35 (10%)	13 (4%)	4	34
1	F	334/338 (99%)	284 (85%)	42 (13%)	8 (2%)	7	46
1	G	334/338 (99%)	283 (85%)	36 (11%)	15 (4%)	3	29
1	H	334/338 (99%)	282 (84%)	40 (12%)	12 (4%)	4	37
1	I	334/338 (99%)	286 (86%)	37 (11%)	11 (3%)	5	39
1	J	334/338 (99%)	287 (86%)	32 (10%)	15 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	334/338 (99%)	280 (84%)	44 (13%)	10 (3%)	5	41
1	L	334/338 (99%)	280 (84%)	41 (12%)	13 (4%)	4	34
All	All	4008/4056 (99%)	3414 (85%)	455 (11%)	139 (4%)	4	38

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLY
1	A	52	PRO
1	A	284	SER
1	B	131	ASP
1	B	187	ALA
1	B	188	LEU
1	C	143	ASP
1	D	52	PRO
1	D	325	ALA
1	E	15	ALA
1	E	94	THR
1	E	297	GLY
1	F	94	THR
1	F	131	ASP
1	F	142	ARG
1	F	143	ASP
1	F	333	LYS
1	G	45	ARG
1	G	51	MET
1	G	52	PRO
1	G	131	ASP
1	G	142	ARG
1	G	194	GLU
1	G	284	SER
1	G	333	LYS
1	H	42	GLY
1	H	51	MET
1	H	52	PRO
1	H	63	LEU
1	H	131	ASP
1	H	325	ALA
1	I	51	MET
1	I	52	PRO
1	I	93	GLY

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Mol	Chain	Res	Type
1	I	142	ARG
1	J	51	MET
1	J	52	PRO
1	J	53	GLY
1	J	131	ASP
1	K	137	VAL
1	L	95	GLY
1	L	333	LYS
1	A	30	ALA
1	A	53	GLY
1	A	146	TYR
1	A	325	ALA
1	A	335	GLY
1	B	93	GLY
1	B	137	VAL
1	B	140	GLU
1	B	142	ARG
1	B	325	ALA
1	C	59	VAL
1	C	284	SER
1	C	296	ALA
1	D	41	PRO
1	D	225	ASP
1	D	284	SER
1	E	225	ASP
1	E	284	SER
1	F	115	GLY
1	F	284	SER
1	G	87	GLU
1	G	93	GLY
1	H	113	ILE
1	I	18	ILE
1	I	143	ASP
1	I	206	ALA
1	I	272	HIS
1	I	284	SER
1	J	45	ARG
1	J	59	VAL
1	J	62	GLU
1	J	142	ARG
1	J	332	ILE
1	K	143	ASP

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Mol	Chain	Res	Type
1	K	209	PHE
1	K	284	SER
1	K	295	THR
1	L	63	LEU
1	L	93	GLY
1	L	131	ASP
1	L	143	ASP
1	L	224	GLY
1	L	325	ALA
1	A	51	MET
1	C	314	ARG
1	E	41	PRO
1	E	45	ARG
1	E	51	MET
1	E	331	TRP
1	F	86	ASP
1	G	250	GLY
1	H	284	SER
1	J	24	ALA
1	K	145	TRP
1	K	296	ALA
1	L	59	VAL
1	L	218	ALA
1	A	10	PRO
1	A	137	VAL
1	A	334	GLU
1	B	333	LYS
1	C	63	LEU
1	C	201	TYR
1	D	51	MET
1	E	114	PHE
1	E	206	ALA
1	G	63	LEU
1	H	142	ARG
1	H	272	HIS
1	I	59	VAL
1	J	63	LEU
1	L	51	MET
1	B	3	VAL
1	B	284	SER
1	D	142	ARG
1	E	44	GLU

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Mol	Chain	Res	Type
1	G	10	PRO
1	I	224	GLY
1	J	220	ALA
1	J	227	ARG
1	J	284	SER
1	K	41	PRO
1	L	24	ALA
1	D	65	ASN
1	D	221	PRO
1	G	57	TRP
1	G	114	PHE
1	H	94	THR
1	J	333	LYS
1	K	51	MET
1	L	141	LYS
1	E	335	GLY
1	H	50	PRO
1	D	211	GLY
1	D	316	GLY
1	B	220	ALA
1	K	52	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	268/270 (99%)	237 (88%)	31 (12%)	7	32
1	B	268/270 (99%)	227 (85%)	41 (15%)	3	20
1	C	268/270 (99%)	232 (87%)	36 (13%)	5	26
1	D	268/270 (99%)	234 (87%)	34 (13%)	5	27
1	E	268/270 (99%)	236 (88%)	32 (12%)	6	30
1	F	268/270 (99%)	236 (88%)	32 (12%)	6	30
1	G	268/270 (99%)	231 (86%)	37 (14%)	4	24
1	H	268/270 (99%)	229 (85%)	39 (15%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	268/270 (99%)	237 (88%)	31 (12%)	7	32
1	J	268/270 (99%)	235 (88%)	33 (12%)	6	29
1	K	268/270 (99%)	240 (90%)	28 (10%)	9	39
1	L	268/270 (99%)	235 (88%)	33 (12%)	6	29
All	All	3216/3240 (99%)	2809 (87%)	407 (13%)	5	27

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	6	PRO
1	A	16	SER
1	A	19	ILE
1	A	40	LYS
1	A	51	MET
1	A	54	ILE
1	A	64	ILE
1	A	77	LYS
1	A	97	TYR
1	A	118	VAL
1	A	140	GLU
1	A	141	LYS
1	A	146	TYR
1	A	152	THR
1	A	182	ARG
1	A	223	PHE
1	A	228	THR
1	A	229	TYR
1	A	234	ARG
1	A	268	LEU
1	A	284	SER
1	A	288	SER
1	A	299	VAL
1	A	303	THR
1	A	304	ILE
1	A	332	ILE
1	A	333	LYS
1	A	334	GLU
1	A	336	LEU
1	B	1	MET

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Mol	Chain	Res	Type
1	B	2	ARG
1	B	3	VAL
1	B	7	THR
1	B	17	LYS
1	B	18	ILE
1	B	19	ILE
1	B	27	GLN
1	B	61	ARG
1	B	62	GLU
1	B	66	HIS
1	B	71	LEU
1	B	73	LEU
1	B	77	LYS
1	B	88	LEU
1	B	90	ASN
1	B	109	LEU
1	B	117	ARG
1	B	118	VAL
1	B	142	ARG
1	B	143	ASP
1	B	144	ARG
1	B	145	TRP
1	B	150	ASP
1	B	195	GLU
1	B	223	PHE
1	B	227	ARG
1	B	229	TYR
1	B	254	VAL
1	B	268	LEU
1	B	271	GLN
1	B	276	VAL
1	B	281	TYR
1	B	283	VAL
1	B	284	SER
1	B	295	THR
1	B	304	ILE
1	B	322	THR
1	B	330	LYS
1	B	333	LYS
1	B	334	GLU
1	C	1	MET
1	C	3	VAL

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Mol	Chain	Res	Type
1	C	4	GLN
1	C	16	SER
1	C	19	ILE
1	C	61	ARG
1	C	69	GLU
1	C	88	LEU
1	C	97	TYR
1	C	109	LEU
1	C	112	GLU
1	C	113	ILE
1	C	117	ARG
1	C	139	LYS
1	C	142	ARG
1	C	144	ARG
1	C	145	TRP
1	C	146	TYR
1	C	150	ASP
1	C	161	VAL
1	C	176	MET
1	C	182	ARG
1	C	227	ARG
1	C	228	THR
1	C	229	TYR
1	C	234	ARG
1	C	242	GLU
1	C	254	VAL
1	C	281	TYR
1	C	283	VAL
1	C	284	SER
1	C	299	VAL
1	C	301	GLU
1	C	303	THR
1	C	304	ILE
1	C	333	LYS
1	D	2	ARG
1	D	7	THR
1	D	13	LEU
1	D	21	ASP
1	D	28	ILE
1	D	40	LYS
1	D	51	MET
1	D	54	ILE

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Mol	Chain	Res	Type
1	D	66	HIS
1	D	71	LEU
1	D	88	LEU
1	D	94	THR
1	D	97	TYR
1	D	100	GLU
1	D	132	HIS
1	D	144	ARG
1	D	146	TYR
1	D	186	ARG
1	D	195	GLU
1	D	215	VAL
1	D	222	LYS
1	D	223	PHE
1	D	227	ARG
1	D	228	THR
1	D	229	TYR
1	D	234	ARG
1	D	268	LEU
1	D	284	SER
1	D	299	VAL
1	D	305	THR
1	D	313	LYS
1	D	330	LYS
1	D	333	LYS
1	D	334	GLU
1	E	2	ARG
1	E	3	VAL
1	E	4	GLN
1	E	44	GLU
1	E	45	ARG
1	E	51	MET
1	E	64	ILE
1	E	76	ASN
1	E	86	ASP
1	E	98	ASP
1	E	113	ILE
1	E	118	VAL
1	E	128	GLU
1	E	140	GLU
1	E	142	ARG
1	E	144	ARG

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Mol	Chain	Res	Type
1	E	152	THR
1	E	153	ILE
1	E	165	GLU
1	E	183	GLU
1	E	185	ARG
1	E	219	SER
1	E	234	ARG
1	E	255	MET
1	E	268	LEU
1	E	281	TYR
1	E	283	VAL
1	E	284	SER
1	E	303	THR
1	E	322	THR
1	E	330	LYS
1	E	334	GLU
1	F	7	THR
1	F	8	THR
1	F	17	LYS
1	F	28	ILE
1	F	59	VAL
1	F	64	ILE
1	F	84	LEU
1	F	109	LEU
1	F	116	ASP
1	F	117	ARG
1	F	118	VAL
1	F	139	LYS
1	F	140	GLU
1	F	142	ARG
1	F	182	ARG
1	F	186	ARG
1	F	214	ARG
1	F	219	SER
1	F	222	LYS
1	F	225	ASP
1	F	228	THR
1	F	229	TYR
1	F	268	LEU
1	F	281	TYR
1	F	283	VAL
1	F	284	SER

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Mol	Chain	Res	Type
1	F	295	THR
1	F	302	ARG
1	F	310	THR
1	F	318	ASP
1	F	322	THR
1	F	332	ILE
1	G	1	MET
1	G	2	ARG
1	G	7	THR
1	G	17	LYS
1	G	19	ILE
1	G	28	ILE
1	G	29	ASP
1	G	51	MET
1	G	61	ARG
1	G	72	SER
1	G	77	LYS
1	G	97	TYR
1	G	98	ASP
1	G	109	LEU
1	G	118	VAL
1	G	128	GLU
1	G	130	THR
1	G	142	ARG
1	G	144	ARG
1	G	161	VAL
1	G	169	ASP
1	G	174	SER
1	G	183	GLU
1	G	207	SER
1	G	223	PHE
1	G	229	TYR
1	G	234	ARG
1	G	238	GLU
1	G	254	VAL
1	G	268	LEU
1	G	295	THR
1	G	303	THR
1	G	305	THR
1	G	318	ASP
1	G	322	THR
1	G	333	LYS

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Mol	Chain	Res	Type
1	G	336	LEU
1	H	1	MET
1	H	2	ARG
1	H	7	THR
1	H	8	THR
1	H	16	SER
1	H	39	VAL
1	H	40	LYS
1	H	45	ARG
1	H	51	MET
1	H	62	GLU
1	H	65	ASN
1	H	73	LEU
1	H	84	LEU
1	H	94	THR
1	H	112	GLU
1	H	127	CYS
1	H	131	ASP
1	H	141	LYS
1	H	142	ARG
1	H	144	ARG
1	H	145	TRP
1	H	152	THR
1	H	171	VAL
1	H	177	MET
1	H	182	ARG
1	H	183	GLU
1	H	214	ARG
1	H	226	ARG
1	H	228	THR
1	H	234	ARG
1	H	255	MET
1	H	268	LEU
1	H	272	HIS
1	H	281	TYR
1	H	283	VAL
1	H	284	SER
1	H	289	LEU
1	H	330	LYS
1	H	333	LYS
1	I	1	MET
1	I	2	ARG

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Mol	Chain	Res	Type
1	I	7	THR
1	I	17	LYS
1	I	40	LYS
1	I	44	GLU
1	I	51	MET
1	I	61	ARG
1	I	63	LEU
1	I	64	ILE
1	I	65	ASN
1	I	66	HIS
1	I	84	LEU
1	I	102	VAL
1	I	113	ILE
1	I	144	ARG
1	I	171	VAL
1	I	195	GLU
1	I	214	ARG
1	I	223	PHE
1	I	229	TYR
1	I	254	VAL
1	I	260	LEU
1	I	268	LEU
1	I	272	HIS
1	I	283	VAL
1	I	284	SER
1	I	295	THR
1	I	299	VAL
1	I	332	ILE
1	I	336	LEU
1	J	1	MET
1	J	2	ARG
1	J	4	GLN
1	J	7	THR
1	J	16	SER
1	J	17	LYS
1	J	19	ILE
1	J	45	ARG
1	J	51	MET
1	J	62	GLU
1	J	63	LEU
1	J	66	HIS
1	J	71	LEU

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Mol	Chain	Res	Type
1	J	73	LEU
1	J	84	LEU
1	J	92	GLU
1	J	100	GLU
1	J	109	LEU
1	J	139	LYS
1	J	146	TYR
1	J	182	ARG
1	J	195	GLU
1	J	223	PHE
1	J	227	ARG
1	J	254	VAL
1	J	256	VAL
1	J	284	SER
1	J	289	LEU
1	J	295	THR
1	J	308	ILE
1	J	309	LEU
1	J	313	LYS
1	J	330	LYS
1	K	7	THR
1	K	28	ILE
1	K	40	LYS
1	K	44	GLU
1	K	45	ARG
1	K	61	ARG
1	K	62	GLU
1	K	66	HIS
1	K	72	SER
1	K	77	LYS
1	K	92	GLU
1	K	112	GLU
1	K	141	LYS
1	K	145	TRP
1	K	151	GLU
1	K	195	GLU
1	K	222	LYS
1	K	223	PHE
1	K	229	TYR
1	K	234	ARG
1	K	252	ASP
1	K	284	SER

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Mol	Chain	Res	Type
1	K	288	SER
1	K	289	LEU
1	K	299	VAL
1	K	301	GLU
1	K	322	THR
1	K	336	LEU
1	L	2	ARG
1	L	7	THR
1	L	16	SER
1	L	17	LYS
1	L	19	ILE
1	L	28	ILE
1	L	51	MET
1	L	61	ARG
1	L	65	ASN
1	L	68	GLU
1	L	83	VAL
1	L	86	ASP
1	L	87	GLU
1	L	88	LEU
1	L	90	ASN
1	L	142	ARG
1	L	145	TRP
1	L	146	TYR
1	L	182	ARG
1	L	183	GLU
1	L	195	GLU
1	L	210	TYR
1	L	222	LYS
1	L	227	ARG
1	L	232	ASP
1	L	234	ARG
1	L	254	VAL
1	L	255	MET
1	L	268	LEU
1	L	281	TYR
1	L	284	SER
1	L	295	THR
1	L	304	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	B	180	GLN
1	B	191	HIS
1	C	324	HIS
1	D	271	GLN
1	E	76	ASN
1	E	230	GLN
1	E	271	GLN
1	F	65	ASN
1	G	27	GLN
1	H	65	ASN
1	H	271	GLN
1	I	90	ASN
1	I	132	HIS
1	I	230	GLN
1	J	65	ASN
1	J	230	GLN
1	J	271	GLN
1	L	282	ASN

### 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

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 ⓘ

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	336/338 (99%)	-0.28	0 100 100	60, 89, 115, 163	0
1	B	336/338 (99%)	-0.34	0 100 100	56, 86, 121, 165	0
1	C	336/338 (99%)	-0.11	0 100 100	51, 83, 116, 160	0
1	D	336/338 (99%)	-0.08	0 100 100	61, 98, 133, 165	0
1	E	336/338 (99%)	-0.20	1 (0%) 94 92	50, 78, 109, 149	0
1	F	336/338 (99%)	-0.26	1 (0%) 94 92	60, 89, 124, 163	0
1	G	336/338 (99%)	0.12	6 (1%) 71 63	58, 88, 120, 163	0
1	H	336/338 (99%)	-0.43	0 100 100	52, 73, 104, 144	0
1	I	336/338 (99%)	-0.33	1 (0%) 94 92	56, 80, 107, 147	0
1	J	336/338 (99%)	-0.13	4 (1%) 81 74	66, 98, 132, 179	0
1	K	336/338 (99%)	0.16	10 (2%) 54 45	72, 109, 137, 184	0
1	L	336/338 (99%)	0.34	8 (2%) 62 53	81, 121, 155, 167	0
All	All	4032/4056 (99%)	-0.13	31 (0%) 87 81	50, 90, 135, 184	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	65	ASN	4.1
1	K	82	GLY	3.0
1	L	142	ARG	3.0
1	K	37	LEU	2.9
1	L	84	LEU	2.9
1	K	39	VAL	2.7
1	K	97	TYR	2.6
1	K	41	PRO	2.6
1	I	65	ASN	2.5
1	L	167	GLY	2.5
1	K	38	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	136	GLY	2.4
1	J	82	GLY	2.3
1	G	75	ILE	2.3
1	J	1	MET	2.3
1	G	39	VAL	2.3
1	L	50	PRO	2.2
1	K	110	ILE	2.2
1	K	65	ASN	2.2
1	L	299	VAL	2.1
1	G	67	VAL	2.1
1	E	75	ILE	2.1
1	F	298	TYR	2.1
1	K	50	PRO	2.1
1	L	199	MET	2.1
1	J	51	MET	2.1
1	K	83	VAL	2.1
1	J	45	ARG	2.0
1	G	42	GLY	2.0
1	G	30	ALA	2.0
1	L	141	LYS	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
2	ZN	I	401	1/1	0.99	0.15	-0.04	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	F	401	1/1	1.00	0.14	-0.37	93,93,93,93	0
2	ZN	I	402	1/1	0.97	0.15	-0.66	106,106,106,106	0
2	ZN	K	401	1/1	0.98	0.10	-0.73	103,103,103,103	0
2	ZN	H	401	1/1	0.98	0.14	-0.78	67,67,67,67	0
2	ZN	K	402	1/1	0.99	0.12	-0.95	126,126,126,126	0
2	ZN	L	401	1/1	0.97	0.07	-1.14	128,128,128,128	0
2	ZN	H	402	1/1	0.99	0.14	-1.22	86,86,86,86	0
2	ZN	C	401	1/1	0.99	0.08	-1.41	92,92,92,92	0
2	ZN	D	401	1/1	0.99	0.08	-1.47	116,116,116,116	0
2	ZN	J	401	1/1	0.99	0.07	-1.66	106,106,106,106	0
2	ZN	L	402	1/1	0.92	0.09	-1.74	130,130,130,130	0
2	ZN	B	401	1/1	0.99	0.08	-1.84	83,83,83,83	0
2	ZN	C	402	1/1	0.99	0.12	-2.03	121,121,121,121	0
2	ZN	B	402	1/1	0.99	0.11	-2.15	127,127,127,127	0
2	ZN	A	401	1/1	0.99	0.08	-2.34	97,97,97,97	0
2	ZN	J	402	1/1	0.99	0.12	-2.54	122,122,122,122	0
2	ZN	G	401	1/1	0.99	0.05	-2.57	78,78,78,78	0
2	ZN	E	401	1/1	0.99	0.07	-2.60	75,75,75,75	0
2	ZN	F	402	1/1	0.99	0.12	-2.69	111,111,111,111	0
2	ZN	D	402	1/1	0.99	0.10	-2.93	113,113,113,113	0
2	ZN	A	402	1/1	0.98	0.09	-3.07	132,132,132,132	0
2	ZN	G	402	1/1	0.96	0.07	-7.20	109,109,109,109	0
2	ZN	E	402	1/1	0.99	0.06	-10.57	93,93,93,93	0

## 6.5 Other polymers

There are no such residues in this entry.