



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 07:25 PM EDT

PDB ID : 2ZHX  
Title : Crystal structure of Uracil-DNA Glycosylase from Mycobacterium tuberculosis in complex with a proteinaceous inhibitor  
Authors : Kaushal, P.S.; Talawar, R.K.; Krishna, P.D.V.; Varshney, U.; Vijayan, M.  
Deposited on : 2008-02-11  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

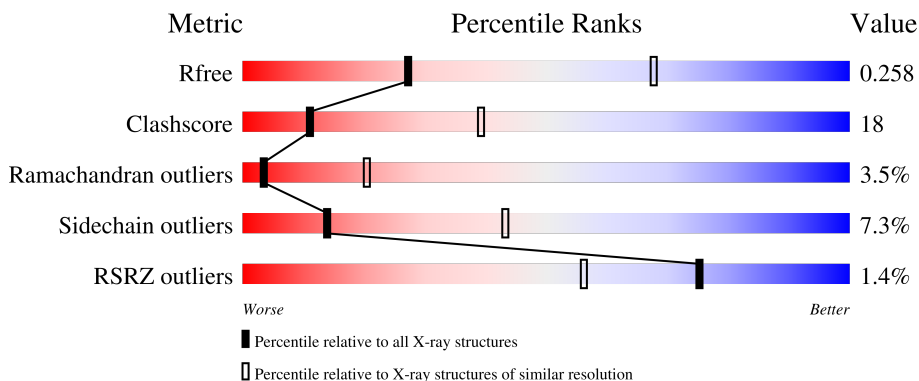
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	238	
1	C	238	
1	E	238	
1	G	238	
1	I	238	

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Mol	Chain	Length	Quality of chain
1	K	238	<p>2% 58% 31% 5% • •</p>
1	M	238	<p>60% 29% 5% • 5%</p>
2	B	84	<p>71% 21% 5% • •</p>
2	D	84	<p>69% 25% • •</p>
2	F	84	<p>% 62% 33% • •</p>
2	H	84	<p>% 75% 19% • •</p>
2	J	84	<p>12% 76% 20% • •</p>
2	L	84	<p>74% 21% • •</p>
2	N	84	<p>11% 68% 27% • • •</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16840 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	Total 1715	C 1095	N 313	O 302	S 5	0	0	0
1	C	225	Total 1709	C 1092	N 310	O 302	S 5	0	0	0
1	E	224	Total 1704	C 1089	N 309	O 301	S 5	0	0	0
1	G	225	Total 1707	C 1091	N 312	O 299	S 5	0	0	0
1	I	225	Total 1705	C 1090	N 310	O 300	S 5	0	0	0
1	K	225	Total 1705	C 1090	N 309	O 301	S 5	0	0	0
1	M	225	Total 1701	C 1088	N 309	O 299	S 5	0	0	0

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P67071
A	-9	HIS	-	expression tag	UNP P67071
A	-8	HIS	-	expression tag	UNP P67071
A	-7	HIS	-	expression tag	UNP P67071
A	-6	HIS	-	expression tag	UNP P67071
A	-5	HIS	-	expression tag	UNP P67071
A	-4	HIS	-	expression tag	UNP P67071
A	-3	GLY	-	expression tag	UNP P67071
A	-2	MET	-	expression tag	UNP P67071
A	-1	ALA	-	expression tag	UNP P67071
A	0	SER	-	expression tag	UNP P67071
C	-10	MET	-	initiating methionine	UNP P67071
C	-9	HIS	-	expression tag	UNP P67071
C	-8	HIS	-	expression tag	UNP P67071
C	-7	HIS	-	expression tag	UNP P67071

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP P67071
C	-5	HIS	-	expression tag	UNP P67071
C	-4	HIS	-	expression tag	UNP P67071
C	-3	GLY	-	expression tag	UNP P67071
C	-2	MET	-	expression tag	UNP P67071
C	-1	ALA	-	expression tag	UNP P67071
C	0	SER	-	expression tag	UNP P67071
E	-10	MET	-	initiating methionine	UNP P67071
E	-9	HIS	-	expression tag	UNP P67071
E	-8	HIS	-	expression tag	UNP P67071
E	-7	HIS	-	expression tag	UNP P67071
E	-6	HIS	-	expression tag	UNP P67071
E	-5	HIS	-	expression tag	UNP P67071
E	-4	HIS	-	expression tag	UNP P67071
E	-3	GLY	-	expression tag	UNP P67071
E	-2	MET	-	expression tag	UNP P67071
E	-1	ALA	-	expression tag	UNP P67071
E	0	SER	-	expression tag	UNP P67071
G	-10	MET	-	initiating methionine	UNP P67071
G	-9	HIS	-	expression tag	UNP P67071
G	-8	HIS	-	expression tag	UNP P67071
G	-7	HIS	-	expression tag	UNP P67071
G	-6	HIS	-	expression tag	UNP P67071
G	-5	HIS	-	expression tag	UNP P67071
G	-4	HIS	-	expression tag	UNP P67071
G	-3	GLY	-	expression tag	UNP P67071
G	-2	MET	-	expression tag	UNP P67071
G	-1	ALA	-	expression tag	UNP P67071
G	0	SER	-	expression tag	UNP P67071
I	-10	MET	-	initiating methionine	UNP P67071
I	-9	HIS	-	expression tag	UNP P67071
I	-8	HIS	-	expression tag	UNP P67071
I	-7	HIS	-	expression tag	UNP P67071
I	-6	HIS	-	expression tag	UNP P67071
I	-5	HIS	-	expression tag	UNP P67071
I	-4	HIS	-	expression tag	UNP P67071
I	-3	GLY	-	expression tag	UNP P67071
I	-2	MET	-	expression tag	UNP P67071
I	-1	ALA	-	expression tag	UNP P67071
I	0	SER	-	expression tag	UNP P67071
K	-10	MET	-	initiating methionine	UNP P67071
K	-9	HIS	-	expression tag	UNP P67071

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-8	HIS	-	expression tag	UNP P67071
K	-7	HIS	-	expression tag	UNP P67071
K	-6	HIS	-	expression tag	UNP P67071
K	-5	HIS	-	expression tag	UNP P67071
K	-4	HIS	-	expression tag	UNP P67071
K	-3	GLY	-	expression tag	UNP P67071
K	-2	MET	-	expression tag	UNP P67071
K	-1	ALA	-	expression tag	UNP P67071
K	0	SER	-	expression tag	UNP P67071
M	-10	MET	-	initiating methionine	UNP P67071
M	-9	HIS	-	expression tag	UNP P67071
M	-8	HIS	-	expression tag	UNP P67071
M	-7	HIS	-	expression tag	UNP P67071
M	-6	HIS	-	expression tag	UNP P67071
M	-5	HIS	-	expression tag	UNP P67071
M	-4	HIS	-	expression tag	UNP P67071
M	-3	GLY	-	expression tag	UNP P67071
M	-2	MET	-	expression tag	UNP P67071
M	-1	ALA	-	expression tag	UNP P67071
M	0	SER	-	expression tag	UNP P67071

- Molecule 2 is a protein called Uracil-DNA glycosylase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			639	402	98	136	3			
2	D	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	F	82	Total	C	N	O	S	0	0	0
			635	399	98	135	3			
2	H	82	Total	C	N	O	S	0	0	0
			628	394	98	133	3			
2	J	82	Total	C	N	O	S	0	0	0
			618	388	97	131	2			
2	L	82	Total	C	N	O	S	0	0	0
			613	387	96	127	3			
2	N	82	Total	C	N	O	S	0	0	0
			595	371	95	127	2			

- Molecule 3 is water.

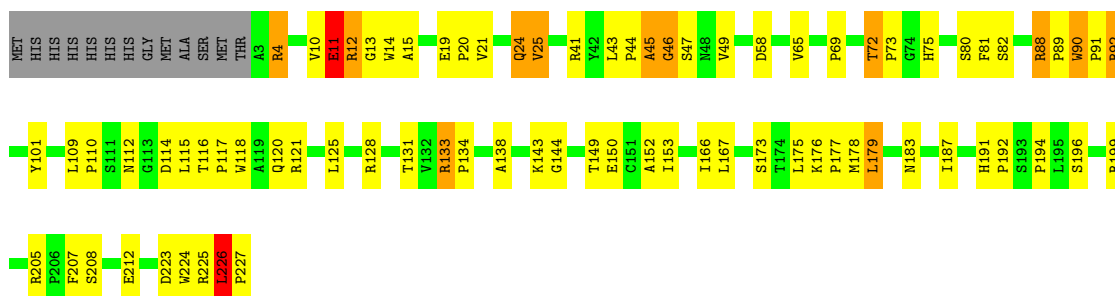
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	23	Total O 23 23	0	0
3	C	50	Total O 50 50	0	0
3	D	46	Total O 46 46	0	0
3	E	52	Total O 52 52	0	0
3	F	16	Total O 16 16	0	0
3	G	42	Total O 42 42	0	0
3	H	25	Total O 25 25	0	0
3	I	41	Total O 41 41	0	0
3	J	20	Total O 20 20	0	0
3	K	57	Total O 57 57	0	0
3	L	20	Total O 20 20	0	0
3	M	42	Total O 42 42	0	0
3	N	16	Total O 16 16	0	0

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

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

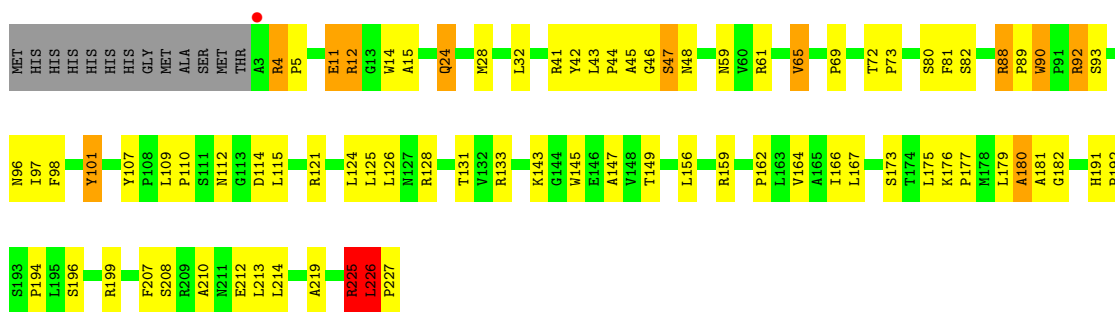
- Molecule 1: Uracil-DNA glycosylase

Chain A: 



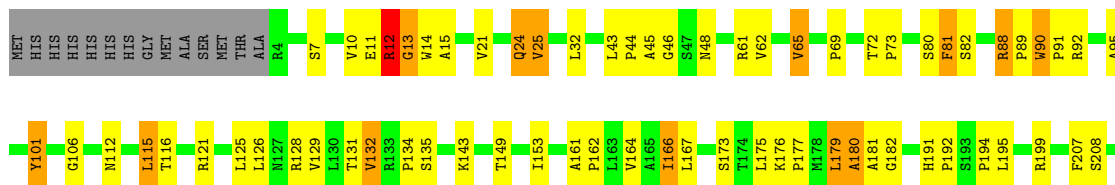
- Molecule 1: Uracil-DNA glycosylase

Chain C: 



- Molecule 1: Uracil-DNA glycosylase

Chain E: 







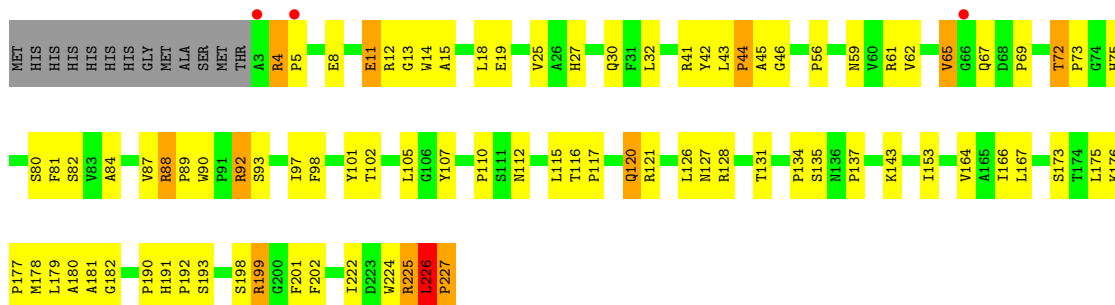
- Molecule 1: Uracil-DNA glycosylase

Chain G: 66% 24% 5% 5%



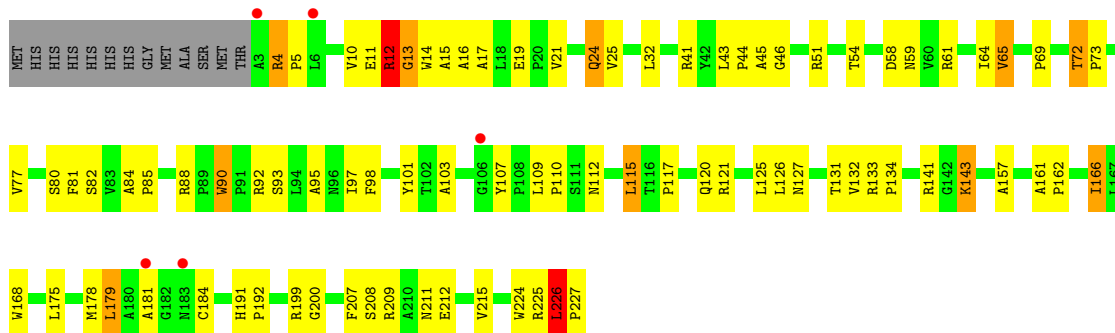
- Molecule 1: Uracil-DNA glycosylase

Chain I: 58% 32% 5% 5%



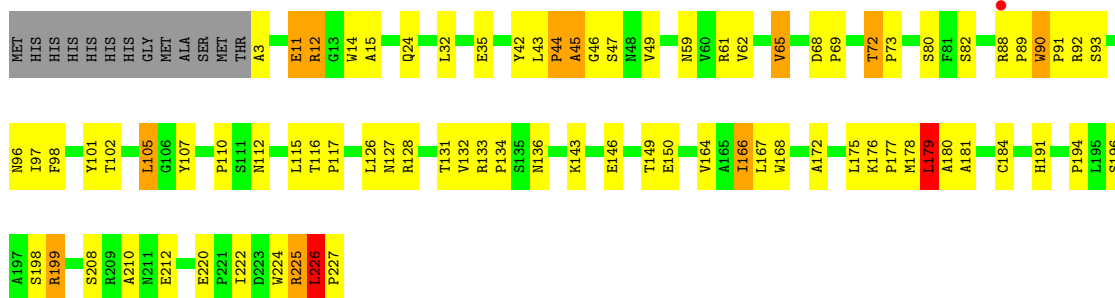
- Molecule 1: Uracil-DNA glycosylase

Chain K: 58% 31% 5% 2%



- Molecule 1: Uracil-DNA glycosylase

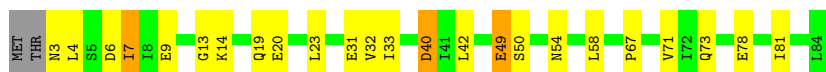
Chain M: 60% 29% 5% 5%



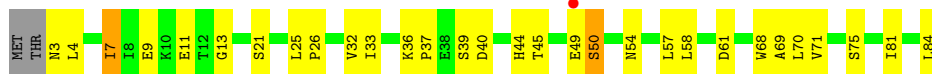
• Molecule 2: Uracil-DNA glycosylase inhibitor



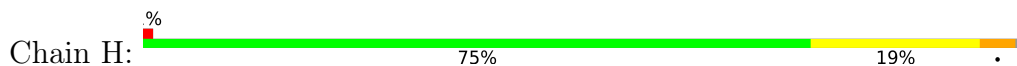
• Molecule 2: Uracil-DNA glycosylase inhibitor



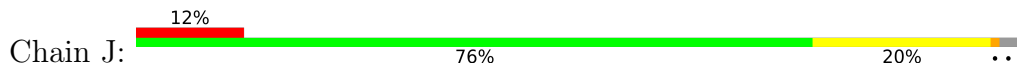
• Molecule 2: Uracil-DNA glycosylase inhibitor



• Molecule 2: Uracil-DNA glycosylase inhibitor



• Molecule 2: Uracil-DNA glycosylase inhibitor



• Molecule 2: Uracil-DNA glycosylase inhibitor





- Molecule 2: Uracil-DNA glycosylase inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.14Å 64.27Å 203.68Å 90.00° 109.72° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-3.10) 97.2 (29.96-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.11Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.276 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	2228 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 i

### 5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.61	0/1766	0.74	0/2416
1	C	0.68	2/1760 (0.1%)	0.77	2/2409 (0.1%)
1	E	0.59	0/1755	0.74	0/2402
1	G	0.61	0/1758	0.71	1/2406 (0.0%)
1	I	0.68	3/1756 (0.2%)	0.72	0/2404
1	K	0.67	2/1756 (0.1%)	0.70	3/2404 (0.1%)
1	M	0.66	2/1752 (0.1%)	0.72	2/2399 (0.1%)
2	B	0.61	0/647	0.66	1/877 (0.1%)
2	D	0.71	2/655 (0.3%)	0.77	1/887 (0.1%)
2	F	0.65	0/643	0.61	0/873
2	H	0.66	0/635	0.63	0/864
2	J	0.79	2/626 (0.3%)	0.65	1/853 (0.1%)
2	L	0.61	1/621 (0.2%)	0.65	1/845 (0.1%)
2	N	1.04	6/602 (1.0%)	0.70	0/823
All	All	0.67	20/16732 (0.1%)	0.71	12/22862 (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	E	0	1
1	K	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	27	GLU	CD-OE2	10.89	1.37	1.25
2	N	27	GLU	CD-OE1	9.87	1.36	1.25
1	I	8	GLU	CD-OE1	8.42	1.34	1.25
2	J	49	GLU	CA-CB	-8.13	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	ARG	CZ-NH2	8.07	1.43	1.33
2	N	57	LEU	CA-CB	-7.84	1.35	1.53
1	K	133	ARG	CZ-NH2	7.37	1.42	1.33
1	I	8	GLU	CD-OE2	7.36	1.33	1.25
1	K	19	GLU	CD-OE1	7.24	1.33	1.25
2	J	84	LEU	C-OXT	7.20	1.37	1.23
2	D	49	GLU	CD-OE1	6.97	1.33	1.25
1	M	3	ALA	C-O	6.42	1.35	1.23
1	M	128	ARG	CZ-NH1	5.60	1.40	1.33
2	D	49	GLU	CD-OE2	5.53	1.31	1.25
1	C	133	ARG	CZ-NH2	5.49	1.40	1.33
2	N	23	LEU	CA-CB	-5.47	1.41	1.53
2	L	78	GLU	CD-OE1	5.40	1.31	1.25
2	N	35	ASN	CG-OD1	5.25	1.35	1.24
1	I	227	PRO	CG-CD	5.08	1.67	1.50
2	N	51	THR	CB-OG1	5.04	1.53	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	K	133	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	K	133	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	M	179	LEU	CA-CB-CG	5.83	128.72	115.30
1	G	179	LEU	CA-CB-CG	5.82	128.70	115.30
1	K	179	LEU	CA-CB-CG	5.63	128.25	115.30
2	J	61	ASP	CB-CA-C	-5.50	99.39	110.40
2	B	4	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	133	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	D	49	GLU	OE1-CD-OE2	-5.23	117.03	123.30
2	L	27	GLU	N-CA-CB	-5.16	101.32	110.60
1	M	128	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	VAL	Peptide
1	K	10	VAL	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	1715	0	1707	88	0
1	C	1709	0	1696	70	0
1	E	1704	0	1691	67	0
1	G	1707	0	1697	65	0
1	I	1705	0	1692	73	0
1	K	1705	0	1690	76	0
1	M	1701	0	1686	76	0
2	B	639	0	630	18	0
2	D	647	0	640	23	0
2	F	635	0	621	18	0
2	H	628	0	606	14	0
2	J	618	0	588	10	0
2	L	613	0	590	9	0
2	N	595	0	549	11	0
3	A	69	0	0	2	0
3	B	23	0	0	0	0
3	C	50	0	0	0	0
3	D	46	0	0	0	0
3	E	52	0	0	2	0
3	F	16	0	0	1	0
3	G	42	0	0	0	0
3	H	25	0	0	0	0
3	I	41	0	0	0	0
3	J	20	0	0	0	0
3	K	57	0	0	1	0
3	L	20	0	0	1	0
3	M	42	0	0	1	0
3	N	16	0	0	0	0
All	All	16840	0	16083	582	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 18.

All (582) 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:G:44:PRO:HG2	1:G:131:THR:HA	1.25	1.13
1:C:44:PRO:HG2	1:C:131:THR:HA	1.27	1.11
1:K:44:PRO:HG2	1:K:131:THR:HA	1.13	1.09
1:A:44:PRO:HG2	1:A:131:THR:HA	1.13	1.07
1:I:44:PRO:HG2	1:I:131:THR:HA	1.32	1.06
1:A:90:TRP:HZ3	1:A:112:ASN:HA	1.19	1.03
1:M:44:PRO:HG2	1:M:131:THR:HA	1.40	1.00
1:E:44:PRO:HG2	1:E:131:THR:HA	1.44	0.99
1:E:11:GLU:HG2	1:E:14:TRP:HD1	1.32	0.93
1:G:12:ARG:HA	1:G:15:ALA:HB2	1.50	0.92
1:G:226:LEU:H	1:G:227:PRO:HD2	1.35	0.91
1:C:90:TRP:HZ3	1:C:112:ASN:HA	1.36	0.90
1:A:90:TRP:CZ3	1:A:112:ASN:HA	2.07	0.89
1:I:226:LEU:H	1:I:227:PRO:HD2	1.37	0.89
1:G:12:ARG:HA	1:G:15:ALA:CB	2.01	0.88
1:A:44:PRO:CG	1:A:131:THR:HA	2.02	0.87
1:C:226:LEU:N	1:C:227:PRO:HD2	1.90	0.87
1:M:90:TRP:CZ3	1:M:112:ASN:HA	2.09	0.87
1:K:44:PRO:CG	1:K:131:THR:HA	2.02	0.86
1:A:82:SER:HB2	1:A:115:LEU:HB2	1.54	0.86
1:M:90:TRP:HZ3	1:M:112:ASN:HA	1.41	0.86
1:I:11:GLU:HG2	1:I:14:TRP:HD1	1.40	0.84
1:G:226:LEU:N	1:G:227:PRO:HD2	1.92	0.84
1:G:44:PRO:CG	1:G:131:THR:HA	2.06	0.83
1:C:208:SER:O	1:C:212:GLU:HG3	1.79	0.82
1:K:11:GLU:HG2	1:K:14:TRP:HD1	1.43	0.82
1:C:90:TRP:CZ3	1:C:112:ASN:HA	2.15	0.82
1:E:44:PRO:CG	1:E:131:THR:HA	2.09	0.82
1:C:12:ARG:HA	1:C:15:ALA:CB	2.10	0.82
1:E:11:GLU:HG2	1:E:14:TRP:CD1	2.14	0.82
1:E:44:PRO:HG3	1:E:69:PRO:HG2	1.61	0.81
1:M:226:LEU:N	1:M:227:PRO:HD2	1.96	0.80
1:K:80:SER:HB2	1:K:125:LEU:HB3	1.60	0.80
1:A:43:LEU:HD11	1:A:73:PRO:HA	1.64	0.80
1:A:176:LYS:N	1:A:177:PRO:HD2	1.94	0.80
1:K:11:GLU:HG3	1:K:12:ARG:O	1.82	0.79
1:I:90:TRP:CZ3	1:I:112:ASN:HA	2.18	0.79
1:E:90:TRP:HZ3	1:E:112:ASN:HA	1.47	0.79
1:C:92:ARG:HA	1:C:92:ARG:HH11	1.47	0.78
1:A:12:ARG:HA	1:A:15:ALA:HB2	1.66	0.78
1:C:226:LEU:H	1:C:227:PRO:HD2	1.49	0.78
1:K:44:PRO:HG3	1:K:69:PRO:HG2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:PRO:CG	1:I:131:THR:HA	2.13	0.77
1:M:12:ARG:HG3	3:M:228:HOH:O	1.85	0.76
1:K:12:ARG:HA	1:K:15:ALA:CB	2.14	0.76
1:I:12:ARG:HA	1:I:15:ALA:CB	2.15	0.76
1:A:175:LEU:O	1:A:179:LEU:HD23	1.85	0.76
1:G:226:LEU:H	1:G:227:PRO:CD	1.98	0.75
1:I:90:TRP:HZ3	1:I:112:ASN:HA	1.47	0.75
1:E:82:SER:HB2	1:E:115:LEU:HB2	1.69	0.75
1:C:4:ARG:H	1:C:5:PRO:HD2	1.50	0.74
1:I:11:GLU:HG2	1:I:14:TRP:CD1	2.22	0.74
1:G:90:TRP:HZ3	1:G:112:ASN:HA	1.52	0.74
1:E:90:TRP:CZ3	1:E:112:ASN:HA	2.23	0.74
1:I:44:PRO:HG3	1:I:69:PRO:HG2	1.69	0.73
1:M:32:LEU:HD21	1:M:131:THR:HG21	1.70	0.73
1:I:92:ARG:HH11	1:I:92:ARG:HA	1.53	0.73
1:C:82:SER:HB2	1:C:115:LEU:HB2	1.69	0.73
1:C:44:PRO:CG	1:C:131:THR:HA	2.14	0.73
1:G:128:ARG:HD3	1:G:175:LEU:HD21	1.69	0.73
1:I:226:LEU:N	1:I:227:PRO:HD2	2.04	0.73
1:M:44:PRO:CG	1:M:131:THR:HA	2.15	0.73
1:K:90:TRP:HZ3	1:K:112:ASN:HA	1.55	0.72
1:G:226:LEU:O	1:G:227:PRO:OXT	2.05	0.72
1:C:44:PRO:HG3	1:C:69:PRO:HG2	1.72	0.72
1:E:92:ARG:HH11	1:E:92:ARG:HA	1.53	0.72
1:G:92:ARG:HH11	1:G:92:ARG:HA	1.55	0.72
1:A:12:ARG:HA	1:A:15:ALA:CB	2.20	0.72
1:C:48:ASN:OD1	1:G:205:ARG:NH1	2.23	0.72
1:A:75:HIS:HE1	2:B:19:GLN:HE21	1.38	0.71
1:E:12:ARG:HA	1:E:15:ALA:CB	2.21	0.71
1:G:90:TRP:CZ3	1:G:112:ASN:HA	2.25	0.71
1:C:226:LEU:H	1:C:227:PRO:CD	2.04	0.71
1:M:82:SER:HB2	1:M:115:LEU:HB2	1.73	0.71
2:H:4:LEU:O	2:H:7:ILE:HG23	1.90	0.70
1:C:180:ALA:O	1:C:182:GLY:N	2.23	0.70
1:G:89:PRO:O	2:H:19:GLN:NE2	2.22	0.70
1:K:12:ARG:HA	1:K:15:ALA:HB2	1.71	0.70
2:F:70:LEU:HD23	2:F:71:VAL:N	2.07	0.70
1:E:11:GLU:HG3	1:E:12:ARG:O	1.90	0.70
1:A:21:VAL:O	1:A:25:VAL:HG12	1.91	0.70
1:K:226:LEU:O	1:K:227:PRO:C	2.30	0.69
1:C:92:ARG:HD2	2:D:54:ASN:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:ILE:HG23	2:H:81:ILE:HG21	1.74	0.69
1:A:92:ARG:HA	1:A:92:ARG:HH11	1.58	0.69
1:G:44:PRO:HG3	1:G:69:PRO:HG2	1.74	0.69
2:J:9:GLU:O	2:J:13:GLY:HA2	1.92	0.69
1:M:225:ARG:CG	1:M:225:ARG:HH21	2.05	0.69
1:C:226:LEU:O	1:C:227:PRO:OXT	2.10	0.68
1:K:82:SER:HB2	1:K:115:LEU:HB2	1.73	0.68
1:A:82:SER:CB	1:A:115:LEU:HB2	2.22	0.68
1:M:226:LEU:HD12	1:M:226:LEU:H	1.59	0.68
1:G:126:LEU:HD11	1:G:149:THR:HG22	1.75	0.68
1:M:208:SER:O	1:M:212:GLU:HG3	1.92	0.68
1:G:11:GLU:HG2	1:G:14:TRP:HD1	1.58	0.68
1:K:208:SER:O	1:K:212:GLU:HG3	1.94	0.68
1:A:226:LEU:O	1:A:227:PRO:OXT	2.12	0.67
1:M:226:LEU:O	1:M:227:PRO:OXT	2.13	0.67
1:I:82:SER:HB2	1:I:115:LEU:HB2	1.75	0.67
1:C:226:LEU:N	1:C:227:PRO:CD	2.58	0.67
1:K:43:LEU:HD11	1:K:73:PRO:HA	1.77	0.66
2:L:4:LEU:O	2:L:7:ILE:HG23	1.96	0.66
2:B:70:LEU:HD23	2:B:71:VAL:N	2.10	0.66
1:G:180:ALA:O	1:G:182:GLY:N	2.27	0.66
1:I:226:LEU:O	1:I:227:PRO:C	2.33	0.66
1:M:11:GLU:HG2	1:M:14:TRP:HD1	1.60	0.65
1:E:92:ARG:NH1	1:E:95:ALA:HB2	2.11	0.65
1:M:226:LEU:N	1:M:227:PRO:CD	2.58	0.65
1:E:226:LEU:N	1:E:227:PRO:CD	2.59	0.65
2:F:4:LEU:O	2:F:7:ILE:HG23	1.97	0.65
1:M:92:ARG:HA	1:M:92:ARG:HH11	1.62	0.65
1:A:44:PRO:HG2	1:A:131:THR:CA	2.08	0.65
1:G:80:SER:O	1:G:82:SER:N	2.29	0.65
1:A:118:TRP:NE1	1:A:224:TRP:HA	2.13	0.64
1:E:226:LEU:H	1:E:227:PRO:CD	2.11	0.64
1:K:93:SER:O	1:K:97:ILE:HG13	1.97	0.64
1:A:44:PRO:HG3	1:A:69:PRO:HG2	1.78	0.64
1:E:101:TYR:HB2	1:E:207:PHE:CE2	2.33	0.64
1:C:12:ARG:HA	1:C:15:ALA:HB3	1.78	0.64
1:I:128:ARG:HD3	1:I:175:LEU:HD21	1.79	0.64
1:C:12:ARG:HA	1:C:15:ALA:HB2	1.79	0.63
1:E:226:LEU:H	1:E:227:PRO:HD3	1.63	0.63
1:K:11:GLU:CG	1:K:12:ARG:O	2.47	0.63
1:I:12:ARG:HA	1:I:15:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LEU:N	1:K:227:PRO:HD2	2.14	0.63
2:D:9:GLU:O	2:D:13:GLY:HA2	1.99	0.63
1:M:93:SER:O	1:M:97:ILE:HG13	1.98	0.62
1:A:90:TRP:O	1:A:92:ARG:NH1	2.32	0.62
1:C:199:ARG:HD2	2:D:32:VAL:HG22	1.81	0.62
2:N:41:ILE:HG21	2:N:58:LEU:HB3	1.81	0.62
1:A:12:ARG:O	1:A:14:TRP:N	2.30	0.62
1:I:11:GLU:O	1:I:12:ARG:HB3	1.99	0.62
1:M:44:PRO:HG3	1:M:69:PRO:HG2	1.81	0.62
2:N:9:GLU:O	2:N:13:GLY:HA2	2.00	0.62
2:B:7:ILE:HD13	2:B:67:PRO:HG3	1.82	0.62
1:C:11:GLU:HG2	1:C:14:TRP:HD1	1.63	0.62
1:A:225:ARG:NH2	1:A:227:PRO:HG2	2.15	0.62
1:K:44:PRO:HG2	1:K:131:THR:CA	2.09	0.62
1:E:88:ARG:HB3	1:E:89:PRO:HD3	1.82	0.62
1:E:12:ARG:HG3	1:E:13:GLY:N	2.14	0.61
1:C:176:LYS:N	1:C:177:PRO:HD2	2.15	0.61
1:E:12:ARG:O	1:E:14:TRP:N	2.32	0.61
1:A:226:LEU:N	1:A:227:PRO:CD	2.64	0.61
1:M:12:ARG:HA	1:M:15:ALA:CB	2.31	0.61
2:N:48:ASP:OD1	2:N:51:THR:HG23	2.00	0.61
1:K:11:GLU:HG2	1:K:14:TRP:CD1	2.32	0.61
1:C:11:GLU:CG	1:C:14:TRP:HD1	2.14	0.61
1:E:11:GLU:CD	1:E:12:ARG:O	2.39	0.61
1:G:226:LEU:N	1:G:227:PRO:CD	2.60	0.60
1:G:208:SER:O	1:G:212:GLU:HG3	2.01	0.60
1:I:11:GLU:CG	1:I:14:TRP:HD1	2.14	0.60
1:K:12:ARG:HG3	1:K:13:GLY:H	1.67	0.60
1:E:106:GLY:HA3	3:E:263:HOH:O	2.02	0.59
1:E:208:SER:O	1:E:212:GLU:HG3	2.01	0.59
2:F:4:LEU:HD21	2:F:57:LEU:HD23	1.84	0.59
1:A:194:PRO:HG2	2:B:45:THR:HG21	1.83	0.59
1:A:226:LEU:H	1:A:227:PRO:CD	2.15	0.59
1:G:90:TRP:O	1:G:92:ARG:NH1	2.35	0.59
1:A:225:ARG:HH22	1:A:227:PRO:HG2	1.67	0.59
1:G:107:TYR:CE1	1:G:225:ARG:HB2	2.37	0.59
1:I:89:PRO:O	2:J:19:GLN:NE2	2.35	0.59
1:K:64:ILE:HG12	1:K:166:ILE:HG12	1.83	0.59
1:G:82:SER:HB2	1:G:115:LEU:HB2	1.84	0.59
1:M:225:ARG:NH2	1:M:227:PRO:HG2	2.17	0.59
1:A:109:LEU:HD12	1:A:110:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:GLU:HG3	1:I:12:ARG:O	2.03	0.58
1:E:12:ARG:HA	1:E:15:ALA:HB3	1.84	0.58
1:K:11:GLU:CD	1:K:12:ARG:O	2.41	0.58
1:A:114:ASP:OD2	1:K:209:ARG:NH1	2.34	0.58
1:A:153:ILE:HD12	1:A:175:LEU:HD23	1.86	0.58
2:D:54:ASN:HB2	2:D:73:GLN:HB3	1.85	0.58
2:J:33:ILE:HG23	2:J:81:ILE:HG21	1.85	0.58
1:E:11:GLU:CG	1:E:12:ARG:O	2.51	0.58
1:C:199:ARG:NH1	1:I:56:PRO:HB3	2.19	0.58
2:B:4:LEU:O	2:B:7:ILE:HG23	2.04	0.58
1:C:199:ARG:HH21	2:D:31:GLU:HG2	1.68	0.58
1:I:93:SER:O	1:I:97:ILE:HG13	2.03	0.57
1:E:153:ILE:HD13	1:E:175:LEU:HD23	1.86	0.57
1:A:179:LEU:HD23	1:A:179:LEU:H	1.69	0.57
1:K:226:LEU:HD12	1:K:226:LEU:H	1.68	0.57
1:A:12:ARG:C	1:A:14:TRP:N	2.57	0.57
2:L:3:ASN:N	2:L:6:ASP:OD2	2.37	0.57
1:M:97:ILE:HD13	1:M:168:TRP:CZ3	2.40	0.57
1:C:82:SER:CB	1:C:115:LEU:HB2	2.34	0.57
1:I:12:ARG:HA	1:I:15:ALA:HB2	1.84	0.57
1:I:62:VAL:HA	1:I:164:VAL:O	2.04	0.57
1:A:12:ARG:HG3	1:A:13:GLY:N	2.18	0.57
1:A:75:HIS:HE1	2:B:19:GLN:NE2	2.02	0.57
1:C:164:VAL:HG11	1:C:210:ALA:HA	1.86	0.57
1:G:44:PRO:HG2	1:G:131:THR:CA	2.17	0.57
1:M:43:LEU:HD13	1:M:134:PRO:HG3	1.86	0.57
1:A:92:ARG:NH2	3:A:238:HOH:O	2.38	0.57
1:C:225:ARG:NH2	1:C:227:PRO:HG2	2.19	0.57
1:M:225:ARG:HH22	1:M:227:PRO:HG2	1.70	0.57
1:I:135:SER:O	1:I:137:PRO:HD3	2.05	0.56
2:D:49:GLU:O	2:D:49:GLU:HG3	2.05	0.56
2:H:25:LEU:HB3	2:H:26:PRO:HD2	1.86	0.56
1:I:82:SER:CB	1:I:115:LEU:HB2	2.35	0.56
1:A:101:TYR:HB2	1:A:207:PHE:CE2	2.41	0.56
1:G:180:ALA:C	1:G:182:GLY:H	2.08	0.56
2:D:7:ILE:HD13	2:D:67:PRO:HG3	1.88	0.56
2:N:61:ASP:C	2:N:63:PRO:HD2	2.26	0.56
1:E:92:ARG:HD2	2:F:54:ASN:OD1	2.06	0.56
1:I:121:ARG:NH1	1:I:224:TRP:O	2.39	0.56
1:I:176:LYS:N	1:I:177:PRO:HD2	2.21	0.56
1:K:12:ARG:HG3	1:K:13:GLY:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LEU:H	1:K:227:PRO:CD	2.19	0.55
1:E:62:VAL:HA	1:E:164:VAL:O	2.05	0.55
1:I:43:LEU:HD11	1:I:73:PRO:HA	1.89	0.55
1:I:41:ARG:O	1:I:134:PRO:HD3	2.07	0.55
1:E:128:ARG:HD3	1:E:175:LEU:HD21	1.88	0.55
1:I:12:ARG:C	1:I:14:TRP:H	2.10	0.55
1:E:226:LEU:O	1:E:227:PRO:C	2.44	0.55
1:G:64:ILE:HG12	1:G:166:ILE:HD13	1.87	0.55
1:A:10:VAL:O	1:A:12:ARG:N	2.40	0.55
1:A:118:TRP:HE1	1:A:224:TRP:HA	1.72	0.55
1:A:128:ARG:HD3	1:A:175:LEU:HD21	1.88	0.55
1:I:12:ARG:C	1:I:14:TRP:N	2.58	0.55
1:C:43:LEU:HD11	1:C:73:PRO:HA	1.90	0.54
1:C:47:SER:HB2	1:G:103:ALA:O	2.07	0.54
1:G:43:LEU:HD11	1:G:73:PRO:HA	1.89	0.54
1:I:67:GLN:O	1:I:127:ASN:HB3	2.07	0.54
1:K:41:ARG:O	1:K:134:PRO:HD3	2.07	0.54
1:A:149:THR:O	1:A:153:ILE:HG13	2.07	0.54
1:G:117:PRO:HA	1:G:120:GLN:HG2	1.88	0.54
1:K:175:LEU:O	1:K:178:MET:HB3	2.08	0.54
2:D:9:GLU:HA	2:D:14:LYS:H	1.72	0.54
1:M:44:PRO:HG2	1:M:131:THR:CA	2.27	0.54
1:M:225:ARG:NH2	1:M:225:ARG:HG3	2.23	0.54
1:K:11:GLU:CG	1:K:14:TRP:HD1	2.17	0.54
1:K:80:SER:CB	1:K:125:LEU:HB3	2.36	0.54
1:M:226:LEU:H	1:M:227:PRO:CD	2.20	0.54
1:K:12:ARG:CG	1:K:13:GLY:N	2.70	0.54
1:C:107:TYR:CE1	1:C:225:ARG:HB2	2.43	0.54
1:A:47:SER:HB3	1:K:103:ALA:O	2.08	0.54
1:C:90:TRP:O	1:C:92:ARG:NH1	2.40	0.54
1:K:117:PRO:HA	1:K:120:GLN:HG2	1.90	0.54
1:K:166:ILE:HD11	1:K:168:TRP:CZ2	2.42	0.54
1:C:12:ARG:O	1:C:14:TRP:N	2.41	0.53
2:D:33:ILE:HD11	2:D:58:LEU:HD22	1.90	0.53
1:K:226:LEU:N	1:K:227:PRO:CD	2.71	0.53
1:C:92:ARG:HH11	1:C:92:ARG:CA	2.17	0.53
1:G:64:ILE:HG12	1:G:166:ILE:CD1	2.38	0.53
2:B:18:ILE:HD13	2:B:44:HIS:HB3	1.89	0.53
1:M:69:PRO:HD2	1:M:132:VAL:HB	1.91	0.53
1:M:82:SER:CB	1:M:115:LEU:HB2	2.37	0.53
1:E:12:ARG:C	1:E:14:TRP:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LEU:H	1:K:227:PRO:HD2	1.73	0.53
1:K:41:ARG:O	1:K:134:PRO:CD	2.56	0.53
1:E:82:SER:CB	1:E:115:LEU:HB2	2.37	0.53
2:D:23:LEU:HB2	2:D:42:LEU:HD23	1.90	0.53
2:N:25:LEU:HB3	2:N:26:PRO:HD2	1.91	0.53
1:C:4:ARG:H	1:C:5:PRO:CD	2.21	0.53
1:C:109:LEU:HD12	1:C:110:PRO:HD2	1.90	0.52
1:E:180:ALA:O	1:E:182:GLY:N	2.42	0.52
1:A:196:SER:O	1:A:199:ARG:HB2	2.09	0.52
1:E:65:VAL:HA	1:E:126:LEU:O	2.08	0.52
1:M:224:TRP:O	1:M:225:ARG:HB3	2.09	0.52
1:G:194:PRO:HG2	2:H:45:THR:HG21	1.90	0.52
1:M:12:ARG:C	1:M:14:TRP:H	2.12	0.52
2:F:58:LEU:HD12	2:F:58:LEU:N	2.25	0.52
1:A:89:PRO:O	2:B:19:GLN:OE1	2.27	0.52
1:E:11:GLU:CG	1:E:14:TRP:HD1	2.13	0.52
1:K:107:TYR:CE1	1:K:225:ARG:HB2	2.44	0.52
1:K:226:LEU:N	1:K:226:LEU:HD12	2.25	0.52
2:F:49:GLU:O	2:F:50:SER:HB3	2.09	0.52
1:G:98:PHE:HA	1:G:101:TYR:HB3	1.92	0.52
1:A:175:LEU:HD12	1:A:175:LEU:N	2.25	0.52
1:C:80:SER:O	1:C:82:SER:N	2.42	0.52
1:I:32:LEU:HB3	1:I:42:TYR:CE2	2.45	0.52
1:G:82:SER:CB	1:G:115:LEU:HB2	2.40	0.51
1:M:11:GLU:CG	1:M:14:TRP:HD1	2.23	0.51
1:A:205:ARG:NH1	1:E:48:ASN:OD1	2.42	0.51
1:C:28:MET:HE2	1:C:145:TRP:CE2	2.45	0.51
2:L:9:GLU:O	2:L:13:GLY:HA2	2.11	0.51
1:M:12:ARG:HA	1:M:15:ALA:HB2	1.90	0.51
1:E:11:GLU:HG3	1:E:14:TRP:HB2	1.93	0.51
2:F:37:PRO:HB3	2:F:68:TRP:CZ2	2.46	0.51
1:M:62:VAL:HA	1:M:164:VAL:O	2.09	0.51
1:M:102:THR:O	1:M:105:LEU:O	2.29	0.51
1:M:194:PRO:HB3	2:N:54:ASN:HD22	1.74	0.51
2:D:23:LEU:HD11	2:D:40:ASP:HB3	1.93	0.51
1:I:88:ARG:HB3	1:I:89:PRO:HD3	1.93	0.51
1:A:175:LEU:O	1:A:179:LEU:CD2	2.55	0.51
1:E:126:LEU:HD11	1:E:149:THR:HG22	1.93	0.51
1:G:24:GLN:OE1	1:G:24:GLN:HA	2.11	0.51
1:K:90:TRP:O	1:K:92:ARG:NH1	2.44	0.51
1:C:124:LEU:HD23	1:C:156:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:ARG:CG	1:M:225:ARG:NH2	2.68	0.51
1:A:11:GLU:CG	1:A:14:TRP:HD1	2.24	0.51
1:C:65:VAL:HA	1:C:126:LEU:O	2.11	0.51
1:I:61:ARG:NH2	1:I:121:ARG:O	2.43	0.50
1:C:12:ARG:C	1:C:14:TRP:N	2.64	0.50
1:E:226:LEU:O	1:E:227:PRO:OXT	2.29	0.50
1:M:88:ARG:HB3	1:M:89:PRO:HD3	1.93	0.50
2:D:71:VAL:HG22	2:D:81:ILE:HG12	1.93	0.50
1:C:12:ARG:HH11	1:C:12:ARG:HG2	1.75	0.50
1:E:176:LYS:N	1:E:177:PRO:HD2	2.27	0.50
2:J:37:PRO:HB3	2:J:68:TRP:CZ2	2.46	0.50
2:L:4:LEU:CD2	2:L:57:LEU:HD23	2.42	0.50
1:M:43:LEU:O	1:M:45:ALA:N	2.44	0.50
1:M:194:PRO:HG2	2:N:45:THR:HG21	1.93	0.50
1:E:12:ARG:HA	1:E:15:ALA:HB2	1.91	0.50
2:H:4:LEU:CD2	2:H:57:LEU:HD23	2.42	0.50
1:K:82:SER:CB	1:K:115:LEU:HB2	2.40	0.50
1:A:80:SER:HB2	1:A:125:LEU:HB3	1.93	0.50
1:E:61:ARG:NH2	1:E:121:ARG:O	2.44	0.50
1:G:190:PRO:O	1:G:201:PHE:HB2	2.11	0.50
1:E:80:SER:O	1:E:82:SER:N	2.44	0.50
1:A:226:LEU:N	1:A:227:PRO:HD2	2.26	0.50
1:M:222:ILE:HG22	1:M:224:TRP:H	1.77	0.50
1:I:226:LEU:H	1:I:227:PRO:CD	2.16	0.49
1:K:191:HIS:CG	1:K:192:PRO:HD2	2.47	0.49
1:K:92:ARG:HA	1:K:92:ARG:HH11	1.77	0.49
1:M:12:ARG:C	1:M:14:TRP:N	2.66	0.49
1:M:32:LEU:O	1:M:35:GLU:HB2	2.12	0.49
1:C:24:GLN:HE21	1:C:147:ALA:HB3	1.77	0.49
2:D:33:ILE:CD1	2:D:58:LEU:HD22	2.42	0.49
1:G:12:ARG:C	1:G:14:TRP:N	2.65	0.49
1:I:128:ARG:CZ	1:I:175:LEU:HD11	2.42	0.49
1:M:126:LEU:HD11	1:M:149:THR:HG22	1.95	0.49
2:D:78:GLU:HB3	1:I:12:ARG:HE	1.78	0.49
1:E:43:LEU:HD11	1:E:73:PRO:HA	1.94	0.49
1:G:24:GLN:O	1:G:28:MET:HG2	2.12	0.49
1:K:12:ARG:C	1:K:14:TRP:N	2.66	0.49
2:L:70:LEU:HD23	2:L:71:VAL:N	2.27	0.49
1:M:167:LEU:HD23	1:M:172:ALA:O	2.11	0.49
1:C:162:PRO:HG2	1:C:219:ALA:HB2	1.94	0.49
2:F:69:ALA:HA	2:F:84:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HG2	1:A:14:TRP:HD1	1.78	0.49
1:A:179:LEU:HD23	1:A:179:LEU:N	2.28	0.49
1:E:80:SER:HB3	1:E:81:PHE:CD1	2.48	0.49
1:E:194:PRO:HG2	2:F:45:THR:HG21	1.93	0.49
1:C:44:PRO:HG3	1:C:69:PRO:CG	2.43	0.48
1:M:168:TRP:HB3	1:M:191:HIS:HA	1.95	0.48
1:M:226:LEU:N	1:M:226:LEU:HD12	2.26	0.48
1:E:24:GLN:HA	1:E:24:GLN:OE1	2.13	0.48
2:J:35:ASN:O	2:J:68:TRP:HH2	1.95	0.48
2:D:4:LEU:O	2:D:4:LEU:HD23	2.12	0.48
1:C:101:TYR:HB2	1:C:207:PHE:CE2	2.49	0.48
1:I:80:SER:O	1:I:82:SER:N	2.44	0.48
1:G:11:GLU:CG	1:G:14:TRP:HD1	2.26	0.48
1:I:27:HIS:O	1:I:30:GLN:HG3	2.14	0.48
1:I:222:ILE:HG22	1:I:224:TRP:H	1.79	0.48
1:A:19:GLU:HB3	1:A:20:PRO:HD3	1.95	0.48
1:K:80:SER:OG	1:K:125:LEU:C	2.51	0.48
1:K:110:PRO:HB3	1:K:226:LEU:HD13	1.94	0.48
1:M:176:LYS:N	1:M:177:PRO:HD2	2.28	0.48
1:K:32:LEU:HD21	1:K:131:THR:HG21	1.96	0.48
1:M:225:ARG:HH21	1:M:225:ARG:HG3	1.75	0.48
1:A:138:ALA:HB3	2:B:62:ALA:HB2	1.96	0.48
1:K:12:ARG:HA	1:K:15:ALA:H	1.77	0.48
1:K:11:GLU:OE1	1:K:12:ARG:O	2.32	0.48
1:E:225:ARG:NH1	3:E:245:HOH:O	2.29	0.47
1:A:118:TRP:CE2	1:A:224:TRP:HE3	2.33	0.47
1:A:133:ARG:HG2	1:A:133:ARG:NH2	2.27	0.47
2:H:11:GLU:HB3	2:H:70:LEU:HD13	1.96	0.47
2:N:37:PRO:HB3	2:N:68:TRP:CZ2	2.48	0.47
1:A:90:TRP:HB2	1:A:91:PRO:HD2	1.96	0.47
1:A:176:LYS:HB3	1:A:177:PRO:HD3	1.96	0.47
1:E:32:LEU:HD11	1:E:131:THR:HG21	1.97	0.47
1:G:194:PRO:HB3	2:H:54:ASN:HD22	1.80	0.47
1:I:198:SER:HA	1:I:202:PHE:HD2	1.78	0.47
1:I:199:ARG:HD2	2:J:32:VAL:HG22	1.97	0.47
2:N:4:LEU:O	2:N:7:ILE:HG23	2.14	0.47
1:A:176:LYS:HB3	1:A:177:PRO:CD	2.44	0.47
2:B:33:ILE:HG23	2:B:81:ILE:HG21	1.96	0.47
2:J:71:VAL:CG1	2:J:79:ASN:HB3	2.45	0.47
1:K:157:ALA:HA	1:K:184:CYS:SG	2.54	0.47
1:A:88:ARG:HB3	1:A:89:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:O	1:A:152:ALA:HB3	2.15	0.47
1:C:61:ARG:NH2	1:C:121:ARG:O	2.48	0.47
1:A:176:LYS:N	1:A:177:PRO:CD	2.70	0.47
1:I:167:LEU:HD23	1:I:173:SER:HA	1.97	0.47
1:E:21:VAL:O	1:E:25:VAL:HG12	2.14	0.47
1:E:175:LEU:O	1:E:179:LEU:HD23	2.14	0.47
1:I:98:PHE:CD1	1:I:110:PRO:HG2	2.50	0.47
1:G:119:ALA:HA	1:G:123:VAL:O	2.15	0.46
1:G:176:LYS:N	1:G:177:PRO:HD2	2.30	0.46
1:K:12:ARG:HA	1:K:15:ALA:HB3	1.97	0.46
1:M:11:GLU:HG2	1:M:14:TRP:CD1	2.45	0.46
2:F:21:SER:OG	2:F:44:HIS:CD2	2.68	0.46
1:K:98:PHE:O	1:K:101:TYR:HB3	2.15	0.46
1:M:222:ILE:HG22	1:M:224:TRP:N	2.31	0.46
1:C:196:SER:O	1:C:199:ARG:HB2	2.14	0.46
1:G:12:ARG:HA	1:G:15:ALA:HB3	1.90	0.46
1:I:12:ARG:HG3	1:I:13:GLY:N	2.30	0.46
1:I:175:LEU:O	1:I:178:MET:HB3	2.15	0.46
1:M:11:GLU:O	1:M:12:ARG:HG2	2.15	0.46
1:M:107:TYR:CE1	1:M:225:ARG:HB2	2.51	0.46
1:M:115:LEU:O	1:M:116:THR:C	2.53	0.46
1:G:80:SER:C	1:G:82:SER:H	2.14	0.46
1:G:226:LEU:O	1:G:227:PRO:C	2.52	0.46
1:M:164:VAL:HG11	1:M:210:ALA:HA	1.97	0.46
2:D:9:GLU:O	2:D:9:GLU:HG2	2.16	0.46
2:H:3:ASN:ND2	2:H:4:LEU:H	2.14	0.46
1:C:226:LEU:O	1:C:227:PRO:C	2.53	0.46
1:G:115:LEU:O	1:G:116:THR:C	2.54	0.46
1:A:133:ARG:HG2	1:A:133:ARG:HH21	1.81	0.46
1:A:11:GLU:C	1:A:12:ARG:O	2.52	0.46
1:A:24:GLN:NE2	1:A:144:GLY:O	2.48	0.46
1:G:117:PRO:HA	1:G:120:GLN:CG	2.46	0.46
1:I:4:ARG:H	1:I:5:PRO:HD2	1.79	0.46
2:F:33:ILE:HG23	2:F:81:ILE:HG21	1.97	0.46
1:G:194:PRO:HB3	2:H:54:ASN:ND2	2.31	0.46
1:M:82:SER:HB2	1:M:115:LEU:HD22	1.98	0.46
1:A:44:PRO:O	1:A:45:ALA:HB3	2.15	0.46
2:F:4:LEU:CD2	2:F:57:LEU:HD23	2.45	0.45
1:K:126:LEU:HG	1:K:127:ASN:O	2.17	0.45
1:C:98:PHE:CD1	1:C:110:PRO:HG2	2.51	0.45
1:M:12:ARG:HA	1:M:15:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HH11	1:A:223:ASP:HB3	1.81	0.45
1:I:180:ALA:O	1:I:182:GLY:N	2.46	0.45
1:K:12:ARG:O	1:K:14:TRP:N	2.48	0.45
1:G:62:VAL:HA	1:G:164:VAL:O	2.17	0.45
1:A:116:THR:N	1:A:117:PRO:HD2	2.31	0.45
1:A:208:SER:O	1:A:212:GLU:HG3	2.17	0.45
1:I:102:THR:O	1:I:105:LEU:O	2.34	0.45
1:I:191:HIS:ND1	1:I:193:SER:HB2	2.32	0.45
1:K:16:ALA:O	1:K:17:ALA:C	2.55	0.45
2:N:48:ASP:CG	2:N:51:THR:HG23	2.36	0.45
1:E:195:LEU:HG	1:E:195:LEU:O	2.17	0.45
1:I:92:ARG:HH11	1:I:92:ARG:CA	2.24	0.45
1:K:181:ALA:HB2	3:K:280:HOH:O	2.16	0.45
1:A:90:TRP:CZ3	1:A:112:ASN:CA	2.90	0.45
2:D:23:LEU:HB2	2:D:42:LEU:CD2	2.47	0.45
1:E:69:PRO:HD3	1:E:129:VAL:O	2.17	0.45
1:M:116:THR:N	1:M:117:PRO:HD2	2.31	0.45
1:A:12:ARG:C	1:A:14:TRP:H	2.14	0.45
1:C:47:SER:CB	1:G:103:ALA:O	2.65	0.45
2:F:9:GLU:O	2:F:13:GLY:HA2	2.17	0.45
2:F:33:ILE:HA	2:F:81:ILE:HD13	1.99	0.45
1:M:98:PHE:HA	1:M:101:TYR:HB3	1.98	0.45
1:G:104:ASP:HA	1:G:205:ARG:HD3	1.99	0.44
1:K:93:SER:HB2	2:L:20:GLU:OE2	2.17	0.44
1:I:191:HIS:CG	1:I:192:PRO:HD2	2.52	0.44
1:C:167:LEU:HD23	1:C:173:SER:HA	1.99	0.44
1:C:191:HIS:CG	1:C:192:PRO:HD2	2.52	0.44
1:I:105:LEU:HD13	1:I:107:TYR:CE1	2.53	0.44
1:A:45:ALA:O	1:A:46:GLY:C	2.56	0.44
1:M:32:LEU:HD22	1:M:42:TYR:CD2	2.53	0.44
1:A:187:ILE:O	1:A:187:ILE:HG13	2.17	0.44
1:A:226:LEU:H	1:A:227:PRO:HD3	1.81	0.44
1:G:21:VAL:O	1:G:25:VAL:HG12	2.17	0.44
2:H:4:LEU:HD21	2:H:57:LEU:HD23	1.99	0.44
1:K:92:ARG:NH1	1:K:95:ALA:HB2	2.32	0.44
1:A:45:ALA:HA	3:A:276:HOH:O	2.17	0.44
1:I:43:LEU:O	1:I:45:ALA:N	2.50	0.44
1:I:115:LEU:O	1:I:116:THR:C	2.53	0.44
1:K:141:ARG:C	1:K:143:LYS:H	2.21	0.44
1:G:44:PRO:HG3	1:G:69:PRO:CG	2.47	0.44
1:C:89:PRO:O	2:D:19:GLN:NE2	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:PRO:HG3	1:E:69:PRO:CG	2.40	0.44
2:L:31:GLU:CD	3:L:101:HOH:O	2.56	0.44
1:G:44:PRO:O	1:G:45:ALA:HB3	2.17	0.44
1:I:190:PRO:O	1:I:201:PHE:HB2	2.18	0.44
1:A:11:GLU:HG3	1:A:12:ARG:O	2.18	0.43
1:K:121:ARG:NH1	1:K:224:TRP:O	2.51	0.43
2:F:25:LEU:HB3	2:F:26:PRO:HD2	2.00	0.43
1:K:110:PRO:HG3	1:K:226:LEU:CD1	2.48	0.43
1:M:226:LEU:H	1:M:227:PRO:HD2	1.74	0.43
1:G:222:ILE:HG22	1:G:224:TRP:N	2.33	0.43
1:M:179:LEU:HD12	1:M:184:CYS:HB3	2.01	0.43
1:A:41:ARG:O	1:A:134:PRO:HD2	2.18	0.43
1:A:226:LEU:O	1:A:227:PRO:C	2.56	0.43
1:I:41:ARG:O	1:I:134:PRO:CD	2.66	0.43
1:I:180:ALA:C	1:I:182:GLY:H	2.21	0.43
1:A:80:SER:O	1:A:82:SER:N	2.44	0.43
2:B:70:LEU:HD23	2:B:71:VAL:H	1.80	0.43
1:C:32:LEU:HB3	1:C:42:TYR:CE2	2.54	0.43
1:C:80:SER:OG	1:C:125:LEU:C	2.56	0.43
2:F:36:LYS:HE3	3:F:100:HOH:O	2.19	0.43
2:J:9:GLU:HA	2:J:14:LYS:H	1.84	0.43
1:K:161:ALA:HA	1:K:162:PRO:HD3	1.83	0.43
2:B:21:SER:OG	2:B:44:HIS:CD2	2.72	0.43
1:G:92:ARG:HD2	2:H:54:ASN:OD1	2.19	0.43
1:M:65:VAL:O	1:M:65:VAL:HG22	2.18	0.43
2:B:45:THR:HG23	2:B:56:MET:CG	2.49	0.43
1:E:90:TRP:HB2	1:E:91:PRO:HD2	2.00	0.43
1:M:225:ARG:HH21	1:M:225:ARG:HG2	1.80	0.43
1:C:126:LEU:HD11	1:C:149:THR:HG22	2.01	0.43
1:E:43:LEU:HD13	1:E:134:PRO:HG3	2.01	0.43
1:G:211:ASN:O	1:G:215:VAL:HG23	2.19	0.43
1:M:146:GLU:O	1:M:150:GLU:HG3	2.19	0.43
1:E:167:LEU:HD23	1:E:173:SER:HA	2.01	0.43
1:G:11:GLU:HG2	1:G:14:TRP:CD1	2.47	0.43
1:M:96:ASN:O	1:M:97:ILE:C	2.56	0.43
1:A:191:HIS:CG	1:A:192:PRO:HD2	2.54	0.42
1:C:98:PHE:HA	1:C:101:TYR:HB3	2.01	0.42
1:M:61:ARG:NH1	1:M:220:GLU:HB2	2.35	0.42
1:A:120:GLN:NE2	1:K:200:GLY:O	2.52	0.42
2:B:7:ILE:HG12	2:B:57:LEU:HD21	2.01	0.42
1:I:222:ILE:HG22	1:I:224:TRP:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:VAL:HA	1:K:126:LEU:O	2.19	0.42
1:K:82:SER:HA	1:K:115:LEU:HD22	2.00	0.42
1:I:18:LEU:O	1:I:19:GLU:C	2.58	0.42
1:I:84:ALA:HB3	1:I:87:VAL:HG23	2.00	0.42
1:M:110:PRO:HA	1:M:227:PRO:HA	2.02	0.42
1:A:226:LEU:H	1:A:226:LEU:HD12	1.84	0.42
1:C:159:ARG:HE	1:C:159:ARG:HB2	1.74	0.42
1:G:11:GLU:CD	1:G:12:ARG:O	2.57	0.42
1:K:61:ARG:NH2	1:K:121:ARG:O	2.52	0.42
1:M:88:ARG:HB3	1:M:89:PRO:CD	2.49	0.42
1:E:88:ARG:HB3	1:E:89:PRO:CD	2.49	0.42
2:H:58:LEU:N	2:H:58:LEU:HD12	2.35	0.42
2:L:33:ILE:HG23	2:L:81:ILE:HG21	2.01	0.42
1:A:183:ASN:OD1	1:A:183:ASN:N	2.52	0.42
1:C:43:LEU:HD21	1:C:73:PRO:HA	2.00	0.42
1:C:96:ASN:O	1:C:97:ILE:C	2.58	0.42
1:E:226:LEU:N	1:E:227:PRO:HD2	2.35	0.42
1:I:72:THR:O	1:I:75:HIS:HB2	2.18	0.42
2:L:11:GLU:HG3	2:L:82:LYS:HZ3	1.84	0.42
1:M:191:HIS:O	1:M:196:SER:OG	2.37	0.42
1:E:199:ARG:HD2	2:F:32:VAL:HG22	2.00	0.42
2:F:39:SER:OG	2:F:40:ASP:N	2.53	0.42
1:A:43:LEU:HD21	1:A:72:THR:C	2.40	0.42
1:A:150:GLU:HG2	1:A:178:MET:HE1	2.01	0.42
1:G:180:ALA:C	1:G:182:GLY:N	2.73	0.42
2:H:37:PRO:HB3	2:H:68:TRP:CZ2	2.55	0.42
1:I:11:GLU:CG	1:I:12:ARG:O	2.68	0.42
1:I:117:PRO:HA	1:I:120:GLN:CG	2.49	0.42
1:I:153:ILE:CD1	1:I:175:LEU:HD23	2.49	0.42
1:M:72:THR:HA	1:M:73:PRO:HD3	1.97	0.41
1:A:110:PRO:HG3	1:A:226:LEU:CD1	2.50	0.41
1:E:80:SER:HB2	1:E:125:LEU:HB3	2.02	0.41
1:I:65:VAL:HA	1:I:126:LEU:O	2.19	0.41
1:C:98:PHE:CE1	1:C:110:PRO:HG2	2.56	0.41
2:J:71:VAL:HG13	2:J:79:ASN:HB3	2.02	0.41
1:M:166:ILE:HD11	1:M:168:TRP:CZ2	2.56	0.41
2:B:60:SER:O	2:B:61:ASP:O	2.38	0.41
1:G:65:VAL:HA	1:G:126:LEU:O	2.21	0.41
1:K:80:SER:HB3	1:K:81:PHE:CD1	2.55	0.41
1:K:84:ALA:HA	1:K:85:PRO:HD3	1.93	0.41
1:A:226:LEU:N	1:A:226:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.97	0.41
2:D:4:LEU:O	2:D:7:ILE:HG23	2.21	0.41
1:I:226:LEU:N	1:I:227:PRO:CD	2.78	0.41
1:A:112:ASN:OD1	1:A:114:ASP:HB3	2.21	0.41
1:E:166:ILE:HD12	1:E:166:ILE:HG21	1.87	0.41
1:G:88:ARG:HB3	1:G:89:PRO:CD	2.50	0.41
1:I:11:GLU:CD	1:I:12:ARG:O	2.59	0.41
1:E:131:THR:O	1:E:132:VAL:HB	2.21	0.41
1:G:12:ARG:CA	1:G:15:ALA:H	2.34	0.41
1:K:98:PHE:HA	1:K:101:TYR:HB3	2.02	0.41
1:M:127:ASN:O	1:M:149:THR:HG21	2.21	0.41
2:B:4:LEU:O	2:B:4:LEU:HD23	2.21	0.41
1:G:24:GLN:HE21	1:G:147:ALA:HB3	1.86	0.41
1:I:11:GLU:CD	1:I:56:PRO:HA	2.41	0.41
1:I:226:LEU:N	1:I:226:LEU:HD12	2.36	0.41
1:M:68:ASP:HB2	1:M:69:PRO:CD	2.51	0.41
1:M:80:SER:O	1:M:82:SER:N	2.53	0.41
1:M:175:LEU:HA	1:M:178:MET:HE3	2.02	0.41
1:C:128:ARG:HD3	1:C:175:LEU:HD21	2.02	0.41
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.94	0.41
1:G:51:ARG:HG2	1:G:79:LEU:HD21	2.03	0.41
1:I:92:ARG:HD2	2:J:54:ASN:CG	2.42	0.41
1:K:101:TYR:HB2	1:K:207:PHE:CE2	2.56	0.41
1:K:211:ASN:O	1:K:215:VAL:HG23	2.21	0.41
2:N:25:LEU:O	2:N:29:VAL:HG23	2.21	0.41
2:B:45:THR:HG23	2:B:56:MET:HG2	2.03	0.40
1:C:194:PRO:HB3	2:D:54:ASN:HD22	1.86	0.40
1:M:133:ARG:HG2	1:M:136:ASN:HB2	2.02	0.40
2:D:3:ASN:HB3	2:D:6:ASP:OD2	2.21	0.40
1:E:11:GLU:CG	1:E:14:TRP:CD1	2.93	0.40
1:E:161:ALA:HA	1:E:162:PRO:HD3	1.92	0.40
1:E:191:HIS:CG	1:E:192:PRO:HD2	2.56	0.40
1:E:226:LEU:N	1:E:226:LEU:HD12	2.37	0.40
1:K:4:ARG:H	1:K:5:PRO:HD2	1.86	0.40
1:K:21:VAL:O	1:K:24:GLN:N	2.53	0.40
1:K:43:LEU:O	1:K:45:ALA:N	2.54	0.40
1:K:109:LEU:HD12	1:K:110:PRO:HD2	2.02	0.40
1:A:167:LEU:HD23	1:A:173:SER:HA	2.03	0.40
1:C:11:GLU:CD	1:C:12:ARG:O	2.59	0.40
1:C:112:ASN:OD1	1:C:114:ASP:HB3	2.21	0.40
1:K:51:ARG:HH12	1:K:77:VAL:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TRP:CD1	1:A:224:TRP:HA	2.56	0.40
1:K:72:THR:HA	1:K:73:PRO:HD3	1.94	0.40
1:A:92:ARG:HD2	2:B:54:ASN:OD1	2.22	0.40
1:C:93:SER:HB2	2:D:20:GLU:OE2	2.21	0.40
2:D:78:GLU:HB3	1:I:12:ARG:NE	2.36	0.40
1:E:212:GLU:HG3	1:E:212:GLU:H	1.63	0.40
1:M:90:TRP:HB2	1:M:91:PRO:HD2	2.03	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	223/238 (94%)	195 (87%)	20 (9%)	8 (4%)	3	20
1	C	223/238 (94%)	189 (85%)	26 (12%)	8 (4%)	3	20
1	E	222/238 (93%)	187 (84%)	24 (11%)	11 (5%)	2	13
1	G	223/238 (94%)	194 (87%)	22 (10%)	7 (3%)	4	23
1	I	223/238 (94%)	193 (86%)	21 (9%)	9 (4%)	3	17
1	K	223/238 (94%)	190 (85%)	26 (12%)	7 (3%)	4	23
1	M	223/238 (94%)	185 (83%)	30 (14%)	8 (4%)	3	20
2	B	80/84 (95%)	68 (85%)	9 (11%)	3 (4%)	3	19
2	D	80/84 (95%)	70 (88%)	8 (10%)	2 (2%)	5	27
2	F	80/84 (95%)	68 (85%)	10 (12%)	2 (2%)	5	27
2	H	80/84 (95%)	69 (86%)	9 (11%)	2 (2%)	5	27
2	J	80/84 (95%)	69 (86%)	9 (11%)	2 (2%)	5	27
2	L	80/84 (95%)	71 (89%)	7 (9%)	2 (2%)	5	27
2	N	80/84 (95%)	73 (91%)	4 (5%)	3 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2120/2254 (94%)	1821 (86%)	225 (11%)	74 (4%)	3	20

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	ASP
1	C	180	ALA
1	C	181	ALA
1	E	180	ALA
1	E	181	ALA
2	F	50	SER
1	G	181	ALA
2	J	61	ASP
1	K	46	GLY
2	L	61	ASP
1	A	11	GLU
1	A	46	GLY
1	C	46	GLY
1	C	226	LEU
2	D	50	SER
1	E	12	ARG
1	E	13	GLY
1	E	45	ALA
1	E	46	GLY
2	F	61	ASP
1	G	45	ALA
1	G	46	GLY
2	H	50	SER
1	I	46	GLY
1	I	81	PHE
1	I	226	LEU
1	K	13	GLY
2	L	50	SER
1	M	181	ALA
2	N	50	SER
1	A	4	ARG
1	A	45	ALA
2	B	50	SER
1	C	4	ARG
1	G	226	LEU
1	I	4	ARG
1	I	181	ALA

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Mol	Chain	Res	Type
1	I	199	ARG
2	J	83	MET
2	N	38	GLU
1	A	226	LEU
1	C	81	PHE
1	C	225	ARG
1	E	81	PHE
1	E	135	SER
1	E	226	LEU
1	K	4	ARG
1	M	180	ALA
1	M	199	ARG
1	A	81	PHE
1	A	88	ARG
1	C	45	ALA
2	D	40	ASP
1	E	88	ARG
1	G	4	ARG
1	G	81	PHE
2	H	63	PRO
1	I	225	ARG
1	K	12	ARG
1	K	88	ARG
1	K	132	VAL
1	K	226	LEU
2	B	62	ALA
1	M	45	ALA
2	N	62	ALA
1	A	49	VAL
1	E	132	VAL
1	M	44	PRO
1	M	46	GLY
1	M	49	VAL
1	G	88	ARG
1	I	44	PRO
1	I	88	ARG
1	M	226	LEU

### 5.3.2 Protein sidechains [i](#)

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	175/186 (94%)	160 (91%)	15 (9%)	10	37
1	C	174/186 (94%)	157 (90%)	17 (10%)	8	29
1	E	174/186 (94%)	160 (92%)	14 (8%)	12	40
1	G	173/186 (93%)	159 (92%)	14 (8%)	11	39
1	I	173/186 (93%)	160 (92%)	13 (8%)	13	42
1	K	173/186 (93%)	158 (91%)	15 (9%)	10	36
1	M	172/186 (92%)	156 (91%)	16 (9%)	9	32
2	B	74/78 (95%)	70 (95%)	4 (5%)	22	53
2	D	76/78 (97%)	75 (99%)	1 (1%)	69	87
2	F	73/78 (94%)	69 (94%)	4 (6%)	21	53
2	H	71/78 (91%)	67 (94%)	4 (6%)	21	52
2	J	68/78 (87%)	67 (98%)	1 (2%)	65	85
2	L	67/78 (86%)	64 (96%)	3 (4%)	27	60
2	N	63/78 (81%)	60 (95%)	3 (5%)	25	58
All	All	1706/1848 (92%)	1582 (93%)	124 (7%)	14	43

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	11	GLU
1	A	12	ARG
1	A	24	GLN
1	A	25	VAL
1	A	58	ASP
1	A	65	VAL
1	A	72	THR
1	A	90	TRP
1	A	92	ARG
1	A	133	ARG
1	A	143	LYS
1	A	166	ILE
1	A	179	LEU
1	A	226	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	3	ASN
2	B	7	ILE
2	B	11	GLU
2	B	35	ASN
1	C	11	GLU
1	C	12	ARG
1	C	24	GLN
1	C	41	ARG
1	C	47	SER
1	C	59	ASN
1	C	65	VAL
1	C	72	THR
1	C	88	ARG
1	C	90	TRP
1	C	92	ARG
1	C	101	TYR
1	C	143	LYS
1	C	166	ILE
1	C	179	LEU
1	C	225	ARG
1	C	226	LEU
2	D	7	ILE
1	E	7	SER
1	E	12	ARG
1	E	24	GLN
1	E	25	VAL
1	E	65	VAL
1	E	72	THR
1	E	90	TRP
1	E	101	TYR
1	E	115	LEU
1	E	116	THR
1	E	143	LYS
1	E	166	ILE
1	E	179	LEU
1	E	226	LEU
2	F	3	ASN
2	F	7	ILE
2	F	11	GLU
2	F	75	SER
1	G	11	GLU
1	G	12	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	24	GLN
1	G	25	VAL
1	G	41	ARG
1	G	65	VAL
1	G	72	THR
1	G	90	TRP
1	G	92	ARG
1	G	101	TYR
1	G	143	LYS
1	G	166	ILE
1	G	225	ARG
1	G	226	LEU
2	H	3	ASN
2	H	7	ILE
2	H	11	GLU
2	H	17	VAL
1	I	11	GLU
1	I	25	VAL
1	I	59	ASN
1	I	65	VAL
1	I	72	THR
1	I	92	ARG
1	I	101	TYR
1	I	120	GLN
1	I	143	LYS
1	I	166	ILE
1	I	179	LEU
1	I	225	ARG
1	I	226	LEU
2	J	7	ILE
1	K	12	ARG
1	K	24	GLN
1	K	25	VAL
1	K	54	THR
1	K	58	ASP
1	K	59	ASN
1	K	65	VAL
1	K	72	THR
1	K	90	TRP
1	K	115	LEU
1	K	143	LYS
1	K	166	ILE

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Mol	Chain	Res	Type
1	K	179	LEU
1	K	199	ARG
1	K	226	LEU
2	L	4	LEU
2	L	7	ILE
2	L	17	VAL
1	M	11	GLU
1	M	12	ARG
1	M	24	GLN
1	M	47	SER
1	M	59	ASN
1	M	65	VAL
1	M	72	THR
1	M	90	TRP
1	M	105	LEU
1	M	143	LYS
1	M	166	ILE
1	M	179	LEU
1	M	198	SER
1	M	199	ARG
1	M	225	ARG
1	M	226	LEU
2	N	7	ILE
2	N	51	THR
2	N	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	120	GLN
2	B	19	GLN
2	B	35	ASN
2	B	44	HIS
1	C	24	GLN
1	C	59	ASN
2	D	3	ASN
1	E	59	ASN
1	E	120	GLN
2	F	44	HIS
1	G	59	ASN
2	H	3	ASN

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Mol	Chain	Res	Type
2	H	35	ASN
1	I	59	ASN
1	I	120	GLN
2	J	44	HIS
1	K	59	ASN
2	L	35	ASN
2	L	44	HIS
1	M	59	ASN
2	N	44	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 monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	225/238 (94%)	-0.24	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	32, 46, 70, 130	0
1	C	225/238 (94%)	-0.25	1 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">84</span>	27, 43, 77, 127	0
1	E	224/238 (94%)	-0.27	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	32, 44, 72, 127	0
1	G	225/238 (94%)	-0.19	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	31, 48, 73, 133	0
1	I	225/238 (94%)	-0.13	3 (1%) <span style="border: 1px solid blue; padding: 2px;">77</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	34, 51, 78, 132	0
1	K	225/238 (94%)	-0.13	5 (2%) <span style="border: 1px solid blue; padding: 2px;">62</span> <span style="border: 1px solid blue; padding: 2px;">41</span>	36, 56, 84, 140	0
1	M	225/238 (94%)	-0.01	1 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">84</span>	40, 63, 89, 139	0
2	B	82/84 (97%)	-0.08	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	40, 56, 91, 110	0
2	D	82/84 (97%)	-0.16	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	34, 52, 80, 109	0
2	F	82/84 (97%)	-0.11	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">61</span>	38, 56, 87, 106	0
2	H	82/84 (97%)	0.13	1 (1%) <span style="border: 1px solid blue; padding: 2px;">79</span> <span style="border: 1px solid blue; padding: 2px;">61</span>	56, 75, 100, 111	0
2	J	82/84 (97%)	0.70	10 (12%) <span style="border: 1px solid red; padding: 2px;">4</span> <span style="border: 1px solid red; padding: 2px;">1</span>	71, 95, 128, 142	0
2	L	82/84 (97%)	0.02	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	62, 82, 116, 149	0
2	N	82/84 (97%)	0.62	9 (10%) <span style="border: 1px solid red; padding: 2px;">5</span> <span style="border: 1px solid red; padding: 2px;">2</span>	82, 103, 125, 151	0
All	All	2148/2254 (95%)	-0.09	31 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">56</span>	27, 54, 102, 151	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	39	SER	5.2
1	I	3	ALA	5.0
1	K	3	ALA	3.7
2	N	49	GLU	3.3
2	J	36	LYS	3.1
2	N	50	SER	3.1
2	J	37	PRO	3.0
1	K	6	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	3	ALA	2.8
1	M	88	ARG	2.8
2	N	3	ASN	2.6
2	F	49	GLU	2.5
2	J	12	THR	2.5
1	K	183	ASN	2.5
2	J	35	ASN	2.5
2	J	68	TRP	2.5
2	H	15	GLN	2.4
1	K	106	GLY	2.3
2	J	51	THR	2.3
2	N	67	PRO	2.2
2	N	68	TRP	2.2
1	I	66	GLY	2.2
2	N	38	GLU	2.2
1	K	181	ALA	2.2
2	J	13	GLY	2.1
2	J	15	GLN	2.1
1	I	5	PRO	2.1
2	J	38	GLU	2.1
2	N	14	LYS	2.0
2	N	6	ASP	2.0
2	J	67	PRO	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.