



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:52 PM GMT

PDB ID : 1VF7  
Title : Crystal structure of the membrane fusion protein, MexA of the multidrug transporter  
Authors : Akama, H.; Matsuura, T.; Kashiwagi, S.; Yoneyama, H.; Tsukihara, T.; Nakagawa, A.; Nakae, T.  
Deposited on : 2004-04-09  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

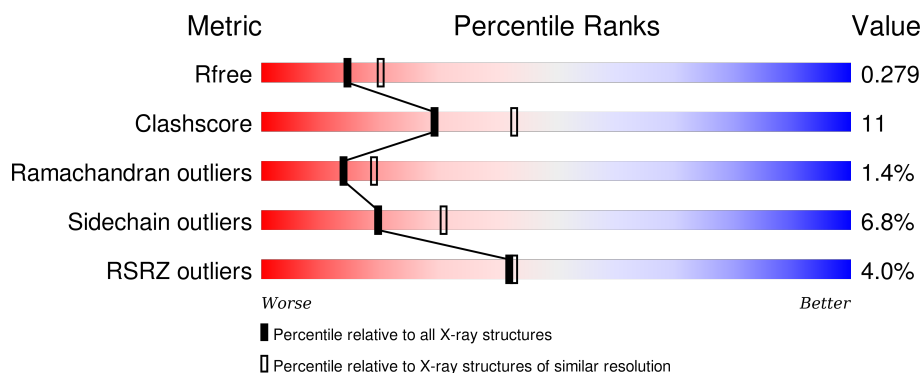
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	369	<div> <div>4%</div> <div>45% 17% • 36%</div> </div>
1	B	369	<div> <div>%</div> <div>47% 13% • 36%</div> </div>
1	C	369	<div> <div>2%</div> <div>49% 15% • 33%</div> </div>
1	D	369	<div> <div>%</div> <div>45% 16% • 36%</div> </div>
1	E	369	<div> <div>4%</div> <div>46% 18% • 32%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	369	
1	G	369	
1	H	369	
1	I	369	
1	J	369	
1	K	369	
1	L	369	
1	M	369	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23655 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 Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1816	1127	327	360	2			
1	B	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	C	246	Total	C	N	O	S	0	0	0
			1885	1173	339	371	2			
1	D	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	E	252	Total	C	N	O	S	0	0	0
			1928	1198	348	380	2			
1	F	233	Total	C	N	O	S	0	0	0
			1788	1110	323	353	2			
1	G	237	Total	C	N	O	S	0	0	0
			1819	1130	327	360	2			
1	H	241	Total	C	N	O	S	0	0	0
			1846	1146	332	366	2			
1	I	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	J	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	K	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			
1	L	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	M	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	CLONING ARTIFACT	UNP P52477
A	-1	GLU	-	CLONING ARTIFACT	UNP P52477
A	0	SER	-	CLONING ARTIFACT	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	CLONING ARTIFACT	UNP P52477
A	361	HIS	-	EXPRESSION TAG	UNP P52477
A	362	HIS	-	EXPRESSION TAG	UNP P52477
A	363	HIS	-	EXPRESSION TAG	UNP P52477
A	364	HIS	-	EXPRESSION TAG	UNP P52477
A	365	HIS	-	EXPRESSION TAG	UNP P52477
A	366	HIS	-	EXPRESSION TAG	UNP P52477
B	-2	ALA	-	CLONING ARTIFACT	UNP P52477
B	-1	GLU	-	CLONING ARTIFACT	UNP P52477
B	0	SER	-	CLONING ARTIFACT	UNP P52477
B	1	SER	-	CLONING ARTIFACT	UNP P52477
B	361	HIS	-	EXPRESSION TAG	UNP P52477
B	362	HIS	-	EXPRESSION TAG	UNP P52477
B	363	HIS	-	EXPRESSION TAG	UNP P52477
B	364	HIS	-	EXPRESSION TAG	UNP P52477
B	365	HIS	-	EXPRESSION TAG	UNP P52477
B	366	HIS	-	EXPRESSION TAG	UNP P52477
C	-2	ALA	-	CLONING ARTIFACT	UNP P52477
C	-1	GLU	-	CLONING ARTIFACT	UNP P52477
C	0	SER	-	CLONING ARTIFACT	UNP P52477
C	1	SER	-	CLONING ARTIFACT	UNP P52477
C	361	HIS	-	EXPRESSION TAG	UNP P52477
C	362	HIS	-	EXPRESSION TAG	UNP P52477
C	363	HIS	-	EXPRESSION TAG	UNP P52477
C	364	HIS	-	EXPRESSION TAG	UNP P52477
C	365	HIS	-	EXPRESSION TAG	UNP P52477
C	366	HIS	-	EXPRESSION TAG	UNP P52477
D	-2	ALA	-	CLONING ARTIFACT	UNP P52477
D	-1	GLU	-	CLONING ARTIFACT	UNP P52477
D	0	SER	-	CLONING ARTIFACT	UNP P52477
D	1	SER	-	CLONING ARTIFACT	UNP P52477
D	361	HIS	-	EXPRESSION TAG	UNP P52477
D	362	HIS	-	EXPRESSION TAG	UNP P52477
D	363	HIS	-	EXPRESSION TAG	UNP P52477
D	364	HIS	-	EXPRESSION TAG	UNP P52477
D	365	HIS	-	EXPRESSION TAG	UNP P52477
D	366	HIS	-	EXPRESSION TAG	UNP P52477
E	-2	ALA	-	CLONING ARTIFACT	UNP P52477
E	-1	GLU	-	CLONING ARTIFACT	UNP P52477
E	0	SER	-	CLONING ARTIFACT	UNP P52477
E	1	SER	-	CLONING ARTIFACT	UNP P52477
E	361	HIS	-	EXPRESSION TAG	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
E	362	HIS	-	EXPRESSION TAG	UNP P52477
E	363	HIS	-	EXPRESSION TAG	UNP P52477
E	364	HIS	-	EXPRESSION TAG	UNP P52477
E	365	HIS	-	EXPRESSION TAG	UNP P52477
E	366	HIS	-	EXPRESSION TAG	UNP P52477
F	-2	ALA	-	CLONING ARTIFACT	UNP P52477
F	-1	GLU	-	CLONING ARTIFACT	UNP P52477
F	0	SER	-	CLONING ARTIFACT	UNP P52477
F	1	SER	-	CLONING ARTIFACT	UNP P52477
F	361	HIS	-	EXPRESSION TAG	UNP P52477
F	362	HIS	-	EXPRESSION TAG	UNP P52477
F	363	HIS	-	EXPRESSION TAG	UNP P52477
F	364	HIS	-	EXPRESSION TAG	UNP P52477
F	365	HIS	-	EXPRESSION TAG	UNP P52477
F	366	HIS	-	EXPRESSION TAG	UNP P52477
G	-2	ALA	-	CLONING ARTIFACT	UNP P52477
G	-1	GLU	-	CLONING ARTIFACT	UNP P52477
G	0	SER	-	CLONING ARTIFACT	UNP P52477
G	1	SER	-	CLONING ARTIFACT	UNP P52477
G	361	HIS	-	EXPRESSION TAG	UNP P52477
G	362	HIS	-	EXPRESSION TAG	UNP P52477
G	363	HIS	-	EXPRESSION TAG	UNP P52477
G	364	HIS	-	EXPRESSION TAG	UNP P52477
G	365	HIS	-	EXPRESSION TAG	UNP P52477
G	366	HIS	-	EXPRESSION TAG	UNP P52477
H	-2	ALA	-	CLONING ARTIFACT	UNP P52477
H	-1	GLU	-	CLONING ARTIFACT	UNP P52477
H	0	SER	-	CLONING ARTIFACT	UNP P52477
H	1	SER	-	CLONING ARTIFACT	UNP P52477
H	361	HIS	-	EXPRESSION TAG	UNP P52477
H	362	HIS	-	EXPRESSION TAG	UNP P52477
H	363	HIS	-	EXPRESSION TAG	UNP P52477
H	364	HIS	-	EXPRESSION TAG	UNP P52477
H	365	HIS	-	EXPRESSION TAG	UNP P52477
H	366	HIS	-	EXPRESSION TAG	UNP P52477
I	-2	ALA	-	CLONING ARTIFACT	UNP P52477
I	-1	GLU	-	CLONING ARTIFACT	UNP P52477
I	0	SER	-	CLONING ARTIFACT	UNP P52477
I	1	SER	-	CLONING ARTIFACT	UNP P52477
I	361	HIS	-	EXPRESSION TAG	UNP P52477
I	362	HIS	-	EXPRESSION TAG	UNP P52477
I	363	HIS	-	EXPRESSION TAG	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
I	364	HIS	-	EXPRESSION TAG	UNP P52477
I	365	HIS	-	EXPRESSION TAG	UNP P52477
I	366	HIS	-	EXPRESSION TAG	UNP P52477
J	-2	ALA	-	CLONING ARTIFACT	UNP P52477
J	-1	GLU	-	CLONING ARTIFACT	UNP P52477
J	0	SER	-	CLONING ARTIFACT	UNP P52477
J	1	SER	-	CLONING ARTIFACT	UNP P52477
J	361	HIS	-	EXPRESSION TAG	UNP P52477
J	362	HIS	-	EXPRESSION TAG	UNP P52477
J	363	HIS	-	EXPRESSION TAG	UNP P52477
J	364	HIS	-	EXPRESSION TAG	UNP P52477
J	365	HIS	-	EXPRESSION TAG	UNP P52477
J	366	HIS	-	EXPRESSION TAG	UNP P52477
K	-2	ALA	-	CLONING ARTIFACT	UNP P52477
K	-1	GLU	-	CLONING ARTIFACT	UNP P52477
K	0	SER	-	CLONING ARTIFACT	UNP P52477
K	1	SER	-	CLONING ARTIFACT	UNP P52477
K	361	HIS	-	EXPRESSION TAG	UNP P52477
K	362	HIS	-	EXPRESSION TAG	UNP P52477
K	363	HIS	-	EXPRESSION TAG	UNP P52477
K	364	HIS	-	EXPRESSION TAG	UNP P52477
K	365	HIS	-	EXPRESSION TAG	UNP P52477
K	366	HIS	-	EXPRESSION TAG	UNP P52477
L	-2	ALA	-	CLONING ARTIFACT	UNP P52477
L	-1	GLU	-	CLONING ARTIFACT	UNP P52477
L	0	SER	-	CLONING ARTIFACT	UNP P52477
L	1	SER	-	CLONING ARTIFACT	UNP P52477
L	361	HIS	-	EXPRESSION TAG	UNP P52477
L	362	HIS	-	EXPRESSION TAG	UNP P52477
L	363	HIS	-	EXPRESSION TAG	UNP P52477
L	364	HIS	-	EXPRESSION TAG	UNP P52477
L	365	HIS	-	EXPRESSION TAG	UNP P52477
L	366	HIS	-	EXPRESSION TAG	UNP P52477
M	-2	ALA	-	CLONING ARTIFACT	UNP P52477
M	-1	GLU	-	CLONING ARTIFACT	UNP P52477
M	0	SER	-	CLONING ARTIFACT	UNP P52477
M	1	SER	-	CLONING ARTIFACT	UNP P52477
M	361	HIS	-	EXPRESSION TAG	UNP P52477
M	362	HIS	-	EXPRESSION TAG	UNP P52477
M	363	HIS	-	EXPRESSION TAG	UNP P52477
M	364	HIS	-	EXPRESSION TAG	UNP P52477
M	365	HIS	-	EXPRESSION TAG	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
M	366	HIS	-	EXPRESSION TAG	UNP P52477

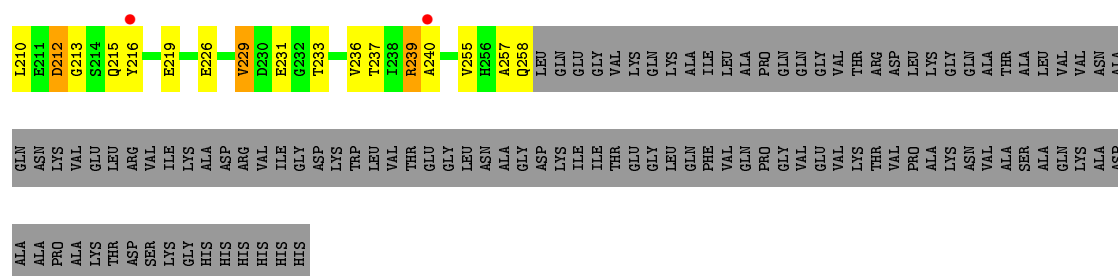




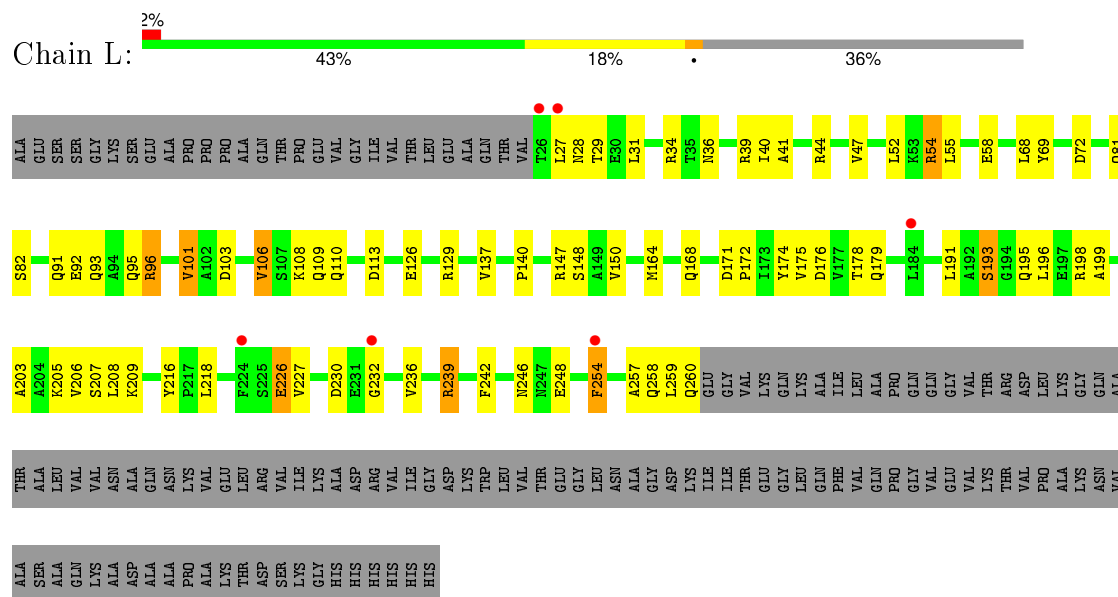




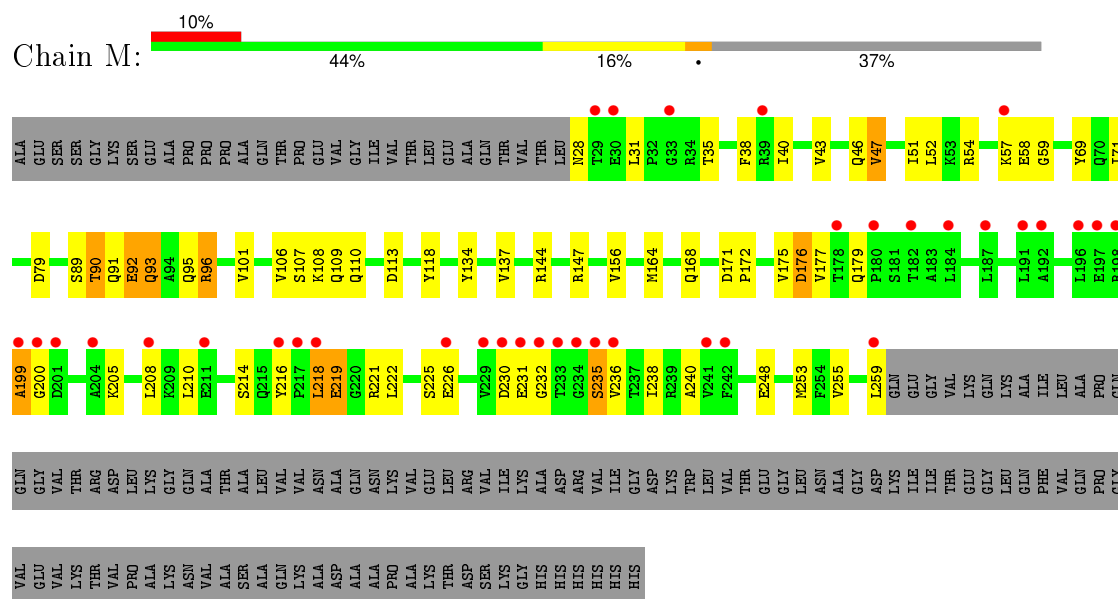




• Molecule 1: Multidrug resistance protein mexA



• Molecule 1: Multidrug resistance protein mexA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.03Å 180.35Å 214.23Å 90.00° 106.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.40) 99.8 (40.00-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.258 , 0.282 0.253 , 0.279	Depositor DCC
$R_{free}$ test set	18428 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.2	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 365653 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.77	0/1840	0.92	7/2495 (0.3%)
1	B	1.17	3/1827 (0.2%)	1.18	16/2478 (0.6%)
1	C	1.09	4/1909 (0.2%)	1.13	13/2588 (0.5%)
1	D	1.22	5/1827 (0.3%)	1.33	23/2478 (0.9%)
1	E	1.05	1/1953 (0.1%)	1.11	14/2648 (0.5%)
1	F	1.05	2/1812 (0.1%)	1.08	12/2457 (0.5%)
1	G	0.77	1/1843 (0.1%)	0.92	6/2500 (0.2%)
1	H	0.89	0/1870	0.98	9/2537 (0.4%)
1	I	1.04	2/1827 (0.1%)	1.11	15/2478 (0.6%)
1	J	0.88	1/1827 (0.1%)	0.99	11/2478 (0.4%)
1	K	0.86	1/1803 (0.1%)	0.93	7/2445 (0.3%)
1	L	0.85	0/1827	0.97	8/2478 (0.3%)
1	M	0.62	0/1803	0.78	3/2445 (0.1%)
All	All	0.96	20/23968 (0.1%)	1.04	144/32505 (0.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ASN	C-O	11.84	1.45	1.23
1	B	248	GLU	CD-OE1	7.55	1.33	1.25
1	C	77	GLU	CD-OE2	6.76	1.33	1.25
1	G	129	ARG	CZ-NH1	6.44	1.41	1.33
1	B	55	LEU	N-CA	5.91	1.58	1.46
1	I	129	ARG	NE-CZ	5.84	1.40	1.33
1	B	150	VAL	CB-CG1	-5.74	1.40	1.52
1	D	129	ARG	NE-CZ	5.70	1.40	1.33
1	D	117	ALA	CA-CB	5.62	1.64	1.52
1	C	129	ARG	NE-CZ	5.51	1.40	1.33
1	C	55	LEU	N-CA	5.44	1.57	1.46
1	F	129	ARG	NE-CZ	5.42	1.40	1.33
1	I	55	LEU	N-CA	5.41	1.57	1.46
1	K	126	GLU	CD-OE2	5.33	1.31	1.25
1	D	43	VAL	CB-CG2	5.24	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	133	ARG	CG-CD	5.19	1.65	1.51
1	E	125	VAL	CB-CG2	-5.14	1.42	1.52
1	F	248	GLU	CD-OE2	5.11	1.31	1.25
1	D	129	ARG	CZ-NH1	5.10	1.39	1.33
1	C	133	ARG	CG-CD	5.03	1.64	1.51

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	C	96	ARG	NE-CZ-NH2	-14.83	112.88	120.30
1	G	133	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	E	54	ARG	NE-CZ-NH2	-13.33	113.64	120.30
1	D	54	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	D	133	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	B	96	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	J	96	ARG	NE-CZ-NH2	-11.47	114.56	120.30
1	B	54	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	L	96	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	I	133	ARG	NE-CZ-NH2	-11.01	114.79	120.30
1	D	129	ARG	NE-CZ-NH1	10.99	125.79	120.30
1	D	96	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	F	129	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	K	96	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	B	246	ASN	C-N-CA	-10.14	96.36	121.70
1	C	129	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	F	54	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	E	54	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	96	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	J	54	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	I	96	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	I	129	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	E	96	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	H	129	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	H	133	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	D	246	ASN	N-CA-C	-8.75	87.38	111.00
1	D	113	ASP	CB-CG-OD2	8.74	126.17	118.30
1	G	133	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	L	54	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	L	96	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	96	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	D	129	ARG	NE-CZ-NH2	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	133	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	K	129	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	133	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	I	129	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	E	133	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	239	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	D	133	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	H	129	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	I	54	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	J	61	ASP	CB-CG-OD2	7.50	125.05	118.30
1	G	129	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	I	172	PRO	N-CA-C	-7.38	92.90	112.10
1	B	79	ASP	CB-CG-OD2	7.27	124.84	118.30
1	D	54	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	96	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	F	129	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	212	ASP	CB-CG-OD2	7.03	124.62	118.30
1	B	212	ASP	CB-CG-OD2	7.02	124.61	118.30
1	E	79	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	54	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	54	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	E	113	ASP	CB-CG-OD2	6.83	124.44	118.30
1	L	129	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	I	133	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	M	79	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	172	PRO	N-CA-C	-6.74	94.59	112.10
1	E	133	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	J	113	ASP	CB-CG-OD2	6.71	124.34	118.30
1	I	61	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	72	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	172	PRO	N-CA-C	-6.67	94.76	112.10
1	C	172	PRO	N-CA-C	-6.58	95.00	112.10
1	B	133	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	F	171	ASP	N-CA-C	-6.54	93.36	111.00
1	A	96	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	F	246	ASN	C-N-CA	-6.33	105.88	121.70
1	C	72	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	129	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	I	96	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	D	201	ASP	CB-CG-OD2	6.22	123.90	118.30
1	H	201	ASP	CB-CG-OD2	6.17	123.86	118.30
1	E	129	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	129	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	J	96	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	J	133	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	F	133	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	171	ASP	CB-CG-OD2	6.04	123.74	118.30
1	D	54	ARG	CG-CD-NE	-6.03	99.13	111.80
1	K	129	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	I	246	ASN	N-CA-C	-5.99	94.82	111.00
1	C	133	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	K	113	ASP	CB-CG-OD2	5.92	123.63	118.30
1	G	129	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	L	103	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	230	ASP	CB-CG-OD2	5.90	123.61	118.30
1	I	201	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	54	ARG	C-N-CA	-5.83	107.12	121.70
1	D	61	ASP	CB-CG-OD2	5.82	123.54	118.30
1	I	212	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	230	ASP	CB-CG-OD2	5.76	123.49	118.30
1	F	133	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	201	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	230	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	172	PRO	N-CA-C	-5.71	97.26	112.10
1	J	212	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	171	ASP	N-CA-CB	5.65	120.77	110.60
1	B	246	ASN	O-C-N	-5.63	113.69	122.70
1	D	106	VAL	CG1-CB-CG2	5.62	119.89	110.90
1	K	212	ASP	CB-CG-OD2	5.62	123.35	118.30
1	I	113	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	54	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	172	PRO	N-CD-CG	-5.58	94.83	103.20
1	J	172	PRO	N-CA-C	-5.58	97.60	112.10
1	C	96	ARG	CG-CD-NE	-5.56	100.12	111.80
1	G	212	ASP	CB-CG-OD2	5.49	123.24	118.30
1	H	113	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	101	VAL	CB-CA-C	-5.47	101.01	111.40
1	C	176	ASP	CB-CG-OD1	5.47	123.22	118.30
1	F	246	ASN	N-CA-C	-5.45	96.30	111.00
1	C	230	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	201	ASP	CB-CG-OD2	5.42	123.17	118.30
1	I	246	ASN	C-N-CA	-5.40	108.20	121.70
1	F	171	ASP	N-CA-CB	5.40	120.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	LYS	CD-CE-NZ	-5.36	99.38	111.70
1	M	96	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	E	171	ASP	N-CA-CB	5.34	120.21	110.60
1	D	54	ARG	O-C-N	-5.33	114.17	122.70
1	L	129	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	H	172	PRO	N-CA-C	-5.30	98.32	112.10
1	J	90	THR	N-CA-CB	-5.29	100.24	110.30
1	I	239	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	171	ASP	N-CA-CB	5.27	120.09	110.60
1	D	230	ASP	CB-CG-OD2	5.27	123.04	118.30
1	H	79	ASP	CB-CG-OD2	5.26	123.04	118.30
1	K	96	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	212	ASP	CB-CG-OD2	5.20	122.97	118.30
1	D	172	PRO	CA-N-CD	5.19	118.96	111.70
1	B	101	VAL	CB-CA-C	-5.18	101.55	111.40
1	C	212	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	89	SER	N-CA-CB	-5.15	102.77	110.50
1	L	113	ASP	CB-CG-OD2	5.14	122.92	118.30
1	J	96	ARG	CG-CD-NE	-5.09	101.11	111.80
1	K	90	THR	N-CA-CB	-5.08	100.65	110.30
1	E	101	VAL	CB-CA-C	-5.06	101.78	111.40
1	E	230	ASP	CB-CG-OD2	5.05	122.84	118.30
1	J	55	LEU	CA-CB-CG	5.04	126.88	115.30
1	M	113	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	201	ASP	CB-CG-OD2	5.02	122.82	118.30
1	L	230	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	103	ASP	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1816	54	0
1	B	1803	0	1807	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1885	0	1902	53	0
1	D	1803	0	1807	42	0
1	E	1928	0	1941	53	0
1	F	1788	0	1789	43	0
1	G	1819	0	1822	39	0
1	H	1846	0	1849	25	0
1	I	1803	0	1807	39	0
1	J	1803	0	1807	43	0
1	K	1779	0	1781	50	0
1	L	1803	0	1807	51	0
1	M	1779	0	1781	43	0
All	All	23655	0	23716	536	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 11.

All (536) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:HG3	1:C:54:ARG:HH11	1.20	1.05
1:H:34:ARG:HH11	1:H:34:ARG:HG2	1.15	1.04
1:I:178:THR:HG22	1:I:237:THR:OG1	1.58	1.02
1:B:90:THR:HG23	1:B:118:TYR:HA	1.41	0.99
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.28	0.99
1:J:90:THR:HG23	1:J:118:TYR:HA	1.42	0.98
1:H:171:ASP:HB3	1:H:172:PRO:HD3	1.47	0.97
1:J:90:THR:CG2	1:J:118:TYR:HA	1.96	0.95
1:L:193:SER:HB2	1:L:195:GLN:NE2	1.80	0.95
1:B:34:ARG:O	1:B:175:VAL:O	1.85	0.95
1:A:226:GLU:HG2	1:A:238:ILE:HA	1.49	0.93
1:I:218:LEU:O	1:I:219:GLU:HB3	1.66	0.93
1:B:175:VAL:O	1:B:176:ASP:HB2	1.68	0.92
1:E:90:THR:HG23	1:E:118:TYR:HA	1.51	0.92
1:F:96:ARG:NH2	1:G:109:GLN:OE1	2.02	0.92
1:K:90:THR:HG23	1:K:118:TYR:HA	1.52	0.90
1:L:193:SER:HB2	1:L:195:GLN:HE21	1.35	0.90
1:F:178:THR:HG22	1:F:237:THR:OG1	1.74	0.88
1:G:206:VAL:HG21	1:G:222:LEU:HB2	1.56	0.88
1:H:109:GLN:OE1	1:I:96:ARG:NH2	2.05	0.88
1:D:90:THR:HG23	1:D:118:TYR:HA	1.55	0.87
1:L:34:ARG:O	1:L:175:VAL:O	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG22	1:D:27:LEU:HG	1.57	0.86
1:C:92:GLU:OE1	1:C:96:ARG:HD3	1.75	0.85
1:A:107:SER:H	1:A:110:GLN:HE21	1.24	0.85
1:A:54:ARG:O	1:A:68:LEU:O	1.94	0.84
1:B:218:LEU:O	1:B:219:GLU:HB3	1.77	0.83
1:L:54:ARG:O	1:L:68:LEU:O	1.96	0.83
1:K:109:GLN:OE1	1:L:96:ARG:NH2	2.12	0.83
1:B:90:THR:CG2	1:B:118:TYR:HA	2.08	0.83
1:J:137:VAL:HG11	1:J:164:MET:CE	2.10	0.82
1:L:254:PHE:H	1:L:254:PHE:HD1	1.27	0.81
1:A:191:LEU:HD11	1:A:198:ARG:HG3	1.62	0.81
1:F:34:ARG:O	1:F:175:VAL:O	1.99	0.80
1:E:144:ARG:HH11	1:E:144:ARG:HB2	1.45	0.80
1:E:218:LEU:O	1:E:219:GLU:HB3	1.81	0.80
1:K:193:SER:O	1:K:195:GLN:N	2.15	0.80
1:H:34:ARG:NH1	1:H:34:ARG:HG2	1.90	0.79
1:L:109:GLN:OE1	1:M:96:ARG:NH2	2.15	0.79
1:K:171:ASP:HB3	1:K:172:PRO:HD3	1.64	0.79
1:A:96:ARG:NH2	1:B:109:GLN:OE1	2.16	0.78
1:J:38:PHE:HB2	1:J:172:PRO:O	1.82	0.78
1:L:226:GLU:CD	1:L:226:GLU:H	1.87	0.78
1:A:34:ARG:HE	1:A:254:PHE:HE2	1.33	0.77
1:K:175:VAL:HG22	1:K:240:ALA:HB3	1.64	0.77
1:M:171:ASP:HB3	1:M:172:PRO:HD3	1.66	0.77
1:E:90:THR:CG2	1:E:118:TYR:HA	2.14	0.76
1:F:137:VAL:HG11	1:F:164:MET:HE3	1.67	0.76
1:B:96:ARG:NH2	1:C:109:GLN:OE1	2.19	0.76
1:E:26:THR:O	1:E:262:GLY:O	2.04	0.76
1:H:171:ASP:HB3	1:H:172:PRO:CD	2.15	0.75
1:K:54:ARG:O	1:K:68:LEU:O	2.03	0.75
1:F:250:LEU:HD11	1:G:226:GLU:HG2	1.68	0.75
1:D:218:LEU:O	1:D:219:GLU:HB3	1.86	0.75
1:K:86:ASN:O	1:K:90:THR:HB	1.87	0.75
1:B:147:ARG:NH2	1:C:176:ASP:OD2	2.19	0.75
1:J:246:ASN:HB2	1:J:248:GLU:HG2	1.69	0.75
1:F:171:ASP:HB3	1:F:172:PRO:HD3	1.69	0.74
1:K:229:VAL:HG12	1:K:236:VAL:HG22	1.69	0.74
1:G:107:SER:H	1:G:110:GLN:HE21	1.35	0.74
1:E:107:SER:H	1:E:110:GLN:HE21	1.34	0.74
1:C:54:ARG:NH1	1:C:54:ARG:HG3	1.99	0.74
1:B:92:GLU:OE1	1:B:96:ARG:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:CG2	1:A:240:ALA:HB3	2.17	0.73
1:K:90:THR:CG2	1:K:118:TYR:HA	2.19	0.73
1:B:171:ASP:O	1:B:244:ASN:HB3	1.89	0.72
1:D:54:ARG:O	1:D:68:LEU:O	2.07	0.72
1:D:107:SER:H	1:D:110:GLN:HE21	1.37	0.72
1:J:107:SER:H	1:J:110:GLN:HE21	1.37	0.72
1:E:96:ARG:NH2	1:F:109:GLN:OE1	2.21	0.72
1:I:239:ARG:NH2	1:J:147:ARG:HH12	1.87	0.72
1:C:107:SER:H	1:C:110:GLN:HE21	1.37	0.72
1:A:107:SER:H	1:A:110:GLN:NE2	1.88	0.71
1:B:54:ARG:O	1:B:68:LEU:O	2.09	0.71
1:L:175:VAL:O	1:L:176:ASP:HB2	1.90	0.71
1:E:250:LEU:HD11	1:F:226:GLU:HG2	1.71	0.71
1:B:215:GLN:NE2	1:B:258:GLN:HE22	1.88	0.71
1:A:171:ASP:HB3	1:A:172:PRO:HD3	1.73	0.71
1:F:137:VAL:HG11	1:F:164:MET:CE	2.22	0.70
1:M:90:THR:HG23	1:M:118:TYR:HA	1.71	0.70
1:G:54:ARG:O	1:G:68:LEU:O	2.10	0.70
1:J:199:ALA:HB2	1:J:205:LYS:HG2	1.72	0.69
1:I:54:ARG:O	1:I:68:LEU:O	2.10	0.69
1:B:171:ASP:HB3	1:B:172:PRO:HD3	1.73	0.69
1:I:171:ASP:O	1:I:172:PRO:C	2.29	0.69
1:J:137:VAL:HG11	1:J:164:MET:HE3	1.75	0.69
1:C:215:GLN:HE22	1:C:258:GLN:HE22	1.38	0.69
1:D:178:THR:HG22	1:D:237:THR:OG1	1.94	0.68
1:K:77:GLU:O	1:K:81:GLN:HG2	1.92	0.68
1:G:91:GLN:O	1:G:95:GLN:HG3	1.92	0.68
1:A:175:VAL:HG22	1:A:240:ALA:HB3	1.75	0.68
1:J:54:ARG:O	1:J:68:LEU:O	2.12	0.68
1:K:210:LEU:HB2	1:K:212:ASP:OD1	1.94	0.68
1:A:129:ARG:NH2	1:A:130:ILE:HD11	2.09	0.67
1:C:54:ARG:CG	1:C:54:ARG:HH11	2.01	0.67
1:B:175:VAL:HG22	1:B:240:ALA:HB3	1.75	0.67
1:I:171:ASP:O	1:I:244:ASN:HB3	1.95	0.67
1:F:147:ARG:NH2	1:G:176:ASP:OD2	2.25	0.67
1:C:171:ASP:HB3	1:C:172:PRO:HD3	1.75	0.67
1:G:107:SER:H	1:G:110:GLN:NE2	1.90	0.67
1:A:206:VAL:HG12	1:A:207:SER:H	1.60	0.67
1:L:199:ALA:HB2	1:L:205:LYS:HG2	1.76	0.67
1:E:212:ASP:O	1:E:214:SER:N	2.28	0.67
1:B:54:ARG:O	1:B:55:LEU:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:GLN:OE1	1:J:96:ARG:NH2	2.27	0.66
1:C:96:ARG:NH2	1:D:109:GLN:OE1	2.28	0.66
1:D:96:ARG:NH2	1:E:109:GLN:OE1	2.28	0.66
1:J:144:ARG:HG3	1:J:144:ARG:HH11	1.59	0.66
1:D:86:ASN:O	1:D:90:THR:HB	1.95	0.66
1:C:107:SER:H	1:C:110:GLN:NE2	1.92	0.66
1:F:216:TYR:CE2	1:F:218:LEU:HB2	2.31	0.66
1:H:27:LEU:HB2	1:H:262:GLY:O	1.95	0.66
1:C:215:GLN:NE2	1:C:258:GLN:HE22	1.94	0.66
1:D:218:LEU:O	1:D:219:GLU:CB	2.43	0.66
1:C:54:ARG:O	1:C:68:LEU:O	2.15	0.65
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.07	0.65
1:G:90:THR:HG23	1:G:118:TYR:HA	1.78	0.65
1:K:171:ASP:HB3	1:K:172:PRO:CD	2.25	0.65
1:J:144:ARG:HG3	1:J:144:ARG:NH1	2.12	0.65
1:E:107:SER:H	1:E:110:GLN:NE2	1.94	0.65
1:L:54:ARG:HD2	1:L:148:SER:HB2	1.78	0.65
1:I:226:GLU:HG2	1:J:250:LEU:HD11	1.77	0.65
1:K:40:ILE:HG12	1:K:168:GLN:HG2	1.79	0.64
1:J:90:THR:HG23	1:J:118:TYR:CA	2.22	0.64
1:J:198:ARG:HH21	1:J:202:ASN:H	1.44	0.64
1:G:198:ARG:HG3	1:G:200:GLY:H	1.62	0.64
1:A:54:ARG:O	1:A:55:LEU:HB2	1.98	0.64
1:F:218:LEU:O	1:F:219:GLU:HB3	1.97	0.64
1:L:91:GLN:HG2	1:L:95:GLN:NE2	2.13	0.64
1:L:254:PHE:CD1	1:L:254:PHE:N	2.66	0.64
1:J:171:ASP:HB3	1:J:172:PRO:CD	2.28	0.63
1:E:216:TYR:CE2	1:E:218:LEU:HB2	2.33	0.63
1:F:175:VAL:O	1:F:176:ASP:HB2	1.97	0.63
1:A:92:GLU:OE1	1:A:96:ARG:HD3	1.99	0.63
1:K:215:GLN:HE22	1:K:258:GLN:HE22	1.45	0.63
1:J:54:ARG:O	1:J:55:LEU:HB2	1.99	0.63
1:E:171:ASP:HB3	1:E:172:PRO:HD3	1.79	0.63
1:I:215:GLN:NE2	1:I:258:GLN:HE22	1.97	0.63
1:C:215:GLN:HE22	1:C:258:GLN:NE2	1.97	0.63
1:D:90:THR:CG2	1:D:118:TYR:HA	2.27	0.62
1:F:171:ASP:O	1:F:172:PRO:C	2.35	0.62
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.07	0.62
1:M:175:VAL:CG2	1:M:240:ALA:HB3	2.30	0.62
1:L:58:GLU:HG2	1:L:147:ARG:HA	1.82	0.62
1:A:186:ARG:O	1:A:190:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:VAL:HG21	1:F:239:ARG:HG2	1.81	0.62
1:D:171:ASP:O	1:D:244:ASN:HB3	1.99	0.61
1:J:107:SER:H	1:J:110:GLN:NE2	1.98	0.61
1:E:86:ASN:O	1:E:90:THR:HB	2.00	0.61
1:J:137:VAL:HG11	1:J:164:MET:HE1	1.82	0.61
1:B:107:SER:H	1:B:110:GLN:NE2	1.97	0.61
1:G:27:LEU:HB2	1:G:261:GLU:HB3	1.82	0.61
1:J:178:THR:HG22	1:J:237:THR:OG1	2.01	0.61
1:K:137:VAL:HG11	1:K:164:MET:HE3	1.82	0.61
1:E:90:THR:HG23	1:E:118:TYR:CA	2.29	0.60
1:A:218:LEU:HD13	1:A:243:PRO:HB2	1.83	0.60
1:L:206:VAL:CG1	1:L:207:SER:N	2.64	0.60
1:M:51:ILE:HD11	1:M:156:VAL:CG1	2.32	0.60
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.65	0.60
1:C:199:ALA:O	1:C:203:ALA:HB3	2.01	0.60
1:M:92:GLU:HA	1:M:95:GLN:HE21	1.67	0.60
1:G:171:ASP:HB3	1:G:172:PRO:HD3	1.84	0.60
1:I:107:SER:H	1:I:110:GLN:HE21	1.49	0.60
1:I:211:GLU:HG2	1:I:254:PHE:O	2.02	0.60
1:D:171:ASP:C	1:D:171:ASP:OD1	2.39	0.60
1:M:175:VAL:HG22	1:M:240:ALA:HB3	1.82	0.60
1:E:126:GLU:OE2	1:E:129:ARG:NH2	2.32	0.60
1:F:170:LEU:O	1:F:171:ASP:O	2.19	0.59
1:I:227:VAL:HG12	1:J:147:ARG:HG3	1.82	0.59
1:D:107:SER:H	1:D:110:GLN:NE2	1.99	0.59
1:H:144:ARG:HH11	1:H:144:ARG:HG3	1.67	0.59
1:B:215:GLN:HE22	1:B:258:GLN:HE22	1.51	0.59
1:M:28:ASN:HA	1:M:259:LEU:HB2	1.82	0.59
1:C:137:VAL:HG11	1:C:164:MET:HE3	1.85	0.59
1:K:90:THR:HG21	1:K:121:SER:OG	2.03	0.59
1:E:54:ARG:O	1:E:56:PHE:N	2.35	0.59
1:B:218:LEU:O	1:B:219:GLU:CB	2.48	0.58
1:E:92:GLU:OE1	1:E:96:ARG:HD3	2.03	0.58
1:L:191:LEU:HG	1:L:198:ARG:HH21	1.68	0.58
1:J:109:GLN:OE1	1:K:96:ARG:NH2	2.36	0.58
1:B:175:VAL:O	1:B:176:ASP:CB	2.40	0.58
1:D:90:THR:HG21	1:D:121:SER:OG	2.03	0.58
1:A:40:ILE:HG12	1:A:168:GLN:HG2	1.85	0.58
1:L:52:LEU:HD22	1:L:72:ASP:HA	1.85	0.58
1:H:216:TYR:CE2	1:H:218:LEU:HB2	2.39	0.58
1:E:86:ASN:ND2	1:E:121:SER:OG	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:ARG:O	1:K:55:LEU:HB2	2.03	0.58
1:G:90:THR:CG2	1:G:118:TYR:HA	2.34	0.58
1:D:215:GLN:HE22	1:D:258:GLN:HE22	1.51	0.58
1:M:90:THR:CG2	1:M:118:TYR:HA	2.32	0.58
1:K:239:ARG:NH2	1:L:147:ARG:HH21	2.01	0.58
1:E:171:ASP:O	1:E:172:PRO:C	2.41	0.57
1:J:86:ASN:O	1:J:90:THR:HB	2.05	0.57
1:B:209:LYS:HE3	1:B:258:GLN:HE21	1.69	0.57
1:K:51:ILE:HD13	1:K:150:VAL:CG1	2.34	0.57
1:M:137:VAL:HG11	1:M:164:MET:HE1	1.86	0.57
1:A:144:ARG:HH22	1:B:225:SER:HB3	1.69	0.57
1:J:193:SER:OG	1:J:195:GLN:HG3	2.05	0.57
1:L:196:LEU:HD11	1:L:259:LEU:HD11	1.87	0.57
1:B:107:SER:H	1:B:110:GLN:HE21	1.53	0.57
1:K:189:ARG:HG2	1:K:189:ARG:HH11	1.69	0.57
1:B:90:THR:HG23	1:B:118:TYR:CA	2.27	0.57
1:K:41:ALA:HB1	1:K:140:PRO:HG2	1.86	0.57
1:C:216:TYR:CE2	1:C:218:LEU:HB2	2.40	0.57
1:D:80:TYR:O	1:D:84:GLN:HG3	2.05	0.56
1:F:101:VAL:CG1	1:F:106:VAL:HG12	2.34	0.56
1:L:206:VAL:HG12	1:L:207:SER:N	2.20	0.56
1:L:101:VAL:HG13	1:L:106:VAL:HG12	1.87	0.56
1:E:246:ASN:O	1:E:248:GLU:N	2.33	0.56
1:C:189:ARG:HH11	1:C:189:ARG:CG	2.17	0.56
1:A:38:PHE:HB2	1:A:172:PRO:O	2.06	0.56
1:L:171:ASP:HB3	1:L:172:PRO:HD3	1.87	0.56
1:B:90:THR:HG21	1:B:121:SER:OG	2.05	0.55
1:C:189:ARG:HH11	1:C:189:ARG:HG2	1.71	0.55
1:C:171:ASP:O	1:C:244:ASN:HB3	2.06	0.55
1:K:175:VAL:CG2	1:K:240:ALA:HB3	2.35	0.55
1:I:184:LEU:O	1:I:188:ARG:HG3	2.07	0.55
1:M:137:VAL:HG11	1:M:164:MET:CE	2.37	0.54
1:M:230:ASP:O	1:M:235:SER:HA	2.07	0.54
1:M:38:PHE:CD1	1:M:172:PRO:HB2	2.42	0.54
1:J:199:ALA:O	1:J:203:ALA:HB3	2.08	0.54
1:C:34:ARG:HA	1:C:253:MET:O	2.07	0.54
1:G:209:LYS:HB2	1:G:258:GLN:NE2	2.23	0.54
1:E:26:THR:HA	1:E:263:VAL:HG12	1.90	0.54
1:B:216:TYR:CE2	1:B:218:LEU:HB2	2.42	0.54
1:F:96:ARG:HH22	1:G:109:GLN:CD	2.06	0.54
1:B:86:ASN:O	1:B:90:THR:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:VAL:HG11	1:I:257:ALA:HB1	1.90	0.54
1:H:34:ARG:HH11	1:H:34:ARG:CG	2.05	0.54
1:J:90:THR:HG21	1:J:121:SER:OG	2.07	0.54
1:K:31:LEU:HB2	1:K:257:ALA:HB3	1.90	0.54
1:A:35:THR:OG1	1:A:253:MET:HB2	2.08	0.54
1:F:171:ASP:HB3	1:F:172:PRO:CD	2.37	0.53
1:E:57:LYS:O	1:E:60:SER:OG	2.23	0.53
1:E:219:GLU:HA	1:E:242:PHE:HE2	1.72	0.53
1:H:86:ASN:ND2	1:H:121:SER:OG	2.41	0.53
1:A:206:VAL:O	1:A:219:GLU:HG3	2.08	0.53
1:G:169:GLN:HE21	1:G:172:PRO:HD2	1.72	0.53
1:B:171:ASP:HB3	1:B:172:PRO:CD	2.39	0.53
1:H:218:LEU:O	1:H:219:GLU:CB	2.57	0.53
1:F:218:LEU:O	1:F:219:GLU:CB	2.55	0.53
1:M:200:GLY:HA3	1:M:221:ARG:HH12	1.73	0.53
1:L:36:ASN:HB3	1:L:174:TYR:HB2	1.90	0.53
1:M:35:THR:HA	1:M:175:VAL:HA	1.91	0.53
1:L:208:LEU:HB2	1:L:242:PHE:CE2	2.42	0.53
1:L:209:LYS:HB2	1:L:258:GLN:NE2	2.24	0.53
1:L:41:ALA:HB1	1:L:140:PRO:HG2	1.90	0.53
1:F:194:GLY:C	1:F:196:LEU:H	2.12	0.53
1:C:171:ASP:C	1:C:171:ASP:OD1	2.48	0.53
1:M:91:GLN:O	1:M:95:GLN:HG3	2.09	0.53
1:J:206:VAL:HG12	1:J:207:SER:N	2.24	0.53
1:E:34:ARG:NH2	1:E:254:PHE:CZ	2.77	0.53
1:M:222:LEU:HD11	1:M:238:ILE:HD12	1.90	0.53
1:I:126:GLU:OE2	1:I:129:ARG:NH2	2.41	0.53
1:I:107:SER:H	1:I:110:GLN:NE2	2.06	0.52
1:G:104:GLN:HB2	1:M:108:LYS:HD3	1.90	0.52
1:F:221:ARG:O	1:F:240:ALA:HA	2.09	0.52
1:I:239:ARG:HH22	1:J:147:ARG:HH12	1.57	0.52
1:B:215:GLN:HE22	1:B:258:GLN:NE2	2.07	0.52
1:I:209:LYS:HB2	1:I:258:GLN:NE2	2.24	0.52
1:K:171:ASP:CB	1:K:172:PRO:HD3	2.36	0.52
1:F:101:VAL:HG12	1:F:106:VAL:HG12	1.90	0.52
1:G:91:GLN:HG2	1:G:95:GLN:HE21	1.76	0.51
1:H:38:PHE:HB2	1:H:172:PRO:O	2.09	0.51
1:M:199:ALA:HB2	1:M:205:LYS:HG3	1.91	0.51
1:C:137:VAL:HG11	1:C:164:MET:CE	2.41	0.51
1:D:250:LEU:HD11	1:E:226:GLU:HG2	1.93	0.51
1:F:171:ASP:O	1:F:244:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:ALA:HB2	1:I:205:LYS:N	2.26	0.51
1:A:129:ARG:NH2	1:A:130:ILE:CD1	2.73	0.51
1:C:171:ASP:HB3	1:C:172:PRO:CD	2.41	0.51
1:E:171:ASP:HB3	1:E:172:PRO:CD	2.41	0.51
1:C:126:GLU:OE2	1:C:129:ARG:NH2	2.43	0.51
1:F:206:VAL:HG12	1:F:242:PHE:HZ	1.74	0.51
1:J:222:LEU:HD11	1:J:238:ILE:HD12	1.92	0.51
1:H:171:ASP:O	1:H:244:ASN:HB3	2.12	0.50
1:K:137:VAL:HG11	1:K:164:MET:CE	2.41	0.50
1:F:209:LYS:HB2	1:F:258:GLN:NE2	2.26	0.50
1:M:171:ASP:CB	1:M:172:PRO:HD3	2.38	0.50
1:F:206:VAL:CG1	1:F:207:SER:N	2.75	0.50
1:M:210:LEU:HD12	1:M:214:SER:HB2	1.93	0.50
1:K:90:THR:HG23	1:K:118:TYR:CA	2.35	0.50
1:I:101:VAL:HG13	1:I:106:VAL:HG23	1.93	0.50
1:H:218:LEU:O	1:H:219:GLU:HB3	2.12	0.50
1:A:206:VAL:HG21	1:A:222:LEU:HB2	1.93	0.50
1:K:31:LEU:HD21	1:K:179:GLN:NE2	2.27	0.50
1:A:30:GLU:HG2	1:A:258:GLN:HG2	1.92	0.50
1:A:209:LYS:HB2	1:A:258:GLN:NE2	2.26	0.50
1:L:226:GLU:HB3	1:L:236:VAL:CG1	2.42	0.50
1:F:250:LEU:CD1	1:G:226:GLU:HG2	2.38	0.50
1:H:144:ARG:CG	1:H:144:ARG:HH11	2.23	0.50
1:E:221:ARG:O	1:E:240:ALA:HA	2.12	0.50
1:L:44:ARG:HH11	1:L:44:ARG:HG2	1.77	0.50
1:L:150:VAL:HG21	1:L:164:MET:HG2	1.94	0.50
1:I:171:ASP:O	1:I:173:ILE:N	2.45	0.50
1:K:206:VAL:HG13	1:K:258:GLN:H	1.77	0.49
1:G:107:SER:OG	1:G:110:GLN:HG3	2.13	0.49
1:I:54:ARG:HD2	1:I:148:SER:HB2	1.93	0.49
1:A:206:VAL:HG11	1:A:257:ALA:HB1	1.93	0.49
1:M:226:GLU:HA	1:M:238:ILE:HG22	1.94	0.49
1:C:80:TYR:O	1:C:84:GLN:HG3	2.13	0.49
1:F:99:LEU:O	1:F:102:ALA:HB3	2.12	0.49
1:J:171:ASP:HB3	1:J:172:PRO:HD3	1.94	0.49
1:G:86:ASN:O	1:G:90:THR:HB	2.12	0.49
1:D:215:GLN:HE22	1:D:258:GLN:NE2	2.10	0.49
1:K:186:ARG:O	1:K:190:GLU:HG3	2.12	0.49
1:L:137:VAL:HG11	1:L:164:MET:HE3	1.95	0.49
1:I:137:VAL:HG11	1:I:164:MET:HE3	1.95	0.49
1:B:247:ASN:H	1:C:188:ARG:HH12	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:174:TYR:CD2	1:L:239:ARG:HD2	2.47	0.49
1:C:171:ASP:O	1:C:244:ASN:N	2.45	0.49
1:E:171:ASP:O	1:E:244:ASN:HB3	2.13	0.49
1:K:51:ILE:CD1	1:K:150:VAL:HG11	2.43	0.49
1:A:129:ARG:HH22	1:A:130:ILE:HD11	1.77	0.49
1:D:171:ASP:O	1:D:172:PRO:C	2.49	0.49
1:G:195:GLN:HG2	1:G:261:GLU:CD	2.34	0.49
1:M:210:LEU:HA	1:M:255:VAL:HG12	1.95	0.48
1:F:171:ASP:CB	1:F:172:PRO:HD3	2.42	0.48
1:C:206:VAL:O	1:C:219:GLU:HB2	2.13	0.48
1:K:183:ALA:O	1:K:187:LEU:HG	2.14	0.48
1:H:51:ILE:HG13	1:H:150:VAL:CG1	2.43	0.48
1:A:38:PHE:CD1	1:A:172:PRO:HB2	2.48	0.48
1:D:147:ARG:HH11	1:E:227:VAL:HG23	1.78	0.48
1:K:39:ARG:HG2	1:K:39:ARG:HH11	1.77	0.48
1:M:46:GLN:HB2	1:M:134:TYR:CD1	2.49	0.48
1:B:144:ARG:NE	1:C:226:GLU:OE1	2.46	0.48
1:M:51:ILE:HD11	1:M:156:VAL:HG11	1.95	0.48
1:G:99:LEU:O	1:G:102:ALA:HB3	2.13	0.48
1:K:171:ASP:CB	1:K:172:PRO:CD	2.92	0.48
1:E:212:ASP:C	1:E:214:SER:H	2.16	0.48
1:M:54:ARG:HG3	1:M:69:TYR:CE2	2.49	0.48
1:E:107:SER:N	1:E:110:GLN:HE21	2.07	0.48
1:E:170:LEU:O	1:E:171:ASP:O	2.31	0.48
1:E:38:PHE:HB2	1:E:172:PRO:O	2.14	0.48
1:F:229:VAL:HG13	1:F:236:VAL:HG22	1.95	0.48
1:I:108:LYS:HD3	1:J:96:ARG:HD2	1.95	0.48
1:K:92:GLU:OE1	1:K:96:ARG:HD3	2.14	0.48
1:A:212:ASP:OD2	1:B:189:ARG:NH2	2.46	0.48
1:C:54:ARG:CG	1:C:54:ARG:NH1	2.66	0.47
1:L:108:LYS:HB3	1:M:96:ARG:HD2	1.97	0.47
1:J:92:GLU:OE1	1:J:96:ARG:HD3	2.15	0.47
1:M:230:ASP:C	1:M:232:GLY:H	2.18	0.47
1:C:186:ARG:NH2	1:C:261:GLU:OE2	2.47	0.47
1:E:189:ARG:HG2	1:E:189:ARG:HH11	1.79	0.47
1:G:216:TYR:CE2	1:G:218:LEU:HB2	2.49	0.47
1:C:171:ASP:O	1:C:244:ASN:CB	2.62	0.47
1:D:231:GLU:OE1	1:D:231:GLU:N	2.48	0.47
1:M:38:PHE:HB2	1:M:172:PRO:O	2.14	0.47
1:C:54:ARG:O	1:C:55:LEU:HB2	2.14	0.47
1:B:209:LYS:HE3	1:B:258:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:TYR:HE2	1:H:218:LEU:HB2	1.78	0.47
1:J:206:VAL:CG1	1:J:207:SER:N	2.78	0.47
1:M:93:GLN:O	1:M:93:GLN:HG3	2.14	0.47
1:J:54:ARG:O	1:J:55:LEU:CB	2.60	0.47
1:A:61:ASP:OD1	1:A:144:ARG:HD2	2.15	0.47
1:K:199:ALA:HB2	1:K:205:LYS:HG3	1.97	0.47
1:M:40:ILE:HG12	1:M:168:GLN:HG2	1.97	0.47
1:E:31:LEU:HD22	1:E:177:VAL:HG11	1.97	0.47
1:L:92:GLU:OE1	1:L:96:ARG:HD3	2.14	0.47
1:C:218:LEU:O	1:C:219:GLU:HG2	2.15	0.47
1:M:47:VAL:HG12	1:M:71:ILE:HD13	1.97	0.47
1:E:171:ASP:O	1:E:173:ILE:N	2.48	0.46
1:A:208:LEU:HB3	1:A:216:TYR:HB3	1.98	0.46
1:H:51:ILE:HG13	1:H:150:VAL:HG11	1.96	0.46
1:A:86:ASN:HD21	1:A:121:SER:HB2	1.80	0.46
1:E:23:GLN:N	1:E:267:ALA:O	2.49	0.46
1:B:227:VAL:HG21	1:B:239:ARG:HD2	1.97	0.46
1:J:200:GLY:HA3	1:J:221:ARG:HH21	1.80	0.46
1:I:239:ARG:NH2	1:J:147:ARG:NH1	2.61	0.46
1:D:206:VAL:HG21	1:D:257:ALA:HB1	1.97	0.46
1:K:209:LYS:HE2	1:K:213:GLY:HA2	1.98	0.46
1:E:230:ASP:HB3	1:E:233:THR:O	2.16	0.46
1:C:209:LYS:HB2	1:C:258:GLN:NE2	2.31	0.46
1:L:40:ILE:HG12	1:L:168:GLN:HG2	1.97	0.46
1:A:46:GLN:HB2	1:A:134:TYR:CD1	2.50	0.46
1:H:254:PHE:N	1:H:254:PHE:CD1	2.83	0.46
1:A:189:ARG:NH1	1:A:189:ARG:CG	2.71	0.46
1:I:54:ARG:O	1:I:55:LEU:HB2	2.15	0.46
1:F:197:GLU:HG3	1:F:260:GLN:NE2	2.30	0.46
1:M:218:LEU:O	1:M:219:GLU:HG2	2.16	0.46
1:I:60:SER:O	1:I:145:ILE:HG22	2.16	0.46
1:B:171:ASP:O	1:B:172:PRO:C	2.50	0.46
1:D:54:ARG:O	1:D:55:LEU:CB	2.62	0.46
1:E:246:ASN:C	1:E:248:GLU:H	2.16	0.46
1:L:106:VAL:HG13	1:L:110:GLN:HB2	1.98	0.45
1:C:181:SER:HB3	1:C:236:VAL:CG2	2.46	0.45
1:J:209:LYS:HB2	1:J:258:GLN:NE2	2.31	0.45
1:D:250:LEU:CD1	1:E:226:GLU:HG2	2.47	0.45
1:I:218:LEU:O	1:I:219:GLU:CB	2.39	0.45
1:M:107:SER:H	1:M:110:GLN:HE21	1.64	0.45
1:G:144:ARG:NH2	1:G:247:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:THR:N	1:L:259:LEU:O	2.48	0.45
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.86	0.45
1:H:221:ARG:O	1:H:240:ALA:HA	2.17	0.45
1:C:250:LEU:HD11	1:D:226:GLU:HG2	1.99	0.45
1:D:144:ARG:HH21	1:E:225:SER:HB2	1.80	0.45
1:L:54:ARG:O	1:L:55:LEU:HB2	2.15	0.45
1:E:96:ARG:HD2	1:F:108:LYS:HD3	1.98	0.45
1:C:33:GLY:HA3	1:C:176:ASP:O	2.17	0.45
1:E:54:ARG:HG2	1:E:54:ARG:O	2.17	0.45
1:K:179:GLN:HE22	1:K:187:LEU:HD11	1.82	0.45
1:B:211:GLU:HB3	1:C:182:THR:HG21	1.98	0.45
1:I:137:VAL:HG11	1:I:164:MET:CE	2.47	0.45
1:G:221:ARG:O	1:G:240:ALA:HA	2.17	0.45
1:I:170:LEU:O	1:I:171:ASP:O	2.34	0.45
1:D:215:GLN:NE2	1:D:258:GLN:HE22	2.13	0.45
1:L:31:LEU:HD22	1:L:179:GLN:NE2	2.31	0.45
1:A:190:GLU:HB3	1:A:195:GLN:HB2	1.98	0.45
1:D:171:ASP:O	1:D:244:ASN:CB	2.65	0.44
1:I:206:VAL:CG1	1:I:207:SER:N	2.80	0.44
1:M:226:GLU:OE2	1:M:236:VAL:HG22	2.17	0.44
1:K:208:LEU:HB3	1:K:216:TYR:HB3	2.00	0.44
1:C:147:ARG:HE	1:D:227:VAL:CG1	2.30	0.44
1:B:247:ASN:N	1:C:188:ARG:HH12	2.16	0.44
1:C:31:LEU:HA	1:C:32:PRO:HD2	1.88	0.44
1:C:219:GLU:HA	1:C:242:PHE:HE2	1.83	0.44
1:J:226:GLU:OE1	1:J:236:VAL:HG13	2.17	0.44
1:D:92:GLU:OE1	1:D:96:ARG:HD3	2.17	0.44
1:G:226:GLU:CD	1:G:226:GLU:H	2.19	0.44
1:K:206:VAL:CG1	1:K:207:SER:N	2.81	0.44
1:E:178:THR:HA	1:E:236:VAL:O	2.16	0.44
1:M:31:LEU:HB3	1:M:177:VAL:HG11	1.99	0.44
1:K:239:ARG:NH2	1:L:147:ARG:NH2	2.66	0.44
1:L:206:VAL:HG11	1:L:257:ALA:HB1	2.00	0.44
1:A:206:VAL:HG12	1:A:207:SER:N	2.32	0.43
1:D:208:LEU:HB2	1:D:242:PHE:CZ	2.53	0.43
1:G:207:SER:HB3	1:G:258:GLN:OE1	2.18	0.43
1:E:221:ARG:NE	1:E:223:GLU:OE2	2.35	0.43
1:G:230:ASP:O	1:G:233:THR:O	2.36	0.43
1:A:54:ARG:O	1:A:55:LEU:CB	2.57	0.43
1:E:250:LEU:CD1	1:F:226:GLU:HG2	2.44	0.43
1:A:144:ARG:NE	1:B:226:GLU:OE2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:ARG:NH1	1:L:44:ARG:HG2	2.33	0.43
1:I:92:GLU:OE2	1:I:96:ARG:NH1	2.51	0.43
1:B:171:ASP:CB	1:B:172:PRO:HD3	2.43	0.43
1:G:169:GLN:HE21	1:G:172:PRO:CD	2.31	0.43
1:C:230:ASP:O	1:C:234:GLY:HA2	2.18	0.43
1:B:91:GLN:O	1:B:95:GLN:HG3	2.18	0.43
1:G:246:ASN:O	1:G:248:GLU:N	2.42	0.43
1:M:106:VAL:HG13	1:M:110:GLN:HB2	2.00	0.43
1:A:174:TYR:CD1	1:A:239:ARG:NH1	2.86	0.43
1:L:226:GLU:N	1:L:226:GLU:CD	2.62	0.43
1:G:233:THR:OG1	1:G:235:SER:HB2	2.18	0.43
1:C:205:LYS:HE3	1:C:219:GLU:OE1	2.19	0.43
1:I:34:ARG:NH2	1:I:252:GLY:O	2.51	0.43
1:A:175:VAL:HG21	1:A:240:ALA:HB3	1.96	0.43
1:B:54:ARG:O	1:B:55:LEU:CB	2.51	0.43
1:H:226:GLU:HA	1:H:238:ILE:HG22	2.00	0.43
1:I:45:PRO:HG3	1:I:156:VAL:HB	2.00	0.43
1:J:171:ASP:O	1:J:172:PRO:C	2.54	0.43
1:L:91:GLN:HG2	1:L:95:GLN:HE21	1.83	0.43
1:H:182:THR:HG21	1:I:211:GLU:HB2	2.00	0.43
1:L:52:LEU:HD12	1:L:52:LEU:HA	1.88	0.43
1:E:211:GLU:HB3	1:E:254:PHE:O	2.18	0.43
1:K:189:ARG:HH11	1:K:189:ARG:CG	2.31	0.42
1:F:101:VAL:HG13	1:F:106:VAL:HG12	2.00	0.42
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.82	0.42
1:J:171:ASP:O	1:J:173:ILE:N	2.52	0.42
1:A:171:ASP:O	1:A:244:ASN:N	2.51	0.42
1:F:196:LEU:HD11	1:F:259:LEU:HD22	2.01	0.42
1:I:44:ARG:CA	1:I:164:MET:HE2	2.49	0.42
1:G:51:ILE:HG13	1:G:150:VAL:CG1	2.49	0.42
1:H:171:ASP:O	1:H:244:ASN:CB	2.67	0.42
1:B:171:ASP:CB	1:B:172:PRO:CD	2.97	0.42
1:K:185:LEU:O	1:K:189:ARG:HG3	2.19	0.42
1:K:38:PHE:HB2	1:K:172:PRO:O	2.18	0.42
1:A:216:TYR:CE2	1:A:218:LEU:HB2	2.54	0.42
1:A:96:ARG:HH22	1:B:109:GLN:CD	2.21	0.42
1:I:54:ARG:O	1:I:55:LEU:CB	2.68	0.42
1:G:218:LEU:O	1:G:219:GLU:HB3	2.18	0.42
1:F:205:LYS:HE2	1:F:205:LYS:HB3	1.69	0.42
1:L:36:ASN:ND2	1:L:176:ASP:OD1	2.53	0.42
1:J:220:GLY:HA3	1:J:242:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:GLU:HA	1:E:242:PHE:CE2	2.54	0.42
1:K:199:ALA:HB2	1:K:205:LYS:CG	2.50	0.42
1:D:203:ALA:HA	1:D:222:LEU:O	2.19	0.42
1:B:186:ARG:O	1:B:190:GLU:HG3	2.20	0.42
1:C:144:ARG:HG3	1:C:144:ARG:NH1	2.35	0.42
1:K:233:THR:HG22	1:K:233:THR:O	2.20	0.42
1:K:177:VAL:O	1:K:237:THR:HA	2.19	0.42
1:A:171:ASP:OD2	1:A:245:PRO:HA	2.20	0.42
1:A:117:ALA:O	1:A:121:SER:HB3	2.20	0.42
1:D:199:ALA:HB2	1:D:205:LYS:N	2.35	0.42
1:F:202:ASN:OD1	1:F:224:PHE:HB2	2.19	0.42
1:A:259:LEU:HA	1:A:259:LEU:HD12	1.90	0.41
1:L:246:ASN:HB2	1:L:248:GLU:HG3	2.01	0.41
1:A:186:ARG:HG2	1:A:190:GLU:OE1	2.19	0.41
1:E:228:SER:HB3	1:E:237:THR:HB	2.02	0.41
1:L:69:TYR:HB2	1:L:137:VAL:HB	2.02	0.41
1:B:171:ASP:OD1	1:B:171:ASP:C	2.59	0.41
1:F:91:GLN:HG2	1:F:95:GLN:NE2	2.34	0.41
1:A:209:LYS:HE2	1:A:213:GLY:HA2	2.02	0.41
1:K:46:GLN:HA	1:K:158:ASN:OD1	2.20	0.41
1:G:98:LYS:HE2	1:G:98:LYS:HB3	1.68	0.41
1:M:109:GLN:HA	1:M:109:GLN:OE1	2.20	0.41
1:F:211:GLU:HG2	1:F:211:GLU:O	2.19	0.41
1:G:119:LEU:HD23	1:G:119:LEU:HA	1.85	0.41
1:D:148:SER:OG	1:D:150:VAL:O	2.37	0.41
1:M:58:GLU:HG2	1:M:147:ARG:HA	2.02	0.41
1:D:183:ALA:O	1:D:187:LEU:HG	2.21	0.41
1:B:90:THR:HG21	1:B:121:SER:CB	2.51	0.41
1:A:216:TYR:HA	1:A:217:PRO:HD3	1.84	0.41
1:G:38:PHE:HB2	1:G:172:PRO:O	2.20	0.41
1:C:44:ARG:CA	1:C:164:MET:HE2	2.51	0.41
1:L:171:ASP:HB3	1:L:172:PRO:CD	2.50	0.41
1:J:139:SER:HA	1:J:140:PRO:HD3	1.88	0.41
1:D:216:TYR:HA	1:D:217:PRO:HD3	1.91	0.41
1:C:153:GLY:O	1:D:44:ARG:HD2	2.21	0.41
1:E:153:GLY:O	1:F:44:ARG:HD2	2.20	0.41
1:D:54:ARG:HD2	1:D:148:SER:HB2	2.03	0.41
1:K:51:ILE:HD11	1:K:150:VAL:HG11	2.01	0.41
1:M:107:SER:H	1:M:110:GLN:NE2	2.19	0.41
1:D:67:GLN:HE22	1:D:70:GLN:NE2	2.19	0.41
1:H:215:GLN:OE1	1:H:258:GLN:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:216:TYR:CE2	1:L:218:LEU:HB2	2.56	0.40
1:K:169:GLN:HE21	1:K:172:PRO:HD2	1.87	0.40
1:L:199:ALA:O	1:L:203:ALA:HB3	2.21	0.40
1:G:193:SER:C	1:G:195:GLN:H	2.24	0.40
1:E:209:LYS:HB2	1:E:258:GLN:NE2	2.36	0.40
1:M:208:LEU:HB3	1:M:216:TYR:HB3	2.03	0.40
1:A:34:ARG:HG2	1:A:254:PHE:CD2	2.56	0.40
1:B:171:ASP:O	1:B:244:ASN:CB	2.65	0.40
1:C:207:SER:OG	1:C:258:GLN:OE1	2.34	0.40
1:M:175:VAL:HG21	1:M:240:ALA:HB3	2.01	0.40
1:M:43:VAL:HG12	1:M:164:MET:CE	2.51	0.40
1:H:227:VAL:HG13	1:I:147:ARG:HG3	2.03	0.40
1:D:221:ARG:O	1:D:240:ALA:HA	2.21	0.40
1:B:191:LEU:HD11	1:B:198:ARG:HG2	2.03	0.40
1:C:51:ILE:HD11	1:C:156:VAL:HG11	2.04	0.40
1:B:34:ARG:HA	1:B:253:MET:O	2.21	0.40
1:D:206:VAL:CG2	1:D:257:ALA:HB1	2.51	0.40
1:F:184:LEU:O	1:F:188:ARG:HG3	2.21	0.40
1:E:205:LYS:HE3	1:E:205:LYS:HB2	1.93	0.40
1:G:30:GLU:HA	1:G:257:ALA:O	2.22	0.40
1:C:144:ARG:HH11	1:C:144:ARG:HG3	1.87	0.40
1:L:28:ASN:HB3	1:L:260:GLN:HG2	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	235/369 (64%)	213 (91%)	19 (8%)	3 (1%)	15	21
1	B	233/369 (63%)	216 (93%)	13 (6%)	4 (2%)	11	14
1	C	244/369 (66%)	236 (97%)	5 (2%)	3 (1%)	16	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	233/369 (63%)	222 (95%)	9 (4%)	2 (1%)	21	30
1	E	250/369 (68%)	232 (93%)	10 (4%)	8 (3%)	5	4
1	F	231/369 (63%)	211 (91%)	17 (7%)	3 (1%)	15	21
1	G	235/369 (64%)	226 (96%)	7 (3%)	2 (1%)	21	30
1	H	239/369 (65%)	228 (95%)	9 (4%)	2 (1%)	24	35
1	I	233/369 (63%)	228 (98%)	2 (1%)	3 (1%)	15	21
1	J	233/369 (63%)	225 (97%)	6 (3%)	2 (1%)	21	30
1	K	230/369 (62%)	208 (90%)	18 (8%)	4 (2%)	11	14
1	L	233/369 (63%)	216 (93%)	16 (7%)	1 (0%)	39	56
1	M	230/369 (62%)	204 (89%)	19 (8%)	7 (3%)	5	4
All	All	3059/4797 (64%)	2865 (94%)	150 (5%)	44 (1%)	14	19

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	VAL
1	E	267	ALA
1	F	29	THR
1	K	194	GLY
1	A	176	ASP
1	C	200	GLY
1	C	232	GLY
1	E	55	LEU
1	E	213	GLY
1	L	232	GLY
1	M	176	ASP
1	M	231	GLU
1	M	235	SER
1	E	232	GLY
1	E	247	ASN
1	E	273	GLN
1	G	212	ASP
1	M	59	GLY
1	B	176	ASP
1	G	213	GLY
1	I	231	GLU
1	J	171	ASP
1	B	219	GLU

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Mol	Chain	Res	Type
1	C	219	GLU
1	F	171	ASP
1	F	219	GLU
1	H	219	GLU
1	I	171	ASP
1	I	219	GLU
1	K	190	GLU
1	K	219	GLU
1	M	248	GLU
1	M	253	MET
1	B	232	GLY
1	D	219	GLU
1	E	171	ASP
1	H	171	ASP
1	M	199	ALA
1	D	194	GLY
1	A	229	VAL
1	J	232	GLY
1	B	171	ASP
1	K	171	ASP
1	E	234	GLY

### 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	191/295 (65%)	174 (91%)	17 (9%)	12	18
1	B	190/295 (64%)	178 (94%)	12 (6%)	22	35
1	C	199/295 (68%)	190 (96%)	9 (4%)	34	52
1	D	190/295 (64%)	179 (94%)	11 (6%)	25	39
1	E	203/295 (69%)	184 (91%)	19 (9%)	11	16
1	F	188/295 (64%)	178 (95%)	10 (5%)	28	44
1	G	192/295 (65%)	174 (91%)	18 (9%)	11	16
1	H	195/295 (66%)	184 (94%)	11 (6%)	26	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	190/295 (64%)	176 (93%)	14 (7%)	17	26
1	J	190/295 (64%)	183 (96%)	7 (4%)	41	62
1	K	187/295 (63%)	174 (93%)	13 (7%)	19	29
1	L	190/295 (64%)	175 (92%)	15 (8%)	15	23
1	M	187/295 (63%)	173 (92%)	14 (8%)	17	26
All	All	2492/3835 (65%)	2322 (93%)	170 (7%)	20	31

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	35	THR
1	A	47	VAL
1	A	66	GLN
1	A	104	GLN
1	A	121	SER
1	A	181	SER
1	A	182	THR
1	A	185	LEU
1	A	189	ARG
1	A	206	VAL
1	A	223	GLU
1	A	225	SER
1	A	226	GLU
1	A	235	SER
1	A	246	ASN
1	A	259	LEU
1	B	27	LEU
1	B	34	ARG
1	B	81	GLN
1	B	89	SER
1	B	90	THR
1	B	93	GLN
1	B	101	VAL
1	B	185	LEU
1	B	186	ARG
1	B	193	SER
1	B	206	VAL
1	B	233	THR
1	C	24	THR

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Mol	Chain	Res	Type
1	C	39	ARG
1	C	54	ARG
1	C	206	VAL
1	C	231	GLU
1	C	235	SER
1	C	247	ASN
1	C	263	VAL
1	C	269	LEU
1	D	47	VAL
1	D	90	THR
1	D	101	VAL
1	D	106	VAL
1	D	197	GLU
1	D	219	GLU
1	D	223	GLU
1	D	226	GLU
1	D	231	GLU
1	D	233	THR
1	D	259	LEU
1	E	31	LEU
1	E	89	SER
1	E	90	THR
1	E	93	GLN
1	E	101	VAL
1	E	106	VAL
1	E	144	ARG
1	E	152	GLU
1	E	175	VAL
1	E	193	SER
1	E	198	ARG
1	E	206	VAL
1	E	219	GLU
1	E	223	GLU
1	E	226	GLU
1	E	231	GLU
1	E	246	ASN
1	E	260	GLN
1	E	272	GLN
1	F	29	THR
1	F	34	ARG
1	F	73	PRO
1	F	92	GLU

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Mol	Chain	Res	Type
1	F	106	VAL
1	F	171	ASP
1	F	185	LEU
1	F	201	ASP
1	F	239	ARG
1	F	247	ASN
1	G	25	VAL
1	G	35	THR
1	G	47	VAL
1	G	89	SER
1	G	90	THR
1	G	98	LYS
1	G	101	VAL
1	G	144	ARG
1	G	150	VAL
1	G	176	ASP
1	G	198	ARG
1	G	207	SER
1	G	212	ASP
1	G	225	SER
1	G	226	GLU
1	G	227	VAL
1	G	235	SER
1	G	261	GLU
1	H	25	VAL
1	H	34	ARG
1	H	63	LYS
1	H	89	SER
1	H	144	ARG
1	H	193	SER
1	H	209	LYS
1	H	226	GLU
1	H	227	VAL
1	H	246	ASN
1	H	254	PHE
1	I	26	THR
1	I	34	ARG
1	I	39	ARG
1	I	89	SER
1	I	92	GLU
1	I	101	VAL
1	I	197	GLU

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Mol	Chain	Res	Type
1	I	198	ARG
1	I	201	ASP
1	I	221	ARG
1	I	225	SER
1	I	226	GLU
1	I	231	GLU
1	I	239	ARG
1	J	34	ARG
1	J	89	SER
1	J	90	THR
1	J	93	GLN
1	J	239	ARG
1	J	248	GLU
1	J	260	GLN
1	K	27	LEU
1	K	39	ARG
1	K	82	SER
1	K	89	SER
1	K	90	THR
1	K	93	GLN
1	K	106	VAL
1	K	176	ASP
1	K	226	GLU
1	K	229	VAL
1	K	231	GLU
1	K	239	ARG
1	K	255	VAL
1	L	27	LEU
1	L	39	ARG
1	L	47	VAL
1	L	81	GLN
1	L	82	SER
1	L	93	GLN
1	L	101	VAL
1	L	106	VAL
1	L	126	GLU
1	L	178	THR
1	L	193	SER
1	L	226	GLU
1	L	227	VAL
1	L	239	ARG
1	L	254	PHE

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Mol	Chain	Res	Type
1	M	47	VAL
1	M	52	LEU
1	M	57	LYS
1	M	89	SER
1	M	90	THR
1	M	92	GLU
1	M	93	GLN
1	M	101	VAL
1	M	144	ARG
1	M	176	ASP
1	M	179	GLN
1	M	218	LEU
1	M	219	GLU
1	M	225	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	66	GLN
1	A	86	ASN
1	A	95	GLN
1	A	110	GLN
1	A	162	ASN
1	A	258	GLN
1	B	46	GLN
1	B	110	GLN
1	B	215	GLN
1	C	36	ASN
1	C	46	GLN
1	C	110	GLN
1	C	162	ASN
1	C	179	GLN
1	C	215	GLN
1	D	28	ASN
1	D	70	GLN
1	D	81	GLN
1	D	110	GLN
1	D	169	GLN
1	D	215	GLN
1	E	86	ASN
1	E	104	GLN

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Mol	Chain	Res	Type
1	E	110	GLN
1	E	162	ASN
1	E	215	GLN
1	F	36	ASN
1	F	81	GLN
1	F	91	GLN
1	F	95	GLN
1	F	127	GLN
1	F	131	ASN
1	F	162	ASN
1	F	260	GLN
1	G	95	GLN
1	G	110	GLN
1	G	169	GLN
1	G	247	ASN
1	G	260	GLN
1	H	36	ASN
1	H	86	ASN
1	H	120	GLN
1	H	215	GLN
1	H	256	HIS
1	I	46	GLN
1	I	104	GLN
1	I	110	GLN
1	I	120	GLN
1	I	215	GLN
1	J	36	ASN
1	J	46	GLN
1	J	104	GLN
1	J	110	GLN
1	J	162	ASN
1	J	215	GLN
1	J	258	GLN
1	J	260	GLN
1	K	120	GLN
1	K	168	GLN
1	K	179	GLN
1	K	215	GLN
1	L	36	ASN
1	L	46	GLN
1	L	95	GLN
1	L	120	GLN

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Mol	Chain	Res	Type
1	L	162	ASN
1	L	195	GLN
1	M	95	GLN
1	M	110	GLN
1	M	179	GLN
1	M	215	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	237/369 (64%)	0.42	16 (6%) 20 20	41, 73, 122, 134	0
1	B	235/369 (63%)	0.18	5 (2%) 67 66	30, 51, 97, 109	0
1	C	246/369 (66%)	0.19	9 (3%) 45 46	29, 51, 92, 110	0
1	D	235/369 (63%)	0.14	2 (0%) 85 85	32, 46, 90, 101	0
1	E	252/369 (68%)	0.29	13 (5%) 31 31	35, 56, 112, 139	0
1	F	233/369 (63%)	0.22	6 (2%) 59 58	36, 56, 99, 106	0
1	G	237/369 (64%)	0.26	13 (5%) 29 29	46, 77, 118, 139	0
1	H	241/369 (65%)	0.08	4 (1%) 73 72	50, 68, 97, 114	0
1	I	235/369 (63%)	0.16	4 (1%) 73 72	35, 52, 95, 105	0
1	J	235/369 (63%)	0.17	6 (2%) 59 58	39, 58, 120, 125	0
1	K	232/369 (62%)	0.19	4 (1%) 73 72	41, 68, 116, 128	0
1	L	235/369 (63%)	0.16	6 (2%) 59 58	45, 69, 113, 120	0
1	M	232/369 (62%)	0.73	36 (15%) 3 3	56, 88, 150, 157	0
All	All	3085/4797 (64%)	0.25	124 (4%) 42 43	29, 64, 118, 157	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	14.1
1	C	268	ILE	7.8
1	E	270	ALA	6.7
1	J	232	GLY	6.6
1	E	272	GLN	6.2
1	A	232	GLY	5.7
1	F	232	GLY	4.9
1	I	26	THR	4.7
1	G	26	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	27	LEU	4.5
1	A	27	LEU	4.4
1	E	268	ILE	4.3
1	M	233	THR	4.3
1	M	182	THR	4.3
1	E	269	LEU	4.2
1	A	26	THR	4.1
1	M	216	TYR	4.1
1	E	273	GLN	4.0
1	L	26	THR	4.0
1	M	242	PHE	3.9
1	M	232	GLY	3.9
1	M	234	GLY	3.9
1	F	185	LEU	3.9
1	A	234	GLY	3.8
1	M	191	LEU	3.8
1	M	199	ALA	3.8
1	L	232	GLY	3.7
1	E	267	ALA	3.7
1	M	235	SER	3.7
1	D	27	LEU	3.7
1	M	259	LEU	3.7
1	B	26	THR	3.7
1	A	201	ASP	3.6
1	M	230	ASP	3.6
1	G	34	ARG	3.5
1	I	231	GLU	3.4
1	C	27	LEU	3.4
1	C	25	VAL	3.4
1	G	25	VAL	3.4
1	A	199	ALA	3.3
1	G	218	LEU	3.3
1	K	191	LEU	3.3
1	M	208	LEU	3.2
1	M	218	LEU	3.2
1	E	271	PRO	3.2
1	L	27	LEU	3.2
1	K	196	LEU	3.1
1	L	254	PHE	3.1
1	M	201	ASP	3.1
1	A	218	LEU	3.0
1	F	231	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	184	LEU	3.0
1	E	232	GLY	3.0
1	J	233	THR	3.0
1	M	200	GLY	3.0
1	B	27	LEU	2.9
1	H	231	GLU	2.9
1	J	27	LEU	2.9
1	M	204	ALA	2.9
1	M	217	PRO	2.8
1	F	28	ASN	2.8
1	J	196	LEU	2.8
1	A	233	THR	2.8
1	M	231	GLU	2.8
1	D	232	GLY	2.8
1	C	232	GLY	2.7
1	M	198	ARG	2.7
1	M	29	THR	2.7
1	M	236	VAL	2.7
1	G	232	GLY	2.7
1	M	33	GLY	2.7
1	M	196	LEU	2.7
1	A	228	SER	2.6
1	C	179	GLN	2.6
1	G	28	ASN	2.6
1	G	211	GLU	2.6
1	A	195	GLN	2.6
1	M	241	VAL	2.5
1	C	269	LEU	2.5
1	M	192	ALA	2.5
1	A	231	GLU	2.5
1	L	184	LEU	2.5
1	M	187	LEU	2.5
1	A	33	GLY	2.5
1	G	27	LEU	2.5
1	M	39	ARG	2.5
1	E	266	LYS	2.4
1	C	266	LYS	2.4
1	I	232	GLY	2.4
1	B	260	GLN	2.4
1	G	215	GLN	2.4
1	M	184	LEU	2.4
1	C	187	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	229	VAL	2.3
1	G	171	ASP	2.3
1	M	211	GLU	2.3
1	M	178	THR	2.3
1	G	208	LEU	2.3
1	K	240	ALA	2.2
1	E	25	VAL	2.2
1	J	231	GLU	2.2
1	G	225	SER	2.2
1	M	226	GLU	2.2
1	L	224	PHE	2.1
1	E	24	THR	2.1
1	C	264	LYS	2.1
1	H	171	ASP	2.1
1	H	25	VAL	2.1
1	M	30	GLU	2.1
1	B	233	THR	2.1
1	F	257	ALA	2.1
1	K	216	TYR	2.1
1	A	184	LEU	2.1
1	J	187	LEU	2.1
1	H	211	GLU	2.0
1	M	57	LYS	2.0
1	A	179	GLN	2.0
1	M	197	GLU	2.0
1	E	263	VAL	2.0
1	B	195	GLN	2.0
1	E	23	GLN	2.0
1	G	248	GLU	2.0
1	M	180	PRO	2.0
1	A	224	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.