



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 07:15 am GMT

PDB ID : 2CB4  
Title : Crystal structure of the catalytic domain of the mosquitocidal toxin from *Bacillus sphaericus*, mutant E197Q  
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.  
Deposited on : 2005-12-29  
Resolution : 2.50 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.

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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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

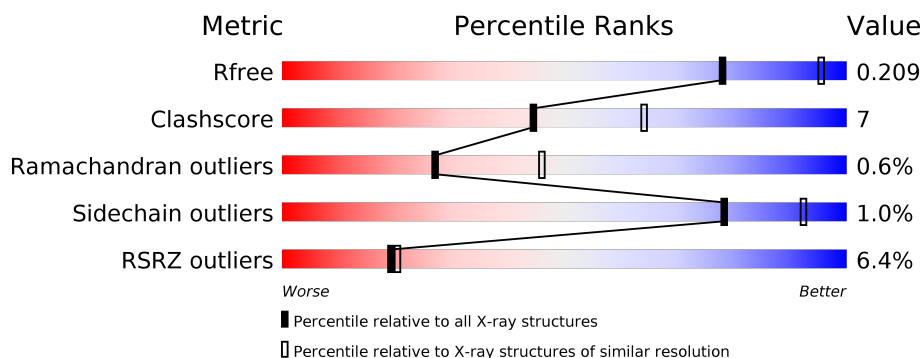
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	291	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	291	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div></div> <div>11%</div> </div> </div>
1	C	291	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	291	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	291	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div></div> <div>11%</div> </div> </div>
1	F	291	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div></div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	291	 3% 76% 12% 11%
1	H	291	 6% 73% 15% 11%
1	I	291	 6% 73% 16% 11%
1	J	291	 3% 74% 14% 11%
1	K	291	 5% 76% 13% 11%
1	L	291	 8% 75% 13% 11%
1	M	291	 6% 76% 13% 11%
1	N	291	 10% 75% 13% 11%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30680 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	B	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	C	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	D	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	E	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	F	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	G	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	H	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	I	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	J	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	K	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	L	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	M	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	N	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLN	GLU	engineered mutation	UNP Q03988

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Chain	Residue	Modelled	Actual	Comment	Reference
B	197	GLN	GLU	engineered mutation	UNP Q03988
C	197	GLN	GLU	engineered mutation	UNP Q03988
D	197	GLN	GLU	engineered mutation	UNP Q03988
E	197	GLN	GLU	engineered mutation	UNP Q03988
F	197	GLN	GLU	engineered mutation	UNP Q03988
G	197	GLN	GLU	engineered mutation	UNP Q03988
H	197	GLN	GLU	engineered mutation	UNP Q03988
I	197	GLN	GLU	engineered mutation	UNP Q03988
J	197	GLN	GLU	engineered mutation	UNP Q03988
K	197	GLN	GLU	engineered mutation	UNP Q03988
L	197	GLN	GLU	engineered mutation	UNP Q03988
M	197	GLN	GLU	engineered mutation	UNP Q03988
N	197	GLN	GLU	engineered mutation	UNP Q03988

- Molecule 2 is water.

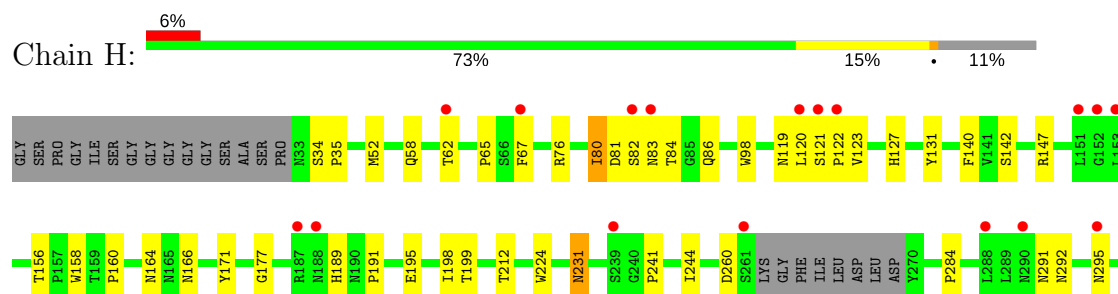
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	108	Total O 108 108	0	0
2	C	120	Total O 120 120	0	0
2	D	114	Total O 114 114	0	0
2	E	82	Total O 82 82	0	0
2	F	81	Total O 81 81	0	0
2	G	96	Total O 96 96	0	0
2	H	86	Total O 86 86	0	0
2	I	109	Total O 109 109	0	0
2	J	112	Total O 112 112	0	0
2	K	80	Total O 80 80	0	0
2	L	92	Total O 92 92	0	0
2	M	93	Total O 93 93	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	84	Total	O	0	0
			84	84		







N298  
ASN  
SER  
GLY  
TYR  
GLN  
ILE  
LYS  
ASN  
LYS

• Molecule 1: MOSQUITOCIDAL TOXIN


Chain I:  6% 73% 16% 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER SER PRO N33 S34 S35 K36 D51 M52 Q58 T62 R63 R64 P65 S66 F67 A68 R76 T84 G85 Q86 E92 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158 T159

P160 M164 N165 N166 Y171 G177 F185 S186 R187 N188 N189 N190 E195 D196 Q197 T212 W224 M231 P241 S242 N243 I244 D260 S261 LYS T84 G85 Q86 E92 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158 T159

ILE  
LYS  
ASN  
LYS

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain J:  3% 74% 14% 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY GLY GLY ALA SER PRO N33 S34 D51 M52 Q58 T62 R63 R64 P65 S66 F67 R76 N83 I87 E92 W98 N119 L120 S121 P122 V123 H127 Y131 F140 V151 S142 R147 T156 P160

M166 Y171 P176 G177 R187 Q197 I198 T199 T212 W224 N231 P232 P241 I244 D260 S261 LYS T84 G85 Q86 E92 W98 N119 L120 S121 P122 V123 H127 Y131 F140 V151 S142 R147 T156 P160


• Molecule 1: MOSQUITOCIDAL TOXIN

Chain K:  5% 76% 13% 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY GLY GLY ALA SER PRO N33 S34 S35 K36 D51 M52 Q58 T62 P65 S66 F67 R76 I80 D81 N82 N83 T84 G85 Q86 I87 Q88 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158

T159 P160 M166 N166 Y171 G177 R187 N188 E195 D196 I198 T212 W224 N231 P241 I244 D260 S261 LYS T84 G85 Q86 E92 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158

• Molecule 1: MOSQUITOCIDAL TOXIN

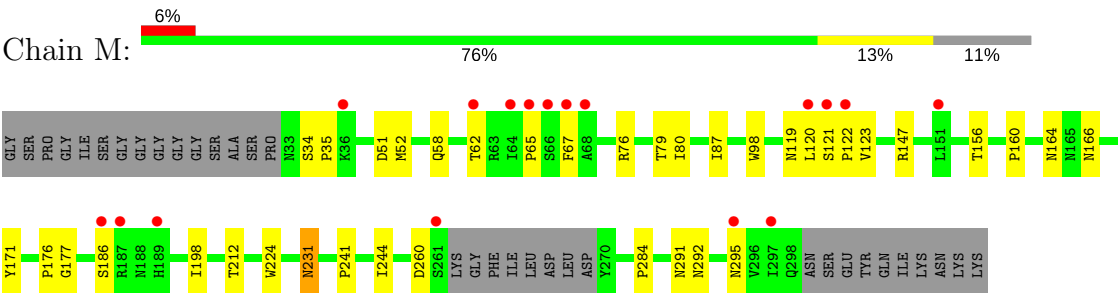
Chain L:  8% 75% 13% 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY GLY GLY ALA SER PRO N33 S34 S35 K36 D51 M52 Q58 T62 P65 S66 F67 R76 D81 S82 N83 T84 G85 Q86 I87 H93 W98 N119 L120 S121 P122 V123 H127 F140 T143 R147 Y148 N149

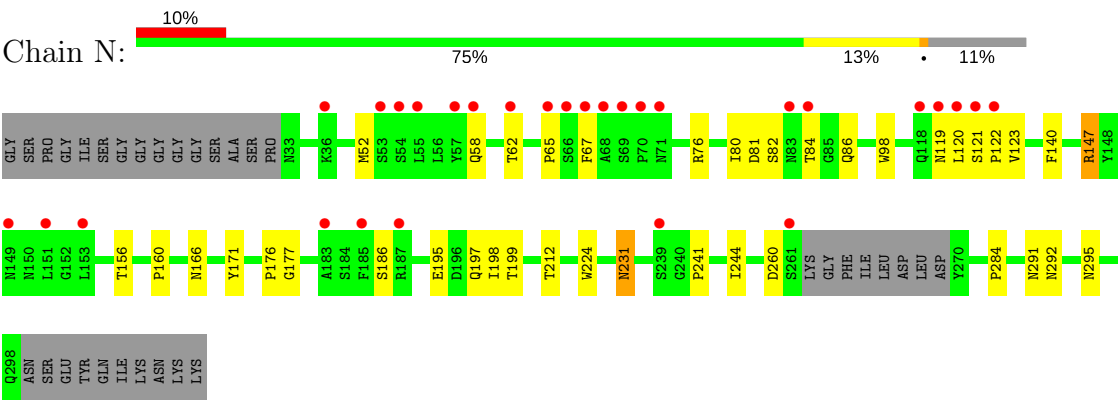
N150 L151 G152 L153 E154 I155 T156 P160 M164 N165 N166 Y171 G177 R187 Q197 I198 T199 T212 W224 N231 N236 P241 I244 D260 S261 LYS T84 G85 Q86 I87 H93 W98 N119 L120 S121 P122 V123 H127 F140 T143 R147 Y148 N149

TYR  
GLN  
ILE  
LYS  
ASN  
LYS

● Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.71Å 143.27Å 135.81Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 99.9 (49.73-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.57 (at 2.51Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, $R_{free}$	0.174 , 0.194 0.192 , 0.209	Depositor DCC
$R_{free}$ test set	8035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.70	0/2149	0.82	2/2928 (0.1%)
1	B	0.71	0/2149	0.80	1/2928 (0.0%)
1	C	0.73	0/2149	0.84	3/2928 (0.1%)
1	D	0.69	0/2149	0.80	1/2928 (0.0%)
1	E	0.71	1/2149 (0.0%)	0.81	0/2928
1	F	0.69	1/2149 (0.0%)	0.83	1/2928 (0.0%)
1	G	0.72	0/2149	0.82	1/2928 (0.0%)
1	H	0.69	0/2149	0.81	1/2928 (0.0%)
1	I	0.70	0/2149	0.82	1/2928 (0.0%)
1	J	0.72	0/2149	0.83	1/2928 (0.0%)
1	K	0.69	0/2149	0.81	1/2928 (0.0%)
1	L	0.68	0/2149	0.81	1/2928 (0.0%)
1	M	0.70	0/2149	0.81	1/2928 (0.0%)
1	N	0.69	0/2149	0.81	1/2928 (0.0%)
All	All	0.70	2/30086 (0.0%)	0.82	16/40992 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	192	PHE	CE1-CZ	5.21	1.47	1.37
1	E	92	GLU	CG-CD	5.19	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ILE	CG1-CB-CG2	-8.96	91.68	111.40
1	C	192	PHE	C-N-CD	-5.92	107.57	120.60
1	A	147	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	147	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	L	147	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	K	147	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	147	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	147	ARG	NE-CZ-NH1	5.05	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	CB-CA-C	-5.05	100.30	110.40
1	D	147	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	N	147	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	H	147	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	M	147	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	I	147	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	147	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	147	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	2095	0	1976	31	1
1	B	2095	0	1976	27	0
1	C	2095	0	1976	36	0
1	D	2095	0	1976	32	0
1	E	2095	0	1976	26	0
1	F	2095	0	1976	26	0
1	G	2095	0	1976	27	1
1	H	2095	0	1976	33	0
1	I	2095	0	1976	33	0
1	J	2095	0	1976	29	1
1	K	2095	0	1976	27	0
1	L	2095	0	1976	30	0
1	M	2095	0	1976	31	0
1	N	2095	0	1976	28	1
2	A	93	0	0	3	0
2	B	108	0	0	3	0
2	C	120	0	0	4	0
2	D	114	0	0	6	0
2	E	82	0	0	2	0
2	F	81	0	0	3	0
2	G	96	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	86	0	0	1	0
2	I	109	0	0	2	0
2	J	112	0	0	3	0
2	K	80	0	0	1	0
2	L	92	0	0	2	0
2	M	93	0	0	2	0
2	N	84	0	0	1	0
All	All	30680	0	27664	404	2

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 7.

All (404) 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:F:241:PRO:HB2	1:F:244:ILE:HD12	1.48	0.96
1:C:241:PRO:HB2	1:C:244:ILE:HD12	1.48	0.96
1:J:241:PRO:HB2	1:J:244:ILE:HD12	1.48	0.96
1:L:241:PRO:HB2	1:L:244:ILE:HD12	1.48	0.96
1:B:241:PRO:HB2	1:B:244:ILE:HD12	1.48	0.96
1:C:87:ILE:HD11	1:C:176:PRO:HD3	1.48	0.95
1:I:241:PRO:HB2	1:I:244:ILE:HD12	1.48	0.95
1:H:241:PRO:HB2	1:H:244:ILE:HD12	1.48	0.95
1:A:241:PRO:HB2	1:A:244:ILE:HD12	1.48	0.94
1:N:241:PRO:HB2	1:N:244:ILE:HD12	1.48	0.94
1:M:241:PRO:HB2	1:M:244:ILE:HD12	1.48	0.93
1:E:241:PRO:HB2	1:E:244:ILE:HD12	1.48	0.93
1:D:241:PRO:HB2	1:D:244:ILE:HD12	1.48	0.93
1:G:241:PRO:HB2	1:G:244:ILE:HD12	1.48	0.92
1:K:241:PRO:HB2	1:K:244:ILE:HD12	1.48	0.92
1:D:76:ARG:HD2	1:D:198:ILE:HG21	1.52	0.91
1:E:244:ILE:HD11	1:E:292:ASN:ND2	1.90	0.86
1:J:76:ARG:HD2	1:J:198:ILE:HG21	1.57	0.86
1:B:76:ARG:HD2	1:B:198:ILE:HG21	1.60	0.83
1:D:76:ARG:HD2	1:D:198:ILE:CG2	2.08	0.83
1:N:244:ILE:HD11	1:N:292:ASN:HD22	1.40	0.83
1:I:292:ASN:HB3	2:I:2075:HOH:O	1.79	0.81
1:A:76:ARG:HD2	1:A:198:ILE:HG21	1.63	0.79
1:B:76:ARG:HD2	1:B:198:ILE:CG2	2.12	0.79
1:C:244:ILE:HD11	1:C:292:ASN:HD22	1.47	0.79
1:H:76:ARG:HD2	1:H:198:ILE:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HD11	1:C:292:ASN:ND2	1.99	0.78
1:F:244:ILE:HD11	1:F:292:ASN:HD22	1.48	0.78
1:M:76:ARG:HD2	1:M:198:ILE:HG21	1.66	0.77
1:M:76:ARG:HD2	1:M:198:ILE:CG2	2.15	0.77
1:E:244:ILE:HD11	1:E:292:ASN:HD22	1.50	0.75
1:F:244:ILE:HD11	1:F:292:ASN:ND2	2.01	0.75
1:M:244:ILE:HD11	1:M:292:ASN:HD22	1.50	0.75
1:A:76:ARG:HD2	1:A:198:ILE:CG2	2.16	0.74
1:H:84:THR:HB	1:H:86:GLN:HG2	1.69	0.73
1:A:292:ASN:OD1	1:H:292:ASN:HB2	1.89	0.73
1:M:87:ILE:CD1	1:M:176:PRO:HD3	2.18	0.73
1:N:244:ILE:HD11	1:N:292:ASN:ND2	2.03	0.73
1:J:76:ARG:HD2	1:J:198:ILE:CG2	2.20	0.72
1:G:76:ARG:HD2	1:G:198:ILE:CG2	2.21	0.71
1:H:76:ARG:HD2	1:H:198:ILE:HG21	1.71	0.71
1:F:292:ASN:HB3	2:F:2056:HOH:O	1.91	0.70
1:C:156:THR:HG21	1:C:284:PRO:HG2	1.74	0.70
1:K:76:ARG:HD2	1:K:198:ILE:CG2	2.21	0.70
1:A:156:THR:HG21	1:A:284:PRO:HG2	1.74	0.70
1:H:81:ASP:OD1	1:H:83:ASN:HB2	1.90	0.70
1:J:244:ILE:HD11	1:J:292:ASN:HD22	1.57	0.70
1:M:156:THR:HG21	1:M:284:PRO:HG2	1.74	0.70
1:G:76:ARG:HD2	1:G:198:ILE:HG21	1.75	0.69
1:L:156:THR:HG21	1:L:284:PRO:HG2	1.74	0.69
1:H:156:THR:HG21	1:H:284:PRO:HG2	1.74	0.69
1:J:156:THR:HG21	1:J:284:PRO:HG2	1.74	0.69
1:K:156:THR:HG21	1:K:284:PRO:HG2	1.74	0.69
1:F:156:THR:HG21	1:F:284:PRO:HG2	1.74	0.69
1:N:156:THR:HG21	1:N:284:PRO:HG2	1.74	0.69
1:N:76:ARG:HD2	1:N:198:ILE:HG21	1.75	0.69
1:I:156:THR:HG21	1:I:284:PRO:HG2	1.74	0.68
1:B:156:THR:HG21	1:B:284:PRO:HG2	1.74	0.68
1:G:244:ILE:HD11	1:G:292:ASN:HD22	1.58	0.68
1:G:156:THR:HG21	1:G:284:PRO:HG2	1.74	0.68
1:E:156:THR:HG21	1:E:284:PRO:HG2	1.74	0.68
1:A:236:ASN:HB2	2:A:2066:HOH:O	1.93	0.68
1:I:76:ARG:HD2	1:I:198:ILE:CG2	2.24	0.67
1:K:76:ARG:HD2	1:K:198:ILE:HG21	1.77	0.67
1:C:87:ILE:HG12	2:C:2022:HOH:O	1.94	0.67
1:J:244:ILE:HD11	1:J:292:ASN:ND2	2.09	0.67
1:D:156:THR:HG21	1:D:284:PRO:HG2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:ILE:HD11	1:G:292:ASN:ND2	2.10	0.67
1:N:76:ARG:HD2	1:N:198:ILE:CG2	2.25	0.66
2:J:2034:HOH:O	1:K:51:ASP:HB2	1.94	0.66
1:D:292:ASN:HB3	2:D:2111:HOH:O	1.94	0.66
1:C:87:ILE:HD11	1:C:176:PRO:CD	2.24	0.66
1:L:76:ARG:HD2	1:L:198:ILE:CG2	2.26	0.65
1:M:244:ILE:HD11	1:M:292:ASN:ND2	2.11	0.65
1:D:244:ILE:HD11	1:D:292:ASN:ND2	2.12	0.64
1:F:76:ARG:HD2	1:F:198:ILE:HG21	1.78	0.64
1:F:76:ARG:HD2	1:F:198:ILE:CG2	2.28	0.64
1:M:87:ILE:HD12	1:M:176:PRO:HD3	1.79	0.64
1:G:164:ASN:HB2	2:G:2042:HOH:O	1.96	0.63
1:E:76:ARG:HD2	1:E:198:ILE:CG2	2.27	0.63
1:H:244:ILE:HD11	1:H:292:ASN:ND2	2.14	0.63
1:L:244:ILE:HD11	1:L:292:ASN:HD22	1.64	0.63
1:C:81:ASP:HB2	1:C:88:GLN:OE1	1.99	0.62
1:A:292:ASN:HB2	1:H:292:ASN:OD1	1.98	0.62
1:L:76:ARG:HD2	1:L:198:ILE:HG21	1.82	0.62
1:I:76:ARG:HD2	1:I:198:ILE:HG21	1.81	0.61
1:H:76:ARG:HD2	1:H:198:ILE:HG23	1.82	0.61
1:C:236:ASN:HB2	2:C:2088:HOH:O	2.02	0.60
1:M:87:ILE:HD11	1:M:176:PRO:HD3	1.82	0.60
1:L:244:ILE:HD11	1:L:292:ASN:ND2	2.17	0.60
1:C:76:ARG:HD2	1:C:198:ILE:HG21	1.84	0.59
1:C:241:PRO:HB2	1:C:244:ILE:CD1	2.29	0.59
1:C:76:ARG:HD2	1:C:198:ILE:CG2	2.32	0.59
1:B:220:ILE:HD11	2:B:2107:HOH:O	2.02	0.59
1:B:241:PRO:HB2	1:B:244:ILE:CD1	2.29	0.59
1:E:76:ARG:HD2	1:E:198:ILE:HG21	1.84	0.58
1:L:241:PRO:HB2	1:L:244:ILE:CD1	2.29	0.58
1:H:241:PRO:HB2	1:H:244:ILE:CD1	2.29	0.58
1:E:241:PRO:HB2	1:E:244:ILE:CD1	2.29	0.57
1:J:241:PRO:HB2	1:J:244:ILE:CD1	2.29	0.57
1:I:244:ILE:HD11	1:I:292:ASN:ND2	2.20	0.57
1:K:241:PRO:HB2	1:K:244:ILE:CD1	2.29	0.56
1:A:292:ASN:HB3	2:A:2059:HOH:O	2.03	0.56
1:C:142:SER:OG	1:C:197:GLN:OE1	2.23	0.56
1:I:58:GLN:O	1:I:62:THR:HG23	2.06	0.56
1:I:92:GLU:H	1:I:92:GLU:CD	2.09	0.56
1:A:58:GLN:O	1:A:62:THR:HG23	2.06	0.56
1:L:58:GLN:O	1:L:62:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:O	1:B:62:THR:HG23	2.06	0.56
1:C:127:HIS:HE1	1:D:51:ASP:OD2	1.88	0.56
1:N:58:GLN:O	1:N:62:THR:HG23	2.06	0.56
1:K:58:GLN:O	1:K:62:THR:HG23	2.06	0.56
1:M:58:GLN:O	1:M:62:THR:HG23	2.06	0.56
1:I:241:PRO:HB2	1:I:244:ILE:CD1	2.29	0.55
1:E:58:GLN:O	1:E:62:THR:HG23	2.06	0.55
1:L:127:HIS:HE1	1:M:51:ASP:OD2	1.89	0.55
1:G:58:GLN:O	1:G:62:THR:HG23	2.06	0.55
1:H:58:GLN:O	1:H:62:THR:HG23	2.06	0.55
1:J:58:GLN:O	1:J:62:THR:HG23	2.06	0.55
1:K:244:ILE:HD11	1:K:292:ASN:ND2	2.22	0.55
1:F:58:GLN:O	1:F:62:THR:HG23	2.06	0.55
1:A:241:PRO:HB2	1:A:244:ILE:CD1	2.29	0.55
1:D:58:GLN:O	1:D:62:THR:HG23	2.06	0.55
1:C:58:GLN:O	1:C:62:THR:HG23	2.06	0.55
1:F:84:THR:HB	1:F:86:GLN:HG3	1.89	0.55
1:E:292:ASN:HB2	1:K:292:ASN:OD1	2.07	0.55
1:C:187:ARG:HH11	1:C:187:ARG:HG2	1.71	0.55
1:D:92:GLU:HB2	2:D:2019:HOH:O	2.07	0.54
1:J:131:TYR:HH	1:J:142:SER:HG	1.49	0.54
1:M:241:PRO:HB2	1:M:244:ILE:CD1	2.29	0.54
1:A:81:ASP:HB3	1:A:84:THR:OG1	2.07	0.54
1:G:241:PRO:HB2	1:G:244:ILE:CD1	2.29	0.54
1:N:84:THR:HB	1:N:86:GLN:HG3	1.89	0.53
1:D:241:PRO:HB2	1:D:244:ILE:CD1	2.29	0.53
1:N:241:PRO:HB2	1:N:244:ILE:CD1	2.29	0.53
1:M:76:ARG:HD2	1:M:198:ILE:HG23	1.90	0.53
1:K:84:THR:OG1	1:K:86:GLN:HB2	2.09	0.53
1:I:244:ILE:HD11	1:I:292:ASN:HD22	1.73	0.52
1:E:164:ASN:HB2	2:E:2040:HOH:O	2.08	0.52
1:I:186:SER:O	1:I:189:HIS:N	2.39	0.52
1:L:164:ASN:HB2	2:L:2040:HOH:O	2.10	0.52
1:I:84:THR:OG1	1:I:86:GLN:HB2	2.09	0.52
1:L:84:THR:OG1	1:L:86:GLN:HB2	2.10	0.52
1:B:142:SER:OG	1:B:197:GLN:OE1	2.27	0.52
1:A:241:PRO:CB	1:A:292:ASN:HD21	2.23	0.52
1:G:76:ARG:HD2	1:G:198:ILE:HG23	1.91	0.51
1:K:76:ARG:HD2	1:K:198:ILE:HG23	1.90	0.51
1:H:164:ASN:HB2	2:H:2041:HOH:O	2.11	0.51
1:I:76:ARG:HD2	1:I:198:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ARG:HD2	1:E:198:ILE:HG23	1.93	0.51
1:F:241:PRO:HB2	1:F:244:ILE:CD1	2.29	0.51
1:C:52:MSE:HA	2:C:2005:HOH:O	2.10	0.51
1:N:292:ASN:HB3	2:N:2052:HOH:O	2.12	0.50
1:H:189:HIS:O	1:H:191:PRO:HD3	2.11	0.50
1:M:80:ILE:HD11	1:M:176:PRO:HB3	1.94	0.50
1:B:231:ASN:HD22	1:B:231:ASN:C	2.16	0.49
1:C:76:ARG:HD3	1:C:177:GLY:O	2.13	0.49
1:L:231:ASN:C	1:L:231:ASN:HD22	2.16	0.49
1:C:232:PRO:HG3	2:C:2085:HOH:O	2.12	0.49
1:F:76:ARG:HD3	1:F:177:GLY:O	2.13	0.49
1:H:76:ARG:HD3	1:H:177:GLY:O	2.13	0.49
1:B:76:ARG:HD3	1:B:177:GLY:O	2.13	0.49
1:D:231:ASN:C	1:D:231:ASN:HD22	2.16	0.49
1:A:241:PRO:CB	1:A:292:ASN:ND2	2.75	0.49
1:E:76:ARG:HD3	1:E:177:GLY:O	2.13	0.49
1:I:185:PHE:HB2	1:I:190:ASN:HB2	1.94	0.49
1:L:76:ARG:HD3	1:L:177:GLY:O	2.13	0.49
1:A:231:ASN:C	1:A:231:ASN:HD22	2.16	0.49
1:F:231:ASN:HD22	1:F:231:ASN:C	2.16	0.49
1:J:285:ASN:HB2	2:J:2105:HOH:O	2.13	0.49
1:J:231:ASN:HD22	1:J:231:ASN:C	2.16	0.49
1:K:231:ASN:C	1:K:231:ASN:HD22	2.16	0.49
1:L:76:ARG:HD2	1:L:198:ILE:HG23	1.94	0.49
1:N:76:ARG:HD3	1:N:177:GLY:O	2.13	0.49
1:D:76:ARG:HD3	1:D:177:GLY:O	2.13	0.49
1:I:76:ARG:HD3	1:I:177:GLY:O	2.13	0.49
1:M:76:ARG:HD3	1:M:177:GLY:O	2.13	0.49
1:H:231:ASN:HD22	1:H:231:ASN:C	2.16	0.48
1:H:291:ASN:HD21	1:H:295:ASN:HD21	1.61	0.48
1:K:177:GLY:HA2	2:K:2004:HOH:O	2.12	0.48
1:M:231:ASN:C	1:M:231:ASN:HD22	2.16	0.48
1:I:231:ASN:HD22	1:I:231:ASN:C	2.16	0.48
1:I:68:ALA:HA	1:I:189:HIS:CB	2.42	0.48
1:G:197:GLN:NE2	2:G:2055:HOH:O	2.46	0.48
1:G:76:ARG:HD3	1:G:177:GLY:O	2.13	0.48
1:J:76:ARG:HD3	1:J:177:GLY:O	2.13	0.48
1:K:291:ASN:HD21	1:K:295:ASN:HD21	1.61	0.48
1:K:76:ARG:HD3	1:K:177:GLY:O	2.13	0.48
1:A:76:ARG:HD3	1:A:177:GLY:O	2.13	0.48
1:C:291:ASN:HD21	1:C:295:ASN:HD21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASN:HD21	1:G:295:ASN:HD21	1.61	0.48
1:K:195:GLU:HG2	1:K:197:GLN:HG3	1.96	0.48
1:D:236:ASN:HB2	2:D:2078:HOH:O	2.13	0.48
1:J:197:GLN:O	1:J:198:ILE:HD13	2.14	0.48
1:N:231:ASN:HD22	1:N:231:ASN:C	2.16	0.48
1:F:291:ASN:HD21	1:F:295:ASN:HD21	1.61	0.48
1:N:291:ASN:HD21	1:N:295:ASN:HD21	1.61	0.48
1:A:241:PRO:HB3	1:A:292:ASN:HD21	1.78	0.48
1:B:76:ARG:HD2	1:B:198:ILE:HG23	1.91	0.48
1:C:231:ASN:C	1:C:231:ASN:HD22	2.16	0.48
1:F:257:ASN:ND2	2:F:2070:HOH:O	2.46	0.48
1:G:292:ASN:HB3	2:G:2061:HOH:O	2.14	0.47
1:H:131:TYR:OH	1:H:142:SER:OG	2.28	0.47
1:I:291:ASN:HD21	1:I:295:ASN:HD21	1.62	0.47
1:L:291:ASN:HD21	1:L:295:ASN:HD21	1.61	0.47
1:L:87:ILE:N	1:L:87:ILE:HD13	2.28	0.47
1:A:51:ASP:OD2	1:G:127:HIS:HE1	1.96	0.47
1:B:244:ILE:HD11	1:B:292:ASN:ND2	2.29	0.47
1:H:127:HIS:HE1	1:I:51:ASP:OD2	1.97	0.47
1:G:231:ASN:C	1:G:231:ASN:HD22	2.16	0.47
1:E:231:ASN:HD22	1:E:231:ASN:C	2.16	0.47
1:K:127:HIS:HE1	1:L:51:ASP:OD2	1.97	0.47
1:J:291:ASN:HD21	1:J:295:ASN:HD21	1.61	0.47
1:C:140:PHE:HB3	1:C:199:THR:CG2	2.44	0.47
1:H:52:MSE:SE	1:H:120:LEU:HD21	2.65	0.47
1:N:52:MSE:SE	1:N:120:LEU:HD21	2.65	0.47
1:D:52:MSE:SE	1:D:120:LEU:HD21	2.65	0.47
2:F:2055:HOH:O	1:J:292:ASN:HB3	2.14	0.47
1:M:164:ASN:HB2	2:M:2042:HOH:O	2.15	0.47
1:E:291:ASN:HD21	1:E:295:ASN:HD21	1.61	0.47
1:I:241:PRO:CB	1:I:292:ASN:ND2	2.78	0.47
1:K:52:MSE:SE	1:K:120:LEU:HD21	2.65	0.47
1:A:291:ASN:HD21	1:A:295:ASN:HD21	1.61	0.46
1:C:171:TYR:CD1	1:C:212:THR:HB	2.51	0.46
1:J:52:MSE:SE	1:J:120:LEU:HD21	2.65	0.46
1:J:171:TYR:CD1	1:J:212:THR:HB	2.51	0.46
1:J:127:HIS:HE1	1:K:51:ASP:OD2	1.98	0.46
1:B:291:ASN:HD21	1:B:295:ASN:HD21	1.61	0.46
1:B:292:ASN:HB3	2:B:2075:HOH:O	2.15	0.46
1:M:291:ASN:HD21	1:M:295:ASN:HD21	1.62	0.46
1:E:171:TYR:CD1	1:E:212:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:MSE:SE	1:M:120:LEU:HD21	2.65	0.46
1:A:164:ASN:HB2	2:A:2040:HOH:O	2.14	0.46
1:I:164:ASN:HB2	2:I:2053:HOH:O	2.16	0.46
1:N:171:TYR:CD1	1:N:212:THR:HB	2.50	0.46
1:A:171:TYR:CD1	1:A:212:THR:HB	2.50	0.46
1:E:52:MSE:SE	1:E:120:LEU:HD21	2.65	0.46
1:F:171:TYR:CD1	1:F:212:THR:HB	2.51	0.46
1:G:52:MSE:SE	1:G:120:LEU:HD21	2.65	0.46
1:I:52:MSE:SE	1:I:120:LEU:HD21	2.65	0.46
1:K:171:TYR:CD1	1:K:212:THR:HB	2.51	0.46
1:L:52:MSE:SE	1:L:120:LEU:HD21	2.65	0.46
1:D:291:ASN:HD21	1:D:295:ASN:HD21	1.61	0.46
1:I:171:TYR:CD1	1:I:212:THR:HB	2.51	0.46
1:B:192:PHE:CG	1:B:278:ALA:HB3	2.51	0.46
1:F:52:MSE:SE	1:F:120:LEU:HD21	2.65	0.46
1:H:171:TYR:CD1	1:H:212:THR:HB	2.51	0.46
1:M:171:TYR:CD1	1:M:212:THR:HB	2.51	0.46
1:A:52:MSE:SE	1:A:120:LEU:HD21	2.65	0.46
1:C:52:MSE:SE	1:C:120:LEU:HD21	2.65	0.46
1:D:171:TYR:CD1	1:D:212:THR:HB	2.51	0.46
1:L:171:TYR:CD1	1:L:212:THR:HB	2.51	0.46
1:A:76:ARG:HD2	1:A:198:ILE:HG23	1.95	0.46
1:D:87:ILE:N	1:D:87:ILE:HD13	2.30	0.46
1:B:52:MSE:SE	1:B:120:LEU:HD21	2.65	0.45
1:E:292:ASN:HB3	2:E:2055:HOH:O	2.16	0.45
1:A:80:ILE:O	1:A:80:ILE:HG22	2.12	0.45
1:B:171:TYR:CD1	1:B:212:THR:HB	2.51	0.45
1:D:76:ARG:HD2	1:D:198:ILE:HG23	1.92	0.45
1:D:65:PRO:HB3	1:D:67:PHE:CE1	2.52	0.45
1:N:140:PHE:HB3	1:N:199:THR:CG2	2.46	0.45
1:C:34:SER:HA	1:C:35:PRO:HD3	1.87	0.45
1:G:171:TYR:CD1	1:G:212:THR:HB	2.51	0.45
1:I:65:PRO:HB3	1:I:67:PHE:CE1	2.52	0.45
1:K:65:PRO:HB3	1:K:67:PHE:CE1	2.52	0.45
1:N:76:ARG:HD2	1:N:198:ILE:HG23	1.98	0.45
1:B:65:PRO:HB3	1:B:67:PHE:CE1	2.52	0.45
1:C:87:ILE:HA	1:C:87:ILE:HD13	1.81	0.45
1:G:65:PRO:HB3	1:G:67:PHE:CE1	2.52	0.45
1:M:65:PRO:HB3	1:M:67:PHE:CE1	2.52	0.45
1:N:80:ILE:CG2	1:N:81:ASP:N	2.80	0.45
1:C:65:PRO:HB3	1:C:67:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:PRO:HB3	1:N:67:PHE:CE1	2.52	0.45
1:N:80:ILE:HG22	1:N:81:ASP:N	2.32	0.45
1:A:65:PRO:HB3	1:A:67:PHE:CE1	2.52	0.44
1:B:74:HIS:HB2	2:B:2006:HOH:O	2.18	0.44
1:H:65:PRO:HB3	1:H:67:PHE:CE1	2.52	0.44
1:A:241:PRO:HG2	1:A:292:ASN:HD22	1.82	0.44
1:C:127:HIS:CE1	1:D:51:ASP:OD2	2.69	0.44
1:L:65:PRO:HB3	1:L:67:PHE:CE1	2.52	0.44
1:B:34:SER:HA	1:B:35:PRO:HD3	1.87	0.44
1:C:212:THR:HG22	1:C:224:TRP:HB2	2.00	0.44
1:I:186:SER:O	1:I:188:ASN:N	2.50	0.44
1:K:158:TRP:CD1	1:K:195:GLU:HA	2.53	0.44
1:B:212:THR:HG22	1:B:224:TRP:HB2	2.00	0.44
1:I:212:THR:HG22	1:I:224:TRP:HB2	2.00	0.44
1:J:87:ILE:HD12	1:J:176:PRO:HD3	2.00	0.44
1:F:65:PRO:HB3	1:F:67:PHE:CE1	2.52	0.44
1:K:121:SER:HB3	1:K:122:PRO:HD2	2.00	0.44
1:N:212:THR:HG22	1:N:224:TRP:HB2	2.00	0.44
1:E:65:PRO:HB3	1:E:67:PHE:CE1	2.52	0.44
1:F:121:SER:HB3	1:F:122:PRO:HD2	2.00	0.44
1:E:212:THR:HG22	1:E:224:TRP:HB2	2.00	0.43
1:H:140:PHE:HB3	1:H:199:THR:CG2	2.47	0.43
1:J:121:SER:HB3	1:J:122:PRO:HD2	2.00	0.43
1:D:121:SER:HB3	1:D:122:PRO:HD2	2.00	0.43
1:M:121:SER:HB3	1:M:122:PRO:HD2	2.00	0.43
1:B:121:SER:HB3	1:B:122:PRO:HD2	2.00	0.43
1:M:212:THR:HG22	1:M:224:TRP:HB2	2.00	0.43
1:J:65:PRO:HB3	1:J:67:PHE:CE1	2.52	0.43
1:L:121:SER:HB3	1:L:122:PRO:HD2	2.00	0.43
1:D:166:ASN:HB3	1:D:260:ASP:OD1	2.19	0.43
1:G:121:SER:HB3	1:G:122:PRO:HD2	2.00	0.43
1:A:121:SER:HB3	1:A:122:PRO:HD2	2.00	0.43
1:J:166:ASN:HB3	1:J:260:ASP:OD1	2.19	0.43
1:A:212:THR:HG22	1:A:224:TRP:HB2	2.00	0.43
1:H:121:SER:HB3	1:H:122:PRO:HD2	2.00	0.43
1:L:236:ASN:HB2	2:L:2063:HOH:O	2.19	0.43
1:M:87:ILE:HD12	1:M:176:PRO:CD	2.48	0.43
1:N:121:SER:HB3	1:N:122:PRO:HD2	2.00	0.43
1:E:166:ASN:HB3	1:E:260:ASP:OD1	2.19	0.43
1:G:166:ASN:HB3	1:G:260:ASP:OD1	2.19	0.43
1:B:166:ASN:HB3	1:B:260:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:HG22	1:D:224:TRP:HB2	2.00	0.43
1:K:212:THR:HG22	1:K:224:TRP:HB2	2.00	0.43
1:M:166:ASN:HB3	1:M:260:ASP:OD1	2.19	0.43
1:B:140:PHE:HB3	1:B:199:THR:CG2	2.49	0.43
1:D:230:ILE:HD12	1:D:230:ILE:HA	1.89	0.43
1:H:212:THR:HG22	1:H:224:TRP:HB2	2.00	0.43
1:L:212:THR:HG22	1:L:224:TRP:HB2	2.00	0.43
1:A:158:TRP:CD1	1:A:195:GLU:HA	2.54	0.42
1:H:166:ASN:HB3	1:H:260:ASP:OD1	2.19	0.42
1:I:127:HIS:HE1	1:J:51:ASP:OD2	2.02	0.42
1:N:166:ASN:HB3	1:N:260:ASP:OD1	2.19	0.42
1:N:80:ILE:HD11	1:N:176:PRO:HB3	1.99	0.42
1:A:166:ASN:HB3	1:A:260:ASP:OD1	2.19	0.42
1:C:121:SER:HB3	1:C:122:PRO:HD2	2.00	0.42
1:I:121:SER:HB3	1:I:122:PRO:HD2	2.00	0.42
1:J:52:MSE:HE2	1:J:52:MSE:HB3	1.78	0.42
1:C:166:ASN:HB3	1:C:260:ASP:OD1	2.19	0.42
1:E:121:SER:HB3	1:E:122:PRO:HD2	2.00	0.42
1:E:230:ILE:HD12	1:E:230:ILE:HA	1.89	0.42
1:F:212:THR:HG22	1:F:224:TRP:HB2	2.00	0.42
1:F:76:ARG:HD2	1:F:198:ILE:HG23	2.01	0.42
1:G:52:MSE:HE2	1:G:52:MSE:HB3	1.78	0.42
1:I:166:ASN:HB3	1:I:260:ASP:OD1	2.19	0.42
1:K:166:ASN:HB3	1:K:260:ASP:OD1	2.19	0.42
1:M:79:THR:C	1:M:80:ILE:HD12	2.40	0.42
1:N:195:GLU:HG2	1:N:197:GLN:HG3	2.01	0.42
1:H:52:MSE:HE2	1:H:52:MSE:HB3	1.78	0.42
1:H:80:ILE:O	1:H:80:ILE:HG22	2.18	0.42
1:D:119:ASN:OD1	1:D:121:SER:HB2	2.20	0.42
1:D:76:ARG:CD	1:D:198:ILE:HG21	2.37	0.42
1:F:230:ILE:HA	1:F:230:ILE:HD12	1.89	0.42
1:H:34:SER:HA	1:H:35:PRO:HD3	1.87	0.42
1:J:212:THR:HG22	1:J:224:TRP:HB2	2.00	0.42
1:N:119:ASN:OD1	1:N:121:SER:HB2	2.20	0.42
1:I:119:ASN:OD1	1:I:121:SER:HB2	2.20	0.42
1:M:34:SER:HA	1:M:35:PRO:HD3	1.87	0.42
1:D:140:PHE:HB3	1:D:199:THR:CG2	2.50	0.42
1:B:52:MSE:HB3	1:B:52:MSE:HE2	1.78	0.42
1:G:212:THR:HG22	1:G:224:TRP:HB2	2.00	0.42
1:J:119:ASN:OD1	1:J:121:SER:HB2	2.20	0.42
1:K:119:ASN:OD1	1:K:121:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:ASN:HB3	1:L:260:ASP:OD1	2.19	0.42
1:M:292:ASN:HB3	2:M:2062:HOH:O	2.20	0.42
1:D:118:GLN:HB2	2:D:2033:HOH:O	2.20	0.41
1:L:127:HIS:CE1	1:M:51:ASP:OD2	2.71	0.41
1:M:119:ASN:OD1	1:M:121:SER:HB2	2.20	0.41
1:D:164:ASN:HB2	2:D:2051:HOH:O	2.20	0.41
1:D:177:GLY:HA2	2:D:2010:HOH:O	2.20	0.41
1:F:166:ASN:HB3	1:F:260:ASP:OD1	2.19	0.41
1:F:34:SER:HA	1:F:35:PRO:HD3	1.87	0.41
1:G:119:ASN:OD1	1:G:121:SER:HB2	2.20	0.41
1:L:143:THR:O	1:L:197:GLN:HA	2.20	0.41
1:C:119:ASN:OD1	1:C:121:SER:HB2	2.20	0.41
1:F:84:THR:CB	1:F:86:GLN:HG3	2.50	0.41
1:I:34:SER:HA	1:I:35:PRO:HD3	1.87	0.41
1:B:98:TRP:CD1	1:B:160:PRO:HD3	2.56	0.41
1:F:119:ASN:OD1	1:F:121:SER:HB2	2.20	0.41
1:H:98:TRP:CD1	1:H:160:PRO:HD3	2.56	0.41
1:M:98:TRP:CD1	1:M:160:PRO:HD3	2.56	0.41
1:B:119:ASN:OD1	1:B:121:SER:HB2	2.20	0.41
1:L:119:ASN:OD1	1:L:121:SER:HB2	2.20	0.41
1:D:34:SER:HA	1:D:35:PRO:HD3	1.87	0.41
1:E:192:PHE:HA	1:E:193:PRO:HD2	1.88	0.41
1:G:230:ILE:HD12	1:G:230:ILE:HA	1.89	0.41
1:J:140:PHE:HB3	1:J:199:THR:CG2	2.50	0.41
1:K:98:TRP:CD1	1:K:160:PRO:HD3	2.56	0.41
1:L:140:PHE:HB3	1:L:199:THR:CG2	2.50	0.41
1:N:98:TRP:CD1	1:N:160:PRO:HD3	2.56	0.41
1:C:76:ARG:HD2	1:C:198:ILE:HG23	2.03	0.41
1:C:98:TRP:CD1	1:C:160:PRO:HD3	2.56	0.41
1:E:119:ASN:OD1	1:E:121:SER:HB2	2.20	0.41
1:G:34:SER:HA	1:G:35:PRO:HD3	1.87	0.41
1:F:98:TRP:CD1	1:F:160:PRO:HD3	2.56	0.41
1:I:158:TRP:CD1	1:I:195:GLU:HA	2.55	0.41
1:E:98:TRP:CD1	1:E:160:PRO:HD3	2.56	0.41
1:H:119:ASN:OD1	1:H:121:SER:HB2	2.20	0.41
1:J:98:TRP:CD1	1:J:160:PRO:HD3	2.56	0.41
1:A:119:ASN:OD1	1:A:121:SER:HB2	2.20	0.40
1:G:98:TRP:CD1	1:G:160:PRO:HD3	2.56	0.40
1:L:98:TRP:CD1	1:L:160:PRO:HD3	2.56	0.40
1:C:147:ARG:HD3	1:C:156:THR:O	2.22	0.40
1:D:147:ARG:HD3	1:D:156:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:TRP:CE2	1:H:195:GLU:HG3	2.55	0.40
1:J:232:PRO:HG3	2:J:2081:HOH:O	2.21	0.40
1:E:52:MSE:HE2	1:E:52:MSE:HB3	1.78	0.40
1:L:147:ARG:HD3	1:L:156:THR:O	2.22	0.40
1:N:147:ARG:HD3	1:N:156:THR:O	2.22	0.40
1:H:158:TRP:CD1	1:H:195:GLU:HA	2.57	0.40
1:I:98:TRP:CD1	1:I:160:PRO:HD3	2.56	0.40
1:A:98:TRP:CD1	1:A:160:PRO:HD3	2.56	0.40
1:C:52:MSE:HG3	1:C:52:MSE:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ASN:N	1:J:286:ASN:ND2[2_557]	2.14	0.06
1:A:151:LEU:CD2	1:N:62:THR:CG2[2_556]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	B	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	C	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	36	57
1	D	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	36	57
1	E	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	F	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	36	57
1	G	254/291 (87%)	241 (95%)	11 (4%)	2 (1%)	21	37
1	H	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	J	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	K	254/291 (87%)	240 (94%)	11 (4%)	3 (1%)	14	26
1	L	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	M	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	N	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	36	57
All	All	3556/4074 (87%)	3363 (95%)	172 (5%)	21 (1%)	27	46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	187	ARG
1	I	187	ARG
1	K	187	ARG
1	J	187	ARG
1	A	187	ARG
1	E	187	ARG
1	K	82	SER
1	A	123	VAL
1	B	123	VAL
1	C	123	VAL
1	D	123	VAL
1	E	123	VAL
1	F	123	VAL
1	G	123	VAL
1	H	123	VAL
1	I	123	VAL
1	J	123	VAL
1	K	123	VAL
1	L	123	VAL
1	M	123	VAL
1	N	123	VAL

### 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	238/257 (93%)	234 (98%)	4 (2%)	63	85
1	B	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	C	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	D	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	E	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	F	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	G	238/257 (93%)	237 (100%)	1 (0%)	92	98
1	H	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	I	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	J	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	K	238/257 (93%)	237 (100%)	1 (0%)	92	98
1	L	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	M	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	N	238/257 (93%)	235 (99%)	3 (1%)	71	89
All	All	3332/3598 (93%)	3300 (99%)	32 (1%)	78	92

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	82	SER
1	A	186	SER
1	A	231	ASN
1	B	186	SER
1	B	231	ASN
1	C	142	SER
1	C	231	ASN
1	D	196	ASP
1	D	197	GLN
1	D	231	ASN
1	E	82	SER
1	E	231	ASN
1	F	82	SER
1	F	197	GLN
1	F	231	ASN
1	G	231	ASN

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Mol	Chain	Res	Type
1	H	80	ILE
1	H	82	SER
1	H	231	ASN
1	I	197	GLN
1	I	231	ASN
1	J	92	GLU
1	J	231	ASN
1	K	231	ASN
1	L	82	SER
1	L	231	ASN
1	M	186	SER
1	M	231	ASN
1	N	82	SER
1	N	186	SER
1	N	231	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	164	ASN
1	A	217	ASN
1	A	231	ASN
1	A	292	ASN
1	A	295	ASN
1	B	127	HIS
1	B	164	ASN
1	B	217	ASN
1	B	231	ASN
1	B	292	ASN
1	B	295	ASN
1	C	127	HIS
1	C	164	ASN
1	C	217	ASN
1	C	231	ASN
1	C	292	ASN
1	C	295	ASN
1	D	127	HIS
1	D	164	ASN
1	D	217	ASN
1	D	228	ASN
1	D	231	ASN

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Mol	Chain	Res	Type
1	D	292	ASN
1	D	295	ASN
1	E	127	HIS
1	E	164	ASN
1	E	217	ASN
1	E	231	ASN
1	E	295	ASN
1	F	127	HIS
1	F	164	ASN
1	F	197	GLN
1	F	217	ASN
1	F	231	ASN
1	F	292	ASN
1	F	295	ASN
1	G	127	HIS
1	G	164	ASN
1	G	217	ASN
1	G	231	ASN
1	G	295	ASN
1	H	127	HIS
1	H	164	ASN
1	H	217	ASN
1	H	231	ASN
1	H	295	ASN
1	I	127	HIS
1	I	164	ASN
1	I	217	ASN
1	I	231	ASN
1	I	292	ASN
1	I	295	ASN
1	J	127	HIS
1	J	164	ASN
1	J	217	ASN
1	J	231	ASN
1	J	295	ASN
1	K	127	HIS
1	K	164	ASN
1	K	217	ASN
1	K	231	ASN
1	K	292	ASN
1	K	295	ASN
1	L	127	HIS

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Mol	Chain	Res	Type
1	L	164	ASN
1	L	217	ASN
1	L	231	ASN
1	L	295	ASN
1	M	127	HIS
1	M	164	ASN
1	M	217	ASN
1	M	231	ASN
1	M	295	ASN
1	N	127	HIS
1	N	164	ASN
1	N	217	ASN
1	N	231	ASN
1	N	292	ASN
1	N	295	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

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	253/291 (86%)	0.23	19 (7%) 14 14	22, 36, 76, 105	0
1	B	253/291 (86%)	0.12	9 (3%) 42 46	21, 35, 72, 96	0
1	C	253/291 (86%)	0.29	16 (6%) 20 21	17, 34, 72, 98	0
1	D	253/291 (86%)	0.20	12 (4%) 31 34	21, 34, 72, 104	0
1	E	253/291 (86%)	0.10	14 (5%) 25 27	21, 35, 74, 106	0
1	F	253/291 (86%)	0.16	18 (7%) 16 16	21, 36, 76, 98	0
1	G	253/291 (86%)	-0.03	9 (3%) 42 46	20, 34, 67, 96	0
1	H	253/291 (86%)	0.08	17 (6%) 18 18	21, 36, 76, 104	0
1	I	253/291 (86%)	0.25	18 (7%) 16 16	21, 35, 72, 108	0
1	J	253/291 (86%)	0.06	10 (3%) 38 41	21, 34, 73, 97	0
1	K	253/291 (86%)	0.14	15 (5%) 22 23	21, 36, 73, 108	0
1	L	253/291 (86%)	0.33	22 (8%) 10 10	21, 36, 75, 101	0
1	M	253/291 (86%)	0.26	17 (6%) 18 18	21, 35, 72, 105	0
1	N	253/291 (86%)	0.34	29 (11%) 5 4	22, 36, 77, 110	0
All	All	3542/4074 (86%)	0.18	225 (6%) 19 20	17, 35, 75, 110	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	PRO	8.8
1	I	122	PRO	8.6
1	N	120	LEU	7.9
1	L	122	PRO	7.8
1	B	83	ASN	7.7
1	F	122	PRO	7.2
1	I	120	LEU	7.1
1	C	122	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	6.3
1	N	122	PRO	5.8
1	I	297	ILE	5.8
1	E	122	PRO	5.8
1	A	83	ASN	5.7
1	G	122	PRO	5.6
1	K	83	ASN	5.6
1	D	120	LEU	5.5
1	M	122	PRO	5.5
1	M	261	SER	5.4
1	H	122	PRO	5.4
1	K	122	PRO	5.3
1	K	120	LEU	5.2
1	M	121	SER	5.1
1	A	122	PRO	5.0
1	C	120	LEU	4.9
1	N	62	THR	4.9
1	H	83	ASN	4.9
1	L	83	ASN	4.9
1	F	120	LEU	4.9
1	G	120	LEU	4.8
1	E	261	SER	4.8
1	M	189	HIS	4.7
1	L	121	SER	4.7
1	C	66	SER	4.7
1	B	120	LEU	4.6
1	I	291	ASN	4.6
1	A	120	LEU	4.4
1	N	58	GLN	4.4
1	J	122	PRO	4.4
1	I	121	SER	4.3
1	N	121	SER	4.3
1	M	67	PHE	4.2
1	J	121	SER	4.2
1	A	82	SER	4.0
1	C	261	SER	3.9
1	N	187	ARG	3.9
1	N	261	SER	3.9
1	L	152	GLY	3.8
1	M	186	SER	3.8
1	N	70	PRO	3.8
1	G	261	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	68	ALA	3.8
1	M	187	ARG	3.8
1	L	151	LEU	3.7
1	F	121	SER	3.7
1	L	261	SER	3.7
1	M	66	SER	3.7
1	H	67	PHE	3.7
1	F	63	ARG	3.7
1	L	67	PHE	3.6
1	B	121	SER	3.6
1	L	120	LEU	3.6
1	L	34	SER	3.6
1	F	62	THR	3.6
1	H	151	LEU	3.5
1	I	63	ARG	3.5
1	F	36	LYS	3.5
1	D	187	ARG	3.5
1	N	83	ASN	3.4
1	E	295	ASN	3.4
1	H	121	SER	3.4
1	H	187	ARG	3.4
1	J	187	ARG	3.4
1	L	153	LEU	3.4
1	K	84	THR	3.4
1	L	36	LYS	3.3
1	N	69	SER	3.3
1	M	120	LEU	3.3
1	A	74	HIS	3.3
1	F	117	ASN	3.3
1	N	119	ASN	3.3
1	N	36	LYS	3.2
1	E	83	ASN	3.2
1	I	290	ASN	3.2
1	C	67	PHE	3.2
1	N	118	GLN	3.2
1	A	151	LEU	3.1
1	I	242	SER	3.1
1	A	297	ILE	3.1
1	I	292	ASN	3.0
1	C	62	THR	3.0
1	C	121	SER	3.0
1	F	65	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	67	PHE	3.0
1	H	82	SER	3.0
1	F	66	SER	3.0
1	H	261	SER	2.9
1	L	290	ASN	2.9
1	N	84	THR	2.9
1	N	54	SER	2.9
1	A	261	SER	2.9
1	K	36	LYS	2.9
1	A	84	THR	2.9
1	H	62	THR	2.9
1	L	84	THR	2.8
1	A	81	ASP	2.8
1	L	81	ASP	2.8
1	C	69	SER	2.8
1	G	121	SER	2.8
1	D	36	LYS	2.8
1	C	71	ASN	2.8
1	M	62	THR	2.8
1	D	70	PRO	2.8
1	E	187	ARG	2.7
1	I	261	SER	2.7
1	F	123	VAL	2.7
1	N	55	LEU	2.7
1	A	36	LYS	2.7
1	A	33	ASN	2.7
1	L	82	SER	2.7
1	F	34	SER	2.7
1	K	81	ASP	2.7
1	L	149	ASN	2.7
1	H	120	LEU	2.6
1	C	58	GLN	2.6
1	K	121	SER	2.6
1	I	62	THR	2.6
1	E	67	PHE	2.6
1	C	242	SER	2.6
1	D	121	SER	2.6
1	L	155	ILE	2.6
1	H	152	GLY	2.6
1	G	297	ILE	2.6
1	M	64	ILE	2.6
1	F	261	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	58	GLN	2.5
1	D	290	ASN	2.5
1	C	191	PRO	2.5
1	A	121	SER	2.5
1	B	242	SER	2.5
1	I	150	ASN	2.5
1	L	291	ASN	2.5
1	A	291	ASN	2.5
1	J	120	LEU	2.4
1	F	270	TYR	2.4
1	A	152	GLY	2.4
1	L	187	ARG	2.4
1	G	187	ARG	2.4
1	K	187	ARG	2.4
1	E	121	SER	2.4
1	E	239	SER	2.4
1	F	82	SER	2.4
1	F	151	LEU	2.4
1	J	261	SER	2.4
1	C	63	ARG	2.4
1	H	153	LEU	2.4
1	H	239	SER	2.3
1	I	243	ASN	2.3
1	N	71	ASN	2.3
1	N	149	ASN	2.3
1	F	67	PHE	2.3
1	A	34	SER	2.3
1	L	150	ASN	2.3
1	H	295	ASN	2.3
1	N	66	SER	2.3
1	K	35	PRO	2.3
1	B	92	GLU	2.3
1	K	291	ASN	2.3
1	M	68	ALA	2.3
1	D	58	GLN	2.3
1	M	151	LEU	2.3
1	M	65	PRO	2.3
1	K	261	SER	2.3
1	B	81	ASP	2.3
1	L	93	HIS	2.3
1	N	153	LEU	2.3
1	A	150	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	295	ASN	2.2
1	K	88	GLN	2.2
1	M	297	ILE	2.2
1	M	36	LYS	2.2
1	J	63	ARG	2.2
1	H	288	LEU	2.2
1	C	292	ASN	2.2
1	N	185	PHE	2.2
1	A	153	LEU	2.2
1	N	57	TYR	2.2
1	B	82	SER	2.2
1	I	123	VAL	2.2
1	E	297	ILE	2.2
1	G	188	ASN	2.2
1	D	68	ALA	2.2
1	E	196	ASP	2.2
1	I	61	SER	2.2
1	J	291	ASN	2.1
1	E	150	ASN	2.1
1	K	80	ILE	2.1
1	D	51	ASP	2.1
1	I	36	LYS	2.1
1	N	183	ALA	2.1
1	G	67	PHE	2.1
1	J	34	SER	2.1
1	N	151	LEU	2.1
1	B	119	ASN	2.1
1	D	292	ASN	2.1
1	F	54	SER	2.1
1	H	188	ASN	2.1
1	K	188	ASN	2.1
1	M	295	ASN	2.1
1	I	298	GLN	2.1
1	G	63	ARG	2.1
1	N	239	SER	2.1
1	E	152	GLY	2.1
1	N	65	PRO	2.0
1	J	83	ASN	2.0
1	K	150	ASN	2.0
1	H	290	ASN	2.0
1	N	53	SER	2.0
1	C	34	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	188	ASN	2.0
1	E	291	ASN	2.0
1	L	33	ASN	2.0
1	E	289	LEU	2.0
1	A	67	PHE	2.0
1	J	67	PHE	2.0
1	C	118	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.