



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:56 PM UTC

PDB ID : 1VF7 / pdb_00001vf7
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

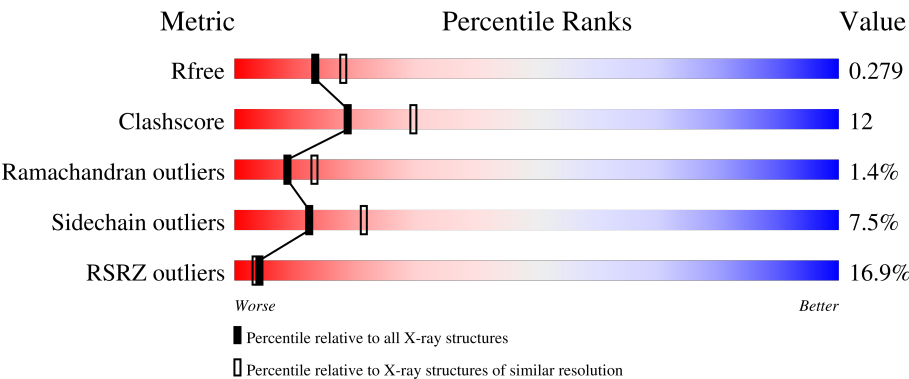
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	369	17% 43% 18% . 36%
1	B	369	6% 48% 12% .. 36%
1	C	369	7% 48% 15% .. 33%
1	D	369	4% 44% 16% .. 36%
1	E	369	8% 45% 18% .. 32%

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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

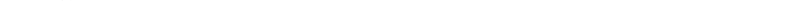
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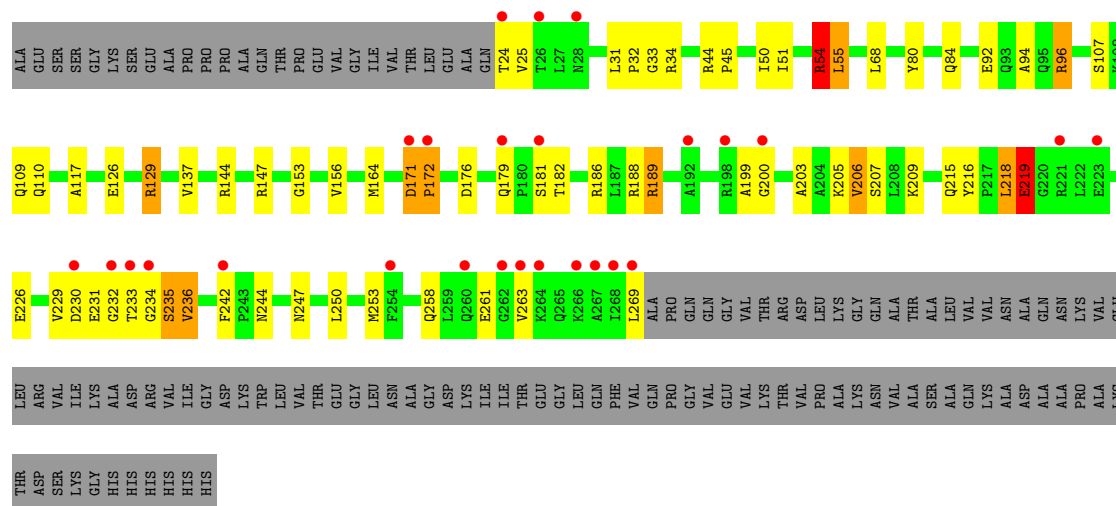
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Chain	Residue	Modelled	Actual	Comment	Reference
M	366	HIS	-	expression tag	UNP P52477

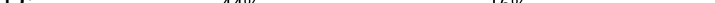
GLY
HIS
HIS
HIS
HIS
HIS
HIS

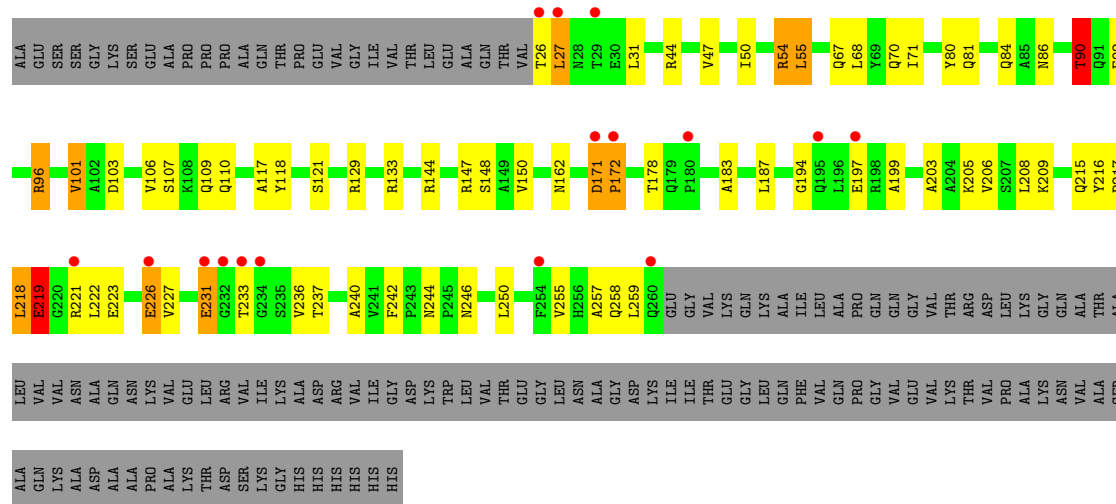
- Molecule 1: Multidrug resistance protein mexA

Chain C:  7% 48% 15% .. 33%

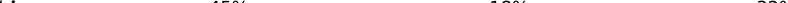


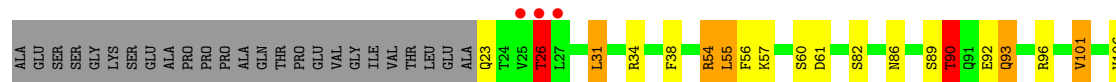
- Molecule 1: Multidrug resistance protein mexA

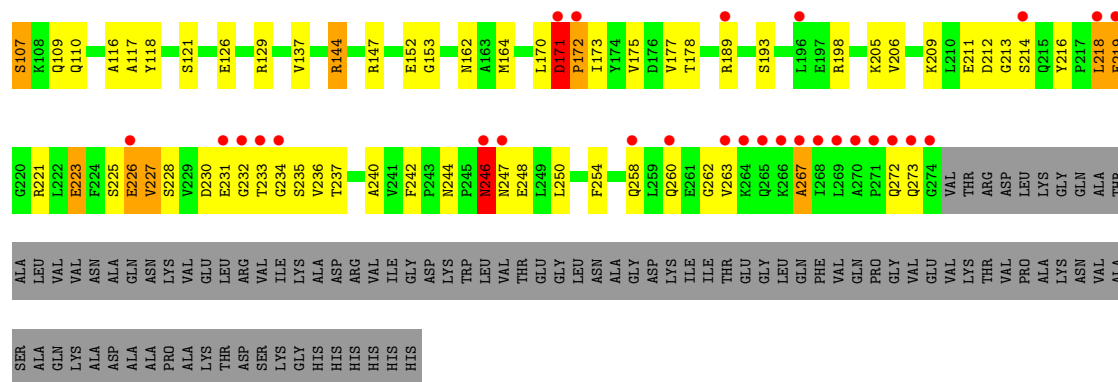
Chain D:  4% 44% 16% 36%



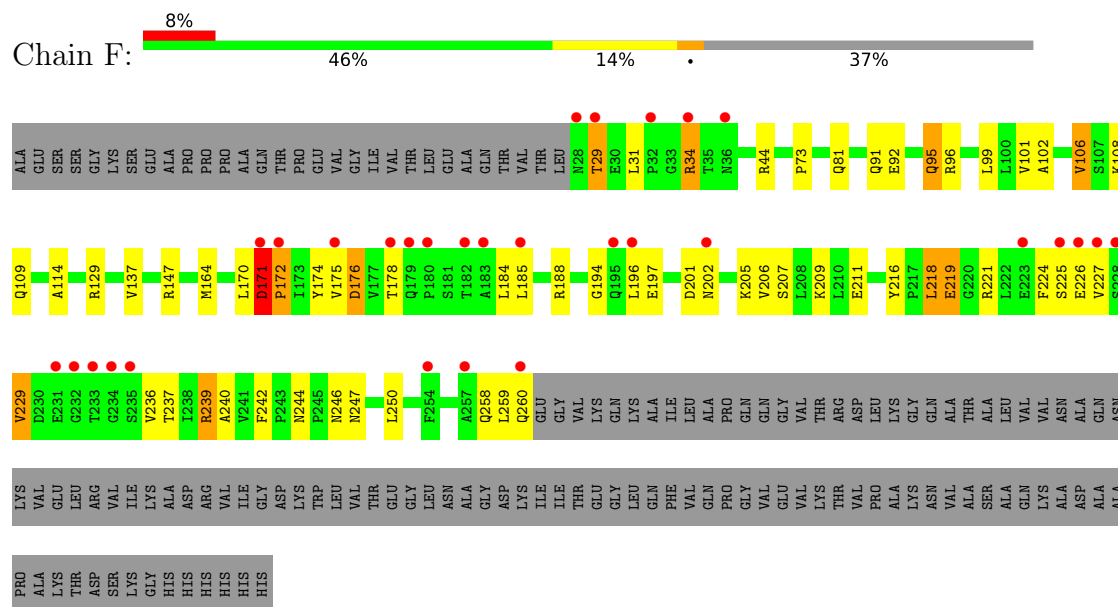
- Molecule 1: Multidrug resistance protein mexA

Chain E: 

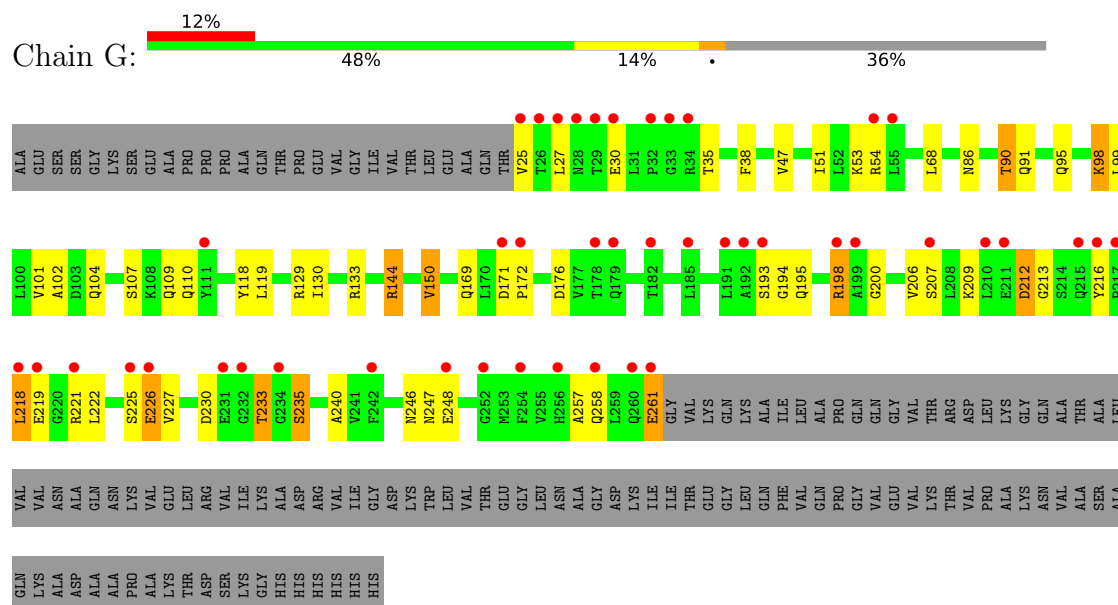




• Molecule 1: Multidrug resistance protein mexA



• Molecule 1: Multidrug resistance protein mexA



Chain H:

Residue	Count	Color
ALA	1	Grey
GLU	1	Grey
SER	1	Grey
SER	1	Grey
GLY	1	Grey
LYS	1	Grey
SER	1	Grey
GLU	1	Grey
ALA	1	Grey
PRO	1	Grey
PRO	1	Grey
PRO	1	Grey
ALA	1	Grey
GLN	1	Grey
THR	1	Grey
PRO	1	Grey
PRO	1	Grey
GLU	1	Grey
VAL	1	Grey
GLY	1	Grey
ILE	1	Grey
VAL	1	Grey
THR	1	Grey
LEU	1	Grey
GLU	1	Grey
ALA	1	Grey
Q23	1	Green
T24	1	Green
V25	1	Orange
T26	1	Yellow
L27	1	Yellow
R34	1	Orange
F38	1	Yellow
T51	1	Yellow
L53	1	Yellow
K53	1	Yellow
K57	1	Yellow
S60	1	Yellow
K63	1	Yellow
Q81	1	Yellow
N86	1	Yellow
S89	1	Yellow
R96	1	Green
S89	1	Yellow
Q109	1	Yellow
S121	1	Yellow
R129	1	Yellow
R140	1	Orange
LYS	1	Grey
GLN	1	Grey
LYS	1	Grey
ILE	1	Grey
LEU	1	Grey
ALA	1	Grey
PRO	1	Grey
GLN	1	Grey
GLY	1	Grey
VAL	1	Grey
THR	1	Grey
ARG	1	Grey
ASP	1	Grey
LEU	1	Grey
LYS	1	Grey
GLY	1	Grey
ALA	1	Grey
ASN	1	Grey
VAL	1	Grey
VAL	1	Grey
ASN	1	Grey
ALA	1	Grey
ASP	1	Grey
ALA	1	Grey
ASN	1	Grey
LYS	1	Grey
VAL	1	Grey
GLU	1	Grey
LEU	1	Grey
ASP	1	Grey
SER	1	Grey
LYS	1	Grey
ILE	1	Grey
GLY	1	Grey
ALA	1	Grey
ASP	1	Grey
ASP	1	Grey
VAL	1	Grey
ILE	1	Grey
GLY	1	Grey
ASP	1	Grey
LYS	1	Grey
TRP	1	Grey
LEU	1	Grey
VAL	1	Grey
THR	1	Grey
GLU	1	Grey
GLY	1	Grey
LEU	1	Grey
ASN	1	Grey
ALA	1	Grey
GLY	1	Grey
ASP	1	Grey
LYS	1	Grey
ILE	1	Grey
THR	1	Grey
GLU	1	Grey
GLY	1	Grey
VAL	1	Grey
THR	1	Grey
GLU	1	Grey
GLN	1	Grey
LYS	1	Grey
ALA	1	Grey
ASP	1	Grey
ALA	1	Grey
ASN	1	Grey
VAL	1	Grey
GLN	1	Grey
VAL	1	Grey
ASN	1	Grey
GLY	1	Grey
LYS	1	Grey
THR	1	Grey
VAL	1	Grey
ASP	1	Grey
GLN	1	Grey
ALA	1	Grey
ASN	1	Grey
GLY	1	Grey
VAL	1	Grey
THR	1	Grey
ARG	1	Grey
ASP	1	Grey
LEU	1	Grey
LYS	1	Grey
GLN	1	Grey
VAL	1	Grey
ASN	1	Grey
ALA	1	Grey
ASP	1	Grey
ALA	1	Grey
ASN	1	Grey
LYS	1	Grey
VAL	1	Grey
GLU	1	Grey
LEU	1	Grey
ASP	1	Grey
SER	1	Grey
LYS	1	Grey
ILE	1	Grey
GLY	1	Grey
ALA	1	Grey
ASP	1	Grey
ASP	1	Grey
VAL	1	Grey
ILE	1	Grey
THR	1	Grey
GLU	1	Grey
GLY	1	Grey
LEU	1	Grey
ASN	1	Grey
ALA	1	Grey
GLY	1	Grey
ASP	1	Grey
LYS	1	Grey
ILE	1	Grey
THR	1	Grey
GLU	1	Grey
GLN	1	Grey
LYS	1	Grey
ALA	1	Grey
ASP	1	Grey
ALA	1	Grey
ASN	1	Grey
VAL	1	Grey
GLN	1	Grey
VAL	1	Grey
ASN	1	Grey

Chain I:

6% 47% 13% 1% 1% 36%

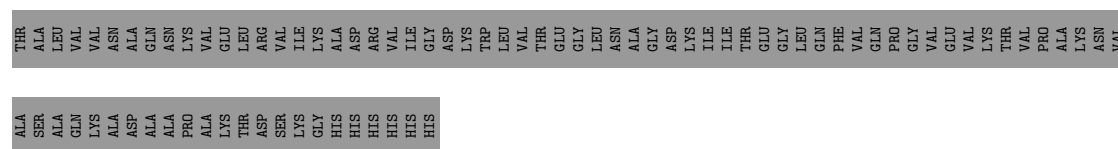
ALA, GLU, SER, SER, GLY, LYS, SER, GLU, ALA, PRO, PRO, PRO, ALA, THR, THR, GLU, VAL, T26, L27, I28, R34, R39, R44, P45, I50, R54, L55, S60, L63, S89, E92, R96, V101, V106, S107, K108, Q109, Q110, E126, R129, V137, I145, G146, R147, S148, V156, M164, L170, D171, P172, I173, T178, Q179, L184, L185, R188, Q195, L196, R197, R198, A199, G200, D201, N202, A203, A204, K205, V206, S207, L208, K209, L210, E211, Q215, L218, E219, S225, E226, V227, S228, E231, Q233, Q1233, T237, I238, R239, N244, P245, N246, G252, R253, F254, A257, Q258, L259, Q260, GLY, GLY, VAL, VAL, LYS, GLN, LYS, ALA, PHE, VAL, GLN, PRO, GLY, VAL, GLU, VAL, LYS, THR, VAL, ASN, VAL, ALA, SER, GLN, LYS, ASP, THR, ASP, ASP, THR, PRO, ALA, LYS, THR, LEU, HIS, HIS, HIS, HIS, ARG, VAL, ILE, GLY, ASP, LYS, TRP, VAL, VAL, GLU, GLY, LEU, ASN, ALA, GLY, LYS, ILE, ILE, THR, GLU, GLY, LEU, GLN, PHE, VAL, GLN, PRO, GLY, VAL, GLU, VAL, LYS, THR, VAL, ASP, THR, VAL, LYS, ASN, VAL, ALA, SER, GLN, LYS, ASP, THR, LYS, VAL, ASP, THR, PRO, ALA, LYS, THR, LEU, HIS, HIS, HIS, HIS, ARG

Chain J:

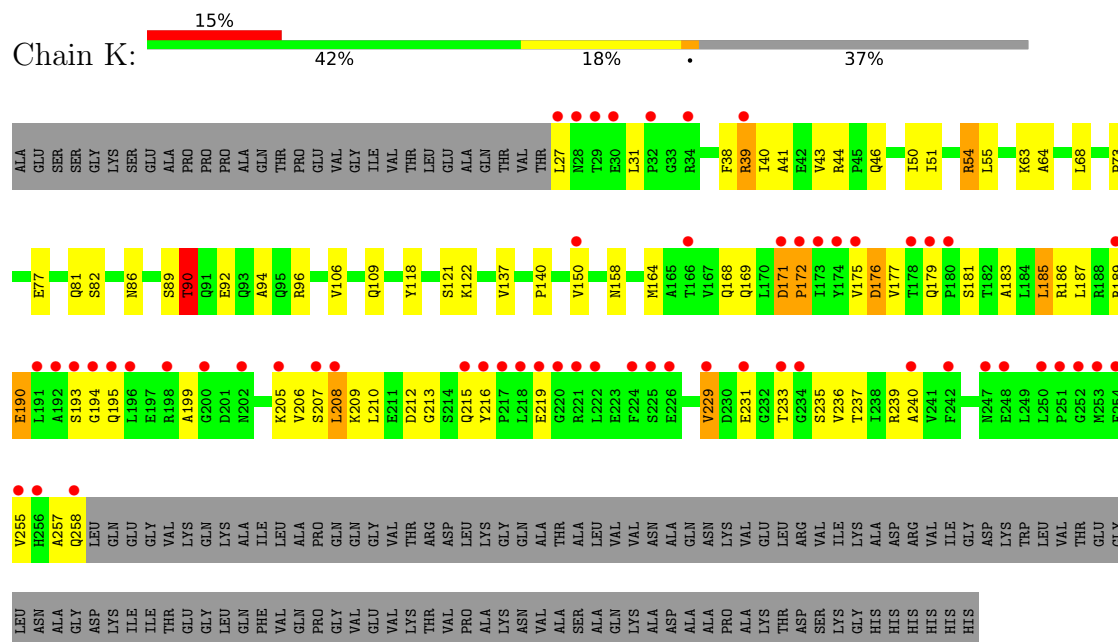
14% 49% 13% 36%

ALA
GLU
SER
SER
GLY
LYS
SER
GLU
GLU
ALA
PRO
PRO
PRO
ALA
GLN
THR
PRO
GLU
VAL
GLY
ILE
VAL
THR
LEU
GLU
ALA
ALA
THR
VAL
T26
L27
N28
T29
P32
F38
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N86
S89
T90
Q91
E92
Q93
R96
V101
S107

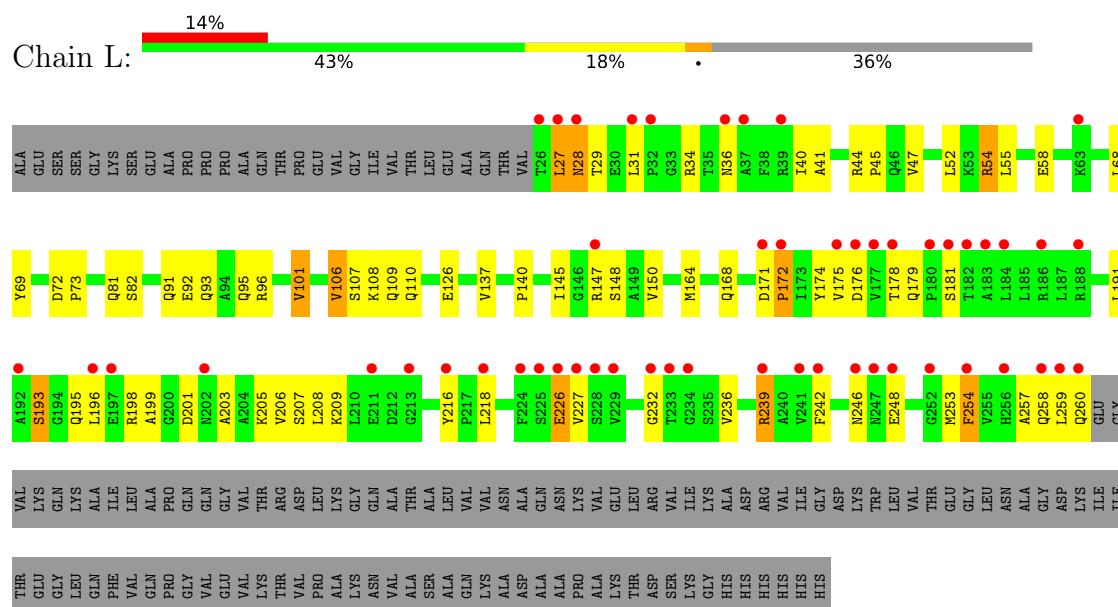
K108
Q109
Q110
Y118
L119
Q120
S121
V137
L138
S139
P140
R144
R147
M164
D171
P172
I173
T178
Q179
P180
S181
T182
L185
R188
R189
E190
L191
A192
G194
L195
L196
E197
R198
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K205
V206
S207
L208
K209
D212
G213
S214
P215



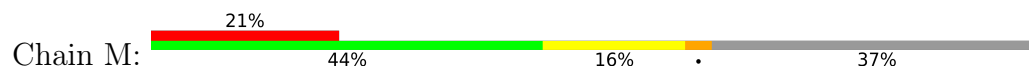
- Molecule 1: Multidrug resistance protein mexA

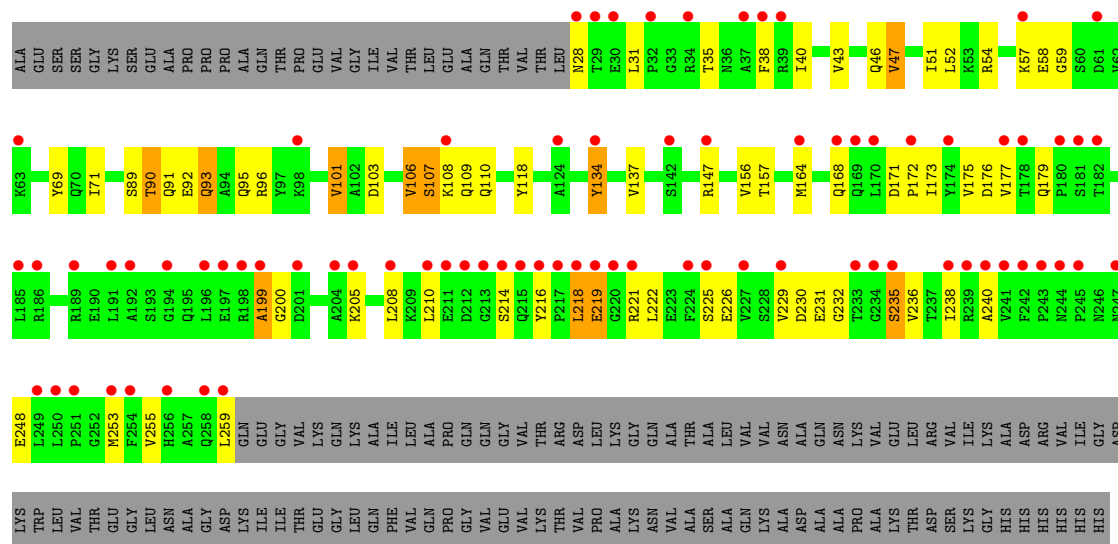


- Molecule 1: Multidrug resistance protein mexA



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.98	1/1840 (0.1%)	1.12	4/2495 (0.2%)
1	B	1.42	12/1827 (0.7%)	1.41	21/2478 (0.8%)
1	C	1.29	5/1909 (0.3%)	1.27	13/2588 (0.5%)
1	D	1.49	8/1827 (0.4%)	1.44	21/2478 (0.8%)
1	E	1.30	4/1953 (0.2%)	1.30	15/2648 (0.6%)
1	F	1.27	4/1812 (0.2%)	1.31	16/2457 (0.7%)
1	G	0.92	2/1843 (0.1%)	1.04	3/2500 (0.1%)
1	H	1.07	1/1870 (0.1%)	1.14	4/2537 (0.2%)
1	I	1.27	6/1827 (0.3%)	1.31	14/2478 (0.6%)
1	J	1.07	4/1827 (0.2%)	1.15	7/2478 (0.3%)
1	K	1.04	4/1803 (0.2%)	1.12	6/2445 (0.2%)
1	L	1.07	2/1827 (0.1%)	1.16	5/2478 (0.2%)
1	M	0.78	0/1803	1.00	2/2445 (0.1%)
All	All	1.17	53/23968 (0.2%)	1.22	131/32505 (0.4%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ASN	C-O	18.19	1.45	1.24
1	B	55	LEU	N-CA	9.28	1.58	1.46
1	C	55	LEU	N-CA	8.55	1.57	1.46
1	I	55	LEU	N-CA	8.51	1.57	1.46
1	D	55	LEU	N-CA	7.56	1.55	1.46
1	D	117	ALA	CA-CB	7.02	1.64	1.53
1	I	129	ARG	NE-CZ	6.91	1.40	1.33
1	B	247	ASN	N-CA	6.88	1.55	1.46
1	I	246	ASN	CA-C	-6.75	1.44	1.52
1	D	129	ARG	NE-CZ	6.74	1.40	1.33
1	K	50	ILE	CA-CB	6.61	1.62	1.54
1	B	73	PRO	N-CA	-6.55	1.42	1.47
1	C	129	ARG	NE-CZ	6.52	1.40	1.33
1	F	171	ASP	CA-C	-6.48	1.44	1.52
1	B	74	ALA	N-CA	6.44	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	129	ARG	NE-CZ	6.40	1.40	1.33
1	G	129	ARG	CZ-NH1	6.20	1.41	1.32
1	F	176	ASP	N-CA	6.09	1.54	1.46
1	B	175	VAL	CA-CB	6.08	1.61	1.55
1	I	50	ILE	CA-CB	6.07	1.61	1.54
1	D	101	VAL	CA-CB	6.00	1.62	1.54
1	B	68	LEU	C-O	-5.98	1.16	1.24
1	D	246	ASN	CA-C	-5.94	1.45	1.52
1	E	82	SER	CA-C	5.91	1.60	1.52
1	B	39	ARG	NE-CZ	5.86	1.39	1.33
1	F	246	ASN	CA-C	-5.86	1.45	1.52
1	J	74	ALA	N-CA	5.85	1.53	1.46
1	J	101	VAL	CA-CB	5.84	1.61	1.54
1	L	73	PRO	CA-C	5.77	1.58	1.52
1	J	55	LEU	N-CA	5.74	1.53	1.46
1	D	50	ILE	CA-CB	5.72	1.62	1.54
1	E	117	ALA	CA-CB	5.62	1.62	1.53
1	E	116	ALA	CA-CB	5.61	1.62	1.53
1	L	145	ILE	CA-CB	5.55	1.60	1.54
1	G	130	ILE	CA-CB	5.51	1.60	1.54
1	B	144	ARG	C-O	5.34	1.30	1.24
1	I	171	ASP	C-O	5.29	1.31	1.24
1	H	129	ARG	NE-CZ	5.29	1.38	1.33
1	E	93	GLN	CA-C	5.29	1.59	1.52
1	B	167	VAL	CA-C	5.25	1.58	1.52
1	B	156	VAL	CA-CB	5.20	1.63	1.54
1	K	90	THR	CA-C	5.17	1.59	1.52
1	C	50	ILE	CA-CB	5.15	1.61	1.54
1	C	94	ALA	N-CA	5.14	1.52	1.46
1	K	73	PRO	CA-C	5.12	1.58	1.52
1	A	55	LEU	N-CA	5.05	1.52	1.46
1	D	255	VAL	CA-CB	5.05	1.61	1.54
1	K	94	ALA	N-CA	5.05	1.52	1.46
1	C	117	ALA	CA-CB	5.05	1.61	1.53
1	J	73	PRO	CA-C	5.03	1.58	1.52
1	I	137	VAL	CA-CB	5.02	1.59	1.54
1	B	164	MET	CA-C	5.02	1.59	1.52
1	B	171	ASP	C-O	5.01	1.30	1.24

All (131) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	ASN	N-CA-C	-13.20	87.38	108.90
1	B	246	ASN	CA-C-N	-13.19	96.36	121.54
1	B	246	ASN	C-N-CA	-13.19	96.36	121.54
1	I	172	PRO	N-CA-C	-11.77	92.90	111.03
1	F	246	ASN	CA-C-N	-11.21	105.88	122.24
1	F	246	ASN	C-N-CA	-11.21	105.88	122.24
1	B	172	PRO	N-CA-C	-10.68	94.59	111.03
1	D	172	PRO	N-CA-C	-10.50	94.76	111.14
1	C	172	PRO	N-CA-C	-10.46	95.00	110.80
1	D	171	ASP	CA-C-N	-9.60	109.87	119.76
1	D	171	ASP	C-N-CA	-9.60	109.87	119.76
1	I	246	ASN	N-CA-C	-9.52	94.82	109.95
1	I	246	ASN	CA-C-N	-9.26	108.20	122.08
1	I	246	ASN	C-N-CA	-9.26	108.20	122.08
1	F	246	ASN	N-CA-C	-8.93	96.30	110.14
1	A	226	GLU	N-CA-C	8.87	123.81	108.02
1	D	27	LEU	N-CA-C	8.56	121.33	109.18
1	E	172	PRO	N-CA-C	-8.45	97.26	110.95
1	H	172	PRO	N-CA-C	-8.26	98.32	111.03
1	J	172	PRO	N-CA-C	-8.24	97.60	110.95
1	B	174	TYR	CA-C-N	-8.13	114.87	123.08
1	B	174	TYR	C-N-CA	-8.13	114.87	123.08
1	E	227	VAL	N-CA-C	-8.11	104.59	113.43
1	L	54	ARG	N-CA-C	7.95	119.72	111.14
1	L	28	ASN	N-CA-C	7.88	121.31	109.25
1	B	218	LEU	N-CA-C	7.87	122.96	113.12
1	I	171	ASP	CA-C-N	-7.75	111.47	119.83
1	I	171	ASP	C-N-CA	-7.75	111.47	119.83
1	F	172	PRO	N-CA-C	-7.69	99.19	111.03
1	B	171	ASP	CA-C-N	-7.65	111.57	119.83
1	B	171	ASP	C-N-CA	-7.65	111.57	119.83
1	E	101	VAL	CB-CA-C	-7.57	101.78	112.22
1	B	54	ARG	CA-C-N	-7.55	107.12	121.54
1	B	54	ARG	C-N-CA	-7.55	107.12	121.54
1	F	171	ASP	N-CA-C	-7.45	93.36	109.81
1	D	96	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	H	218	LEU	N-CA-C	7.39	122.35	113.12
1	F	171	ASP	CA-C-N	-7.11	112.15	119.83
1	F	171	ASP	C-N-CA	-7.11	112.15	119.83
1	F	174	TYR	CA-C-N	-7.04	115.97	123.08
1	F	174	TYR	C-N-CA	-7.04	115.97	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ARG	NE-CZ-NH2	-7.02	112.88	119.20
1	D	101	VAL	CB-CA-C	-6.95	101.01	112.26
1	B	101	VAL	CB-CA-C	-6.84	101.55	112.16
1	I	218	LEU	N-CA-C	6.69	121.58	112.68
1	C	233	THR	N-CA-C	-6.62	100.03	109.96
1	B	246	ASN	O-C-N	-6.60	113.69	122.14
1	L	27	LEU	N-CA-C	6.53	120.86	113.02
1	G	133	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	C	235	SER	N-CA-C	6.48	118.38	110.41
1	J	90	THR	N-CA-CB	-6.48	100.24	110.28
1	K	172	PRO	N-CA-C	-6.46	101.07	111.14
1	L	172	PRO	N-CA-C	-6.46	101.07	111.14
1	I	101	VAL	N-CA-CB	6.42	119.27	110.54
1	B	55	LEU	N-CA-C	6.37	124.37	110.80
1	B	175	VAL	N-CA-C	6.34	117.02	111.56
1	E	26	THR	N-CA-C	6.32	117.97	111.14
1	F	218	LEU	N-CA-C	6.29	121.05	112.68
1	D	54	ARG	CA-C-N	-6.28	109.55	121.54
1	D	54	ARG	C-N-CA	-6.28	109.55	121.54
1	C	54	ARG	CA-C-N	-6.26	109.58	121.54
1	C	54	ARG	C-N-CA	-6.26	109.58	121.54
1	K	90	THR	N-CA-CB	-6.22	100.65	110.22
1	E	55	LEU	N-CA-C	6.20	124.02	110.80
1	E	171	ASP	CA-C-N	-6.20	112.79	119.98
1	E	171	ASP	C-N-CA	-6.20	112.79	119.98
1	E	54	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	E	218	LEU	N-CA-C	6.18	120.90	112.68
1	D	246	ASN	O-C-N	6.11	130.57	123.30
1	D	90	THR	N-CA-CB	-6.07	100.95	110.30
1	D	54	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	C	179	GLN	N-CA-C	6.03	113.56	108.13
1	C	218	LEU	N-CA-C	5.98	121.09	113.55
1	D	218	LEU	N-CA-C	5.95	120.55	113.12
1	B	90	THR	N-CA-CB	-5.88	101.17	110.28
1	D	133	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	D	54	ARG	CG-CD-NE	-5.85	99.13	112.00
1	D	171	ASP	N-CA-CB	5.84	120.77	110.37
1	I	54	ARG	CA-C-N	-5.83	110.40	121.54
1	I	54	ARG	C-N-CA	-5.83	110.40	121.54
1	H	227	VAL	CB-CA-C	5.82	116.18	111.06
1	E	101	VAL	N-CA-CB	5.80	119.28	110.58
1	A	246	ASN	N-CA-C	-5.72	102.02	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	N-CA-CB	5.71	117.69	111.41
1	B	162	ASN	N-CA-C	5.70	119.21	110.20
1	D	103	ASP	CB-CA-C	-5.62	100.37	110.37
1	D	172	PRO	CB-CA-C	5.61	118.69	111.46
1	K	235	SER	N-CA-C	5.60	117.30	110.41
1	F	171	ASP	N-CA-CB	5.59	120.31	110.37
1	F	172	PRO	N-CD-CG	-5.58	94.83	103.20
1	E	171	ASP	N-CA-CB	5.53	120.21	110.37
1	D	54	ARG	O-C-N	-5.52	114.17	122.28
1	K	54	ARG	CA-C-N	-5.51	115.33	125.02
1	K	54	ARG	C-N-CA	-5.51	115.33	125.02
1	D	71	ILE	N-CA-C	-5.50	100.51	108.87
1	J	120	GLN	N-CA-C	5.50	117.27	111.28
1	B	171	ASP	N-CA-CB	5.46	120.09	110.37
1	K	208	LEU	N-CA-C	5.44	117.25	108.34
1	C	171	ASP	CA-C-N	-5.41	114.22	119.90
1	C	171	ASP	C-N-CA	-5.41	114.22	119.90
1	J	54	ARG	CA-C-N	-5.41	111.22	121.54
1	J	54	ARG	C-N-CA	-5.41	111.22	121.54
1	C	96	ARG	CG-CD-NE	-5.40	100.12	112.00
1	I	172	PRO	CB-CA-C	5.40	118.44	111.64
1	E	107	SER	N-CA-C	5.39	117.48	110.53
1	E	90	THR	N-CA-CB	-5.37	101.96	110.28
1	I	27	LEU	N-CA-C	5.32	117.95	109.65
1	B	96	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	E	162	ASN	N-CA-C	5.29	118.23	109.46
1	F	95	GLN	N-CA-C	-5.26	105.71	111.82
1	I	55	LEU	N-CA-C	5.26	122.01	110.80
1	C	25	VAL	N-CA-C	5.22	116.23	108.46
1	J	55	LEU	N-CA-C	5.22	121.91	110.80
1	F	225	SER	CA-C-N	5.19	128.22	120.90
1	F	225	SER	C-N-CA	5.19	128.22	120.90
1	E	246	ASN	N-CA-C	-5.18	100.72	109.07
1	D	162	ASN	N-CA-C	5.17	118.25	109.76
1	J	96	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	L	107	SER	N-CA-C	5.15	117.18	110.53
1	G	194	GLY	N-CA-C	-5.14	108.52	115.36
1	M	134	TYR	N-CA-C	5.14	119.03	112.87
1	C	55	LEU	N-CA-C	5.11	121.69	110.80
1	B	171	ASP	N-CA-C	-5.11	98.52	109.81
1	I	101	VAL	CB-CA-C	-5.10	105.25	112.14
1	A	143	GLY	N-CA-C	5.09	116.90	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	N-CA-C	5.09	116.90	108.20
1	H	25	VAL	N-CA-C	5.09	116.92	108.99
1	F	114	ALA	N-CA-C	-5.03	105.88	111.36
1	B	54	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	G	218	LEU	N-CA-C	5.01	119.47	112.90
1	M	107	SER	N-CA-C	5.01	116.80	110.33

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	57	0
1	B	1803	0	1807	50	0
1	C	1885	0	1902	56	0
1	D	1803	0	1807	42	0
1	E	1928	0	1941	56	0
1	F	1788	0	1789	45	0
1	G	1819	0	1822	39	0
1	H	1846	0	1849	28	0
1	I	1803	0	1807	42	0
1	J	1803	0	1807	42	0
1	K	1779	0	1781	56	0
1	L	1803	0	1807	55	0
1	M	1779	0	1781	45	0
All	All	23655	0	23716	562	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 12.

All (562) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:ARG:HG2	1:H:34:ARG:HH11	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:HG3	1:A:189:ARG:HH11	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:F:137:VAL:HG11	1:F:164:MET:HE1	1.52	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
1:D:26:THR:HG22	1:D:27:LEU:HG	1.57	0.86
1:J:137:VAL:HG11	1:J:164:MET:HE1	1.57	0.85
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:L:226:GLU:CD	1:L:226:GLU:H	1.87	0.82
1:J:137:VAL:HG11	1:J:164:MET:CE	2.10	0.82
1:L:254:PHE:HD1	1:L:254:PHE:H	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:HG2	1:H:34:ARG:NH1	1.90	0.79
1:L:109:GLN:OE1	1:M:96:ARG:NH2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:137:VAL:HG11	1:C:164:MET:HE1	1.66	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: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:F:250:LEU:HD11	1:G:226:GLU:HG2	1.68	0.75
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: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:HG3	1:C:54:ARG:NH1	1.99	0.74
1:I:171:ASP:O	1:I:172:PRO:C	2.29	0.74
1:B:92:GLU:OE1	1:B:96:ARG:HD3	1.88	0.73
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:E:96:ARG:NH2	1:F:109:GLN:OE1	2.21	0.72
1:J:107:SER:H	1:J:110:GLN:HE21	1.37	0.72
1:C:107:SER:H	1:C:110:GLN:HE21	1.37	0.72
1:I:239:ARG:NH2	1:J:147:ARG:HH12	1.87	0.72
1:M:137:VAL:HG11	1:M:164:MET:HE1	1.71	0.71
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:E:250:LEU:HD11	1:F:226:GLU:HG2	1.71	0.71
1:L:175:VAL:O	1:L:176:ASP:HB2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:VAL:HG11	1:I:164:MET:HE1	1.73	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:I:54:ARG:O	1:I:68:LEU:O	2.10	0.69
1:J:199:ALA:HB2	1:J:205:LYS:HG2	1.72	0.69
1:B:171:ASP:HB3	1:B:172:PRO:HD3	1.73	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:B:175:VAL:HG22	1:B:240:ALA:HB3	1.75	0.67
1:C:54:ARG:HH11	1:C:54:ARG:CG	2.01	0.67
1:C:171:ASP:HB3	1:C:172:PRO:HD3	1.75	0.67
1:F:147:ARG:NH2	1:G:176:ASP:OD2	2.25	0.67
1:I:171:ASP:O	1:I:244:ASN:HB3	1.95	0.67
1:A:206:VAL:HG12	1:A:207:SER:H	1.60	0.67
1:G:107:SER:H	1:G:110:GLN:NE2	1.90	0.67
1:E:212:ASP:O	1:E:214:SER:N	2.28	0.67
1:F:171:ASP:O	1:F:172:PRO:C	2.35	0.67
1:K:181:SER:HB2	1:L:253:MET:HE3	1.77	0.67
1:L:199:ALA:HB2	1:L:205:LYS:HG2	1.76	0.67
1:B:54:ARG:O	1:B:55:LEU:HB2	1.94	0.66
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:J:144:ARG:HG3	1:J:144:ARG:NH1	2.12	0.65
1:K:171:ASP:HB3	1:K:172:PRO:CD	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:SER:H	1:E:110:GLN:NE2	1.94	0.65
1:I:226:GLU:HG2	1:J:250:LEU:HD11	1.77	0.65
1:L:54:ARG:HD2	1:L:148:SER:HB2	1.78	0.65
1:D:171:ASP:C	1:D:171:ASP:OD1	2.39	0.64
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:F:96:ARG:HH22	1:G:109:GLN:CD	2.06	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:K:137:VAL:HG11	1:K:164:MET:HE1	1.80	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:A:92:GLU:OE1	1:A:96:ARG:HD3	1.99	0.63
1:F:175:VAL:O	1:F:176:ASP:HB2	1.97	0.63
1:K:215:GLN:HE22	1:K:258:GLN:HE22	1.45	0.63
1:C:44:ARG:C	1:C:164:MET:HE2	2.24	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:E:171:ASP:O	1:E:172:PRO:C	2.41	0.62
1:I:44:ARG:C	1:I:164:MET:HE2	2.23	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:A:186:ARG:O	1:A:190:GLU:HG3	2.00	0.62
1:F:227:VAL:HG21	1:F:239:ARG:HG2	1.81	0.62
1:L:58:GLU:HG2	1:L:147:ARG:HA	1.82	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: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:J:54:ARG:O	1:J:55:LEU:HB2	1.99	0.60
1:A:218:LEU:HD13	1:A:243:PRO:HB2	1.83	0.60
1:E:90:THR:HG23	1:E:118:TYR:CA	2.29	0.60
1:I:45:PRO:N	1:I:164:MET:HE2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:VAL:CG1	1:L:207:SER:N	2.64	0.60
1:C:199:ALA:O	1:C:203:ALA:HB3	2.01	0.60
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.65	0.60
1:M:51:ILE:HD11	1:M:156:VAL:CG1	2.32	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:E:126:GLU:OE2	1:E:129:ARG:NH2	2.32	0.60
1:M:175:VAL:HG22	1:M:240:ALA:HB3	1.82	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:HG3	1:H:144:ARG:HH11	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:E:54:ARG:O	1:E:56:PHE:N	2.35	0.59
1:K:90:THR:HG21	1:K:121:SER:OG	2.03	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:J:109:GLN:OE1	1:K:96:ARG:NH2	2.36	0.58
1:L:191:LEU:HG	1:L:198:ARG:HH21	1.68	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:H:216:TYR:CE2	1:H:218:LEU:HB2	2.39	0.58
1:L:52:LEU:HD22	1:L:72:ASP:HA	1.85	0.58
1:E:86:ASN:ND2	1:E:121:SER:OG	2.37	0.58
1:K:54:ARG:O	1:K:55:LEU:HB2	2.03	0.58
1:D:215:GLN:HE22	1:D:258:GLN:HE22	1.51	0.58
1:G:90:THR:CG2	1:G:118:TYR:HA	2.34	0.58
1:K:239:ARG:NH2	1:L:147:ARG:HH21	2.01	0.58
1:M:90:THR:CG2	1:M:118:TYR:HA	2.32	0.58
1:F:194:GLY:C	1:F:196:LEU:H	2.12	0.57
1:C:171:ASP:OD1	1:C:171:ASP:C	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:SER:H	1:B:110:GLN:HE21	1.53	0.57
1:K:189:ARG:HH11	1:K:189:ARG:HG2	1.69	0.57
1:B:90:THR:HG23	1:B:118:TYR:CA	2.27	0.57
1:C:216:TYR:CE2	1:C:218:LEU:HB2	2.40	0.57
1:K:41:ALA:HB1	1:K:140:PRO:HG2	1.86	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:E:246:ASN:O	1:E:248:GLU:N	2.33	0.56
1:L:101:VAL:HG13	1:L:106:VAL:HG12	1.87	0.56
1:L:206:VAL:HG12	1:L:207:SER:N	2.20	0.56
1:K:43:VAL:HG12	1:K:164:MET:HE3	1.88	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:230:ASP:O	1:M:235:SER:HA	2.07	0.54
1:M:43:VAL:HG12	1:M:164:MET:HE3	1.89	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:J:199:ALA:O	1:J:203:ALA:HB3	2.08	0.54
1:M:38:PHE:CD1	1:M:172:PRO:HB2	2.42	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:M:137:VAL:HG11	1:M:164:MET:CE	2.37	0.54
1:B:86:ASN:O	1:B:90:THR:HB	2.07	0.54
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:D:171:ASP:O	1:D:172:PRO:C	2.49	0.53
1:E:57:LYS:O	1:E:60:SER:OG	2.23	0.53
1:F:171:ASP:HB3	1:F:172:PRO:CD	2.37	0.53
1:E:219:GLU:HA	1:E:242:PHE:HE2	1.72	0.53
1:G:195:GLN:HG2	1:G:261:GLU:CD	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:35:THR:HA	1:M:175:VAL:HA	1.91	0.53
1:E:212:ASP:C	1:E:214:SER:H	2.16	0.53
1:L:41:ALA:HB1	1:L:140:PRO:HG2	1.90	0.53
1:E:246:ASN:C	1:E:248:GLU:H	2.16	0.53
1:E:34:ARG:NH2	1:E:254:PHE:CZ	2.77	0.53
1:I:126:GLU:OE2	1:I:129:ARG:NH2	2.41	0.53
1:J:206:VAL:HG12	1:J:207:SER:N	2.24	0.53
1:M:91:GLN:O	1:M:95:GLN:HG3	2.09	0.53
1:M:222:LEU:HD11	1:M:238:ILE:HD12	1.90	0.53
1:C:45:PRO:N	1:C:164:MET:HE2	2.23	0.52
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:M:230:ASP:C	1:M:232:GLY:H	2.18	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: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
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:126:GLU:OE2	1:C:129:ARG:NH2	2.43	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: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:L:45:PRO:N	1:L:164:MET:HE2	2.26	0.50
1:F:209:LYS:HB2	1:F:258:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:171:ASP:O	1:B:172:PRO:C	2.50	0.50
1:F:206:VAL:CG1	1:F:207:SER:N	2.75	0.50
1:L:226:GLU:CD	1:L:226:GLU:N	2.62	0.50
1:M:171:ASP:CB	1:M:172:PRO:HD3	2.38	0.50
1:M:210:LEU:HD12	1:M:214:SER:HB2	1.93	0.50
1:E:137:VAL:HG11	1:E:164:MET:HE1	1.93	0.50
1:I:101:VAL:HG13	1:I:106:VAL:HG23	1.93	0.50
1:K:90:THR:HG23	1:K:118:TYR:CA	2.35	0.50
1:B:253:MET:HE2	1:C:182:THR:HG22	1.93	0.50
1:H:218:LEU:O	1:H:219:GLU:HB3	2.12	0.50
1:A:30:GLU:HG2	1:A:258:GLN:HG2	1.92	0.50
1:A:206:VAL:HG21	1:A:222:LEU:HB2	1.93	0.50
1:A:209:LYS:HB2	1:A:258:GLN:NE2	2.26	0.50
1:K:31:LEU:HD21	1:K:179:GLN:NE2	2.27	0.50
1:E:221:ARG:O	1:E:240:ALA:HA	2.12	0.50
1:F:250:LEU:CD1	1:G:226:GLU:HG2	2.38	0.50
1:H:144:ARG:HH11	1:H:144:ARG:CG	2.23	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:L:226:GLU:HB3	1:L:236:VAL:CG1	2.42	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:A:206:VAL:HG11	1:A:257:ALA:HB1	1.93	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:I:54:ARG:HD2	1:I:148:SER:HB2	1.93	0.49
1:M:226:GLU:HA	1:M:238:ILE:HG22	1.94	0.49
1:D:215:GLN:HE22	1:D:258:GLN:NE2	2.10	0.49
1:G:86:ASN:O	1:G:90:THR:HB	2.12	0.49
1:J:171:ASP:HB3	1:J:172:PRO:HD3	1.94	0.49
1:K:186:ARG:O	1:K:190:GLU:HG3	2.12	0.49
1:B:247:ASN:H	1:C:188:ARG:HH12	1.60	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:L:174:TYR:CD2	1:L:239:ARG:HD2	2.47	0.49
1:A:129:ARG:HH22	1:A:130:ILE:HD11	1.77	0.49
1:M:210:LEU:HA	1:M:255:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:VAL:O	1:C:219:GLU:HB2	2.13	0.48
1:F:171:ASP:CB	1:F:172:PRO:HD3	2.42	0.48
1:H:51:ILE:HG13	1:H:150:VAL:CG1	2.43	0.48
1:K:183:ALA:O	1:K:187:LEU:HG	2.14	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:HH11	1:K:39:ARG:HG2	1.77	0.48
1:B:144:ARG:NE	1:C:226:GLU:OE1	2.46	0.48
1:G:226:GLU:CD	1:G:226:GLU:H	2.19	0.48
1:M:46:GLN:HB2	1:M:134:TYR:CD1	2.49	0.48
1:G:99:LEU:O	1:G:102:ALA:HB3	2.13	0.48
1:M:51:ILE:HD11	1:M:156:VAL:HG11	1.95	0.48
1:K:171:ASP:CB	1:K:172:PRO:CD	2.92	0.48
1:M:54:ARG:HG3	1:M:69:TYR:CE2	2.49	0.48
1:E:38:PHE:HB2	1:E:172:PRO:O	2.14	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:H:248:GLU:O	1:H:253:MET:HE1	2.12	0.48
1:F:229:VAL:HG13	1:F:236:VAL:HG22	1.95	0.48
1:A:212:ASP:OD2	1:B:189:ARG:NH2	2.46	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:C:54:ARG:NH1	1:C:54:ARG:CG	2.66	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:J:92:GLU:OE1	1:J:96:ARG:HD3	2.15	0.47
1:L:108:LYS:HB3	1:M:96:ARG:HD2	1.97	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:B:209:LYS:HE3	1:B:258:GLN:NE2	2.30	0.47
1:C:54:ARG:O	1:C:55:LEU:HB2	2.14	0.47
1:H:216:TYR:HE2	1:H:218:LEU:HB2	1.78	0.47
1:M:93:GLN:O	1:M:93:GLN:HG3	2.14	0.47
1:A:61:ASP:OD1	1:A:144:ARG:HD2	2.15	0.47
1:C:137:VAL:HG11	1:C:164:MET:CE	2.41	0.47
1:E:31:LEU:HD22	1:E:177:VAL:HG11	1.97	0.47
1:J:54:ARG:O	1:J:55:LEU:CB	2.60	0.47
1:J:171:ASP:O	1:J:172:PRO:C	2.54	0.47
1:J:206:VAL:CG1	1:J:207:SER:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:96:ARG:HH22	1:B:109:GLN:CD	2.21	0.47
1:C:218:LEU:O	1:C:219:GLU:HG2	2.15	0.47
1:L:92:GLU:OE1	1:L:96:ARG:HD3	2.14	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:86:ASN:HD21	1:A:121:SER:HB2	1.80	0.46
1:A:208:LEU:HB3	1:A:216:TYR:HB3	1.98	0.46
1:B:227:VAL:HG21	1:B:239:ARG:HD2	1.97	0.46
1:E:23:GLN:N	1:E:267:ALA:O	2.49	0.46
1:H:51:ILE:HG13	1:H:150:VAL:HG11	1.96	0.46
1:J:200:GLY:HA3	1:J:221:ARG:HH21	1.80	0.46
1:D:206:VAL:HG21	1:D:257:ALA:HB1	1.97	0.46
1:E:230:ASP:HB3	1:E:233:THR:O	2.16	0.46
1:I:239:ARG:NH2	1:J:147:ARG:NH1	2.61	0.46
1:K:209:LYS:HE2	1:K:213:GLY:HA2	1.98	0.46
1:A:46:GLN:HB2	1:A:134:TYR:CD1	2.50	0.46
1:C:209:LYS:HB2	1:C:258:GLN:NE2	2.31	0.46
1:H:254:PHE:N	1:H:254:PHE:CD1	2.83	0.46
1:L:40:ILE:HG12	1:L:168:GLN:HG2	1.97	0.46
1:B:171:ASP:OD1	1:B:171:ASP:C	2.59	0.46
1:A:189:ARG:CG	1:A:189:ARG:NH1	2.71	0.46
1:F:197:GLU:HG3	1:F:260:GLN:NE2	2.30	0.46
1:I:54:ARG:O	1:I:55:LEU:HB2	2.15	0.46
1:I:60:SER:O	1:I:145:ILE:HG22	2.16	0.46
1:M:218:LEU:O	1:M:219:GLU:HG2	2.16	0.46
1:D:54:ARG:O	1:D:55:LEU:CB	2.62	0.46
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:L:106:VAL:HG13	1:L:110:GLN:HB2	1.98	0.45
1:D:250:LEU:CD1	1:E:226:GLU:HG2	2.47	0.45
1:H:57:LYS:O	1:H:60:SER:OG	2.24	0.45
1:G:144:ARG:NH2	1:G:247:ASN:HD22	2.14	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:C:218:LEU:HD23	1:C:218:LEU:HA	1.86	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:H:221:ARG:O	1:H:240:ALA:HA	2.17	0.45
1:L:29:THR:N	1:L:259:LEU:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG11	1:A:164:MET:HE1	1.97	0.45
1:E:96:ARG:HD2	1:F:108:LYS:HD3	1.98	0.45
1:L:54:ARG:O	1:L:55:LEU:HB2	2.15	0.45
1:B:211:GLU:HB3	1:C:182:THR:HG21	1.98	0.45
1:C:33:GLY:HA3	1:C:176:ASP:O	2.17	0.45
1:E:54:ARG:O	1:E:54:ARG:HG2	2.17	0.45
1:G:193:SER:C	1:G:195:GLN:H	2.24	0.45
1:K:179:GLN:HE22	1:K:187:LEU:HD11	1.82	0.45
1:G:221:ARG:O	1:G:240:ALA:HA	2.17	0.45
1:D:215:GLN:NE2	1:D:258:GLN:HE22	2.13	0.45
1:I:170:LEU:O	1:I:171:ASP:O	2.34	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:I:215:GLN:HE22	1:I:258:GLN:CD	2.25	0.44
1:L:137:VAL:HG11	1:L:164:MET:HE1	1.99	0.44
1:C:147:ARG:HE	1:D:227:VAL:CG1	2.30	0.44
1:K:208:LEU:HB3	1:K:216:TYR:HB3	2.00	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:E:178:THR:HA	1:E:236:VAL:O	2.16	0.44
1:I:199:ALA:HB2	1:I:204:ALA:C	2.43	0.44
1:K:206:VAL:CG1	1:K:207:SER:N	2.81	0.44
1:K:44:ARG:C	1:K:164:MET:HE2	2.43	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:M:101:VAL:C	1:M:103:ASP:H	2.26	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:E:221:ARG:NE	1:E:223:GLU:OE2	2.35	0.43
1:G:207:SER:HB3	1:G:258:GLN:OE1	2.18	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:A:144:ARG:NE	1:B:226:GLU:OE2	2.35	0.43
1:E:250:LEU:CD1	1:F:226:GLU:HG2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:ARG:HG2	1:L:44:ARG:NH1	2.33	0.43
1:B:91:GLN:O	1:B:95:GLN:HG3	2.18	0.43
1:B:171:ASP:CB	1:B:172:PRO:HD3	2.43	0.43
1:C:230:ASP:O	1:C:234:GLY:HA2	2.18	0.43
1:G:169:GLN:HE21	1:G:172:PRO:CD	2.31	0.43
1:I:92:GLU:OE2	1:I:96:ARG:NH1	2.51	0.43
1:G:246:ASN:O	1:G:248:GLU:N	2.42	0.43
1:A:174:TYR:CD1	1:A:239:ARG:NH1	2.86	0.43
1:M:106:VAL:HG13	1:M:110:GLN:HB2	2.00	0.43
1:G:233:THR:OG1	1:G:235:SER:HB2	2.18	0.43
1:A:64:ALA:HB2	1:A:141:ILE:C	2.44	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:E:211:GLU:HB3	1:E:254:PHE:O	2.18	0.43
1:F:44:ARG:C	1:F:164:MET:HE2	2.44	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:L:91:GLN:HG2	1:L:95:GLN:HE21	1.83	0.43
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.82	0.42
1:F:101:VAL:HG13	1:F:106:VAL:HG12	2.00	0.42
1:K:189:ARG:HH11	1:K:189:ARG:CG	2.31	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:G:51:ILE:HG13	1:G:150:VAL:CG1	2.49	0.42
1:J:171:ASP:O	1:J:173:ILE:N	2.52	0.42
1:K:109:GLN:CD	1:L:96:ARG:HH22	2.23	0.42
1:B:96:ARG:HH22	1:C:109:GLN:CD	2.23	0.42
1:B:171:ASP:CB	1:B:172:PRO:CD	2.97	0.42
1:H:171:ASP:O	1:H:244:ASN:CB	2.67	0.42
1:K:185:LEU:O	1:K:189:ARG:HG3	2.19	0.42
1:A:216:TYR:CE2	1:A:218:LEU:HB2	2.54	0.42
1:K:38:PHE:HB2	1:K:172:PRO:O	2.18	0.42
1:K:63:LYS:O	1:K:64:ALA:C	2.62	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:J:220:GLY:HA3	1:J:242:PHE:CE2	2.55	0.42
1:L:36:ASN:ND2	1:L:176:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:203:ALA:HA	1:D:222:LEU:O	2.19	0.42
1:E:219:GLU:HA	1:E:242:PHE:CE2	2.54	0.42
1:K:177:VAL:O	1:K:237:THR:HA	2.19	0.42
1:K:199:ALA:HB2	1:K:205:LYS:CG	2.50	0.42
1:K:233:THR:HG22	1:K:233:THR:O	2.20	0.42
1:A:117:ALA:O	1:A:121:SER:HB3	2.20	0.42
1:A:171:ASP:OD2	1:A:245:PRO:HA	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:HD12	1:A:259:LEU:HA	1.90	0.41
1:H:171:ASP:O	1:H:172:PRO:C	2.61	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:L:201:ASP:C	1:L:203:ALA:H	2.29	0.41
1:A:209:LYS:HE2	1:A:213:GLY:HA2	2.02	0.41
1:F:91:GLN:HG2	1:F:95:GLN:NE2	2.34	0.41
1:F:171:ASP:C	1:F:171:ASP:OD1	2.63	0.41
1:F:211:GLU:O	1:F:211:GLU:HG2	2.19	0.41
1:G:98:LYS:HB3	1:G:98:LYS:HE2	1.68	0.41
1:K:46:GLN:HA	1:K:158:ASN:OD1	2.20	0.41
1:M:109:GLN:OE1	1:M:109:GLN:HA	2.20	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:D:183:ALA:O	1:D:187:LEU:HG	2.21	0.41
1:M:58:GLU:HG2	1:M:147:ARG:HA	2.02	0.41
1:A:216:TYR:HA	1:A:217:PRO:HD3	1.84	0.41
1:B:90:THR:HG21	1:B:121:SER:CB	2.51	0.41
1:C:153:GLY:O	1:D:44:ARG:HD2	2.21	0.41
1:D:216:TYR:HA	1:D:217:PRO:HD3	1.91	0.41
1:E:153:GLY:O	1:F:44:ARG:HD2	2.20	0.41
1:G:38:PHE:HB2	1:G:172:PRO:O	2.20	0.41
1:I:137:VAL:HG11	1:I:164:MET:CE	2.47	0.41
1:I:226:GLU:CD	1:I:226:GLU:H	2.28	0.41
1:J:139:SER:HA	1:J:140:PRO:HD3	1.88	0.41
1:L:171:ASP:HB3	1:L:172:PRO:CD	2.50	0.41
1:D:54:ARG:HD2	1:D:148:SER:HB2	2.03	0.41
1:D:67:GLN:HE22	1:D:70:GLN:NE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:GLN:OE1	1:H:258:GLN:OE1	2.39	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:K:175:VAL:O	1:K:176:ASP:C	2.62	0.40
1:L:216:TYR:CE2	1:L:218:LEU:HB2	2.56	0.40
1:E:61:ASP:CG	1:E:144:ARG:HH12	2.28	0.40
1:E:209:LYS:HB2	1:E:258:GLN:NE2	2.36	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: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: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:C:207:SER:OG	1:C:258:GLN:OE1	2.34	0.40
1:D:221:ARG:O	1:D:240:ALA:HA	2.21	0.40
1:E:233:THR:C	1:E:235:SER:H	2.29	0.40
1:H:227:VAL:HG13	1:I:147:ARG:HG3	2.03	0.40
1:M:43:VAL:HG12	1:M:164:MET:CE	2.51	0.40
1:M:175:VAL:HG21	1:M:240:ALA:HB3	2.01	0.40
1:A:63:LYS:O	1:A:64:ALA:C	2.65	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:E:205:LYS:HE3	1:E:205:LYS:HB2	1.93	0.40
1:F:184:LEU:O	1:F:188:ARG:HG3	2.21	0.40
1:G:30:GLU:HA	1:G:257:ALA:O	2.22	0.40
1:C:144:ARG:HG3	1:C:144:ARG:HH11	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%)	9	14
1	B	233/369 (63%)	216 (93%)	13 (6%)	4 (2%)	7	10
1	C	244/369 (66%)	236 (97%)	5 (2%)	3 (1%)	10	16
1	D	233/369 (63%)	222 (95%)	9 (4%)	2 (1%)	14	22
1	E	250/369 (68%)	232 (93%)	10 (4%)	8 (3%)	3	3
1	F	231/369 (63%)	211 (91%)	17 (7%)	3 (1%)	9	14
1	G	235/369 (64%)	226 (96%)	7 (3%)	2 (1%)	14	22
1	H	239/369 (65%)	228 (95%)	9 (4%)	2 (1%)	16	25
1	I	233/369 (63%)	228 (98%)	2 (1%)	3 (1%)	9	14
1	J	233/369 (63%)	225 (97%)	6 (3%)	2 (1%)	14	22
1	K	230/369 (62%)	208 (90%)	18 (8%)	4 (2%)	7	10
1	L	233/369 (63%)	216 (93%)	16 (7%)	1 (0%)	30	43
1	M	230/369 (62%)	204 (89%)	19 (8%)	7 (3%)	3	3
All	All	3059/4797 (64%)	2865 (94%)	150 (5%)	44 (1%)	9	13

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

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Mol	Chain	Res	Type
1	I	231	GLU
1	J	171	ASP
1	B	219	GLU
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%)	170 (89%)	21 (11%)	6	9
1	B	190/295 (64%)	178 (94%)	12 (6%)	16	29
1	C	199/295 (68%)	187 (94%)	12 (6%)	17	31
1	D	190/295 (64%)	175 (92%)	15 (8%)	11	19
1	E	203/295 (69%)	182 (90%)	21 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	188/295 (64%)	175 (93%)	13 (7%)	14	24
1	G	192/295 (65%)	175 (91%)	17 (9%)	9	15
1	H	195/295 (66%)	180 (92%)	15 (8%)	12	20
1	I	190/295 (64%)	179 (94%)	11 (6%)	18	32
1	J	190/295 (64%)	183 (96%)	7 (4%)	30	51
1	K	187/295 (63%)	175 (94%)	12 (6%)	16	28
1	L	190/295 (64%)	175 (92%)	15 (8%)	11	19
1	M	187/295 (63%)	172 (92%)	15 (8%)	11	19
All	All	2492/3835 (65%)	2306 (92%)	186 (8%)	12	21

All (186) 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	53	LYS
1	A	66	GLN
1	A	86	ASN
1	A	104	GLN
1	A	130	ILE
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	227	VAL
1	A	229	VAL
1	A	235	SER
1	A	246	ASN
1	A	259	LEU
1	B	27	LEU
1	B	81	GLN
1	B	89	SER
1	B	90	THR
1	B	101	VAL

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Mol	Chain	Res	Type
1	B	171	ASP
1	B	175	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
1	C	54	ARG
1	C	189	ARG
1	C	206	VAL
1	C	219	GLU
1	C	229	VAL
1	C	231	GLU
1	C	235	SER
1	C	236	VAL
1	C	247	ASN
1	C	263	VAL
1	C	269	LEU
1	D	31	LEU
1	D	47	VAL
1	D	81	GLN
1	D	90	THR
1	D	101	VAL
1	D	106	VAL
1	D	197	GLU
1	D	209	LYS
1	D	219	GLU
1	D	223	GLU
1	D	226	GLU
1	D	231	GLU
1	D	233	THR
1	D	236	VAL
1	D	259	LEU
1	E	26	THR
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

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Mol	Chain	Res	Type
1	E	147	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	31	LEU
1	F	34	ARG
1	F	73	PRO
1	F	81	GLN
1	F	92	GLU
1	F	106	VAL
1	F	171	ASP
1	F	185	LEU
1	F	201	ASP
1	F	229	VAL
1	F	239	ARG
1	F	247	ASN
1	G	25	VAL
1	G	35	THR
1	G	47	VAL
1	G	53	LYS
1	G	90	THR
1	G	98	LYS
1	G	101	VAL
1	G	144	ARG
1	G	150	VAL
1	G	198	ARG
1	G	212	ASP
1	G	225	SER
1	G	226	GLU
1	G	227	VAL
1	G	233	THR
1	G	235	SER

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Mol	Chain	Res	Type
1	G	261	GLU
1	H	25	VAL
1	H	34	ARG
1	H	63	LYS
1	H	81	GLN
1	H	89	SER
1	H	144	ARG
1	H	150	VAL
1	H	185	LEU
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	H	260	GLN
1	I	26	THR
1	I	39	ARG
1	I	89	SER
1	I	92	GLU
1	I	101	VAL
1	I	185	LEU
1	I	197	GLU
1	I	201	ASP
1	I	225	SER
1	I	226	GLU
1	I	231	GLU
1	J	89	SER
1	J	90	THR
1	J	93	GLN
1	J	238	ILE
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	106	VAL
1	K	122	LYS
1	K	176	ASP

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Mol	Chain	Res	Type
1	K	185	LEU
1	K	229	VAL
1	K	231	GLU
1	K	255	VAL
1	L	27	LEU
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	181	SER
1	L	193	SER
1	L	226	GLU
1	L	227	VAL
1	L	239	ARG
1	L	254	PHE
1	M	47	VAL
1	M	52	LEU
1	M	57	LYS
1	M	89	SER
1	M	90	THR
1	M	93	GLN
1	M	101	VAL
1	M	106	VAL
1	M	157	THR
1	M	173	ILE
1	M	179	GLN
1	M	218	LEU
1	M	219	GLU
1	M	225	SER
1	M	229	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	70	GLN
1	A	84	GLN
1	A	86	ASN

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	110	GLN
1	A	162	ASN
1	A	202	ASN
1	A	256	HIS
1	A	260	GLN
1	B	28	ASN
1	B	84	GLN
1	B	110	GLN
1	B	179	GLN
1	B	215	GLN
1	C	36	ASN
1	C	67	GLN
1	C	70	GLN
1	C	84	GLN
1	C	110	GLN
1	C	115	ASN
1	C	127	GLN
1	C	179	GLN
1	C	215	GLN
1	C	256	HIS
1	D	28	ASN
1	D	70	GLN
1	D	81	GLN
1	D	110	GLN
1	D	127	GLN
1	D	169	GLN
1	D	215	GLN
1	D	260	GLN
1	E	84	GLN
1	E	86	ASN
1	E	110	GLN
1	E	127	GLN
1	E	162	ASN
1	E	168	GLN
1	E	215	GLN
1	E	256	HIS
1	F	28	ASN
1	F	36	ASN
1	F	81	GLN
1	F	95	GLN
1	F	127	GLN

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Mol	Chain	Res	Type
1	F	162	ASN
1	F	260	GLN
1	G	36	ASN
1	G	95	GLN
1	G	104	GLN
1	G	110	GLN
1	G	169	GLN
1	G	247	ASN
1	G	260	GLN
1	H	36	ASN
1	H	81	GLN
1	H	84	GLN
1	H	86	ASN
1	H	120	GLN
1	H	179	GLN
1	H	215	GLN
1	H	256	HIS
1	H	260	GLN
1	I	81	GLN
1	I	84	GLN
1	I	93	GLN
1	I	110	GLN
1	I	120	GLN
1	I	127	GLN
1	I	195	GLN
1	I	215	GLN
1	J	81	GLN
1	J	84	GLN
1	J	110	GLN
1	J	162	ASN
1	J	168	GLN
1	J	195	GLN
1	J	215	GLN
1	J	258	GLN
1	J	260	GLN
1	K	46	GLN
1	K	84	GLN
1	K	95	GLN
1	K	120	GLN
1	K	168	GLN
1	K	169	GLN
1	K	179	GLN

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Mol	Chain	Res	Type
1	K	215	GLN
1	L	28	ASN
1	L	36	ASN
1	L	46	GLN
1	L	81	GLN
1	L	95	GLN
1	L	104	GLN
1	L	115	ASN
1	L	120	GLN
1	L	127	GLN
1	L	162	ASN
1	L	168	GLN
1	L	195	GLN
1	L	256	HIS
1	M	46	GLN
1	M	84	GLN
1	M	95	GLN
1	M	104	GLN
1	M	110	GLN
1	M	120	GLN
1	M	160	GLN
1	M	168	GLN
1	M	169	GLN
1	M	179	GLN
1	M	215	GLN
1	M	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	237/369 (64%)	1.51	64 (27%) 1 1	41, 73, 122, 134	0
1	B	235/369 (63%)	0.60	23 (9%) 13 10	30, 51, 97, 109	0
1	C	246/369 (66%)	0.62	26 (10%) 11 8	29, 51, 92, 110	0
1	D	235/369 (63%)	0.34	16 (6%) 23 20	32, 46, 90, 101	0
1	E	252/369 (68%)	0.77	31 (12%) 8 6	35, 56, 112, 139	0
1	F	233/369 (63%)	0.72	30 (12%) 7 5	36, 56, 99, 106	0
1	G	237/369 (64%)	1.15	45 (18%) 3 2	46, 77, 118, 139	0
1	H	241/369 (65%)	0.89	26 (10%) 11 8	50, 68, 97, 114	0
1	I	235/369 (63%)	0.47	22 (9%) 14 11	35, 52, 95, 105	0
1	J	235/369 (63%)	0.98	51 (21%) 2 2	39, 58, 120, 125	0
1	K	232/369 (62%)	1.13	57 (24%) 2 1	41, 68, 116, 128	0
1	L	235/369 (63%)	1.14	52 (22%) 2 2	45, 69, 113, 120	0
1	M	232/369 (62%)	1.81	78 (33%) 1 1	56, 88, 150, 157	0
All	All	3085/4797 (64%)	0.93	521 (16%) 4 3	29, 64, 118, 157	0

All (521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	11.8
1	L	27	LEU	11.6
1	A	227	VAL	11.5
1	E	274	GLY	11.3
1	G	25	VAL	11.0
1	A	27	LEU	10.9
1	K	27	LEU	10.0
1	E	269	LEU	9.2
1	J	27	LEU	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLY	8.8
1	C	269	LEU	7.1
1	A	26	THR	6.9
1	L	26	THR	6.7
1	M	254	PHE	6.7
1	M	32	PRO	6.5
1	H	263	VAL	6.5
1	C	24	THR	6.3
1	E	266	LYS	6.2
1	L	254	PHE	6.1
1	G	26	THR	6.0
1	B	26	THR	5.8
1	M	229	VAL	5.6
1	E	271	PRO	5.6
1	J	26	THR	5.6
1	A	229	VAL	5.6
1	G	27	LEU	5.5
1	J	232	GLY	5.3
1	M	243	PRO	5.3
1	B	260	GLN	5.3
1	D	27	LEU	5.2
1	D	260	GLN	5.1
1	M	216	TYR	5.1
1	M	225	SER	5.0
1	F	226	GLU	5.0
1	F	180	PRO	5.0
1	A	233	THR	4.9
1	K	231	GLU	4.9
1	E	270	ALA	4.8
1	F	260	GLN	4.8
1	H	171	ASP	4.7
1	C	268	ILE	4.7
1	J	233	THR	4.7
1	L	232	GLY	4.6
1	M	39	ARG	4.6
1	I	260	GLN	4.6
1	E	264	LYS	4.6
1	M	234	GLY	4.6
1	B	254	PHE	4.6
1	K	254	PHE	4.5
1	C	179	GLN	4.5
1	E	272	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	26	THR	4.4
1	H	25	VAL	4.4
1	M	235	SER	4.4
1	A	195	GLN	4.4
1	G	171	ASP	4.4
1	L	181	SER	4.3
1	J	260	GLN	4.2
1	I	27	LEU	4.2
1	D	231	GLU	4.2
1	E	263	VAL	4.2
1	K	221	ARG	4.2
1	I	26	THR	4.2
1	M	227	VAL	4.2
1	M	185	LEU	4.2
1	M	242	PHE	4.2
1	K	192	ALA	4.1
1	M	218	LEU	4.1
1	M	256	HIS	4.1
1	A	232	GLY	4.0
1	H	24	THR	4.0
1	G	32	PRO	4.0
1	G	232	GLY	4.0
1	L	234	GLY	4.0
1	E	247	ASN	4.0
1	M	29	THR	4.0
1	M	192	ALA	3.9
1	M	259	LEU	3.9
1	A	198	ARG	3.9
1	J	171	ASP	3.9
1	M	217	PRO	3.9
1	G	254	PHE	3.9
1	J	220	GLY	3.9
1	G	221	ARG	3.9
1	M	239	ARG	3.9
1	M	196	LEU	3.9
1	J	180	PRO	3.9
1	F	254	PHE	3.8
1	B	186	ARG	3.8
1	A	217	PRO	3.8
1	K	29	THR	3.8
1	M	240	ALA	3.8
1	J	226	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	226	GLU	3.7
1	M	247	ASN	3.7
1	A	224	PHE	3.7
1	H	234	GLY	3.7
1	K	258	GLN	3.7
1	A	228	SER	3.7
1	L	252	GLY	3.7
1	M	205	LYS	3.7
1	K	178	THR	3.6
1	A	226	GLU	3.6
1	F	183	ALA	3.6
1	B	200	GLY	3.6
1	J	218	LEU	3.6
1	E	268	ILE	3.6
1	A	172	PRO	3.6
1	C	171	ASP	3.6
1	I	231	GLU	3.6
1	C	266	LYS	3.6
1	A	179	GLN	3.6
1	J	195	GLN	3.6
1	J	32	PRO	3.6
1	K	248	GLU	3.6
1	A	254	PHE	3.5
1	L	248	GLU	3.5
1	M	221	ARG	3.5
1	M	211	GLU	3.5
1	A	218	LEU	3.5
1	F	232	GLY	3.5
1	C	26	THR	3.5
1	C	181	SER	3.5
1	C	28	ASN	3.4
1	A	39	ARG	3.4
1	B	233	THR	3.4
1	H	26	THR	3.4
1	K	32	PRO	3.4
1	A	171	ASP	3.4
1	E	273	GLN	3.4
1	A	185	LEU	3.4
1	L	32	PRO	3.4
1	G	234	GLY	3.4
1	J	254	PHE	3.4
1	L	28	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	185	LEU	3.4
1	M	233	THR	3.4
1	E	25	VAL	3.3
1	K	196	LEU	3.3
1	C	200	GLY	3.3
1	E	267	ALA	3.3
1	G	261	GLU	3.3
1	G	28	ASN	3.3
1	I	226	GLU	3.3
1	L	197	GLU	3.3
1	J	185	LEU	3.3
1	F	171	ASP	3.3
1	M	198	ARG	3.3
1	A	197	GLU	3.3
1	A	213	GLY	3.3
1	J	182	THR	3.3
1	M	182	THR	3.3
1	A	32	PRO	3.2
1	L	211	GLU	3.2
1	D	234	GLY	3.2
1	K	194	GLY	3.2
1	G	260	GLN	3.2
1	J	179	GLN	3.2
1	M	38	PHE	3.2
1	E	172	PRO	3.2
1	H	23	GLN	3.2
1	J	221	ARG	3.2
1	K	225	SER	3.2
1	F	202	ASN	3.2
1	J	245	PRO	3.2
1	F	29	THR	3.2
1	G	258	GLN	3.2
1	J	196	LEU	3.2
1	K	180	PRO	3.2
1	H	232	GLY	3.2
1	A	225	SER	3.1
1	E	214	SER	3.1
1	E	171	ASP	3.1
1	M	174	TYR	3.1
1	L	239	ARG	3.1
1	I	185	LEU	3.1
1	C	232	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	179	GLN	3.1
1	K	195	GLN	3.1
1	E	231	GLU	3.1
1	K	256	HIS	3.1
1	G	207	SER	3.1
1	L	247	ASN	3.1
1	L	178	THR	3.1
1	K	218	LEU	3.1
1	M	181	SER	3.1
1	J	247	ASN	3.1
1	A	33	GLY	3.1
1	C	264	LYS	3.0
1	F	231	GLU	3.0
1	G	219	GLU	3.0
1	J	231	GLU	3.0
1	J	227	VAL	3.0
1	F	179	GLN	3.0
1	M	180	PRO	3.0
1	M	34	ARG	3.0
1	M	194	GLY	3.0
1	J	219	GLU	3.0
1	L	172	PRO	3.0
1	K	198	ARG	3.0
1	L	225	SER	3.0
1	L	228	SER	3.0
1	E	26	THR	3.0
1	F	178	THR	3.0
1	D	171	ASP	3.0
1	M	28	ASN	3.0
1	M	241	VAL	2.9
1	K	247	ASN	2.9
1	K	250	LEU	2.9
1	G	242	PHE	2.9
1	L	171	ASP	2.9
1	M	61	ASP	2.9
1	E	233	THR	2.9
1	G	198	ARG	2.9
1	M	251	PRO	2.9
1	L	184	LEU	2.9
1	G	248	GLU	2.9
1	G	191	LEU	2.9
1	A	176	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	28	ASN	2.8
1	I	225	SER	2.8
1	C	263	VAL	2.8
1	J	29	THR	2.8
1	F	28	ASN	2.8
1	K	28	ASN	2.8
1	M	238	ILE	2.8
1	K	150	VAL	2.8
1	H	172	PRO	2.8
1	C	260	GLN	2.8
1	L	176	ASP	2.8
1	E	232	GLY	2.8
1	C	172	PRO	2.8
1	M	245	PRO	2.8
1	M	191	LEU	2.8
1	M	253	MET	2.8
1	E	226	GLU	2.8
1	G	192	ALA	2.8
1	K	240	ALA	2.8
1	D	197	GLU	2.8
1	E	260	GLN	2.8
1	M	258	GLN	2.8
1	K	174	TYR	2.7
1	K	251	PRO	2.7
1	H	221	ARG	2.7
1	M	189	ARG	2.7
1	A	38	PHE	2.7
1	J	59	GLY	2.7
1	G	216	TYR	2.7
1	G	199	ALA	2.7
1	M	199	ALA	2.7
1	H	96	ARG	2.7
1	I	254	PHE	2.7
1	A	237	THR	2.7
1	L	260	GLN	2.7
1	J	234	GLY	2.7
1	B	28	ASN	2.7
1	G	34	ARG	2.7
1	H	231	GLU	2.7
1	A	247	ASN	2.6
1	K	189	ARG	2.6
1	J	222	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	259	LEU	2.6
1	M	250	LEU	2.6
1	A	260	GLN	2.6
1	B	171	ASP	2.6
1	B	232	GLY	2.6
1	H	213	GLY	2.6
1	M	147	ARG	2.6
1	H	86	ASN	2.6
1	J	229	VAL	2.6
1	L	241	VAL	2.6
1	A	120	GLN	2.6
1	K	171	ASP	2.6
1	J	188	ARG	2.6
1	J	217	PRO	2.6
1	G	218	LEU	2.6
1	L	227	VAL	2.6
1	L	229	VAL	2.6
1	A	37	ALA	2.6
1	A	240	ALA	2.6
1	J	205	LYS	2.6
1	H	144	ARG	2.6
1	J	194	GLY	2.6
1	J	213	GLY	2.6
1	L	39	ARG	2.6
1	A	175	VAL	2.6
1	F	195	GLN	2.6
1	I	195	GLN	2.6
1	A	193	SER	2.6
1	A	257	ALA	2.6
1	G	217	PRO	2.5
1	C	242	PHE	2.5
1	J	191	LEU	2.5
1	F	227	VAL	2.5
1	M	215	GLN	2.5
1	F	235	SER	2.5
1	A	180	PRO	2.5
1	F	172	PRO	2.5
1	J	248	GLU	2.5
1	K	222	LEU	2.5
1	A	199	ALA	2.5
1	C	192	ALA	2.5
1	K	193	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	54	ARG	2.5
1	C	234	GLY	2.5
1	M	197	GLU	2.5
1	A	184	LEU	2.5
1	B	196	LEU	2.5
1	J	242	PHE	2.5
1	I	28	ASN	2.5
1	K	229	VAL	2.5
1	L	177	VAL	2.5
1	A	204	ALA	2.5
1	K	166	THR	2.5
1	M	178	THR	2.5
1	B	172	PRO	2.5
1	L	180	PRO	2.5
1	A	234	GLY	2.5
1	I	171	ASP	2.5
1	E	196	LEU	2.5
1	M	57	LYS	2.5
1	A	221	ARG	2.5
1	J	198	ARG	2.5
1	F	257	ALA	2.5
1	M	204	ALA	2.5
1	G	29	THR	2.5
1	C	262	GLY	2.4
1	K	200	GLY	2.4
1	K	205	LYS	2.4
1	K	216	TYR	2.4
1	I	259	LEU	2.4
1	D	195	GLN	2.4
1	I	179	GLN	2.4
1	H	254	PHE	2.4
1	M	224	PHE	2.4
1	M	177	VAL	2.4
1	H	199	ALA	2.4
1	K	253	MET	2.4
1	G	182	THR	2.4
1	A	223	GLU	2.4
1	F	234	GLY	2.4
1	J	212	ASP	2.4
1	B	195	GLN	2.4
1	E	27	LEU	2.4
1	M	169	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	254	PHE	2.4
1	K	242	PHE	2.4
1	J	181	SER	2.4
1	M	214	SER	2.4
1	A	169	GLN	2.4
1	B	185	LEU	2.4
1	L	186	ARG	2.4
1	L	216	TYR	2.4
1	A	63	LYS	2.4
1	J	190	GLU	2.4
1	L	233	THR	2.4
1	A	194	GLY	2.4
1	A	201	ASP	2.4
1	F	34	ARG	2.4
1	M	168	GLN	2.4
1	M	210	LEU	2.4
1	I	227	VAL	2.4
1	K	202	ASN	2.4
1	M	124	ALA	2.4
1	K	226	GLU	2.4
1	M	30	GLU	2.4
1	A	178	THR	2.3
1	I	172	PRO	2.3
1	E	234	GLY	2.3
1	A	40	ILE	2.3
1	B	198	ARG	2.3
1	C	221	ARG	2.3
1	A	215	GLN	2.3
1	C	230	ASP	2.3
1	L	224	PHE	2.3
1	M	63	LYS	2.3
1	F	36	ASN	2.3
1	G	30	GLU	2.3
1	K	219	GLU	2.3
1	M	37	ALA	2.3
1	F	233	THR	2.3
1	I	228	SER	2.3
1	D	232	GLY	2.3
1	G	33	GLY	2.3
1	B	179	GLN	2.3
1	G	179	GLN	2.3
1	A	196	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	210	LEU	2.3
1	G	256	HIS	2.3
1	H	191	LEU	2.3
1	I	196	LEU	2.3
1	H	53	LYS	2.3
1	A	248	GLU	2.3
1	H	248	GLU	2.3
1	B	180	PRO	2.3
1	D	180	PRO	2.3
1	G	172	PRO	2.3
1	D	29	THR	2.3
1	G	178	THR	2.3
1	C	198	ARG	2.3
1	K	191	LEU	2.3
1	M	201	ASP	2.3
1	A	261	GLU	2.3
1	B	219	GLU	2.3
1	F	223	GLU	2.3
1	K	215	GLN	2.3
1	M	142	SER	2.3
1	C	254	PHE	2.3
1	J	38	PHE	2.3
1	B	189	ARG	2.3
1	D	221	ARG	2.3
1	F	32	PRO	2.3
1	M	172	PRO	2.3
1	L	246	ASN	2.2
1	M	186	ARG	2.3
1	J	204	ALA	2.2
1	M	244	ASN	2.2
1	C	233	THR	2.2
1	H	151	THR	2.2
1	I	178	THR	2.2
1	I	232	GLY	2.2
1	K	220	GLY	2.2
1	M	108	LYS	2.2
1	B	231	GLU	2.2
1	G	211	GLU	2.2
1	K	224	PHE	2.2
1	A	241	VAL	2.2
1	H	155	LEU	2.2
1	G	225	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	219	GLU	2.2
1	K	39	ARG	2.2
1	A	236	VAL	2.2
1	B	229	VAL	2.2
1	F	175	VAL	2.2
1	J	172	PRO	2.2
1	M	98	LYS	2.2
1	L	196	LEU	2.2
1	L	213	GLY	2.2
1	M	170	LEU	2.2
1	M	213	GLY	2.2
1	M	220	GLY	2.2
1	G	54	ARG	2.2
1	B	95	GLN	2.2
1	A	29	THR	2.2
1	D	233	THR	2.2
1	F	182	THR	2.2
1	K	233	THR	2.2
1	A	235	SER	2.2
1	F	225	SER	2.2
1	J	214	SER	2.2
1	G	226	GLU	2.2
1	B	209	LYS	2.2
1	L	36	ASN	2.1
1	L	183	ALA	2.1
1	G	252	GLY	2.1
1	I	233	THR	2.1
1	K	173	ILE	2.1
1	E	189	ARG	2.1
1	K	30	GLU	2.1
1	K	207	SER	2.1
1	D	172	PRO	2.1
1	K	172	PRO	2.1
1	L	256	HIS	2.1
1	E	265	GLN	2.1
1	G	55	LEU	2.1
1	L	218	LEU	2.1
1	M	249	LEU	2.1
1	A	77	GLU	2.1
1	M	219	GLU	2.1
1	G	193	SER	2.1
1	J	225	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	164	MET	2.1
1	G	215	GLN	2.1
1	C	267	ALA	2.1
1	E	246	ASN	2.1
1	K	252	GLY	2.1
1	L	31	LEU	2.1
1	M	208	LEU	2.1
1	H	233	THR	2.1
1	C	223	GLU	2.1
1	G	231	GLU	2.1
1	L	226	GLU	2.1
1	M	134	TYR	2.1
1	E	258	GLN	2.1
1	L	258	GLN	2.1
1	A	177	VAL	2.1
1	K	175	VAL	2.1
1	L	175	VAL	2.1
1	L	37	ALA	2.1
1	A	170	LEU	2.1
1	A	202	ASN	2.1
1	G	185	LEU	2.1
1	H	247	ASN	2.1
1	I	202	ASN	2.1
1	L	202	ASN	2.1
1	K	34	ARG	2.1
1	K	234	GLY	2.1
1	J	197	GLU	2.1
1	J	223	GLU	2.1
1	A	205	LYS	2.1
1	L	63	LYS	2.1
1	M	212	ASP	2.1
1	K	255	VAL	2.0
1	L	242	PHE	2.0
1	L	188	ARG	2.0
1	L	192	ALA	2.0
1	J	202	ASN	2.0
1	H	209	LYS	2.0
1	G	111	TYR	2.0
1	F	228	SER	2.0
1	H	245	PRO	2.0
1	J	258	GLN	2.0
1	I	188	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	224	PHE	2.0
1	L	147	ARG	2.0
1	E	218	LEU	2.0
1	F	196	LEU	2.0
1	J	192	ALA	2.0
1	K	208	LEU	2.0
1	L	182	THR	2.0
1	K	217	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.