Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 03:36 PM EDT

PDB ID	:	4KSL
Title	:	Gumby/Fam105B in complex with linear di-ubiquitin
Authors	:	Juang, Y.-C.; Ceccarelli, D.F.; Sicheri, F.
Deposited on	:	2013-05-17
Resolution	:	2.83 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 (i) 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 (i)) were used in the production of this report:

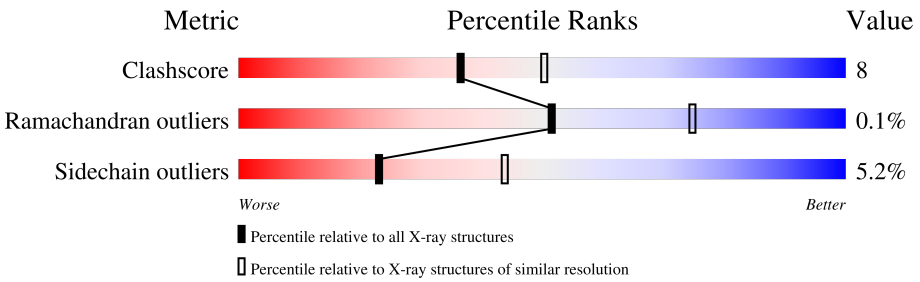
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.83 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))
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	276	77% 18% 5%
1	B	276	74% 21% 5%
1	E	276	72% 21% • 5%
1	G	276	75% 19% • 5%
1	I	276	80% 14% • 5%
1	K	276	79% 17% • •
1	M	276	70% 22% • 6%
1	O	276	76% 21% • •

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Mol	Chain	Length	Quality of chain
1	Q	276	76% 17% 5%
1	S	276	67% 26% 5%
1	U	276	66% 27% 5%
1	W	276	71% 22% 6%
2	C	156	81% 12%
2	D	156	78% 14%
2	F	156	72% 20%
2	H	156	77% 15%
2	J	156	71% 22%
2	L	156	76% 19%
2	N	156	75% 16% 5%
2	P	156	75% 18%
2	R	156	69% 24%
2	T	156	79% 13%
2	V	156	71% 24%
2	X	156	76% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40089 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 Protein FAM105B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2157	1379	367	398	13	0	0	0
1	B	263	2157	1379	367	398	13	0	0	0
1	E	262	2149	1375	365	396	13	0	0	0
1	G	261	2140	1370	364	393	13	0	0	0
1	I	262	2149	1375	365	396	13	0	0	0
1	K	270	2210	1414	376	407	13	0	0	0
1	M	260	2128	1362	363	390	13	0	0	0
1	O	270	2210	1414	376	407	13	0	0	0
1	Q	261	2140	1370	364	393	13	0	0	0
1	S	263	2153	1377	366	397	13	0	0	0
1	U	261	2140	1370	364	393	13	0	0	0
1	W	260	2132	1366	363	390	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP Q96BN8
A	78	SER	-	expression tag	UNP Q96BN8
A	129	ALA	CYS	engineered mutation	UNP Q96BN8
B	77	GLY	-	expression tag	UNP Q96BN8
B	78	SER	-	expression tag	UNP Q96BN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	129	ALA	CYS	engineered mutation	UNP Q96BN8
E	77	GLY	-	expression tag	UNP Q96BN8
E	78	SER	-	expression tag	UNP Q96BN8
E	129	ALA	CYS	engineered mutation	UNP Q96BN8
G	77	GLY	-	expression tag	UNP Q96BN8
G	78	SER	-	expression tag	UNP Q96BN8
G	129	ALA	CYS	engineered mutation	UNP Q96BN8
I	77	GLY	-	expression tag	UNP Q96BN8
I	78	SER	-	expression tag	UNP Q96BN8
I	129	ALA	CYS	engineered mutation	UNP Q96BN8
K	77	GLY	-	expression tag	UNP Q96BN8
K	78	SER	-	expression tag	UNP Q96BN8
K	129	ALA	CYS	engineered mutation	UNP Q96BN8
M	77	GLY	-	expression tag	UNP Q96BN8
M	78	SER	-	expression tag	UNP Q96BN8
M	129	ALA	CYS	engineered mutation	UNP Q96BN8
O	77	GLY	-	expression tag	UNP Q96BN8
O	78	SER	-	expression tag	UNP Q96BN8
O	129	ALA	CYS	engineered mutation	UNP Q96BN8
Q	77	GLY	-	expression tag	UNP Q96BN8
Q	78	SER	-	expression tag	UNP Q96BN8
Q	129	ALA	CYS	engineered mutation	UNP Q96BN8
S	77	GLY	-	expression tag	UNP Q96BN8
S	78	SER	-	expression tag	UNP Q96BN8
S	129	ALA	CYS	engineered mutation	UNP Q96BN8
U	77	GLY	-	expression tag	UNP Q96BN8
U	78	SER	-	expression tag	UNP Q96BN8
U	129	ALA	CYS	engineered mutation	UNP Q96BN8
W	77	GLY	-	expression tag	UNP Q96BN8
W	78	SER	-	expression tag	UNP Q96BN8
W	129	ALA	CYS	engineered mutation	UNP Q96BN8

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	149	1183	746	204	231	2	0	0	0
			Total	C	N	O	S			
2	C	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	F	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	H	149	1183	746	204	231	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	L	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	N	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	P	149	1183	746	204	231	2	0	0	0
			Total	C	N	O	S			
2	R	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	T	149	1183	746	204	231	2	0	0	0
			Total	C	N	O	S			
2	V	150	1187	748	205	232	2	0	0	0
			Total	C	N	O	S			
2	X	149	1183	746	204	231	2	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P0CG48
D	-2	ALA	-	expression tag	UNP P0CG48
D	-1	MET	-	expression tag	UNP P0CG48
C	-3	GLY	-	expression tag	UNP P0CG48
C	-2	ALA	-	expression tag	UNP P0CG48
C	-1	MET	-	expression tag	UNP P0CG48
F	-3	GLY	-	expression tag	UNP P0CG48
F	-2	ALA	-	expression tag	UNP P0CG48
F	-1	MET	-	expression tag	UNP P0CG48
H	-3	GLY	-	expression tag	UNP P0CG48
H	-2	ALA	-	expression tag	UNP P0CG48
H	-1	MET	-	expression tag	UNP P0CG48
J	-3	GLY	-	expression tag	UNP P0CG48
J	-2	ALA	-	expression tag	UNP P0CG48
J	-1	MET	-	expression tag	UNP P0CG48
L	-3	GLY	-	expression tag	UNP P0CG48
L	-2	ALA	-	expression tag	UNP P0CG48
L	-1	MET	-	expression tag	UNP P0CG48
N	-3	GLY	-	expression tag	UNP P0CG48
N	-2	ALA	-	expression tag	UNP P0CG48
N	-1	MET	-	expression tag	UNP P0CG48
P	-3	GLY	-	expression tag	UNP P0CG48
P	-2	ALA	-	expression tag	UNP P0CG48

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	MET	-	expression tag	UNP P0CG48
R	-3	GLY	-	expression tag	UNP P0CG48
R	-2	ALA	-	expression tag	UNP P0CG48
R	-1	MET	-	expression tag	UNP P0CG48
T	-3	GLY	-	expression tag	UNP P0CG48
T	-2	ALA	-	expression tag	UNP P0CG48
T	-1	MET	-	expression tag	UNP P0CG48
V	-3	GLY	-	expression tag	UNP P0CG48
V	-2	ALA	-	expression tag	UNP P0CG48
V	-1	MET	-	expression tag	UNP P0CG48
X	-3	GLY	-	expression tag	UNP P0CG48
X	-2	ALA	-	expression tag	UNP P0CG48
X	-1	MET	-	expression tag	UNP P0CG48

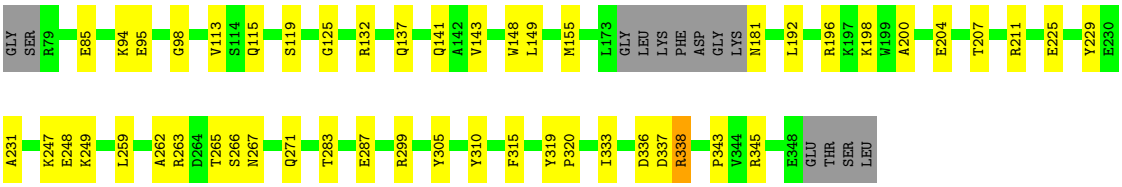
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

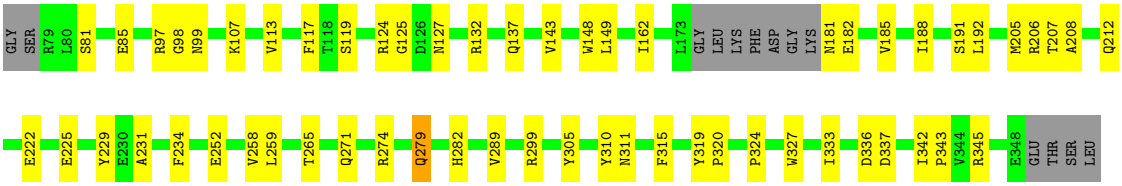
• Molecule 1: Protein FAM105B

Chain A: 77% 18% 5%



• Molecule 1: Protein FAM105B

Chain B: 74% 21% 5%

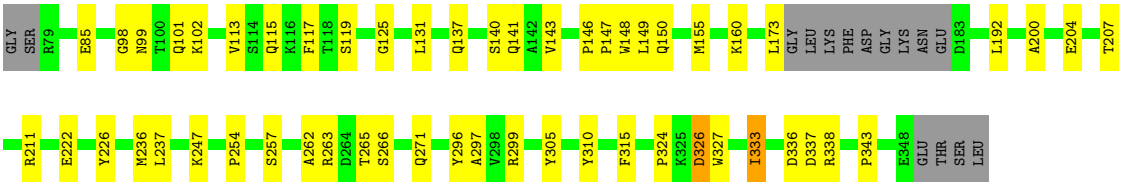


• Molecule 1: Protein FAM105B

Chain E: 72% 21% • 5%

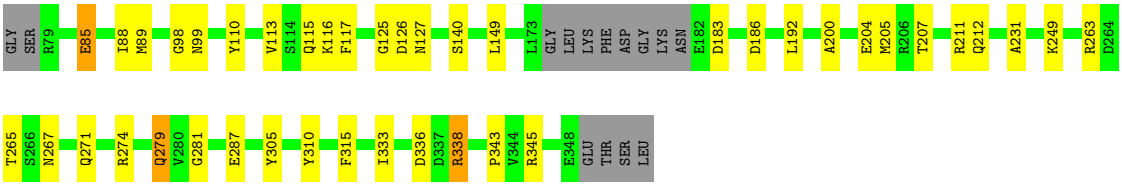
• Molecule 1: Protein FAM105B

Chain G: 75% 19% • 5%



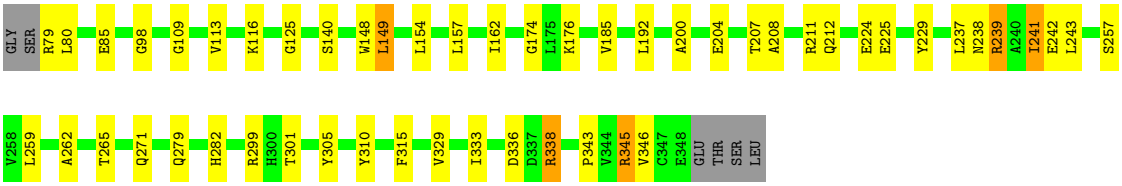
- Molecule 1: Protein FAM105B

Chain I:



- Molecule 1: Protein FAM105B

Chain K:

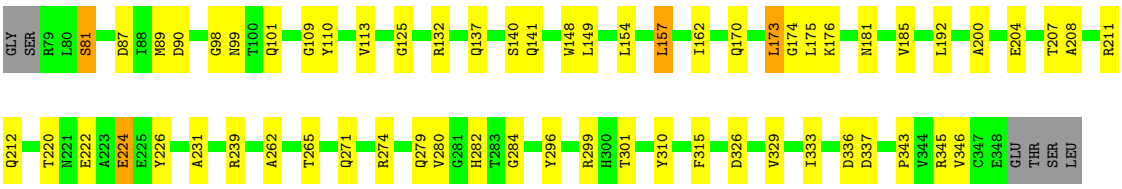


- Molecule 1: Protein FAM105B

Chain M:

- Molecule 1: Protein FAM105B

Chain O:



- Molecule 1: Protein FAM105B

Chain Q: 76% 17% • 5%

GLY SER R79 R97 G98 N99 F117 G125 D126 N127 Y128 A129 A130 L131 L135 F136 Q137 S140 Q141 W148 L149 M155 L161 L173 GLY LEU LYS PHE ASP GLY LYS ASN GLU D183 L184 V185 D186 K187 L192 T193 R196 A200 E204 M205 R206 T207

R211 N221 E222 A223 E224 E225 Y229 E230 A231 L243 P254 S257 V258 A262 T265 R299 Q303 Y310 F315 Y319 P320 D326 T331 L332 I333 R338 I342 P343 E348 GLU THR SER LEU

• Molecule 1: Protein FAM105B

Chain S: 67% 26% • 5%

GLY SER R79 I88 M89 R97 G98 N99 T100 Q101 G109 Y110 V113 F117 G125 D126 N127 Y128 Q137 Q141 A142 V143 W148 L149 L157 P158 E159 K160 L161 I162 Y165 N166 W167 I168 W171 K172 L173 G174 LEU LYS PHE ASP GLY LYS ASN E182 D183 L184

V185 D186 K187 E190 S191 L192 R196 A200 E204 M205 R206 T207 R211 E217 L218 F219 T220 E224 E225 Y226 S227 L228 Y229 E230 A231 V232 K233 L237 N238 R239 A240 I241 K247 E248 K249 G250 K251 A262 P269 H276 L277 V280 G281 L293 R299

H300 T301 Y310 F315 V329 I333 D336 D337 R338 P343 V344 R345 V346 C347 E348 GLU THR SER LEU

• Molecule 1: Protein FAM105B

Chain U: 66% 27% • 5%

GLY SER R79 L80 S81 M89 D90 Y91 C92 K93 R97 G98 G109 V113 S114 Q115 K116 F117 R122 G125 D126 N127 Q137 S140 Q141 A142 V143 G144 L145 P146 P147 W148 L149 Y165 N166 W167 I168 K169 Q170 W171 K172 L173 GLY LEU LYS PHE ASP GLY LYS ASN GLU

D183 D186 K187 S191 L194 A200 E204 M205 R206 T207 R211 E222 A223 E224 E225 Y226 S227 L228 Y229 E230 A231 L243 Y244 N245 K249 E252 V253 P254 S257 A262 T265 N275 Q279 T283 R299 Q303 V304 Y305 Y310 F315

Y319 P320 T321 D322 D326 V330 T331 L332 I333 D336 D337 R338 I342 P343 V344 R345 V346 C347 E348 GLU THR SER LEU

• Molecule 1: Protein FAM105B

Chain W: 71% 22% • 6%

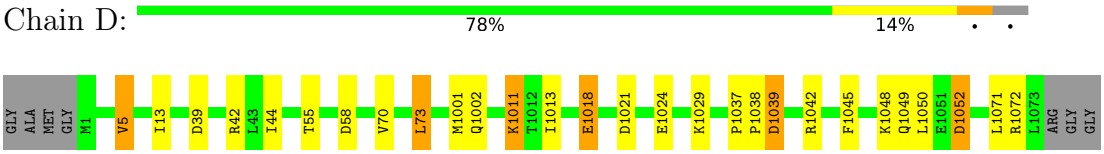
GLY SER R79 K94 E95 W96 R97 G98 G109 V113 S114 Q115 K116 G125 D126 N127 Y128 A129 A130 L131 Q137 S140 Q141 A142 V143 E159 K164 Y165 N166 W167 I168 K169 Q170 L173 GLY LEU LYS PHE ASP GLY LYS ASN GLU ASP L184 K189 L192 T193 L194

A200 E204 M205 R206 T207 R211 N221 E222 A223 E224 E225 Y226 S227 L228 A231 M236 L237 A240 V258 L259 A262 T265 P269 G270 Q271 L272 L273 R274 H282 L293 T301 Y305 Y310 F315 Y319 P320 V329 V330 I333

D336 D337 R338 I342 P343 V344 R345 E348 GLU THR SER LEU

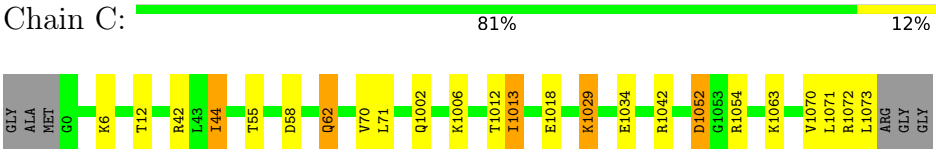
• Molecule 2: Polyubiquitin-C

Chain D:



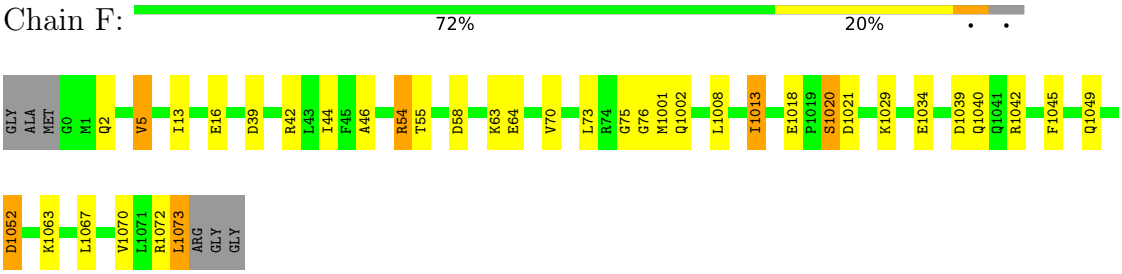
• Molecule 2: Polyubiquitin-C

Chain C:



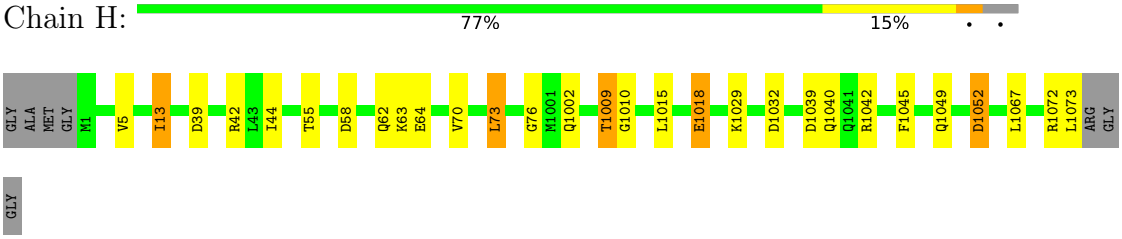
• Molecule 2: Polyubiquitin-C

Chain F:



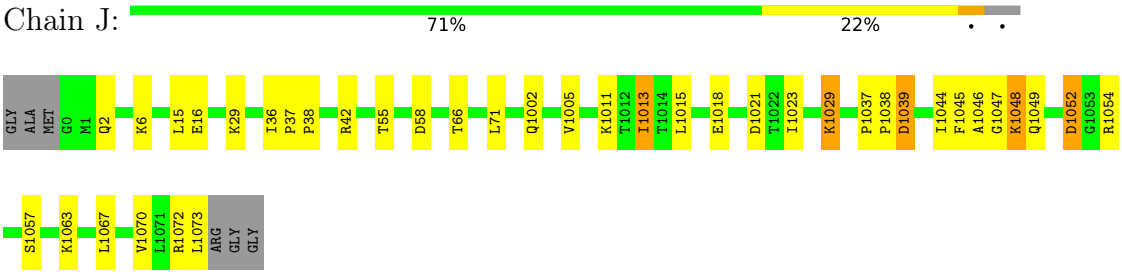
• Molecule 2: Polyubiquitin-C

Chain H:



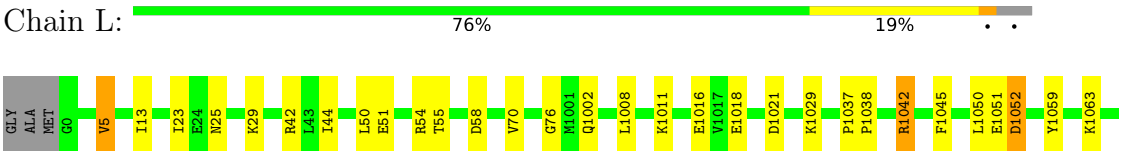
• Molecule 2: Polyubiquitin-C

Chain J:



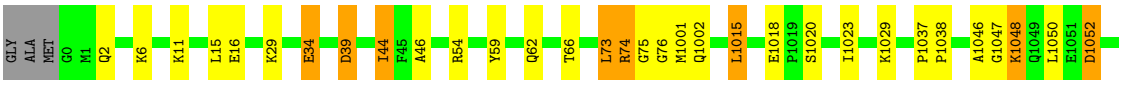
• Molecule 2: Polyubiquitin-C

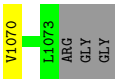
Chain L:



• Molecule 2: Polyubiquitin-C

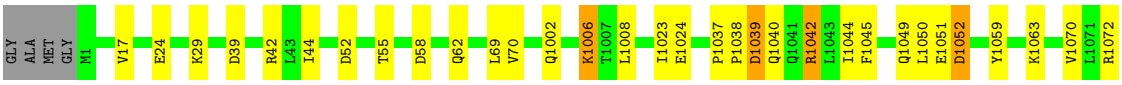
Chain N:





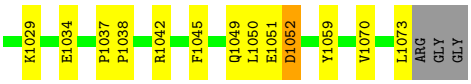
• Molecule 2: Polyubiquitin-C

Chain P:



• Molecule 2: Polyubiquitin-C

Chain R:

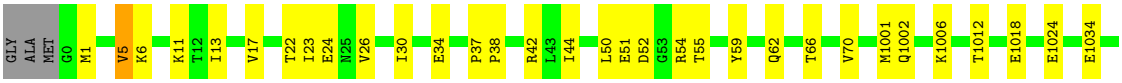


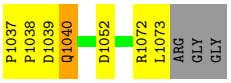
• Molecule 2: Polyubiquitin-C

Chain T:

• Molecule 2: Polyubiquitin-C

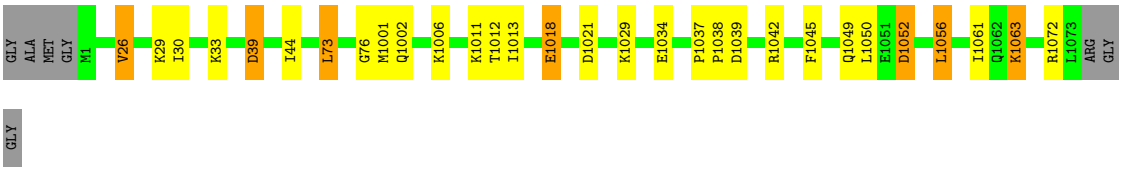
Chain V:





• Molecule 2: Polyubiquitin-C

Chain X:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	183.62Å 186.09Å 219.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.83	Depositor
% Data completeness (in resolution range)	96.7 (50.00-2.83)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.224 , 0.254	Depositor
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.336	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
Total number of atoms	40089	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9919e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.28	0/2204	0.51	0/2981
1	B	0.27	0/2204	0.50	0/2981
1	E	0.28	0/2196	0.50	0/2970
1	G	0.28	0/2187	0.52	0/2958
1	I	0.27	0/2196	0.49	0/2970
1	K	0.28	0/2259	0.51	0/3054
1	M	0.28	0/2175	0.52	0/2941
1	O	0.28	0/2259	0.51	0/3054
1	Q	0.29	0/2187	0.51	0/2958
1	S	0.29	0/2200	0.51	0/2975
1	U	0.28	0/2187	0.51	0/2958
1	W	0.28	0/2179	0.51	0/2947
2	C	0.26	0/1200	0.52	0/1616
2	D	0.25	0/1196	0.51	0/1611
2	F	0.25	0/1200	0.52	0/1616
2	H	0.26	0/1196	0.53	0/1611
2	J	0.26	0/1200	0.53	0/1616
2	L	0.27	0/1200	0.52	0/1616
2	N	0.28	0/1200	0.53	0/1616
2	P	0.27	0/1196	0.52	0/1611
2	R	0.27	0/1200	0.52	0/1616
2	T	0.25	0/1196	0.51	0/1611
2	V	0.26	0/1200	0.56	0/1616
2	X	0.26	0/1196	0.53	0/1611
All	All	0.27	0/40813	0.51	0/55114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2157	0	2152	34	0
1	B	2157	0	2152	36	0
1	E	2149	0	2146	46	0
1	G	2140	0	2140	33	0
1	I	2149	0	2146	32	0
1	K	2210	0	2209	35	0
1	M	2128	0	2128	49	0
1	O	2210	0	2209	46	0
1	Q	2140	0	2140	34	0
1	S	2153	0	2149	59	0
1	U	2140	0	2140	50	0
1	W	2132	0	2136	48	0
2	C	1187	0	1240	14	0
2	D	1183	0	1237	23	0
2	F	1187	0	1240	21	0
2	H	1183	0	1237	18	0
2	J	1187	0	1240	26	0
2	L	1187	0	1240	18	0
2	N	1187	0	1240	22	0
2	P	1183	0	1237	23	0
2	R	1187	0	1240	27	0
2	T	1183	0	1237	14	0
2	V	1187	0	1240	24	0
2	X	1183	0	1237	24	0
All	All	40089	0	40712	641	0

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

All (641) 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)
2:V:1039:ASP:O	2:V:1072:ARG:NH1	1.96	0.98
1:A:98:GLY:HA2	1:K:207:THR:HA	1.47	0.97
1:G:207:THR:HA	1:I:98:GLY:HA2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLY:HA2	1:U:207:THR:HA	1.45	0.97
1:I:207:THR:HA	1:W:98:GLY:HA2	1.48	0.95
1:A:207:THR:HA	1:Q:98:GLY:HA2	1.48	0.95
1:E:207:THR:HA	1:M:98:GLY:HA2	1.46	0.95
2:X:1042:ARG:HH11	2:X:1072:ARG:HH21	1.13	0.94
1:B:98:GLY:HA2	1:O:207:THR:HA	1.48	0.94
1:G:98:GLY:HA2	1:W:207:THR:HA	1.48	0.92
1:O:98:GLY:HA2	1:S:207:THR:HA	1.53	0.91
1:K:98:GLY:HA2	1:Q:207:THR:HA	1.52	0.91
1:M:125:GLY:HA3	2:N:1002:GLN:HG2	1.53	0.90
1:B:125:GLY:HA3	2:C:1002:GLN:HG2	1.55	0.87
1:U:125:GLY:HA3	2:V:1002:GLN:HG2	1.57	0.87
1:B:207:THR:HA	1:S:98:GLY:HA2	1.56	0.87
1:A:125:GLY:HA3	2:D:1002:GLN:HG2	1.57	0.87
1:B:336:ASP:OD1	2:C:1029:LYS:NZ	2.09	0.86
2:D:1042:ARG:HH11	2:D:1072:ARG:HH21	1.19	0.85
1:K:125:GLY:HA3	2:L:1002:GLN:HG2	1.57	0.85
2:X:1039:ASP:O	2:X:1072:ARG:NH1	2.09	0.85
1:M:286:LEU:O	2:N:74:ARG:O	1.96	0.83
2:T:1042:ARG:NH1	2:T:1049:GLN:OE1	2.11	0.83
1:M:207:THR:HA	1:U:98:GLY:HA2	1.60	0.82
1:E:116:LYS:HG2	1:M:115:GLN:HE22	1.43	0.82
1:O:125:GLY:HA3	2:P:1002:GLN:HG2	1.58	0.82
1:I:125:GLY:HA3	2:J:1002:GLN:HG2	1.61	0.82
1:G:125:GLY:HA3	2:H:1002:GLN:HG2	1.61	0.81
1:S:125:GLY:HA3	2:T:1002:GLN:HG2	1.61	0.81
2:D:1039:ASP:O	2:D:1072:ARG:NH1	2.13	0.81
1:A:115:GLN:HE22	1:K:116:LYS:HG2	1.47	0.79
1:E:125:GLY:HA3	2:F:1002:GLN:HG2	1.64	0.79
2:R:1042:ARG:NH1	2:R:1049:GLN:OE1	2.15	0.78
1:Q:125:GLY:HA3	2:R:1002:GLN:HG2	1.66	0.78
1:I:336:ASP:OD1	2:J:1029:LYS:NZ	2.16	0.78
2:V:5:VAL:HG13	2:V:13:ILE:HB	1.64	0.78
2:D:5:VAL:HG13	2:D:13:ILE:HB	1.67	0.77
1:Q:206:ARG:H	1:Q:206:ARG:HD2	1.49	0.76
1:U:279:GLN:OE1	1:U:283:THR:OG1	2.03	0.76
1:O:140:SER:O	1:O:211:ARG:NH1	2.16	0.76
1:I:140:SER:O	1:I:211:ARG:NH1	2.19	0.75
1:Q:155:MET:HE2	1:Q:196:ARG:HE	1.52	0.75
2:R:63:LYS:HG2	2:R:64:GLU:HG3	1.69	0.74
2:L:23:ILE:HD13	2:L:50:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:GLN:O	1:I:115:GLN:NE2	2.19	0.74
1:Q:140:SER:O	1:Q:211:ARG:NH1	2.20	0.74
1:M:115:GLN:O	1:U:115:GLN:NE2	2.21	0.73
2:J:1054:ARG:HH22	1:O:271:GLN:HE21	1.37	0.73
1:W:125:GLY:HA3	2:X:1002:GLN:HG2	1.70	0.72
1:S:149:LEU:HD21	1:S:196:ARG:HA	1.72	0.72
1:E:338:ARG:HA	2:F:75:GLY:HA2	1.71	0.72
1:K:140:SER:O	1:K:211:ARG:NH1	2.22	0.72
2:H:1040:GLN:OE1	1:W:206:ARG:NH2	2.23	0.71
1:E:137:GLN:HE22	1:E:342:ILE:HG23	1.54	0.71
1:Q:137:GLN:HE22	1:Q:342:ILE:HG23	1.56	0.71
1:I:338:ARG:NH1	2:J:1021:ASP:OD2	2.24	0.71
2:L:5:VAL:HG23	2:L:13:ILE:HB	1.72	0.70
2:D:1042:ARG:NH2	2:D:1049:GLN:OE1	2.25	0.70
1:E:338:ARG:NH1	2:F:1021:ASP:OD1	2.25	0.70
1:I:274:ARG:O	1:I:279:GLN:NE2	2.25	0.70
1:Q:254:PRO:O	1:Q:257:SER:OG	2.07	0.70
2:F:5:VAL:HG13	2:F:13:ILE:HB	1.73	0.70
1:O:170:GLN:HG2	1:O:274:ARG:HG2	1.75	0.68
1:E:326:ASP:OD1	1:E:326:ASP:N	2.25	0.68
1:W:159:GLU:H	1:W:189:LYS:HZ1	1.40	0.67
1:Q:243:LEU:HD21	1:Q:257:SER:HB2	1.76	0.67
1:E:116:LYS:HG2	1:M:115:GLN:NE2	2.09	0.67
2:C:62:GLN:HE22	2:F:46:ALA:HA	1.60	0.67
1:G:140:SER:O	1:G:211:ARG:NH1	2.26	0.67
1:I:116:LYS:HG2	1:W:115:GLN:NE2	2.10	0.67
1:U:172:LYS:HD3	1:U:173:LEU:H	1.60	0.66
2:J:15:LEU:HD22	2:J:29:LYS:HG3	1.78	0.66
2:H:1009:THR:OG1	2:H:1010:GLY:N	2.29	0.66
1:S:345:ARG:HG2	1:S:346:VAL:H	1.60	0.65
2:D:1042:ARG:HH11	2:D:1072:ARG:NH2	1.94	0.65
1:W:140:SER:O	1:W:211:ARG:NH1	2.26	0.65
1:E:345:ARG:HG2	1:E:346:VAL:H	1.62	0.65
2:F:1040:GLN:OE1	1:U:206:ARG:NH2	2.30	0.65
1:A:115:GLN:NE2	1:K:116:LYS:HG2	2.12	0.65
1:U:97:ARG:NH1	2:V:1034:GLU:OE1	2.30	0.65
2:V:11:LYS:NZ	2:V:34:GLU:OE1	2.31	0.64
2:J:1049:GLN:HB3	1:O:176:LYS:HG3	1.80	0.64
1:B:274:ARG:O	1:B:279:GLN:NE2	2.31	0.64
1:S:184:LEU:HA	1:S:187:LYS:HD2	1.78	0.64
1:S:249:LYS:HE3	1:S:251:LYS:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1005:VAL:HB	2:J:1013:ILE:HG13	1.79	0.63
1:M:124:ARG:NH1	1:M:226:TYR:OH	2.31	0.63
2:X:73:LEU:HD13	2:X:1018:GLU:HG3	1.80	0.63
1:W:97:ARG:NH1	2:X:1034:GLU:OE1	2.32	0.62
2:F:63:LYS:HG2	2:F:64:GLU:HG3	1.82	0.62
2:N:46:ALA:HA	2:P:62:GLN:HE22	1.64	0.62
1:S:336:ASP:OD2	2:T:1029:LYS:NZ	2.26	0.62
1:G:99:ASN:HB2	1:W:143:VAL:HG12	1.81	0.61
1:S:173:LEU:HD21	1:S:187:LYS:HD3	1.83	0.61
1:I:116:LYS:HG2	1:W:115:GLN:HE22	1.65	0.61
1:G:297:ALA:O	1:G:299:ARG:NH1	2.34	0.61
2:H:63:LYS:HG2	2:H:64:GLU:HG3	1.82	0.61
1:W:271:GLN:HG2	1:W:274:ARG:NH2	2.15	0.61
2:C:55:THR:OG1	2:C:58:ASP:OD2	2.13	0.61
2:H:73:LEU:HD23	2:H:1018:GLU:HG3	1.82	0.60
1:M:139:MET:HG2	1:M:199:TRP:CE3	2.36	0.60
1:W:338:ARG:NH1	2:X:1021:ASP:OD2	2.34	0.60
2:C:6:LYS:HG2	2:C:12:THR:HG22	1.82	0.60
1:G:333:ILE:HG22	1:G:343:PRO:HD3	1.84	0.60
1:M:336:ASP:OD2	2:N:1029:LYS:NZ	2.26	0.60
1:U:140:SER:O	1:U:211:ARG:NE	2.24	0.60
1:A:247:LYS:NZ	1:A:248:GLU:OE2	2.34	0.59
1:E:345:ARG:HG2	1:E:346:VAL:N	2.17	0.59
1:M:326:ASP:OD2	1:M:326:ASP:N	2.29	0.59
1:U:168:ILE:H	1:U:168:ILE:HD12	1.67	0.59
2:T:22:THR:HA	2:T:55:THR:HA	1.84	0.59
1:U:165:TYR:HB2	1:U:168:ILE:HD11	1.84	0.59
1:K:239:ARG:NH2	1:K:242:GLU:OE2	2.34	0.59
1:O:173:LEU:HD23	1:O:173:LEU:H	1.68	0.59
2:D:1024:GLU:HG2	2:D:1052:ASP:HB3	1.85	0.59
2:F:1018:GLU:OE1	2:F:1020:SER:OG	2.16	0.59
1:W:159:GLU:N	1:W:189:LYS:HZ1	2.01	0.59
1:U:117:PHE:CD1	1:U:343:PRO:HB2	2.38	0.58
1:K:345:ARG:HG2	1:K:346:VAL:H	1.66	0.58
1:M:146:PRO:HD3	1:M:199:TRP:NE1	2.19	0.58
1:S:182:GLU:HB3	1:S:187:LYS:HE3	1.85	0.58
2:X:1042:ARG:HH11	2:X:1072:ARG:NH2	1.93	0.58
2:H:1042:ARG:NH1	2:H:1049:GLN:OE1	2.37	0.58
1:S:148:TRP:CG	1:S:299:ARG:HD2	2.39	0.58
1:S:345:ARG:HG2	1:S:346:VAL:N	2.19	0.58
1:W:200:ALA:O	1:W:204:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LEU:HD23	1:E:231:ALA:HB1	1.86	0.58
2:P:1023:ILE:HB	2:P:1052:ASP:HA	1.84	0.57
1:Q:129:ALA:HB3	2:R:76:GLY:HA2	1.86	0.57
1:E:333:ILE:HG13	1:E:343:PRO:HD3	1.86	0.57
1:O:137:GLN:O	1:O:141:GLN:HG2	2.04	0.57
1:Q:243:LEU:CD2	1:Q:257:SER:HB2	2.33	0.57
2:J:1046:ALA:HB3	2:J:1048:LYS:HE3	1.86	0.57
1:S:281:GLY:O	2:T:1063:LYS:NZ	2.37	0.57
1:E:140:SER:O	1:E:211:ARG:NH1	2.34	0.57
1:W:168:ILE:HD12	1:W:237:LEU:HD21	1.86	0.57
2:P:1024:GLU:HG3	2:P:1052:ASP:HB3	1.87	0.57
1:Q:310:TYR:HA	1:Q:315:PHE:CD2	2.39	0.57
2:R:73:LEU:HD23	2:R:1018:GLU:HG3	1.86	0.56
2:D:73:LEU:HD13	2:D:1018:GLU:HG3	1.88	0.56
1:E:262:ALA:HB3	2:F:44:ILE:HD13	1.87	0.56
1:G:326:ASP:OD1	1:G:326:ASP:N	2.35	0.56
1:M:194:LEU:HD21	1:M:224:GLU:HB3	1.86	0.56
1:M:338:ARG:HD2	2:N:1018:GLU:HB2	1.87	0.56
2:N:1046:ALA:HB3	2:N:1048:LYS:HE3	1.87	0.56
1:U:148:TRP:CG	1:U:299:ARG:HD2	2.41	0.56
1:A:338:ARG:NH1	2:D:1021:ASP:OD2	2.39	0.56
2:D:1045:PHE:HB3	2:D:1050:LEU:HD21	1.87	0.56
1:K:336:ASP:OD1	2:L:1029:LYS:NZ	2.33	0.56
1:K:345:ARG:HG2	1:K:346:VAL:N	2.21	0.56
1:G:200:ALA:O	1:G:204:GLU:HG2	2.06	0.56
2:P:1040:GLN:NE2	2:P:1072:ARG:O	2.37	0.56
1:S:168:ILE:HD12	1:S:237:LEU:HD21	1.87	0.56
2:N:15:LEU:HD22	2:N:29:LYS:HG3	1.88	0.56
2:X:39:ASP:OD1	2:X:39:ASP:N	2.31	0.55
2:L:1051:GLU:HG2	2:L:1059:TYR:OH	2.06	0.55
1:E:99:ASN:HB2	1:U:143:VAL:HG12	1.88	0.55
1:E:113:VAL:HG22	1:E:305:TYR:CD1	2.41	0.55
2:J:1072:ARG:O	2:J:1073:LEU:HB2	2.06	0.55
1:O:265:THR:O	1:O:271:GLN:HB3	2.07	0.55
1:W:129:ALA:HB3	2:X:76:GLY:HA2	1.87	0.55
2:F:1045:PHE:HB2	2:F:1067:LEU:HD22	1.89	0.55
2:T:16:GLU:O	2:T:29:LYS:NZ	2.40	0.55
1:G:113:VAL:HG22	1:G:305:TYR:CD2	2.42	0.55
1:Q:99:ASN:ND2	1:Q:99:ASN:O	2.39	0.55
1:K:333:ILE:HG13	1:K:343:PRO:HD3	1.88	0.55
1:E:310:TYR:HA	1:E:315:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:224:GLU:O	1:U:228:LEU:HG	2.07	0.54
1:E:200:ALA:O	1:E:204:GLU:HG2	2.08	0.54
1:W:222:GLU:HB3	1:W:226:TYR:CE2	2.42	0.54
1:S:310:TYR:HA	1:S:315:PHE:CD1	2.42	0.54
1:E:336:ASP:O	1:E:338:ARG:N	2.41	0.54
1:E:137:GLN:O	1:E:141:GLN:HG2	2.08	0.54
1:O:148:TRP:CD1	1:O:299:ARG:HD2	2.43	0.54
1:W:113:VAL:HG22	1:W:305:TYR:CD1	2.43	0.54
1:U:91:TYR:OH	1:U:122:ARG:NH2	2.37	0.54
2:V:23:ILE:HB	2:V:52:ASP:HA	1.89	0.54
1:Q:117:PHE:CD1	1:Q:343:PRO:HB2	2.43	0.54
1:U:113:VAL:HG22	1:U:305:TYR:CD1	2.42	0.54
1:M:145:LEU:HA	1:M:199:TRP:HE1	1.73	0.54
1:S:137:GLN:O	1:S:141:GLN:HG2	2.08	0.54
1:S:182:GLU:HB3	1:S:187:LYS:CE	2.38	0.54
1:B:259:LEU:HD23	2:C:44:ILE:HD11	1.88	0.54
1:S:262:ALA:HB3	2:T:44:ILE:HD13	1.90	0.54
1:A:113:VAL:HG22	1:A:305:TYR:CD2	2.43	0.53
1:G:336:ASP:OD1	2:H:1029:LYS:NZ	2.27	0.53
1:U:137:GLN:O	1:U:141:GLN:HG2	2.09	0.53
1:Q:243:LEU:HD21	1:Q:257:SER:CB	2.37	0.53
1:Q:338:ARG:NH1	2:R:1021:ASP:OD2	2.41	0.53
1:K:113:VAL:HG22	1:K:305:TYR:CD1	2.44	0.53
2:X:1011:LYS:HG2	2:X:1012:THR:H	1.74	0.53
1:M:162:ILE:HD13	1:M:185:VAL:HG22	1.89	0.53
1:O:99:ASN:HB2	1:S:143:VAL:HG12	1.90	0.53
1:O:262:ALA:HB3	2:P:44:ILE:HD13	1.89	0.53
2:V:1024:GLU:HG2	2:V:1052:ASP:HB3	1.91	0.53
1:E:333:ILE:HD11	1:E:343:PRO:HB3	1.91	0.52
1:G:262:ALA:HB3	2:H:44:ILE:HD13	1.90	0.52
2:P:1051:GLU:HG2	2:P:1059:TYR:OH	2.09	0.52
1:W:224:GLU:O	1:W:228:LEU:HG	2.10	0.52
1:B:188:ILE:HD13	1:B:234:PHE:CD1	2.45	0.52
2:C:1042:ARG:HB3	2:C:1070:VAL:HG22	1.90	0.52
1:S:217:GLU:O	1:S:220:THR:OG1	2.28	0.52
1:I:265:THR:O	1:I:271:GLN:HB3	2.09	0.52
2:N:1052:ASP:N	2:N:1052:ASP:OD2	2.42	0.52
1:A:137:GLN:O	1:A:141:GLN:HG2	2.09	0.52
1:B:124:ARG:NH1	1:B:222:GLU:OE2	2.40	0.52
2:P:1045:PHE:HB3	2:P:1050:LEU:HD21	1.91	0.52
1:U:310:TYR:HA	1:U:315:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1042:ARG:CZ	2:X:1049:GLN:HE22	2.22	0.52
1:A:310:TYR:HA	1:A:315:PHE:CD1	2.45	0.51
1:G:148:TRP:CD1	1:G:299:ARG:HG3	2.45	0.51
2:F:54:ARG:NH1	2:F:58:ASP:OD1	2.44	0.51
1:S:333:ILE:HG13	1:S:343:PRO:HD3	1.91	0.51
1:U:333:ILE:HG13	1:U:343:PRO:HD3	1.92	0.51
1:G:310:TYR:HA	1:G:315:PHE:CD1	2.45	0.51
1:S:97:ARG:NH1	2:T:1034:GLU:OE1	2.44	0.51
1:U:191:SER:HB3	1:U:231:ALA:HB2	1.93	0.51
1:Q:148:TRP:CG	1:Q:299:ARG:HD2	2.46	0.51
1:S:224:GLU:O	1:S:228:LEU:HG	2.10	0.51
1:G:137:GLN:O	1:G:141:GLN:HG2	2.10	0.51
1:B:192:LEU:HD23	1:B:231:ALA:HB1	1.93	0.51
1:E:141:GLN:HA	1:E:211:ARG:NH1	2.26	0.51
2:R:1024:GLU:CG	2:R:1052:ASP:HB3	2.41	0.51
1:W:159:GLU:HB2	1:W:189:LYS:HZ3	1.75	0.51
1:W:310:TYR:HA	1:W:315:PHE:CD1	2.45	0.51
1:K:310:TYR:HA	1:K:315:PHE:CD1	2.46	0.51
1:Q:200:ALA:O	1:Q:204:GLU:HG2	2.11	0.51
1:U:165:TYR:HB2	1:U:168:ILE:CD1	2.41	0.51
1:M:263:ARG:HB2	1:M:266:SER:HB3	1.93	0.50
1:A:192:LEU:HD23	1:A:231:ALA:HB1	1.93	0.50
2:F:1042:ARG:NH1	2:F:1049:GLN:OE1	2.44	0.50
1:I:281:GLY:O	2:J:1063:LYS:NZ	2.44	0.50
1:S:162:ILE:HD12	1:S:185:VAL:HG22	1.92	0.50
2:T:1005:VAL:HB	2:T:1013:ILE:HG13	1.93	0.50
1:B:97:ARG:NH1	2:C:1034:GLU:OE1	2.44	0.50
2:C:1006:LYS:HG3	2:C:1012:THR:HG22	1.93	0.50
1:E:265:THR:O	1:E:271:GLN:HB3	2.11	0.50
1:K:262:ALA:HB3	2:L:44:ILE:HD13	1.94	0.50
2:N:39:ASP:OD2	2:N:39:ASP:N	2.45	0.50
2:R:42:ARG:HB3	2:R:70:VAL:O	2.11	0.50
1:K:157:LEU:HD21	1:K:238:ASN:CG	2.32	0.50
1:K:241:ILE:HG13	1:K:242:GLU:N	2.26	0.50
1:S:89:MET:HE3	1:S:110:TYR:O	2.12	0.50
1:W:137:GLN:O	1:W:141:GLN:HG2	2.12	0.50
1:B:107:LYS:HE3	1:O:346:VAL:HG11	1.93	0.50
1:B:113:VAL:HG22	1:B:305:TYR:CD1	2.46	0.50
1:A:333:ILE:HD11	1:A:343:PRO:HB3	1.94	0.50
2:J:1015:LEU:HD22	2:J:1029:LYS:HG2	1.93	0.50
1:M:117:PHE:CD1	1:M:343:PRO:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:117:PHE:CD1	1:S:343:PRO:HB2	2.47	0.50
2:V:23:ILE:HD13	2:V:51:GLU:O	2.12	0.50
1:W:164:LYS:HE3	1:W:165:TYR:CZ	2.47	0.50
2:N:6:LYS:HE2	2:N:66:THR:HG21	1.93	0.50
1:A:94:LYS:HE3	1:A:95:GLU:OE2	2.12	0.49
1:E:85:GLU:HB2	1:E:119:SER:HB3	1.93	0.49
2:F:1072:ARG:O	2:F:1073:LEU:HB3	2.13	0.49
1:M:137:GLN:O	1:M:141:GLN:HG2	2.12	0.49
1:M:265:THR:O	1:M:271:GLN:HB3	2.12	0.49
1:O:192:LEU:HD23	1:O:231:ALA:HB1	1.94	0.49
1:O:310:TYR:HA	1:O:315:PHE:CD2	2.46	0.49
2:R:1024:GLU:HG2	2:R:1052:ASP:HB3	1.94	0.49
1:K:237:LEU:O	1:K:241:ILE:HG23	2.12	0.49
1:A:148:TRP:CD1	1:A:299:ARG:HD2	2.47	0.49
1:A:265:THR:O	1:A:271:GLN:HB3	2.13	0.49
1:I:200:ALA:O	1:I:204:GLU:HG2	2.12	0.49
1:S:159:GLU:OE1	1:S:185:VAL:HG11	2.13	0.49
2:V:24:GLU:HG3	2:V:52:ASP:HB3	1.94	0.49
1:A:262:ALA:HB3	2:D:44:ILE:HD13	1.95	0.49
2:F:1013:ILE:HD13	2:F:1034:GLU:HG3	1.94	0.49
1:I:310:TYR:HA	1:I:315:PHE:CD1	2.47	0.49
2:R:11:LYS:NZ	2:R:34:GLU:OE1	2.45	0.49
1:B:265:THR:O	1:B:271:GLN:HB3	2.12	0.49
1:B:310:TYR:HA	1:B:315:PHE:CD1	2.47	0.49
2:F:55:THR:OG1	2:F:58:ASP:OD2	2.19	0.49
2:H:1052:ASP:N	2:H:1052:ASP:OD1	2.46	0.49
1:K:148:TRP:CG	1:K:299:ARG:HD2	2.48	0.49
2:P:24:GLU:OE1	2:P:52:ASP:HB3	2.13	0.49
1:E:336:ASP:OD2	2:F:1029:LYS:NZ	2.42	0.49
1:O:81:SER:HB2	1:O:132:ARG:HD3	1.95	0.49
2:X:1045:PHE:HB3	2:X:1050:LEU:HD21	1.94	0.49
1:W:262:ALA:HB3	2:X:44:ILE:HD13	1.94	0.49
1:I:89:MET:HE3	1:I:110:TYR:O	2.12	0.49
1:Q:148:TRP:CD1	1:Q:299:ARG:HD2	2.47	0.49
1:Q:262:ALA:HB3	2:R:44:ILE:HD13	1.94	0.49
1:U:171:TRP:HD1	1:U:187:LYS:HZ3	1.61	0.49
2:V:6:LYS:HE2	2:V:66:THR:HG21	1.95	0.49
1:E:137:GLN:NE2	1:E:342:ILE:HG23	2.26	0.49
1:K:125:GLY:HA3	2:L:1002:GLN:CG	2.37	0.49
2:T:42:ARG:HB3	2:T:70:VAL:O	2.13	0.49
2:T:55:THR:OG1	2:T:56:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:333:ILE:HG13	1:W:343:PRO:HD3	1.95	0.49
2:H:1042:ARG:HG3	2:H:1072:ARG:HH21	1.78	0.48
1:M:155:MET:HE3	1:M:193:THR:HA	1.95	0.48
1:S:186:ASP:O	1:S:190:GLU:HG3	2.13	0.48
1:B:117:PHE:CD1	1:B:343:PRO:HB2	2.48	0.48
1:B:225:GLU:HG2	1:B:229:TYR:CZ	2.48	0.48
2:N:11:LYS:NZ	2:N:34:GLU:OE2	2.33	0.48
2:P:1039:ASP:OD2	2:P:1039:ASP:N	2.46	0.48
1:B:85:GLU:HB2	1:B:119:SER:HB3	1.95	0.48
1:G:265:THR:O	1:G:271:GLN:HB3	2.12	0.48
1:Q:243:LEU:C	1:Q:243:LEU:HD23	2.33	0.48
1:I:89:MET:HE3	1:I:110:TYR:C	2.34	0.48
2:L:23:ILE:HD12	2:L:51:GLU:O	2.13	0.48
1:O:162:ILE:HD12	1:O:185:VAL:HG22	1.95	0.48
1:S:157:LEU:HD12	1:S:160:LYS:HE2	1.95	0.48
1:I:117:PHE:CD1	1:I:343:PRO:HB2	2.48	0.48
2:L:25:ASN:O	2:L:29:LYS:HG3	2.14	0.48
1:A:225:GLU:HG2	1:A:229:TYR:CZ	2.49	0.48
1:O:301:THR:HB	1:O:329:VAL:HG22	1.94	0.48
1:U:200:ALA:O	1:U:204:GLU:HG2	2.14	0.48
1:W:222:GLU:HB3	1:W:226:TYR:HE2	1.77	0.48
1:G:117:PHE:CD1	1:G:343:PRO:HB2	2.49	0.48
1:B:206:ARG:O	1:S:98:GLY:HA2	2.13	0.48
1:E:143:VAL:HG12	1:M:99:ASN:HB2	1.95	0.48
1:B:181:ASN:OD1	1:B:182:GLU:HG3	2.14	0.47
1:M:155:MET:HE2	1:M:196:ARG:HE	1.79	0.47
1:O:333:ILE:HG13	1:O:343:PRO:HD3	1.96	0.47
2:X:1052:ASP:OD1	2:X:1052:ASP:N	2.47	0.47
1:M:311:ASN:O	1:M:311:ASN:ND2	2.42	0.47
2:P:1042:ARG:HG3	2:P:1072:ARG:HH22	1.80	0.47
1:U:222:GLU:HB3	1:U:226:TYR:CE2	2.49	0.47
1:K:148:TRP:CD1	1:K:299:ARG:HD2	2.49	0.47
1:Q:97:ARG:NH1	2:R:1034:GLU:OE1	2.47	0.47
1:Q:303:GLN:O	1:Q:331:THR:HA	2.14	0.47
2:D:1024:GLU:CG	2:D:1052:ASP:HB3	2.43	0.47
1:O:141:GLN:HA	1:O:211:ARG:NH1	2.29	0.47
1:S:192:LEU:HD13	1:S:231:ALA:HB1	1.97	0.47
2:V:26:VAL:O	2:V:30:ILE:HG13	2.14	0.47
2:V:50:LEU:HG	2:V:59:TYR:CZ	2.49	0.47
1:E:148:TRP:CD1	1:E:299:ARG:HD2	2.50	0.47
1:O:148:TRP:CG	1:O:299:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1042:ARG:HB3	2:R:1070:VAL:HG22	1.97	0.47
1:S:301:THR:HB	1:S:329:VAL:HG22	1.95	0.47
1:U:254:PRO:O	1:U:257:SER:OG	2.26	0.47
1:M:333:ILE:HD11	1:M:343:PRO:HB3	1.96	0.47
1:M:333:ILE:HG13	1:M:343:PRO:HD3	1.97	0.47
1:Q:137:GLN:O	1:Q:141:GLN:HG2	2.13	0.47
2:R:1045:PHE:HB3	2:R:1050:LEU:HD21	1.97	0.47
1:S:162:ILE:HG22	1:S:168:ILE:HB	1.96	0.47
1:S:338:ARG:NH1	2:T:1021:ASP:OD1	2.47	0.47
1:W:265:THR:O	1:W:271:GLN:HB3	2.15	0.47
1:I:192:LEU:HD23	1:I:231:ALA:HB1	1.97	0.47
1:W:282:HIS:HA	2:X:1063:LYS:NZ	2.30	0.47
2:J:1045:PHE:HB2	2:J:1067:LEU:HD22	1.96	0.47
1:S:171:TRP:CH2	1:S:277:LEU:HD21	2.50	0.47
2:C:1072:ARG:HD3	2:C:1073:LEU:HD13	1.97	0.46
1:I:333:ILE:HG13	1:I:343:PRO:HD3	1.97	0.46
1:M:148:TRP:CD1	1:M:299:ARG:HD2	2.50	0.46
2:P:55:THR:OG1	2:P:58:ASP:OD2	2.31	0.46
1:I:113:VAL:HG22	1:I:305:TYR:CD1	2.50	0.46
1:U:183:ASP:HB3	1:U:186:ASP:HB2	1.97	0.46
1:W:126:ASP:O	1:W:127:ASN:HB2	2.16	0.46
2:J:1052:ASP:OD2	2:J:1052:ASP:N	2.48	0.46
2:L:42:ARG:HB3	2:L:70:VAL:O	2.15	0.46
2:L:1016:GLU:O	2:L:1029:LYS:NZ	2.49	0.46
1:E:263:ARG:NH1	1:E:287:GLU:OE2	2.47	0.46
1:G:115:GLN:NE2	1:W:115:GLN:O	2.42	0.46
1:K:333:ILE:HD11	1:K:343:PRO:HB3	1.96	0.46
2:V:42:ARG:HB3	2:V:70:VAL:O	2.16	0.46
1:A:333:ILE:HG13	1:A:343:PRO:HD3	1.96	0.46
1:E:97:ARG:NH1	2:F:1034:GLU:OE1	2.49	0.46
2:P:1042:ARG:HD2	2:P:1044:ILE:HD11	1.97	0.46
1:E:131:LEU:HD21	1:E:236:MET:HE1	1.98	0.46
2:P:1052:ASP:OD2	2:P:1052:ASP:N	2.48	0.46
1:U:345:ARG:HG2	1:U:346:VAL:H	1.80	0.46
1:W:94:LYS:HE3	1:W:95:GLU:OE1	2.16	0.46
1:I:267:ASN:HB2	1:I:271:GLN:OE1	2.15	0.46
2:R:23:ILE:HD12	2:R:54:ARG:O	2.15	0.46
1:U:126:ASP:O	1:U:127:ASN:HB2	2.16	0.46
1:W:127:ASN:OD1	2:X:1001:MET:HB3	2.16	0.46
1:A:336:ASP:OD2	2:D:1029:LYS:NZ	2.29	0.46
1:E:126:ASP:O	1:E:127:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:ARG:HB3	2:H:70:VAL:O	2.15	0.46
2:J:1044:ILE:HD11	1:O:175:LEU:HD12	1.96	0.46
2:V:22:THR:HA	2:V:55:THR:HA	1.97	0.46
1:W:125:GLY:O	2:X:1001:MET:HA	2.16	0.46
1:K:301:THR:HB	1:K:329:VAL:HG22	1.96	0.46
1:W:109:GLY:O	1:W:113:VAL:HG23	2.16	0.46
1:E:99:ASN:HB3	1:U:211:ARG:NH1	2.31	0.45
1:E:187:LYS:HD2	1:E:187:LYS:HA	1.81	0.45
2:R:1011:LYS:HD2	2:R:1011:LYS:HA	1.67	0.45
1:W:131:LEU:HD21	1:W:236:MET:HE1	1.98	0.45
1:E:117:PHE:CD1	1:E:343:PRO:HB2	2.52	0.45
1:K:282:HIS:HA	2:L:1063:LYS:NZ	2.30	0.45
2:N:1023:ILE:HB	2:N:1052:ASP:HA	1.99	0.45
1:S:126:ASP:OD2	1:S:226:TYR:OH	2.34	0.45
2:L:1052:ASP:N	2:L:1052:ASP:OD1	2.50	0.45
1:W:141:GLN:HA	1:W:211:ARG:NH1	2.32	0.45
1:W:221:ASN:ND2	1:W:224:GLU:OE1	2.49	0.45
1:I:126:ASP:O	1:I:127:ASN:HB2	2.17	0.45
1:M:145:LEU:HA	1:M:199:TRP:NE1	2.31	0.45
1:O:89:MET:HE3	1:O:110:TYR:C	2.37	0.45
1:O:280:VAL:HA	1:O:284:GLY:O	2.17	0.45
1:B:324:PRO:HG2	1:B:327:TRP:CE2	2.52	0.45
1:W:336:ASP:OD1	2:X:1029:LYS:NZ	2.29	0.45
1:B:99:ASN:HB3	1:O:211:ARG:HH21	1.81	0.45
1:K:162:ILE:HD12	1:K:185:VAL:HG22	1.98	0.45
1:K:174:GLY:N	2:N:1047:GLY:O	2.36	0.45
1:K:338:ARG:NH1	2:L:1021:ASP:OD2	2.49	0.45
1:M:148:TRP:CG	1:M:299:ARG:HD2	2.51	0.45
2:R:5:VAL:O	2:R:13:ILE:HG13	2.16	0.45
2:T:1013:ILE:H	2:T:1013:ILE:HG12	1.61	0.45
2:V:1:MET:HG2	2:V:17:VAL:O	2.16	0.45
2:X:26:VAL:O	2:X:30:ILE:HG13	2.17	0.45
1:A:287:GLU:OE2	2:D:42:ARG:NH2	2.49	0.45
2:F:42:ARG:HB3	2:F:70:VAL:O	2.16	0.45
2:R:3:ILE:HD13	2:R:15:LEU:HB2	1.98	0.45
1:O:125:GLY:HA3	2:P:1002:GLN:CG	2.40	0.45
1:O:200:ALA:O	1:O:204:GLU:HG2	2.17	0.45
2:P:1042:ARG:HG3	2:P:1072:ARG:NH2	2.30	0.45
1:U:89:MET:O	1:U:93:LYS:HG3	2.17	0.45
1:A:200:ALA:O	1:A:204:GLU:HG2	2.17	0.45
1:M:206:ARG:NH2	2:V:1040:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:162:ILE:CD1	1:S:185:VAL:HG22	2.46	0.45
1:S:226:TYR:N	1:S:226:TYR:CD2	2.85	0.45
2:N:1015:LEU:HG	2:N:1029:LYS:HD3	1.99	0.45
1:Q:225:GLU:HG2	1:Q:229:TYR:CZ	2.52	0.45
1:U:137:GLN:HG2	1:U:330:VAL:HB	1.99	0.45
1:S:88:ILE:HG23	1:S:89:MET:HE2	1.99	0.44
2:J:36:ILE:HG21	2:J:71:LEU:HD11	1.99	0.44
2:J:1039:ASP:OD1	2:J:1039:ASP:N	2.50	0.44
1:M:113:VAL:HG22	1:M:305:TYR:CD1	2.53	0.44
2:R:1052:ASP:OD1	2:R:1052:ASP:N	2.51	0.44
1:U:225:GLU:HG2	1:U:229:TYR:CE2	2.52	0.44
1:U:265:THR:O	1:U:275:ASN:ND2	2.40	0.44
2:V:6:LYS:HA	2:V:11:LYS:O	2.17	0.44
2:R:1051:GLU:HG2	2:R:1059:TYR:OH	2.18	0.44
2:D:1039:ASP:OD2	2:D:1039:ASP:N	2.42	0.44
1:I:333:ILE:HD11	1:I:343:PRO:HB3	1.99	0.44
2:J:1054:ARG:NH2	1:O:271:GLN:HE21	2.09	0.44
1:A:132:ARG:NE	1:A:225:GLU:OE1	2.37	0.44
2:D:1042:ARG:NH1	2:D:1072:ARG:HH21	2.00	0.44
1:G:324:PRO:HG2	1:G:327:TRP:CE2	2.53	0.44
2:L:1037:PRO:HA	2:L:1038:PRO:HD3	1.84	0.44
1:Q:126:ASP:O	1:Q:127:ASN:HB2	2.18	0.44
2:D:42:ARG:HB3	2:D:70:VAL:O	2.18	0.44
2:F:1052:ASP:OD1	2:F:1052:ASP:N	2.51	0.44
1:Q:206:ARG:HG2	1:Q:207:THR:N	2.32	0.44
1:B:319:TYR:HA	1:B:320:PRO:HA	1.85	0.44
1:K:109:GLY:O	1:K:113:VAL:HG23	2.18	0.44
1:K:208:ALA:O	1:K:212:GLN:HG3	2.18	0.44
1:M:162:ILE:HD12	1:M:185:VAL:HG13	2.00	0.44
1:O:98:GLY:HA2	1:S:206:ARG:O	2.18	0.44
1:O:99:ASN:HB3	1:S:211:ARG:NH1	2.32	0.44
1:S:226:TYR:N	1:S:226:TYR:HD2	2.15	0.44
2:T:1052:ASP:N	2:T:1052:ASP:OD1	2.51	0.44
1:M:220:THR:O	1:M:222:GLU:HG3	2.17	0.44
1:O:109:GLY:O	1:O:113:VAL:HG23	2.18	0.44
1:Q:192:LEU:HD23	1:Q:231:ALA:HB1	1.98	0.44
1:S:89:MET:HE3	1:S:110:TYR:C	2.38	0.44
1:A:85:GLU:HB2	1:A:119:SER:HB3	1.99	0.44
1:E:99:ASN:HB3	1:U:211:ARG:HH11	1.83	0.44
2:P:42:ARG:HB3	2:P:70:VAL:O	2.17	0.44
1:Q:221:ASN:HD21	1:Q:223:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB2	1:A:271:GLN:OE1	2.18	0.43
1:B:143:VAL:HG12	1:S:99:ASN:HB2	1.98	0.43
2:C:1052:ASP:OD2	2:C:1052:ASP:N	2.51	0.43
1:E:148:TRP:CG	1:E:299:ARG:HD2	2.54	0.43
1:E:287:GLU:OE2	2:F:42:ARG:NH2	2.51	0.43
1:G:296:TYR:O	1:G:299:ARG:HD3	2.17	0.43
1:K:243:LEU:HD23	1:K:257:SER:HB3	2.00	0.43
1:S:89:MET:HE1	1:S:110:TYR:HB3	2.00	0.43
1:U:109:GLY:O	1:U:113:VAL:HG23	2.18	0.43
1:U:225:GLU:HG2	1:U:229:TYR:CZ	2.53	0.43
1:G:98:GLY:HA2	1:W:206:ARG:O	2.18	0.43
2:J:2:GLN:NE2	2:J:16:GLU:OE2	2.44	0.43
2:N:44:ILE:O	2:N:44:ILE:HG13	2.18	0.43
1:A:263:ARG:NH1	1:A:287:GLU:OE2	2.51	0.43
1:E:303:GLN:O	1:E:331:THR:HA	2.19	0.43
1:S:219:PHE:CD1	1:S:225:GLU:HG3	2.53	0.43
1:U:303:GLN:O	1:U:331:THR:HA	2.18	0.43
1:W:301:THR:HB	1:W:329:VAL:HG22	2.00	0.43
1:G:222:GLU:O	1:G:226:TYR:HD1	2.01	0.43
2:J:37:PRO:HA	2:J:38:PRO:HD3	1.86	0.43
2:J:1023:ILE:HB	2:J:1052:ASP:HA	2.00	0.43
2:N:1048:LYS:H	2:N:1048:LYS:HG3	1.61	0.43
1:S:161:LEU:HD21	1:S:241:ILE:HD12	2.00	0.43
1:U:243:LEU:HD11	1:U:254:PRO:HD2	2.00	0.43
2:V:1037:PRO:HA	2:V:1038:PRO:HD3	1.88	0.43
1:G:254:PRO:O	1:G:257:SER:HB3	2.19	0.43
1:K:148:TRP:CZ3	1:K:149:LEU:HG	2.54	0.43
1:Q:333:ILE:HG13	1:Q:343:PRO:HD3	2.00	0.43
1:W:240:ALA:HB2	1:W:293:LEU:HD11	2.00	0.43
2:X:1042:ARG:NH1	2:X:1072:ARG:HH21	1.97	0.43
1:B:282:HIS:HA	2:C:1063:LYS:NZ	2.33	0.43
1:E:115:GLN:NE2	1:U:116:LYS:HG2	2.33	0.43
2:H:1045:PHE:HB2	2:H:1067:LEU:HD22	1.99	0.43
2:H:1073:LEU:HD23	2:H:1073:LEU:HA	1.84	0.43
1:S:165:TYR:O	1:S:168:ILE:HG12	2.18	0.43
1:B:81:SER:HB2	1:B:132:ARG:HD3	2.01	0.43
1:O:282:HIS:HA	2:P:1063:LYS:NZ	2.33	0.43
2:V:1072:ARG:HG3	2:V:1073:LEU:H	1.82	0.43
1:B:162:ILE:HD12	1:B:185:VAL:HG22	2.00	0.43
1:E:194:LEU:HD21	1:E:224:GLU:HB3	2.00	0.43
1:G:131:LEU:HD21	1:G:236:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:THR:OG1	2:H:58:ASP:OD1	2.34	0.43
1:O:222:GLU:HB3	1:O:226:TYR:CE2	2.53	0.43
1:M:225:GLU:HG2	1:M:229:TYR:CE2	2.54	0.43
1:S:239:ARG:HD2	1:S:239:ARG:HA	1.76	0.43
2:V:54:ARG:HD2	2:V:59:TYR:OH	2.19	0.43
1:E:276:HIS:O	1:E:280:VAL:HG23	2.19	0.43
2:L:1042:ARG:HB2	2:L:1070:VAL:HG22	2.01	0.43
1:M:309:LYS:O	1:M:315:PHE:HD1	2.02	0.43
2:D:1011:LYS:HE2	2:D:1011:LYS:HB2	1.83	0.42
1:B:333:ILE:HD11	1:B:343:PRO:HB3	2.01	0.42
1:B:333:ILE:HG13	1:B:343:PRO:HD3	2.01	0.42
2:C:1013:ILE:HD13	2:C:1034:GLU:HG3	2.00	0.42
1:G:85:GLU:HB2	1:G:119:SER:HB3	2.01	0.42
2:H:5:VAL:HB	2:H:13:ILE:HG12	2.00	0.42
1:I:287:GLU:OE1	2:J:42:ARG:NH2	2.51	0.42
2:P:1024:GLU:CG	2:P:1052:ASP:HB3	2.49	0.42
1:Q:319:TYR:HA	1:Q:320:PRO:HA	1.86	0.42
1:W:192:LEU:HD13	1:W:231:ALA:HB1	2.01	0.42
1:W:319:TYR:HA	1:W:320:PRO:HA	1.88	0.42
2:J:6:LYS:HE2	2:J:66:THR:HG21	2.01	0.42
1:M:200:ALA:O	1:M:204:GLU:HG2	2.19	0.42
2:V:37:PRO:HA	2:V:38:PRO:HD3	1.84	0.42
2:N:2:GLN:NE2	2:N:16:GLU:OE2	2.51	0.42
2:X:1037:PRO:HA	2:X:1038:PRO:HD3	1.85	0.42
1:M:165:TYR:HB3	1:M:167:TRP:NE1	2.34	0.42
1:S:109:GLY:O	1:S:113:VAL:HG23	2.19	0.42
1:B:148:TRP:CG	1:B:299:ARG:HD2	2.55	0.42
1:G:141:GLN:HA	1:G:211:ARG:NH1	2.34	0.42
1:K:200:ALA:O	1:K:204:GLU:HG2	2.19	0.42
2:L:55:THR:OG1	2:L:58:ASP:OD1	2.38	0.42
2:N:1037:PRO:HA	2:N:1038:PRO:HD3	1.87	0.42
1:U:333:ILE:HD11	1:U:343:PRO:HB3	2.02	0.42
1:I:88:ILE:HG23	1:I:89:MET:HE2	2.02	0.42
1:Q:131:LEU:O	1:Q:135:LEU:HB2	2.19	0.42
1:Q:155:MET:HE3	1:Q:193:THR:HA	2.02	0.42
1:U:262:ALA:HB3	2:V:44:ILE:HD13	2.01	0.42
1:A:143:VAL:HG12	1:A:211:ARG:HH12	1.85	0.42
1:A:225:GLU:HG2	1:A:229:TYR:CE2	2.55	0.42
1:K:79:ARG:HG2	1:K:80:LEU:N	2.35	0.42
1:A:263:ARG:HB2	1:A:266:SER:HB3	2.01	0.42
2:C:42:ARG:HB3	2:C:70:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:ASP:O	1:G:337:ASP:HB2	2.20	0.42
1:O:181:ASN:O	1:O:185:VAL:HG23	2.20	0.42
1:K:225:GLU:HG2	1:K:229:TYR:CZ	2.54	0.42
1:O:87:ASP:HB3	1:O:90:ASP:HB2	2.02	0.42
1:S:158:PRO:O	1:S:162:ILE:HD13	2.19	0.42
1:U:165:TYR:HB3	1:U:167:TRP:NE1	2.34	0.42
2:V:5:VAL:HG22	2:V:13:ILE:HD12	2.02	0.42
1:G:263:ARG:HB2	1:G:266:SER:HB3	2.02	0.42
2:L:1045:PHE:HB3	2:L:1050:LEU:HD21	2.02	0.42
1:O:336:ASP:O	1:O:337:ASP:HB2	2.19	0.42
2:R:28:ALA:O	2:R:31:GLN:HB3	2.20	0.42
1:U:169:LYS:HE3	1:U:169:LYS:HB2	1.93	0.42
2:D:1052:ASP:OD1	2:D:1052:ASP:N	2.53	0.41
1:B:279:GLN:H	1:B:279:GLN:HG2	1.62	0.41
1:M:327:TRP:HA	1:M:328:PRO:HD3	1.94	0.41
1:U:145:LEU:HA	1:U:146:PRO:HD3	1.92	0.41
1:B:208:ALA:O	1:B:212:GLN:HG3	2.21	0.41
1:M:186:ASP:OD1	1:M:186:ASP:N	2.53	0.41
1:M:208:ALA:O	1:M:212:GLN:HG3	2.20	0.41
1:M:276:HIS:O	1:M:279:GLN:HG2	2.18	0.41
2:R:1016:GLU:O	2:R:1029:LYS:NZ	2.46	0.41
1:U:319:TYR:HA	1:U:320:PRO:HA	1.87	0.41
2:D:1037:PRO:HA	2:D:1038:PRO:HD3	1.86	0.41
2:J:71:LEU:HD13	2:J:71:LEU:HA	1.84	0.41
1:O:224:GLU:H	1:O:224:GLU:HG2	1.59	0.41
2:V:1006:LYS:HG3	2:V:1012:THR:HG22	2.02	0.41
1:E:222:GLU:O	1:E:226:TYR:HD2	2.02	0.41
2:J:55:THR:OG1	2:J:58:ASP:OD2	2.38	0.41
2:J:1037:PRO:HA	2:J:1038:PRO:HD3	1.90	0.41
1:M:125:GLY:HA3	2:N:1002:GLN:CG	2.39	0.41
1:M:146:PRO:HD3	1:M:199:TRP:CE2	2.55	0.41
2:P:17:VAL:HG12	2:P:29:LYS:HE3	2.01	0.41
2:P:1006:LYS:O	2:P:1006:LYS:HG3	2.21	0.41
1:S:276:HIS:O	1:S:280:VAL:HG23	2.21	0.41
1:B:127:ASN:ND2	1:B:282:HIS:O	2.43	0.41
1:I:85:GLU:H	1:I:85:GLU:HG3	1.39	0.41
1:O:326:ASP:OD1	1:O:326:ASP:N	2.50	0.41
1:I:263:ARG:NH1	1:I:287:GLU:OE1	2.53	0.41
1:K:265:THR:O	1:K:271:GLN:HB3	2.19	0.41
1:M:191:SER:HB3	1:M:231:ALA:HB2	2.02	0.41
1:S:336:ASP:O	1:S:337:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:141:GLN:HA	1:Q:211:ARG:NH1	2.35	0.41
1:S:165:TYR:HB3	1:S:167:TRP:NE1	2.36	0.41
1:W:342:ILE:HA	1:W:343:PRO:HD2	1.97	0.41
2:D:55:THR:OG1	2:D:58:ASP:OD1	2.39	0.41
1:G:143:VAL:HG12	1:I:99:ASN:HB2	2.03	0.41
2:P:1042:ARG:HD3	2:P:1049:GLN:CD	2.41	0.41
1:U:336:ASP:O	1:U:337:ASP:HB2	2.21	0.41
2:X:1042:ARG:HG2	2:X:1049:GLN:NE2	2.36	0.41
1:A:198:LYS:HD3	1:A:198:LYS:HA	1.92	0.41
1:E:162:ILE:HD12	1:E:185:VAL:HG22	2.03	0.41
1:G:102:LYS:HG2	2:H:1032:ASP:OD2	2.21	0.41
1:I:249:LYS:HB3	1:I:249:LYS:HE2	1.88	0.41
1:M:119:SER:HB2	1:M:344:VAL:HB	2.03	0.41
1:M:127:ASN:OD1	2:N:1001:MET:HB2	2.21	0.41
1:O:157:LEU:HD12	1:O:157:LEU:HA	1.89	0.41
2:R:55:THR:OG1	2:R:58:ASP:OD2	2.38	0.41
2:R:1037:PRO:HA	2:R:1038:PRO:HD3	1.90	0.41
1:S:171:TRP:HZ3	1:S:237:LEU:HD22	1.85	0.41
1:S:200:ALA:O	1:S:204:GLU:HG2	2.21	0.41
1:U:137:GLN:OE1	1:U:342:ILE:HG23	2.21	0.41
1:U:245:ASN:O	1:U:249:LYS:HG2	2.21	0.41
2:X:29:LYS:NZ	2:X:33:LYS:HE2	2.36	0.41
2:X:1056:LEU:HD12	2:X:1061:ILE:HD12	2.02	0.41
1:A:125:GLY:O	2:D:1001:MET:HA	2.21	0.41
1:B:336:ASP:O	1:B:337:ASP:HB2	2.21	0.41
1:I:116:LYS:NZ	1:W:115:GLN:HE22	2.19	0.41
1:I:183:ASP:OD1	1:I:186:ASP:HB2	2.20	0.41
1:K:279:GLN:OE1	1:K:279:GLN:N	2.54	0.41
2:R:37:PRO:HA	2:R:38:PRO:HD3	1.86	0.41
2:R:72:ARG:O	2:R:72:ARG:HG2	2.21	0.41
1:W:167:TRP:CH2	1:W:269:PRO:HB2	2.56	0.41
1:B:148:TRP:CD1	1:B:299:ARG:HD2	2.55	0.40
1:G:146:PRO:HA	1:G:147:PRO:HD3	1.92	0.40
2:N:54:ARG:HD2	2:N:59:TYR:OH	2.21	0.40
1:W:137:GLN:HG2	1:W:330:VAL:HB	2.02	0.40
1:A:155:MET:CE	1:A:196:ARG:HE	2.34	0.40
1:A:249:LYS:HB3	1:A:249:LYS:HE2	1.88	0.40
1:M:109:GLY:O	1:M:113:VAL:HG23	2.21	0.40
1:S:128:TYR:HE1	1:S:233:LYS:HD2	1.85	0.40
1:M:165:TYR:HB2	1:M:168:ILE:HD13	2.04	0.40
2:R:23:ILE:HD13	2:R:51:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:170:GLN:HG3	1:W:170:GLN:O	2.21	0.40
1:A:319:TYR:HA	1:A:320:PRO:HA	1.86	0.40
1:A:336:ASP:O	1:A:337:ASP:HB2	2.22	0.40
1:B:137:GLN:OE1	1:B:342:ILE:HG23	2.22	0.40
1:E:324:PRO:HG2	1:E:327:TRP:CE2	2.57	0.40
2:F:2:GLN:NE2	2:F:16:GLU:OE2	2.53	0.40
2:H:1015:LEU:HD22	2:H:1029:LYS:HD3	2.04	0.40
1:M:319:TYR:HA	1:M:320:PRO:HA	1.91	0.40
2:N:73:LEU:HD13	2:N:1018:GLU:HG3	2.03	0.40
1:O:154:LEU:O	1:O:157:LEU:HB2	2.22	0.40
1:O:208:ALA:O	1:O:212:GLN:HG3	2.21	0.40
2:P:1037:PRO:HA	2:P:1038:PRO:HD3	1.88	0.40
2:D:1048:LYS:HE3	2:D:1048:LYS:HB3	1.93	0.40
1:B:191:SER:HB3	1:B:231:ALA:HB2	2.02	0.40
1:G:338:ARG:O	2:H:76:GLY:N	2.55	0.40
1:I:279:GLN:H	1:I:279:GLN:HG2	1.66	0.40
2:J:1047:GLY:O	1:O:174:GLY:N	2.41	0.40
1:O:89:MET:HE1	1:O:110:TYR:HB3	2.04	0.40
1:O:173:LEU:H	1:O:173:LEU:CD2	2.34	0.40
1:O:239:ARG:NH1	1:O:296:TYR:O	2.54	0.40
1:S:167:TRP:CH2	1:S:269:PRO:HB2	2.56	0.40
1:S:225:GLU:HG2	1:S:229:TYR:CZ	2.55	0.40
1:U:326:ASP:OD1	1:U:326:ASP:N	2.39	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	259/276 (94%)	253 (98%)	6 (2%)	0	100	100
1	B	259/276 (94%)	253 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	258/276 (94%)	247 (96%)	9 (4%)	2 (1%)	19	38
1	G	257/276 (93%)	248 (96%)	9 (4%)	0	100	100
1	I	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	K	268/276 (97%)	261 (97%)	7 (3%)	0	100	100
1	M	256/276 (93%)	247 (96%)	9 (4%)	0	100	100
1	O	268/276 (97%)	259 (97%)	9 (3%)	0	100	100
1	Q	257/276 (93%)	250 (97%)	7 (3%)	0	100	100
1	S	259/276 (94%)	250 (96%)	9 (4%)	0	100	100
1	U	257/276 (93%)	246 (96%)	11 (4%)	0	100	100
1	W	256/276 (93%)	249 (97%)	7 (3%)	0	100	100
2	C	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
2	D	147/156 (94%)	143 (97%)	4 (3%)	0	100	100
2	F	148/156 (95%)	145 (98%)	2 (1%)	1 (1%)	22	42
2	H	147/156 (94%)	143 (97%)	3 (2%)	1 (1%)	22	42
2	J	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
2	L	148/156 (95%)	145 (98%)	2 (1%)	1 (1%)	22	42
2	N	148/156 (95%)	144 (97%)	2 (1%)	2 (1%)	11	24
2	P	147/156 (94%)	143 (97%)	4 (3%)	0	100	100
2	R	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
2	T	147/156 (94%)	144 (98%)	3 (2%)	0	100	100
2	V	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
2	X	147/156 (94%)	143 (97%)	4 (3%)	0	100	100
All	All	4883/5184 (94%)	4744 (97%)	132 (3%)	7 (0%)	51	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	337	ASP
2	N	75	GLY
2	L	76	GLY
1	E	335	GLU
2	N	76	GLY
2	H	1009	THR
2	F	76	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/244 (96%)	228 (97%)	6 (3%)	46	70
1	B	234/244 (96%)	226 (97%)	8 (3%)	37	62
1	E	233/244 (96%)	222 (95%)	11 (5%)	26	50
1	G	232/244 (95%)	221 (95%)	11 (5%)	26	50
1	I	233/244 (96%)	226 (97%)	7 (3%)	41	65
1	K	239/244 (98%)	228 (95%)	11 (5%)	27	51
1	M	230/244 (94%)	219 (95%)	11 (5%)	25	49
1	O	239/244 (98%)	230 (96%)	9 (4%)	33	59
1	Q	232/244 (95%)	217 (94%)	15 (6%)	17	33
1	S	233/244 (96%)	224 (96%)	9 (4%)	32	58
1	U	232/244 (95%)	221 (95%)	11 (5%)	26	50
1	W	231/244 (95%)	219 (95%)	12 (5%)	23	44
2	C	135/137 (98%)	126 (93%)	9 (7%)	16	32
2	D	135/137 (98%)	126 (93%)	9 (7%)	16	32
2	F	135/137 (98%)	122 (90%)	13 (10%)	8	17
2	H	135/137 (98%)	128 (95%)	7 (5%)	23	44
2	J	135/137 (98%)	126 (93%)	9 (7%)	16	32
2	L	135/137 (98%)	127 (94%)	8 (6%)	19	37
2	N	135/137 (98%)	123 (91%)	12 (9%)	9	20
2	P	135/137 (98%)	127 (94%)	8 (6%)	19	37
2	R	135/137 (98%)	128 (95%)	7 (5%)	23	44
2	T	135/137 (98%)	124 (92%)	11 (8%)	11	24
2	V	135/137 (98%)	130 (96%)	5 (4%)	34	59
2	X	135/137 (98%)	126 (93%)	9 (7%)	16	32
All	All	4422/4572 (97%)	4194 (95%)	228 (5%)	23	44

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	181	ASN
1	A	259	LEU
1	A	283	THR
1	A	338	ARG
1	A	345	ARG
2	D	5	VAL
2	D	39	ASP
2	D	73	LEU
2	D	1011	LYS
2	D	1013	ILE
2	D	1018	GLU
2	D	1039	ASP
2	D	1052	ASP
2	D	1071	LEU
1	B	149	LEU
1	B	205	MET
1	B	252	GLU
1	B	258	VAL
1	B	279	GLN
1	B	289	VAL
1	B	311	ASN
1	B	345	ARG
2	C	44	ILE
2	C	62	GLN
2	C	71	LEU
2	C	1013	ILE
2	C	1018	GLU
2	C	1029	LYS
2	C	1052	ASP
2	C	1054	ARG
2	C	1071	LEU
1	E	149	LEU
1	E	211	ARG
1	E	221	ASN
1	E	224	GLU
1	E	235	LEU
1	E	249	LYS
1	E	257	SER
1	E	326	ASP
1	E	338	ARG
1	E	344	VAL
1	E	345	ARG

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Mol	Chain	Res	Type
2	F	5	VAL
2	F	39	ASP
2	F	54	ARG
2	F	73	LEU
2	F	1001	MET
2	F	1008	LEU
2	F	1013	ILE
2	F	1020	SER
2	F	1039	ASP
2	F	1052	ASP
2	F	1063	LYS
2	F	1070	VAL
2	F	1073	LEU
1	G	101	GLN
1	G	149	LEU
1	G	150	GLN
1	G	155	MET
1	G	160	LYS
1	G	173	LEU
1	G	192	LEU
1	G	237	LEU
1	G	247	LYS
1	G	326	ASP
1	G	333	ILE
2	H	13	ILE
2	H	39	ASP
2	H	62	GLN
2	H	73	LEU
2	H	1018	GLU
2	H	1039	ASP
2	H	1052	ASP
1	I	85	GLU
1	I	149	LEU
1	I	205	MET
1	I	212	GLN
1	I	279	GLN
1	I	338	ARG
1	I	345	ARG
2	J	1011	LYS
2	J	1013	ILE
2	J	1018	GLU
2	J	1029	LYS

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Mol	Chain	Res	Type
2	J	1039	ASP
2	J	1048	LYS
2	J	1052	ASP
2	J	1057	SER
2	J	1070	VAL
1	K	85	GLU
1	K	149	LEU
1	K	154	LEU
1	K	176	LYS
1	K	192	LEU
1	K	224	GLU
1	K	239	ARG
1	K	241	ILE
1	K	259	LEU
1	K	338	ARG
1	K	345	ARG
2	L	5	VAL
2	L	54	ARG
2	L	1008	LEU
2	L	1011	LYS
2	L	1018	GLU
2	L	1042	ARG
2	L	1052	ASP
2	L	1073	LEU
1	M	155	MET
1	M	186	ASP
1	M	205	MET
1	M	216	ASP
1	M	224	GLU
1	M	239	ARG
1	M	279	GLN
1	M	311	ASN
1	M	326	ASP
1	M	345	ARG
1	M	348	GLU
2	N	34	GLU
2	N	39	ASP
2	N	44	ILE
2	N	62	GLN
2	N	73	LEU
2	N	74	ARG
2	N	1015	LEU

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Mol	Chain	Res	Type
2	N	1020	SER
2	N	1048	LYS
2	N	1050	LEU
2	N	1052	ASP
2	N	1070	VAL
1	O	81	SER
1	O	101	GLN
1	O	149	LEU
1	O	157	LEU
1	O	173	LEU
1	O	220	THR
1	O	224	GLU
1	O	279	GLN
1	O	345	ARG
2	P	39	ASP
2	P	69	LEU
2	P	1006	LYS
2	P	1008	LEU
2	P	1039	ASP
2	P	1042	ARG
2	P	1052	ASP
2	P	1070	VAL
1	Q	99	ASN
1	Q	135	LEU
1	Q	149	LEU
1	Q	155	MET
1	Q	161	LEU
1	Q	185	VAL
1	Q	186	ASP
1	Q	187	LYS
1	Q	205	MET
1	Q	206	ARG
1	Q	258	VAL
1	Q	265	THR
1	Q	326	ASP
1	Q	331	THR
1	Q	338	ARG
2	R	3	ILE
2	R	13	ILE
2	R	73	LEU
2	R	1009	THR
2	R	1011	LYS

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Mol	Chain	Res	Type
2	R	1052	ASP
2	R	1073	LEU
1	S	101	GLN
1	S	149	LEU
1	S	162	ILE
1	S	192	LEU
1	S	220	THR
1	S	247	LYS
1	S	293	LEU
1	S	338	ARG
1	S	345	ARG
2	T	29	LYS
2	T	39	ASP
2	T	55	THR
2	T	63	LYS
2	T	1008	LEU
2	T	1011	LYS
2	T	1012	THR
2	T	1013	ILE
2	T	1039	ASP
2	T	1052	ASP
2	T	1070	VAL
1	U	81	SER
1	U	149	LEU
1	U	169	LYS
1	U	172	LYS
1	U	194	LEU
1	U	205	MET
1	U	252	GLU
1	U	322	ASP
1	U	326	ASP
1	U	338	ARG
1	U	345	ARG
2	V	5	VAL
2	V	62	GLN
2	V	1001	MET
2	V	1018	GLU
2	V	1040	GLN
1	W	116	LYS
1	W	192	LEU
1	W	194	LEU
1	W	205	MET

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Mol	Chain	Res	Type
1	W	224	GLU
1	W	258	VAL
1	W	259	LEU
1	W	265	THR
1	W	272	LEU
1	W	293	LEU
1	W	338	ARG
1	W	345	ARG
2	X	26	VAL
2	X	39	ASP
2	X	73	LEU
2	X	1006	LYS
2	X	1013	ILE
2	X	1018	GLU
2	X	1052	ASP
2	X	1056	LEU
2	X	1063	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	E	115	GLN
1	E	137	GLN
1	E	221	ASN
1	M	115	GLN
1	Q	137	GLN
1	W	115	GLN
1	W	288	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.