



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:51 pm BST

PDB ID : 4QRM
Title : crystal structure of a binary complex of FliM-FliG middle domains from T.maritima
Authors : Crane, B.R.; Sircar, R.
Deposited on : 2014-07-01
Resolution : 4.32 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

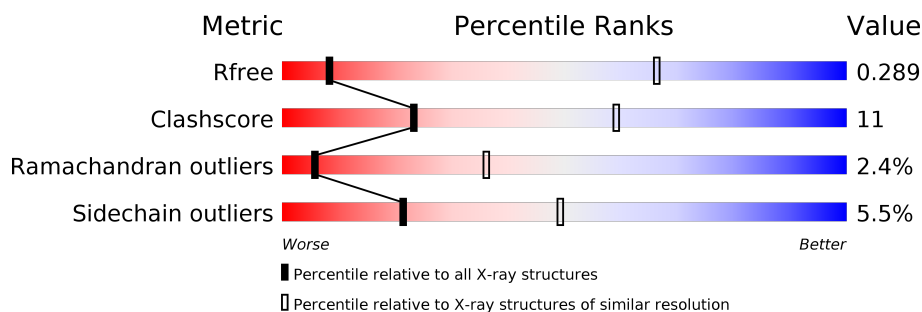
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	183	64% 32% . .
1	C	183	67% 31% ..
1	E	183	64% 32% .
1	G	183	65% 32% .
1	I	183	68% 31% .
1	K	183	74% 23% .
1	M	183	69% 29% .

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Mol	Chain	Length	Quality of chain
1	O	183	 71%26%.
1	Q	183	 67%32%..
1	S	183	 67%30%..
1	U	183	 64%32%.
2	B	75	 61%36%..
2	D	75	 80%20%
2	F	75	 75%23%.
2	H	75	 77%23%
2	J	75	 81%17%.
2	L	75	 69%28%.
2	N	75	 81%17%.
2	P	75	 71%25%..
2	R	75	 67%32%.
2	T	75	 69%27%.
2	V	75	 53%41%5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22777 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 Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	C	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	E	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	G	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	I	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	K	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	M	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	O	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	Q	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	S	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			
1	U	183	Total	C	N	O	S	0	0	0
			1483	968	231	276	8			

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			584	375	98	110	1			
2	D	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	F	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	J	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	L	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	N	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	P	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	R	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	T	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			
2	V	75	Total	C	N	O	S	0	0	0
			588	377	99	111	1			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
B	114	SER	-	EXPRESSION TAG	UNP Q9WY63
B	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
B	116	MET	-	EXPRESSION TAG	UNP Q9WY63
D	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
D	114	SER	-	EXPRESSION TAG	UNP Q9WY63
D	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
D	116	MET	-	EXPRESSION TAG	UNP Q9WY63
F	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
F	114	SER	-	EXPRESSION TAG	UNP Q9WY63
F	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
F	116	MET	-	EXPRESSION TAG	UNP Q9WY63
H	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
H	114	SER	-	EXPRESSION TAG	UNP Q9WY63
H	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
H	116	MET	-	EXPRESSION TAG	UNP Q9WY63
J	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
J	114	SER	-	EXPRESSION TAG	UNP Q9WY63
J	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
J	116	MET	-	EXPRESSION TAG	UNP Q9WY63
L	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
L	114	SER	-	EXPRESSION TAG	UNP Q9WY63
L	115	HIS	-	EXPRESSION TAG	UNP Q9WY63

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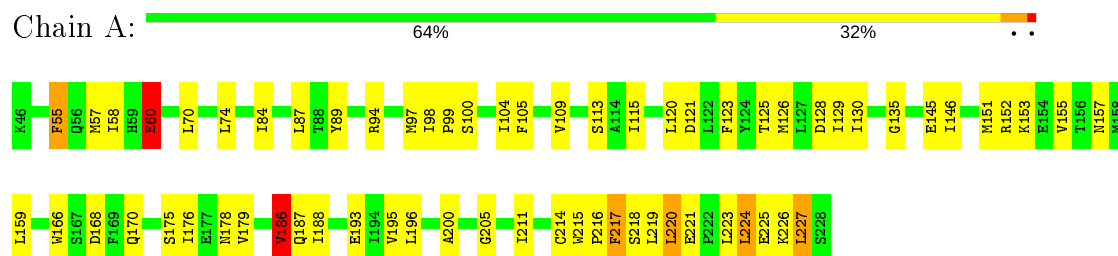
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Chain	Residue	Modelled	Actual	Comment	Reference
L	116	MET	-	EXPRESSION TAG	UNP Q9WY63
N	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
N	114	SER	-	EXPRESSION TAG	UNP Q9WY63
N	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
N	116	MET	-	EXPRESSION TAG	UNP Q9WY63
P	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
P	114	SER	-	EXPRESSION TAG	UNP Q9WY63
P	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
P	116	MET	-	EXPRESSION TAG	UNP Q9WY63
R	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
R	114	SER	-	EXPRESSION TAG	UNP Q9WY63
R	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
R	116	MET	-	EXPRESSION TAG	UNP Q9WY63
T	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
T	114	SER	-	EXPRESSION TAG	UNP Q9WY63
T	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
T	116	MET	-	EXPRESSION TAG	UNP Q9WY63
V	113	GLY	-	EXPRESSION TAG	UNP Q9WY63
V	114	SER	-	EXPRESSION TAG	UNP Q9WY63
V	115	HIS	-	EXPRESSION TAG	UNP Q9WY63
V	116	MET	-	EXPRESSION TAG	UNP Q9WY63

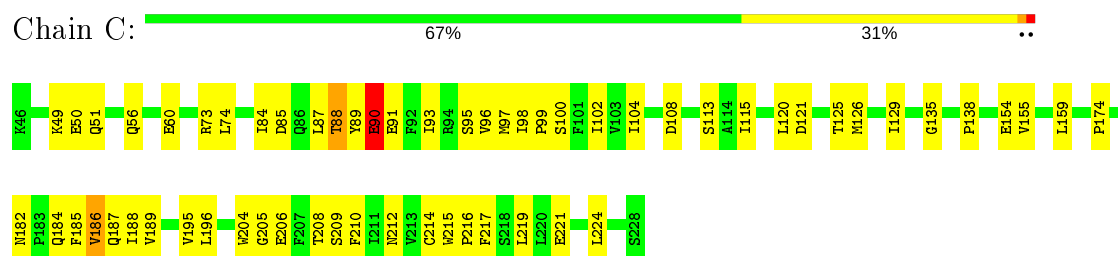
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

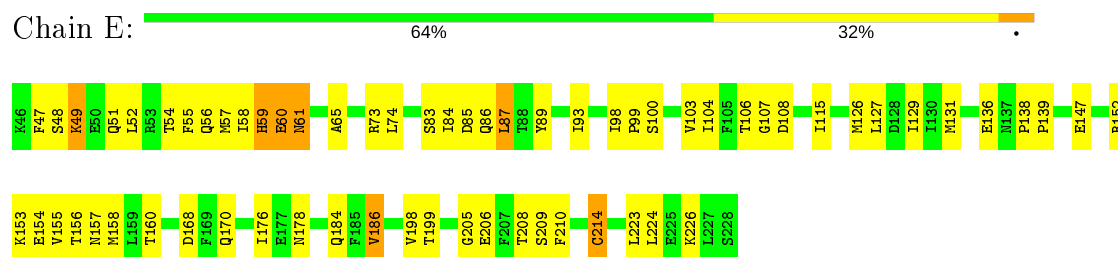
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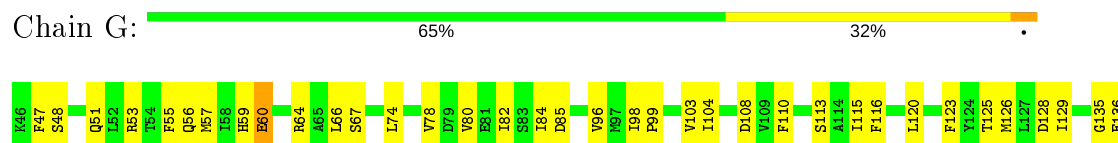
• Molecule 1: Flagellar motor switch protein FliM

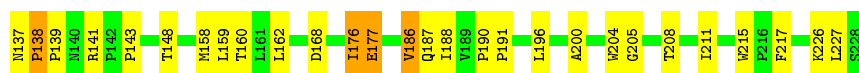


• Molecule 1: Flagellar motor switch protein FliM

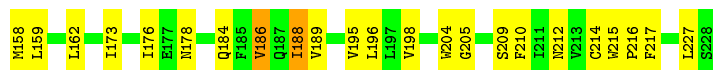


• Molecule 1: Flagellar motor switch protein FliM

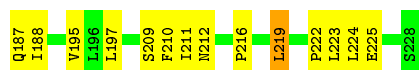
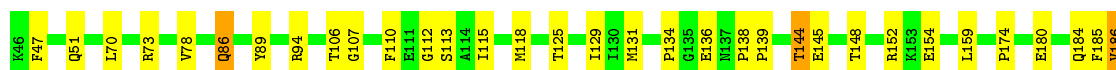




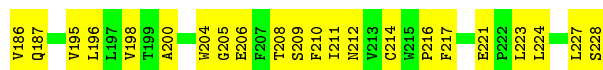
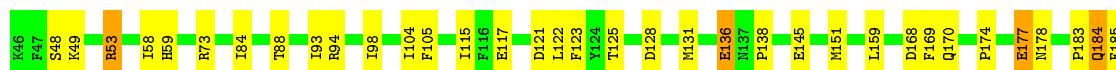
- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM



- Molecule 1: Flagellar motor switch protein FliM





• Molecule 1: Flagellar motor switch protein FliM



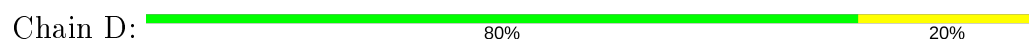
• Molecule 1: Flagellar motor switch protein FliM



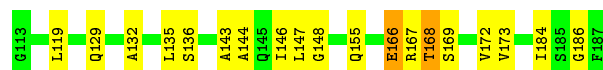
• Molecule 2: Flagellar motor switch protein FliG



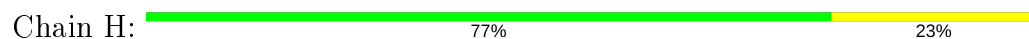
• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG

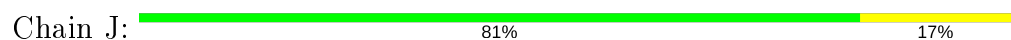


• Molecule 2: Flagellar motor switch protein FliG





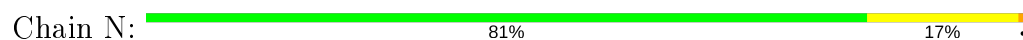
- Molecule 2: Flagellar motor switch protein FliG



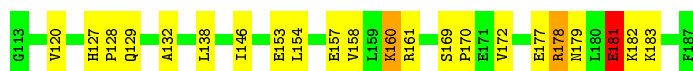
- Molecule 2: Flagellar motor switch protein FliG



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- Molecule 2: Flagellar motor switch protein FliG



- Molecule 2: Flagellar motor switch protein FliG



G113	V117	Q118	L119	V120	M121	H127	P128	Q129	A132	L135	S136	A143	I146	E152	E153	L154	E157	V158	L159	K160	R161	I162	E166	R167	T168	S169	V172	V173	K174	E175	I176	E177	R178	M179	L180	E181	K182	K183	I184	S185	G186	F187
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.40Å 216.25Å 262.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.18 – 4.32 49.98 – 4.31	Depositor EDS
% Data completeness (in resolution range)	89.7 (44.18-4.32) 88.5 (49.98-4.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.209 , 0.291 0.213 , 0.289	Depositor DCC
R_{free} test set	2000 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22777	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.04% 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 [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	0.29	0/1521	0.50	0/2069
1	C	0.29	0/1521	0.46	0/2069
1	E	0.27	0/1521	0.46	0/2069
1	G	0.27	0/1521	0.46	0/2069
1	I	0.29	0/1521	0.44	0/2069
1	K	0.27	0/1521	0.47	0/2069
1	M	0.29	0/1521	0.47	0/2069
1	O	0.27	0/1521	0.44	0/2069
1	Q	0.27	0/1521	0.44	0/2069
1	S	0.30	0/1521	0.48	0/2069
1	U	0.27	0/1521	0.49	0/2069
2	B	0.43	0/593	0.53	0/805
2	D	0.26	0/597	0.46	0/810
2	F	0.26	0/597	0.45	0/810
2	H	0.25	0/597	0.49	0/810
2	J	0.26	0/597	0.48	0/810
2	L	0.27	0/597	0.48	0/810
2	N	0.26	0/597	0.44	0/810
2	P	0.26	0/597	0.54	0/810
2	R	0.28	0/597	0.44	0/810
2	T	0.29	0/597	0.52	0/810
2	V	0.25	0/597	0.51	0/810
All	All	0.28	0/23294	0.47	0/31664

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	GLU	Peptide
1	E	59	HIS	Peptide
1	G	176	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1483	0	1471	47	0
1	C	1483	0	1471	40	0
1	E	1483	0	1471	38	0
1	G	1483	0	1471	32	0
1	I	1483	0	1471	28	0
1	K	1483	0	1471	28	0
1	M	1483	0	1471	32	0
1	O	1483	0	1471	32	0
1	Q	1483	0	1471	34	0
1	S	1483	0	1471	34	0
1	U	1483	0	1471	39	0
2	B	584	0	610	22	0
2	D	588	0	613	8	0
2	F	588	0	613	12	0
2	H	588	0	613	9	0
2	J	588	0	613	7	0
2	L	588	0	613	18	0
2	N	588	0	613	12	0
2	P	588	0	613	19	0
2	R	588	0	613	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	588	0	613	20	0
2	V	588	0	613	23	0
All	All	22777	0	22921	514	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (514) 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:I:48:SER:HB3	1:I:51:GLN:HG2	1.49	0.95
1:E:170:GLN:HG3	1:E:223:LEU:HD11	1.61	0.83
1:A:221:GLU:HA	1:A:224:LEU:HB2	1.63	0.81
1:C:195:VAL:HG22	1:C:216:PRO:HA	1.66	0.78
1:Q:68:THR:HG21	1:S:68:THR:HG21	1.66	0.77
1:U:78:VAL:HG21	1:U:204:TRP:HB3	1.67	0.76
1:A:84:ILE:HD11	1:A:196:LEU:HD11	1.68	0.76
1:C:115:ILE:HB	1:C:214:CYS:HB3	1.67	0.75
1:G:104:ILE:HG22	1:G:115:ILE:HG22	1.67	0.75
1:C:88:THR:OG1	1:C:89:TYR:N	2.17	0.74
1:S:91:GLU:O	1:S:95:SER:N	2.20	0.73
1:I:96:VAL:HG11	1:I:102:ILE:HD11	1.70	0.73
1:A:196:LEU:HB3	1:A:215:TRP:HB2	1.72	0.72
2:V:176:ILE:HA	2:V:179:ASN:HB2	1.72	0.71
1:G:53:ARG:O	1:G:57:MET:N	2.19	0.70
2:P:129:GLN:HA	2:P:161:ARG:NH2	2.06	0.70
2:V:177:GLU:HG3	2:V:178:ARG:H	1.55	0.70
2:B:180:LEU:C	2:B:182:LYS:H	1.95	0.70
1:Q:131:MET:HG2	2:R:172:VAL:HG21	1.74	0.69
1:Q:195:VAL:HG22	1:Q:216:PRO:HA	1.74	0.69
2:T:154:LEU:O	2:T:158:VAL:N	2.24	0.69
1:M:131:MET:HG2	2:N:172:VAL:HG21	1.75	0.69
1:E:73:ARG:NH2	1:E:154:GLU:OE1	2.26	0.69
1:Q:48:SER:OG	1:Q:49:LYS:N	2.24	0.68
2:P:128:PRO:O	2:P:161:ARG:NH2	2.26	0.68
1:K:136:GLU:OE2	2:L:127:HIS:NE2	2.27	0.67
1:G:176:ILE:HG13	1:G:177:GLU:HG2	1.76	0.67
1:I:195:VAL:HG22	1:I:216:PRO:HA	1.77	0.67
1:G:48:SER:HB2	1:G:51:GLN:HG2	1.77	0.67
2:P:160:LYS:HZ3	2:P:161:ARG:HB3	1.59	0.66
2:B:144:ALA:HB1	2:T:159:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:157:GLU:HA	2:P:160:LYS:HG2	1.78	0.66
1:C:221:GLU:HA	1:C:224:LEU:HB2	1.78	0.66
1:M:104:ILE:HG22	1:M:115:ILE:HG12	1.77	0.65
1:C:74:LEU:HD21	1:C:126:MET:HG2	1.77	0.65
2:P:178:ARG:HB3	2:P:181:GLU:HG3	1.79	0.65
1:U:117:GLU:HB3	1:U:212:ASN:HB2	1.78	0.65
1:A:219:LEU:HD22	1:A:220:LEU:HG	1.77	0.65
1:E:153:LYS:O	1:E:157:ASN:ND2	2.29	0.65
1:C:159:LEU:HD23	1:C:174:PRO:HB2	1.79	0.64
1:G:200:ALA:HB3	1:G:211:ILE:HB	1.80	0.64
1:C:73:ARG:NH2	1:C:154:GLU:OE1	2.31	0.64
1:K:195:VAL:HG22	1:K:216:PRO:HA	1.80	0.64
2:T:147:LEU:HD21	2:T:159:LEU:HD21	1.79	0.64
1:M:117:GLU:HB3	1:M:212:ASN:HB2	1.80	0.63
1:M:145:GLU:OE2	2:N:183:LYS:NZ	2.24	0.63
1:E:47:PHE:HB2	1:E:86:GLN:HE21	1.61	0.63
1:M:224:LEU:O	1:M:228:SER:OG	2.13	0.63
2:R:144:ALA:O	2:R:148:GLY:N	2.31	0.63
1:C:91:GLU:O	1:C:95:SER:N	2.27	0.63
1:M:121:ASP:HA	1:M:138:PRO:HB3	1.79	0.63
1:E:104:ILE:HD11	1:E:178:ASN:HB3	1.80	0.63
1:S:112:GLY:HA3	1:S:219:LEU:HD11	1.79	0.63
1:G:74:LEU:HD21	1:G:126:MET:HG2	1.81	0.62
1:O:84:ILE:HD11	1:O:196:LEU:HD11	1.80	0.62
1:S:88:THR:HB	1:S:90:GLU:H	1.63	0.62
1:C:104:ILE:HG22	1:C:115:ILE:HG12	1.81	0.62
2:F:119:LEU:HD22	2:F:146:ILE:HD13	1.82	0.62
2:P:178:ARG:O	2:P:181:GLU:HB2	2.00	0.62
2:F:168:THR:OG1	2:F:169:SER:N	2.33	0.61
2:B:176:ILE:O	2:B:180:LEU:N	2.32	0.61
2:L:129:GLN:HA	2:L:161:ARG:HD3	1.80	0.61
1:U:86:GLN:HG2	1:U:196:LEU:HA	1.83	0.61
1:A:57:MET:C	1:A:60:GLU:HG2	2.21	0.61
2:B:184:ILE:HB	2:B:187:PHE:CZ	2.35	0.61
1:C:216:PRO:HG2	1:C:219:LEU:HD13	1.81	0.61
1:I:106:THR:OG1	1:I:107:GLY:N	2.33	0.61
1:O:200:ALA:HB3	1:O:211:ILE:HB	1.83	0.61
1:M:59:HIS:CD2	1:M:198:VAL:HG21	2.36	0.61
2:V:180:LEU:HB2	2:V:187:PHE:CD1	2.35	0.60
1:O:74:LEU:HD21	1:O:126:MET:HG2	1.82	0.60
2:N:178:ARG:HA	2:N:181:GLU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:OE2	1:A:218:SER:N	2.34	0.60
1:S:49:LYS:HB2	1:S:53:ARG:HH22	1.66	0.60
1:E:103:VAL:HG21	1:E:155:VAL:HG21	1.83	0.60
1:U:152:ARG:HA	1:U:155:VAL:HG22	1.84	0.60
1:A:176:ILE:HD11	1:A:179:VAL:HG22	1.83	0.59
1:C:96:VAL:HG11	1:C:102:ILE:HD11	1.83	0.59
1:U:104:ILE:HG22	1:U:115:ILE:HG12	1.84	0.59
1:G:103:VAL:O	1:G:116:PHE:N	2.34	0.59
1:O:115:ILE:HB	1:O:214:CYS:HB2	1.84	0.59
1:I:128:ASP:HB3	1:I:135:GLY:HA2	1.85	0.59
1:A:170:GLN:HG3	1:A:223:LEU:HD13	1.86	0.58
1:S:186:VAL:HG23	1:S:187:GLN:H	1.68	0.58
1:S:131:MET:HG2	2:T:172:VAL:HG21	1.86	0.58
2:B:147:LEU:HD21	2:B:159:LEU:HD12	1.86	0.58
1:U:57:MET:HA	1:U:60:GLU:HB2	1.83	0.58
2:V:119:LEU:HD13	2:V:146:ILE:HD11	1.85	0.58
1:S:89:TYR:HE1	1:S:187:GLN:HA	1.69	0.58
1:Q:73:ARG:NH1	1:Q:154:GLU:OE1	2.37	0.58
2:B:118:GLN:NE2	2:B:183:LYS:O	2.36	0.58
2:P:127:HIS:CD2	2:P:128:PRO:HD2	2.39	0.58
2:B:180:LEU:O	2:B:182:LYS:N	2.37	0.57
2:P:153:GLU:O	2:P:157:GLU:N	2.29	0.57
1:I:209:SER:OG	1:I:210:PHE:N	2.36	0.57
2:N:170:PRO:HB3	1:O:227:LEU:HD13	1.85	0.57
2:V:172:VAL:HA	2:V:175:GLU:HB2	1.87	0.57
1:U:89:TYR:CZ	1:U:188:ILE:HG22	2.40	0.57
1:K:197:LEU:HD11	1:K:212:ASN:HB2	1.85	0.57
1:Q:145:GLU:HG3	2:R:179:ASN:HD21	1.69	0.57
1:C:212:ASN:OD1	1:C:212:ASN:N	2.35	0.57
1:E:115:ILE:HB	1:E:214:CYS:HB2	1.87	0.57
1:U:104:ILE:HD11	1:U:178:ASN:HB3	1.87	0.57
1:G:53:ARG:NH2	1:G:56:GLN:OE1	2.39	0.56
2:V:154:LEU:O	2:V:158:VAL:N	2.35	0.56
1:U:121:ASP:O	1:U:125:THR:OG1	2.23	0.56
1:Q:74:LEU:HD21	1:Q:126:MET:HG2	1.87	0.56
1:U:116:PHE:HD2	1:U:213:VAL:HG22	1.71	0.56
2:V:169:SER:HB3	2:V:172:VAL:HG12	1.88	0.56
1:S:51:GLN:HG3	1:S:224:LEU:HD11	1.88	0.56
1:S:106:THR:OG1	1:S:107:GLY:N	2.40	0.55
1:I:54:THR:HG21	1:I:227:LEU:HD21	1.88	0.55
1:U:55:PHE:HA	1:U:58:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HG22	1:A:115:ILE:HG12	1.89	0.55
1:S:92:PHE:HA	1:S:95:SER:HB3	1.87	0.55
1:K:222:PRO:HG2	1:K:223:LEU:HD12	1.88	0.55
1:C:56:GLN:O	1:C:60:GLU:HB2	2.06	0.55
1:M:183:PRO:O	1:M:186:VAL:HG22	2.06	0.55
2:T:162:ILE:HA	2:T:165:LEU:HD23	1.88	0.55
1:A:146:ILE:HD11	2:B:122:PHE:HZ	1.71	0.55
2:L:129:GLN:HG2	2:L:161:ARG:HD3	1.88	0.55
1:O:113:SER:HB2	1:O:188:ILE:HG21	1.89	0.55
2:T:166:GLU:N	2:T:166:GLU:OE1	2.37	0.55
1:U:195:VAL:HG22	1:U:216:PRO:HA	1.89	0.55
1:K:73:ARG:NH2	1:K:154:GLU:OE1	2.34	0.54
1:Q:51:GLN:HE22	1:Q:224:LEU:HD21	1.72	0.54
2:D:180:LEU:O	2:D:182:LYS:N	2.41	0.54
1:E:61:ASN:O	1:E:65:ALA:N	2.38	0.54
2:F:144:ALA:O	2:F:148:GLY:N	2.40	0.54
1:Q:162:LEU:HD21	1:Q:215:TRP:HZ2	1.73	0.54
2:V:174:LYS:C	2:V:177:GLU:HG2	2.28	0.54
2:P:132:ALA:HB3	2:P:161:ARG:HH12	1.71	0.54
1:Q:96:VAL:HG11	1:Q:102:ILE:HD11	1.88	0.54
1:Q:83:SER:HB3	1:Q:199:THR:HB	1.90	0.54
1:U:88:THR:HG22	1:U:90:GLU:H	1.72	0.54
2:P:120:VAL:HG22	2:P:146:ILE:HG23	1.89	0.53
1:M:122:LEU:HD23	1:M:211:ILE:HD11	1.90	0.53
1:E:136:GLU:OE1	1:E:136:GLU:N	2.41	0.53
2:L:147:LEU:O	2:L:155:GLN:NE2	2.40	0.53
1:Q:110:PHE:HB3	1:Q:219:LEU:HD11	1.91	0.53
2:T:169:SER:O	2:T:172:VAL:HG12	2.09	0.53
1:A:100:SER:HA	1:A:120:LEU:HG	1.91	0.53
1:A:217:PHE:O	1:A:219:LEU:HB2	2.08	0.53
1:E:54:THR:HG22	1:E:58:ILE:HD11	1.89	0.53
1:I:100:SER:HA	1:I:120:LEU:HG	1.91	0.53
1:I:188:ILE:HG13	1:I:189:VAL:HG13	1.91	0.53
1:M:209:SER:OG	1:M:210:PHE:N	2.41	0.53
1:S:89:TYR:CE1	1:S:187:GLN:HA	2.43	0.53
1:I:85:ASP:OD1	1:I:86:GLN:N	2.40	0.53
1:K:106:THR:OG1	1:K:107:GLY:N	2.42	0.53
2:V:157:GLU:HA	2:V:160:LYS:HB3	1.89	0.53
1:C:87:LEU:HB3	1:C:90:GLU:OE2	2.08	0.53
1:Q:104:ILE:HG22	1:Q:115:ILE:HG12	1.91	0.52
1:S:195:VAL:HG22	1:S:216:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:GLN:NE2	1:K:224:LEU:O	2.42	0.52
2:T:116:MET:SD	2:T:145:GLN:NE2	2.82	0.52
1:A:115:ILE:HB	1:A:214:CYS:HB3	1.90	0.52
2:R:120:VAL:HG22	2:R:146:ILE:HG23	1.90	0.52
1:U:61:ASN:HA	1:U:64:ARG:HG2	1.91	0.52
1:K:89:TYR:HE1	1:K:187:GLN:HA	1.74	0.52
1:O:196:LEU:HB3	1:O:215:TRP:HB2	1.92	0.52
1:A:128:ASP:OD1	1:A:135:GLY:N	2.36	0.52
1:O:51:GLN:HA	1:O:54:THR:HG22	1.92	0.52
1:A:89:TYR:HE1	1:A:187:GLN:HA	1.74	0.52
2:B:127:HIS:CD2	2:B:128:PRO:HD2	2.45	0.52
2:D:169:SER:O	2:D:172:VAL:HG22	2.09	0.52
1:E:57:MET:O	1:E:60:GLU:HB3	2.09	0.52
1:M:84:ILE:HD11	1:M:196:LEU:HD11	1.92	0.52
1:C:113:SER:HB2	1:C:188:ILE:HG12	1.92	0.52
1:E:209:SER:OG	1:E:210:PHE:N	2.42	0.52
2:F:167:ARG:NH1	2:F:168:THR:O	2.43	0.52
2:T:159:LEU:HA	2:T:162:ILE:HD11	1.91	0.52
1:K:131:MET:HG2	2:L:172:VAL:HG11	1.91	0.51
1:K:51:GLN:HE21	1:K:225:GLU:HG3	1.75	0.51
1:C:88:THR:N	1:C:90:GLU:OE2	2.42	0.51
1:A:200:ALA:HB3	1:A:211:ILE:HB	1.91	0.51
2:T:158:VAL:O	2:T:162:ILE:HG13	2.10	0.51
1:G:55:PHE:O	1:G:59:HIS:ND1	2.31	0.51
1:K:118:MET:HG3	1:K:211:ILE:HD11	1.93	0.51
1:E:54:THR:O	1:E:58:ILE:HG13	2.10	0.51
1:U:155:VAL:HA	1:U:158:MET:HB3	1.93	0.51
1:E:59:HIS:NE2	1:E:198:VAL:HG21	2.25	0.51
2:L:147:LEU:HD11	2:L:155:GLN:HA	1.91	0.51
2:T:132:ALA:HB1	2:T:162:ILE:HG23	1.93	0.51
1:A:220:LEU:O	1:A:224:LEU:N	2.44	0.51
2:L:135:LEU:HA	2:L:138:LEU:HB2	1.93	0.51
1:Q:178:ASN:OD1	1:Q:179:VAL:N	2.44	0.51
1:S:87:LEU:HB3	1:S:90:GLU:HG3	1.93	0.51
2:V:160:LYS:HE2	2:V:161:ARG:HG3	1.93	0.51
1:A:152:ARG:HA	1:A:155:VAL:HG22	1.93	0.51
2:H:179:ASN:HA	2:H:181:GLU:HG3	1.93	0.51
1:E:47:PHE:HA	1:E:51:GLN:HE21	1.76	0.50
1:S:73:ARG:NH2	1:S:154:GLU:OE1	2.43	0.50
1:M:131:MET:O	2:N:129:GLN:NE2	2.41	0.50
1:M:195:VAL:HG22	1:M:216:PRO:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:132:GLY:O	2:V:129:GLN:NE2	2.45	0.50
1:C:188:ILE:HG23	1:C:189:VAL:HG22	1.93	0.50
2:V:182:LYS:HB2	2:V:183:LYS:HG3	1.93	0.50
2:B:180:LEU:C	2:B:182:LYS:N	2.62	0.50
1:U:189:VAL:HG22	1:U:190:PRO:HD2	1.94	0.50
1:E:73:ARG:NH1	1:G:168:ASP:OD2	2.44	0.50
2:H:147:LEU:HG	2:H:155:GLN:HG3	1.93	0.50
2:F:147:LEU:O	2:F:155:GLN:NE2	2.45	0.49
1:O:55:PHE:CE2	1:O:220:LEU:HD21	2.47	0.49
2:R:139:ASP:HB3	2:R:142:VAL:HB	1.94	0.49
2:D:180:LEU:HG	2:D:184:ILE:HD13	1.93	0.49
1:O:134:PRO:HD3	2:P:161:ARG:HD3	1.94	0.49
1:U:112:GLY:HA3	1:U:219:LEU:HD11	1.93	0.49
2:L:117:VAL:O	2:L:121:ASN:ND2	2.45	0.49
1:S:196:LEU:HB3	1:S:215:TRP:HB2	1.93	0.49
1:U:120:LEU:HA	1:U:123:PHE:HB3	1.95	0.49
1:A:113:SER:HB2	1:A:188:ILE:HG12	1.94	0.49
1:S:50:GLU:HG3	1:S:51:GLN:HG2	1.94	0.49
1:M:98:ILE:HG23	1:M:183:PRO:HD2	1.94	0.49
1:Q:168:ASP:OD1	1:S:73:ARG:NH1	2.46	0.49
1:I:59:HIS:CD2	1:I:198:VAL:HG21	2.47	0.49
1:O:159:LEU:HD23	1:O:174:PRO:HB2	1.95	0.49
1:C:121:ASP:OD2	1:C:121:ASP:N	2.46	0.49
1:U:78:VAL:HG11	1:U:204:TRP:HB2	1.94	0.49
1:A:70:LEU:O	1:A:74:LEU:N	2.46	0.49
1:C:74:LEU:HA	1:C:129:ILE:HG21	1.95	0.49
1:G:59:HIS:O	1:G:82:ILE:HG13	2.13	0.49
2:R:151:PRO:HG2	2:R:153:GLU:HG2	1.94	0.49
1:E:47:PHE:HB2	1:E:86:GLN:NE2	2.28	0.48
1:I:76:THR:OG1	1:I:77:PHE:N	2.46	0.48
1:O:76:THR:OG1	1:O:77:PHE:N	2.46	0.48
1:E:52:LEU:HD11	1:E:86:GLN:NE2	2.27	0.48
2:P:129:GLN:HA	2:P:161:ARG:CZ	2.43	0.48
1:I:115:ILE:HB	1:I:214:CYS:HB3	1.95	0.48
1:A:123:PHE:CE1	1:A:151:MET:HG2	2.48	0.48
1:C:121:ASP:O	1:C:125:THR:OG1	2.20	0.48
1:S:90:GLU:OE1	1:S:90:GLU:N	2.46	0.48
1:Q:46:LYS:HA	1:Q:194:ILE:HG21	1.94	0.48
1:A:105:PHE:CG	1:A:159:LEU:HD21	2.49	0.48
2:H:169:SER:O	2:H:172:VAL:HG22	2.13	0.48
1:A:104:ILE:HD11	1:A:178:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:LEU:HD23	1:K:174:PRO:HB2	1.95	0.48
2:T:153:GLU:HG2	2:T:154:LEU:HG	1.96	0.48
1:K:70:LEU:HD23	1:K:78:VAL:HG11	1.96	0.48
1:S:49:LYS:O	1:S:53:ARG:NH2	2.47	0.48
1:U:63:GLY:O	1:U:67:SER:OG	2.23	0.48
1:C:209:SER:OG	1:C:210:PHE:N	2.46	0.48
1:K:148:THR:O	1:K:152:ARG:N	2.47	0.48
1:M:200:ALA:HB3	1:M:211:ILE:HB	1.96	0.48
1:E:131:MET:O	2:F:129:GLN:NE2	2.44	0.47
2:V:120:VAL:HG22	2:V:146:ILE:HA	1.96	0.47
1:C:73:ARG:HA	1:C:73:ARG:HE	1.79	0.47
2:P:169:SER:O	2:P:172:VAL:HG22	2.14	0.47
1:U:71:SER:OG	1:U:77:PHE:O	2.22	0.47
2:B:158:VAL:O	2:B:162:ILE:HG13	2.14	0.47
1:U:100:SER:HA	1:U:120:LEU:HG	1.97	0.47
1:C:88:THR:OG1	1:C:90:GLU:HG3	2.13	0.47
2:V:180:LEU:HD13	2:V:187:PHE:CD2	2.49	0.47
1:G:108:ASP:N	1:G:108:ASP:OD1	2.46	0.47
1:G:137:ASN:OD1	2:H:161:ARG:NH2	2.47	0.47
2:H:147:LEU:HD23	2:J:159:LEU:HD11	1.96	0.47
1:E:57:MET:SD	2:H:167:ARG:NH1	2.88	0.47
1:K:144:THR:OG1	1:K:145:GLU:N	2.47	0.47
2:N:174:LYS:HA	2:N:177:GLU:CD	2.35	0.47
1:C:84:ILE:HD11	1:C:196:LEU:HD11	1.95	0.47
1:A:153:LYS:O	1:A:157:ASN:ND2	2.43	0.47
1:C:186:VAL:HG23	1:C:187:GLN:H	1.80	0.47
1:C:204:TRP:O	1:C:206:GLU:N	2.48	0.47
1:G:60:GLU:OE2	1:G:64:ARG:NH2	2.48	0.47
1:Q:186:VAL:HG23	1:Q:187:GLN:H	1.80	0.47
1:S:88:THR:HA	1:S:194:ILE:HA	1.95	0.47
2:L:132:ALA:HB1	2:L:162:ILE:HG12	1.97	0.46
2:L:172:VAL:O	2:L:176:ILE:HG13	2.14	0.46
1:M:177:GLU:N	1:M:177:GLU:OE1	2.48	0.46
1:A:195:VAL:HG22	1:A:216:PRO:HA	1.96	0.46
1:A:224:LEU:HA	1:A:226:LYS:HD2	1.98	0.46
1:M:159:LEU:HD23	1:M:174:PRO:HB2	1.97	0.46
1:O:81:GLU:HB3	1:O:201:SER:HB2	1.97	0.46
2:P:177:GLU:C	2:P:179:ASN:H	2.18	0.46
2:R:184:ILE:HB	2:R:187:PHE:CE2	2.51	0.46
1:U:61:ASN:HD21	1:U:165:ALA:HA	1.81	0.46
1:E:74:LEU:HD21	1:E:126:MET:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:94:ARG:HH22	1:U:98:ILE:HD11	1.79	0.46
1:A:146:ILE:HD11	2:B:122:PHE:CZ	2.51	0.46
1:Q:169:PHE:HB3	1:Q:227:LEU:HD11	1.97	0.46
1:Q:51:GLN:HA	1:Q:54:THR:HG22	1.96	0.46
1:A:155:VAL:O	1:A:159:LEU:HB2	2.16	0.46
1:C:125:THR:HG21	1:C:204:TRP:HZ2	1.81	0.46
2:D:158:VAL:O	2:D:162:ILE:HG13	2.16	0.46
1:I:103:VAL:HG11	1:I:176:ILE:HD12	1.98	0.46
1:Q:106:THR:OG1	1:Q:107:GLY:N	2.47	0.46
1:A:226:LYS:HA	1:A:226:LYS:HD2	1.68	0.46
1:O:122:LEU:HD23	1:O:211:ILE:HD11	1.98	0.46
1:Q:200:ALA:HB3	1:Q:211:ILE:HB	1.97	0.46
1:A:89:TYR:CE1	1:A:187:GLN:HA	2.50	0.46
1:Q:160:THR:HG21	1:S:160:THR:HG21	1.98	0.46
2:D:152:GLU:HA	2:D:155:GLN:HB2	1.98	0.45
1:E:51:GLN:NE2	1:E:224:LEU:HD21	2.30	0.45
1:E:83:SER:HB3	1:E:199:THR:HB	1.98	0.45
2:F:135:LEU:HD22	2:F:143:ALA:HA	1.97	0.45
1:K:125:THR:O	1:K:129:ILE:HG12	2.15	0.45
1:K:86:GLN:H	1:K:86:GLN:HG3	1.62	0.45
1:O:146:ILE:HG22	2:P:179:ASN:ND2	2.32	0.45
2:V:181:GLU:HB3	2:V:182:LYS:H	1.58	0.45
1:C:98:ILE:HA	1:C:99:PRO:HA	1.80	0.45
1:I:195:VAL:HG11	1:I:214:CYS:SG	2.56	0.45
1:O:56:GLN:O	1:O:60:GLU:HB2	2.17	0.45
1:Q:105:PHE:CD1	1:Q:159:LEU:HD21	2.52	0.45
1:I:104:ILE:HD11	1:I:178:ASN:HB3	1.99	0.45
1:I:123:PHE:CE1	1:I:151:MET:HG2	2.52	0.45
2:J:119:LEU:HD13	2:J:146:ILE:HD11	1.97	0.45
1:K:186:VAL:HG23	1:K:187:GLN:H	1.82	0.45
2:R:154:LEU:HB3	2:R:158:VAL:HG23	1.99	0.45
1:A:121:ASP:O	1:A:125:THR:OG1	2.31	0.45
1:K:209:SER:OG	1:K:210:PHE:N	2.50	0.45
1:E:98:ILE:HA	1:E:99:PRO:HA	1.78	0.45
2:V:172:VAL:O	2:V:176:ILE:HG13	2.17	0.45
1:A:58:ILE:HA	1:A:58:ILE:HD12	1.80	0.45
1:Q:84:ILE:HD11	1:Q:196:LEU:HD11	1.98	0.45
1:M:117:GLU:OE1	1:M:212:ASN:ND2	2.46	0.45
1:M:48:SER:OG	1:M:49:LYS:N	2.49	0.45
1:O:102:ILE:HG12	1:O:117:GLU:OE1	2.17	0.45
2:T:175:GLU:O	2:T:179:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:180:LEU:O	2:T:184:ILE:HG22	2.17	0.45
1:C:49:LYS:HG3	1:C:51:GLN:N	2.33	0.45
1:Q:195:VAL:HG11	1:Q:214:CYS:SG	2.57	0.45
2:R:127:HIS:CD2	2:R:128:PRO:HD2	2.53	0.45
2:B:182:LYS:HE2	2:B:183:LYS:HB2	1.98	0.44
1:C:49:LYS:C	1:C:51:GLN:H	2.21	0.44
2:V:127:HIS:CD2	2:V:128:PRO:HD2	2.52	0.44
1:I:125:THR:HG21	1:I:204:TRP:HZ2	1.83	0.44
2:N:174:LYS:NZ	2:N:178:ARG:HH12	2.16	0.44
1:O:122:LEU:HD13	1:O:204:TRP:CH2	2.52	0.44
1:U:77:PHE:O	1:U:78:VAL:HG22	2.16	0.44
1:E:153:LYS:HA	1:E:156:THR:HB	2.00	0.44
2:F:132:ALA:O	2:F:136:SER:OG	2.32	0.44
2:T:152:GLU:O	2:T:155:GLN:N	2.50	0.44
1:U:80:VAL:HG22	1:U:202:VAL:HA	1.99	0.44
1:A:126:MET:O	1:A:130:ILE:HG12	2.17	0.44
1:A:186:VAL:HG23	1:A:187:GLN:H	1.83	0.44
2:D:178:ARG:HA	2:D:178:ARG:HD3	1.77	0.44
1:S:188:ILE:HG23	1:S:189:VAL:HG13	1.98	0.44
1:E:152:ARG:CZ	1:E:176:ILE:HD11	2.48	0.44
1:I:120:LEU:HD23	1:I:120:LEU:HA	1.81	0.44
1:O:98:ILE:HA	1:O:99:PRO:HA	1.72	0.44
1:O:146:ILE:HG22	2:P:179:ASN:HD22	1.82	0.44
2:P:183:LYS:HA	2:P:183:LYS:HD3	1.89	0.44
1:Q:169:PHE:HA	2:T:170:PRO:HB2	1.99	0.44
1:A:57:MET:HG2	1:A:60:GLU:OE1	2.18	0.44
2:B:174:LYS:HA	2:B:177:GLU:HB3	1.99	0.44
1:E:85:ASP:HB3	1:E:87:LEU:HD12	2.00	0.44
1:G:186:VAL:HG23	1:G:187:GLN:H	1.82	0.44
2:R:169:SER:HA	2:R:170:PRO:HD3	1.89	0.44
2:T:180:LEU:HB3	2:T:184:ILE:HG21	2.00	0.44
1:A:55:PHE:O	1:A:58:ILE:HG22	2.18	0.44
1:A:98:ILE:HA	1:A:99:PRO:HA	1.73	0.44
2:J:147:LEU:HD11	2:J:155:GLN:HA	2.00	0.44
1:K:89:TYR:CZ	1:K:188:ILE:HG22	2.52	0.44
1:M:53:ARG:CZ	1:M:228:SER:HB2	2.47	0.44
1:Q:155:VAL:O	1:Q:159:LEU:HB2	2.18	0.44
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.86	0.43
1:A:125:THR:O	1:A:129:ILE:HG12	2.17	0.43
1:C:155:VAL:O	1:C:159:LEU:HB2	2.18	0.43
1:G:190:PRO:HA	1:G:191:PRO:HD3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:GLU:HA	2:B:180:LEU:HB2	1.99	0.43
1:I:74:LEU:O	1:I:76:THR:HG22	2.18	0.43
2:J:158:VAL:O	2:J:162:ILE:HG13	2.18	0.43
1:O:209:SER:OG	1:O:210:PHE:N	2.51	0.43
1:S:128:ASP:HB3	1:S:135:GLY:HA2	2.00	0.43
1:I:125:THR:HG21	1:I:204:TRP:CZ2	2.53	0.43
2:L:158:VAL:O	2:L:162:ILE:HG13	2.18	0.43
1:Q:169:PHE:HB3	1:Q:227:LEU:HD21	2.01	0.43
1:C:90:GLU:OE1	1:C:91:GLU:N	2.51	0.43
2:F:169:SER:O	2:F:172:VAL:HG12	2.18	0.43
1:G:136:GLU:O	1:G:138:PRO:HD3	2.18	0.43
1:I:62:PHE:CE1	1:I:162:LEU:HB3	2.53	0.43
2:L:127:HIS:O	2:L:131:ILE:HG13	2.18	0.43
2:L:169:SER:HB3	2:L:172:VAL:HB	1.99	0.43
1:U:98:ILE:HA	1:U:99:PRO:HA	1.75	0.43
1:E:89:TYR:CZ	1:E:93:ILE:HD13	2.54	0.43
1:G:120:LEU:HA	1:G:123:PHE:HB3	2.01	0.43
1:I:108:ASP:OD1	1:I:108:ASP:N	2.51	0.43
2:J:169:SER:HA	2:J:170:PRO:HD3	1.80	0.43
1:O:155:VAL:O	1:O:159:LEU:N	2.51	0.43
1:M:168:ASP:CG	1:O:73:ARG:HH12	2.21	0.43
1:O:98:ILE:H	1:O:98:ILE:HG13	1.61	0.43
1:S:108:ASP:N	1:S:108:ASP:OD1	2.50	0.43
1:U:55:PHE:CD2	1:U:58:ILE:HD11	2.53	0.43
1:E:138:PRO:HA	1:E:139:PRO:HD2	1.95	0.43
1:G:162:LEU:HD21	1:G:215:TRP:HZ2	1.84	0.43
2:N:117:VAL:HG13	1:S:185:PHE:CE2	2.54	0.43
1:S:59:HIS:CE1	1:S:166:TRP:HE1	2.36	0.43
2:B:155:GLN:O	2:B:159:LEU:HB2	2.19	0.43
2:B:169:SER:HA	2:B:170:PRO:HD3	1.79	0.43
2:B:182:LYS:HB3	2:B:182:LYS:NZ	2.34	0.43
1:G:84:ILE:HD11	1:G:196:LEU:HD11	2.00	0.43
2:R:183:LYS:HD2	2:R:183:LYS:HA	1.78	0.43
2:B:182:LYS:HG2	2:B:183:LYS:HG3	2.00	0.43
1:M:125:THR:HG21	1:M:204:TRP:HZ2	1.84	0.43
1:M:204:TRP:O	1:M:206:GLU:N	2.52	0.43
1:Q:195:VAL:HG13	1:Q:215:TRP:C	2.38	0.43
1:M:73:ARG:HA	1:M:73:ARG:HD2	1.86	0.43
1:O:74:LEU:O	1:O:76:THR:N	2.50	0.43
1:U:195:VAL:HG13	1:U:215:TRP:C	2.39	0.43
2:L:174:LYS:HA	2:L:177:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:165:LEU:HD11	2:N:168:THR:HG22	2.00	0.42
1:U:125:THR:O	1:U:129:ILE:HG12	2.19	0.42
1:G:98:ILE:HD12	1:G:99:PRO:HA	2.01	0.42
1:I:155:VAL:HA	1:I:158:MET:HB3	2.00	0.42
1:K:73:ARG:HA	1:K:73:ARG:HE	1.83	0.42
1:S:113:SER:OG	1:S:177:GLU:OE1	2.37	0.42
1:U:117:GLU:OE1	1:U:212:ASN:ND2	2.51	0.42
2:R:144:ALA:HA	2:R:147:LEU:HB3	2.00	0.42
1:E:131:MET:HG2	2:F:172:VAL:HG21	2.00	0.42
1:I:117:GLU:HB3	1:I:212:ASN:HB2	2.02	0.42
1:S:198:VAL:HB	1:S:213:VAL:HB	2.01	0.42
1:U:92:PHE:CE1	1:U:197:LEU:HD13	2.54	0.42
2:V:135:LEU:HD22	2:V:143:ALA:HA	2.02	0.42
2:B:140:PRO:N	2:B:141:PRO:HD2	2.34	0.42
1:O:138:PRO:HA	1:O:139:PRO:HD2	1.97	0.42
1:Q:97:MET:O	1:Q:100:SER:HB2	2.20	0.42
1:U:144:THR:H	1:U:147:GLU:HB2	1.84	0.42
1:A:97:MET:HB2	1:A:97:MET:HE3	1.73	0.42
1:C:182:ASN:HB3	1:C:185:PHE:CD2	2.55	0.42
1:S:120:LEU:HD23	1:S:120:LEU:HA	1.87	0.42
1:E:127:LEU:HD21	1:E:147:GLU:HG2	2.01	0.42
1:G:113:SER:HB2	1:G:188:ILE:HD11	2.00	0.42
1:K:159:LEU:HA	1:K:159:LEU:HD12	1.91	0.42
1:M:169:PHE:CD2	2:P:170:PRO:HG2	2.54	0.42
1:A:109:VAL:HG21	1:A:170:GLN:OE1	2.20	0.42
1:A:217:PHE:C	1:A:219:LEU:HB2	2.40	0.42
1:E:86:GLN:O	1:E:87:LEU:HG	2.20	0.42
1:M:105:PHE:CG	1:M:159:LEU:HD21	2.55	0.42
1:M:170:GLN:NE2	1:M:227:LEU:HD22	2.34	0.42
1:U:196:LEU:HB3	1:U:215:TRP:HB2	2.02	0.42
2:B:139:ASP:OD1	2:B:141:PRO:HG2	2.20	0.42
1:A:58:ILE:HG13	1:A:166:TRP:CD1	2.54	0.41
1:C:196:LEU:HB3	1:C:215:TRP:HB2	2.00	0.41
1:G:66:LEU:HD23	1:G:80:VAL:HG11	2.02	0.41
1:U:61:ASN:N	1:U:61:ASN:OD1	2.48	0.41
2:V:117:VAL:O	2:V:121:ASN:HB2	2.20	0.41
1:E:48:SER:OG	1:E:49:LYS:N	2.52	0.41
1:G:67:SER:OG	1:G:78:VAL:O	2.32	0.41
2:V:160:LYS:HG2	2:V:161:ARG:HG3	2.03	0.41
1:A:168:ASP:OD1	1:C:73:ARG:NH1	2.53	0.41
1:C:97:MET:O	1:C:100:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:PRO:HA	1:G:139:PRO:HD2	1.99	0.41
1:G:143:PRO:HB2	1:G:148:THR:HG23	2.03	0.41
1:I:74:LEU:HD21	1:I:126:MET:HG2	2.03	0.41
1:K:113:SER:HB2	1:K:188:ILE:HD11	2.01	0.41
1:M:123:PHE:CE1	1:M:151:MET:HG2	2.56	0.41
1:M:221:GLU:C	1:M:223:LEU:H	2.23	0.41
1:M:136:GLU:HB2	2:N:161:ARG:HH22	1.85	0.41
2:R:127:HIS:HB3	2:R:130:THR:OG1	2.21	0.41
1:G:226:LYS:HB3	1:G:227:LEU:HD12	2.02	0.41
2:N:174:LYS:HZ1	2:N:178:ARG:HH12	1.67	0.41
1:Q:104:ILE:HD11	1:Q:178:ASN:HB3	2.03	0.41
1:E:93:ILE:HA	1:E:93:ILE:HD12	1.94	0.41
2:J:154:LEU:HA	2:J:154:LEU:HD23	1.78	0.41
1:K:138:PRO:HA	1:K:139:PRO:HD2	1.95	0.41
2:T:155:GLN:O	2:T:159:LEU:HG	2.20	0.41
1:U:108:ASP:OD1	1:U:109:VAL:N	2.53	0.41
1:A:74:LEU:HD22	1:A:129:ILE:HG13	2.03	0.41
1:A:87:LEU:O	1:A:195:VAL:N	2.53	0.41
1:M:177:GLU:CD	1:M:178:ASN:H	2.23	0.41
1:K:70:LEU:HB3	1:K:78:VAL:HG21	2.03	0.41
1:M:183:PRO:C	1:M:185:PHE:H	2.23	0.41
1:Q:221:GLU:N	1:Q:222:PRO:HD2	2.36	0.41
2:D:139:ASP:HB3	2:D:141:PRO:HD2	2.02	0.41
1:G:125:THR:HG21	1:G:204:TRP:HZ2	1.86	0.41
2:H:147:LEU:HD11	2:H:155:GLN:HA	2.02	0.41
1:O:51:GLN:NE2	1:O:224:LEU:HD21	2.35	0.41
1:Q:207:PHE:CZ	1:Q:209:SER:HB2	2.55	0.41
1:O:217:PHE:CG	1:O:218:SER:N	2.89	0.41
2:T:127:HIS:CD2	2:T:128:PRO:HD2	2.56	0.41
1:U:123:PHE:CE1	1:U:151:MET:HG2	2.56	0.41
2:J:130:THR:O	2:J:134:VAL:HG23	2.20	0.41
2:L:182:LYS:HG3	2:L:182:LYS:H	1.62	0.41
1:S:121:ASP:N	1:S:121:ASP:OD1	2.54	0.41
2:T:169:SER:HB3	2:T:172:VAL:HB	2.03	0.41
2:D:150:LEU:HD22	2:D:154:LEU:HD12	2.03	0.41
1:E:106:THR:OG1	1:E:107:GLY:N	2.54	0.41
1:G:74:LEU:HA	1:G:129:ILE:HG21	2.02	0.41
1:K:224:LEU:HD12	1:K:224:LEU:HA	1.89	0.41
1:S:113:SER:HB2	1:S:188:ILE:HG12	2.02	0.41
1:S:123:PHE:CE1	1:S:151:MET:HG3	2.56	0.41
1:S:98:ILE:HA	1:S:99:PRO:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:TYR:CE1	1:C:93:ILE:HD12	2.55	0.40
1:E:160:THR:HG21	1:G:160:THR:HG21	2.03	0.40
2:F:184:ILE:HG22	2:F:186:GLY:H	1.86	0.40
2:H:174:LYS:HD2	2:H:177:GLU:HG3	2.01	0.40
1:I:195:VAL:HG13	1:I:215:TRP:O	2.21	0.40
1:I:98:ILE:HA	1:I:99:PRO:HA	1.80	0.40
2:L:137:TYR:OH	2:L:168:THR:HG21	2.22	0.40
2:L:166:GLU:H	2:L:166:GLU:HG2	1.73	0.40
1:C:195:VAL:HG11	1:C:214:CYS:SG	2.61	0.40
2:H:183:LYS:HG2	2:H:184:ILE:HD12	2.03	0.40
1:K:86:GLN:HB2	1:K:86:GLN:HE21	1.60	0.40
2:B:169:SER:O	2:B:172:VAL:HG12	2.21	0.40
1:C:120:LEU:HD23	1:C:120:LEU:HA	1.93	0.40
1:E:56:GLN:HE21	1:E:84:ILE:HG22	1.86	0.40
2:F:166:GLU:HG2	2:F:166:GLU:H	1.70	0.40
1:G:128:ASP:CG	1:G:135:GLY:HA2	2.42	0.40
1:G:98:ILE:HA	1:G:99:PRO:HA	1.80	0.40
2:P:154:LEU:HA	2:P:154:LEU:HD23	1.76	0.40
1:Q:54:THR:O	1:Q:58:ILE:HG13	2.21	0.40
2:V:158:VAL:O	2:V:162:ILE:HG13	2.21	0.40
1:C:100:SER:HA	1:C:120:LEU:HG	2.03	0.40
1:E:74:LEU:HA	1:E:129:ILE:HG21	2.03	0.40
2:L:129:GLN:CA	2:L:161:ARG:HD3	2.51	0.40
2:V:132:ALA:O	2:V:136:SER:OG	2.35	0.40
1:U:75:ARG:HH22	2:V:166:GLU:CD	2.24	0.40
1:A:226:LYS:HE3	1:A:227:LEU:HD22	2.03	0.40
1:K:112:GLY:HA3	1:K:219:LEU:HG	2.03	0.40
2:N:169:SER:HB2	2:N:172:VAL:HG12	2.03	0.40
1:O:136:GLU:H	1:O:136:GLU:CD	2.25	0.40
1:O:161:LEU:HD23	1:O:161:LEU:HA	1.88	0.40
1:O:220:LEU:O	1:O:224:LEU:N	2.37	0.40
1:O:223:LEU:HG	1:O:226:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/183 (99%)	164 (91%)	14 (8%)	3 (2%)	9	43
1	C	181/183 (99%)	165 (91%)	11 (6%)	5 (3%)	5	33
1	E	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	4	30
1	G	181/183 (99%)	159 (88%)	19 (10%)	3 (2%)	9	43
1	I	181/183 (99%)	170 (94%)	9 (5%)	2 (1%)	14	52
1	K	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	9	43
1	M	181/183 (99%)	163 (90%)	13 (7%)	5 (3%)	5	33
1	O	181/183 (99%)	157 (87%)	19 (10%)	5 (3%)	5	33
1	Q	181/183 (99%)	166 (92%)	10 (6%)	5 (3%)	5	33
1	S	181/183 (99%)	161 (89%)	13 (7%)	7 (4%)	3	26
1	U	181/183 (99%)	158 (87%)	17 (9%)	6 (3%)	4	30
2	B	72/75 (96%)	67 (93%)	3 (4%)	2 (3%)	5	33
2	D	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	11	47
2	F	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	11	47
2	H	73/75 (97%)	62 (85%)	9 (12%)	2 (3%)	5	34
2	J	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	11	47
2	L	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
2	N	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	11	47
2	P	73/75 (97%)	62 (85%)	7 (10%)	4 (6%)	2	21
2	R	73/75 (97%)	65 (89%)	6 (8%)	2 (3%)	5	34
2	T	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	11	47
2	V	73/75 (97%)	63 (86%)	7 (10%)	3 (4%)	3	25
All	All	2793/2838 (98%)	2508 (90%)	217 (8%)	68 (2%)	6	36

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	C	90	GLU
2	D	181	GLU
1	E	60	GLU

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Mol	Chain	Res	Type
1	G	177	GLU
1	M	53	ARG
1	M	136	GLU
2	N	177	GLU
1	O	144	THR
1	O	217	PHE
1	S	50	GLU
1	S	90	GLU
2	T	153	GLU
1	U	78	VAL
1	U	190	PRO
1	A	186	VAL
2	B	181	GLU
1	C	205	GLY
1	E	49	LYS
1	E	186	VAL
2	F	166	GLU
1	G	205	GLY
1	I	186	VAL
1	I	205	GLY
1	M	187	GLN
1	M	205	GLY
1	O	187	GLN
1	Q	49	LYS
1	Q	186	VAL
2	R	153	GLU
1	S	88	THR
1	S	136	GLU
1	S	225	GLU
2	V	185	SER
2	B	182	LYS
1	E	61	ASN
2	J	185	SER
1	K	144	THR
2	P	182	LYS
2	R	166	GLU
1	U	77	PHE
1	U	186	VAL
1	U	205	GLY
2	V	128	PRO
1	C	50	GLU
1	E	226	LYS

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Mol	Chain	Res	Type
2	H	166	GLU
1	K	185	PHE
1	M	184	GLN
2	P	181	GLU
1	Q	144	THR
1	Q	226	LYS
1	K	134	PRO
1	O	205	GLY
2	P	178	ARG
2	V	182	LYS
1	E	205	GLY
1	G	138	PRO
2	H	115	HIS
1	S	205	GLY
1	C	135	GLY
1	Q	138	PRO
1	S	186	VAL
1	A	205	GLY
1	C	138	PRO
1	O	186	VAL
2	P	158	VAL
1	U	134	PRO

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	170/170 (100%)	160 (94%)	10 (6%)	19	47
1	C	170/170 (100%)	162 (95%)	8 (5%)	26	53
1	E	170/170 (100%)	159 (94%)	11 (6%)	17	44
1	G	170/170 (100%)	159 (94%)	11 (6%)	17	44
1	I	170/170 (100%)	158 (93%)	12 (7%)	14	41
1	K	170/170 (100%)	161 (95%)	9 (5%)	22	50
1	M	170/170 (100%)	160 (94%)	10 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	170/170 (100%)	162 (95%)	8 (5%)	26	53
1	Q	170/170 (100%)	161 (95%)	9 (5%)	22	50
1	S	170/170 (100%)	154 (91%)	16 (9%)	8	30
1	U	170/170 (100%)	159 (94%)	11 (6%)	17	44
2	B	67/67 (100%)	64 (96%)	3 (4%)	27	54
2	D	67/67 (100%)	67 (100%)	0	100	100
2	F	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	H	67/67 (100%)	64 (96%)	3 (4%)	27	54
2	J	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	L	67/67 (100%)	64 (96%)	3 (4%)	27	54
2	N	67/67 (100%)	66 (98%)	1 (2%)	65	80
2	P	67/67 (100%)	64 (96%)	3 (4%)	27	54
2	R	67/67 (100%)	63 (94%)	4 (6%)	19	46
2	T	67/67 (100%)	64 (96%)	3 (4%)	27	54
2	V	67/67 (100%)	63 (94%)	4 (6%)	19	46
All	All	2607/2607 (100%)	2464 (94%)	143 (6%)	21	49

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	60	GLU
1	A	94	ARG
1	A	145	GLU
1	A	175	SER
1	A	186	VAL
1	A	217	PHE
1	A	220	LEU
1	A	224	LEU
1	A	227	LEU
2	B	116	MET
2	B	168	THR
2	B	179	ASN
1	C	85	ASP
1	C	88	THR
1	C	90	GLU
1	C	108	ASP

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Mol	Chain	Res	Type
1	C	184	GLN
1	C	186	VAL
1	C	208	THR
1	C	217	PHE
1	E	55	PHE
1	E	87	LEU
1	E	100	SER
1	E	108	ASP
1	E	158	MET
1	E	168	ASP
1	E	184	GLN
1	E	186	VAL
1	E	206	GLU
1	E	208	THR
1	E	214	CYS
2	F	168	THR
2	F	173	VAL
1	G	47	PHE
1	G	60	GLU
1	G	85	ASP
1	G	96	VAL
1	G	110	PHE
1	G	141	ARG
1	G	158	MET
1	G	159	LEU
1	G	186	VAL
1	G	208	THR
1	G	217	PHE
2	H	130	THR
2	H	157	GLU
2	H	160	LYS
1	I	53	ARG
1	I	93	ILE
1	I	94	ARG
1	I	110	PHE
1	I	119	ARG
1	I	159	LEU
1	I	173	ILE
1	I	184	GLN
1	I	186	VAL
1	I	188	ILE
1	I	196	LEU

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Mol	Chain	Res	Type
1	I	217	PHE
2	J	119	LEU
2	J	171	GLU
1	K	47	PHE
1	K	86	GLN
1	K	94	ARG
1	K	110	PHE
1	K	115	ILE
1	K	180	GLU
1	K	184	GLN
1	K	186	VAL
1	K	219	LEU
2	L	155	GLN
2	L	173	VAL
2	L	182	LYS
1	M	58	ILE
1	M	88	THR
1	M	93	ILE
1	M	94	ARG
1	M	128	ASP
1	M	177	GLU
1	M	184	GLN
1	M	208	THR
1	M	214	CYS
1	M	217	PHE
2	N	138	LEU
1	O	98	ILE
1	O	119	ARG
1	O	178	ASN
1	O	186	VAL
1	O	208	THR
1	O	219	LEU
1	O	220	LEU
1	O	227	LEU
2	P	138	LEU
2	P	160	LYS
2	P	181	GLU
1	Q	55	PHE
1	Q	77	PHE
1	Q	93	ILE
1	Q	108	ASP
1	Q	111	GLU

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Mol	Chain	Res	Type
1	Q	152	ARG
1	Q	186	VAL
1	Q	206	GLU
1	Q	214	CYS
2	R	119	LEU
2	R	153	GLU
2	R	168	THR
2	R	180	LEU
1	S	46	LYS
1	S	47	PHE
1	S	49	LYS
1	S	55	PHE
1	S	83	SER
1	S	85	ASP
1	S	88	THR
1	S	90	GLU
1	S	91	GLU
1	S	140	ASN
1	S	180	GLU
1	S	186	VAL
1	S	208	THR
1	S	214	CYS
1	S	221	GLU
1	S	228	SER
2	T	145	GLN
2	T	150	LEU
2	T	179	ASN
1	U	57	MET
1	U	85	ASP
1	U	86	GLN
1	U	136	GLU
1	U	146	ILE
1	U	159	LEU
1	U	186	VAL
1	U	189	VAL
1	U	192	ASN
1	U	194	ILE
1	U	214	CYS
2	V	121	ASN
2	V	152	GLU
2	V	160	LYS
2	V	168	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
2	B	118	GLN
2	B	127	HIS
1	C	86	GLN
1	C	187	GLN
2	D	179	ASN
1	E	51	GLN
1	E	86	GLN
1	I	157	ASN
1	K	51	GLN
1	K	86	GLN
1	K	170	GLN
2	L	121	ASN
2	L	155	GLN
2	P	115	HIS
2	R	179	ASN
2	T	145	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.