



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:10 AM UTC

PDB ID : 5YK3 / pdb_00005yk3
Title : human Ragulator complex
Authors : Wu, G.; Mu, Z.
Deposited on : 2017-10-12
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

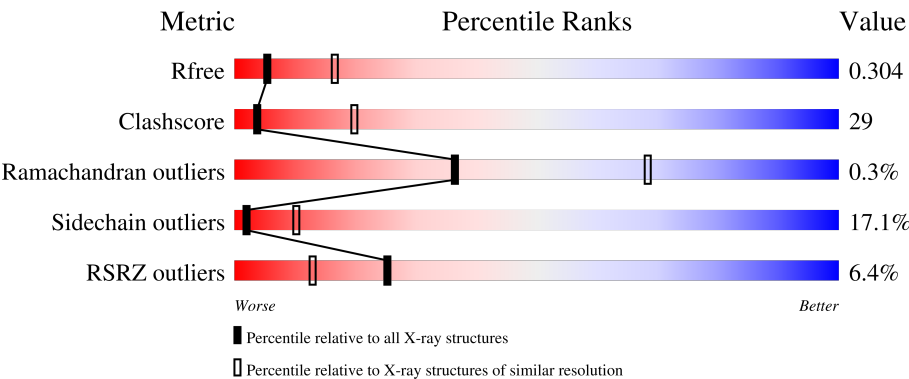
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	124	2% 68% 24% 7% .
1	m	124	2% 74% 23% .
2	G	125	8% 58% 28% 12% .
2	l	125	6% 56% 36% 7% .
3	o	90	3% 78% 18% ..

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Mol	Chain	Length	Quality of chain
4	n	88	
5	k	85	
6	C	123	
7	B	125	
8	E	91	
8	J	91	
9	D	96	
10	A	85	
10	F	85	
11	I	99	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11608 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 Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	m	124	Total	C	N	O	S	0	0	0
			941	606	154	180	1			
1	H	124	Total	C	N	O	S	0	0	0
			957	615	161	180	1			

- Molecule 2 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	124	Total	C	N	O	S	0	0	0
			928	586	159	176	7			
2	G	123	Total	C	N	O	S	0	0	0
			903	567	152	178	6			

- Molecule 3 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	o	90	Total	C	N	O	S	0	0	0
			657	402	114	134	7			

- Molecule 4 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	n	88	Total	C	N	O	S	0	0	0
			630	395	114	119	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	5	ALA	-	expression tag	UNP Q0VGL1
n	7	ALA	GLN	engineered mutation	UNP Q0VGL1

- Molecule 5 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	85	Total	C	N	O	S	0	0	0
			658	420	113	124	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	77	ALA	-	expression tag	UNP Q6IAA8
k	78	ALA	-	expression tag	UNP Q6IAA8

- Molecule 6 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	123	Total	C	N	O	S	0	0	0
			951	612	160	178	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	-	expression tag	UNP Q9UHA4

- Molecule 7 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	125	Total	C	N	O	S	0	0	0
			916	574	157	179	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP Q9Y2Q5
B	2	ALA	-	expression tag	UNP Q9Y2Q5
B	3	ALA	-	expression tag	UNP Q9Y2Q5
B	122	ALA	VAL	engineered mutation	UNP Q9Y2Q5
B	125	ALA	SER	engineered mutation	UNP Q9Y2Q5

- Molecule 8 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			
8	J	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			

- Molecule 9 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	96	Total	C	N	O	S	0	0	0
			715	448	130	135	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP Q0VGL1
D	3	THR	-	expression tag	UNP Q0VGL1

- Molecule 10 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	85	Total	C	N	O	S	0	0	0
			665	423	117	124	1			
10	F	85	Total	C	N	O	S	0	0	0
			665	423	117	124	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ALA	-	expression tag	UNP Q6IAA8
F	77	ALA	-	expression tag	UNP Q6IAA8

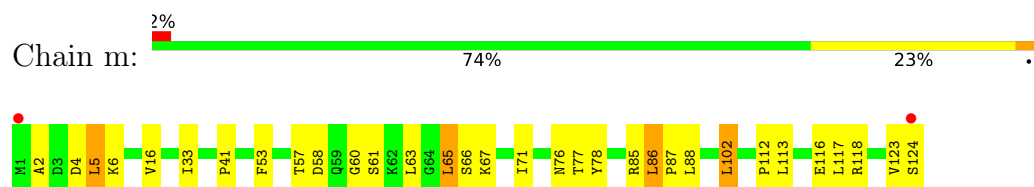
- Molecule 11 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	95	Total	C	N	O	S	0	0	0
			690	433	124	131	2			

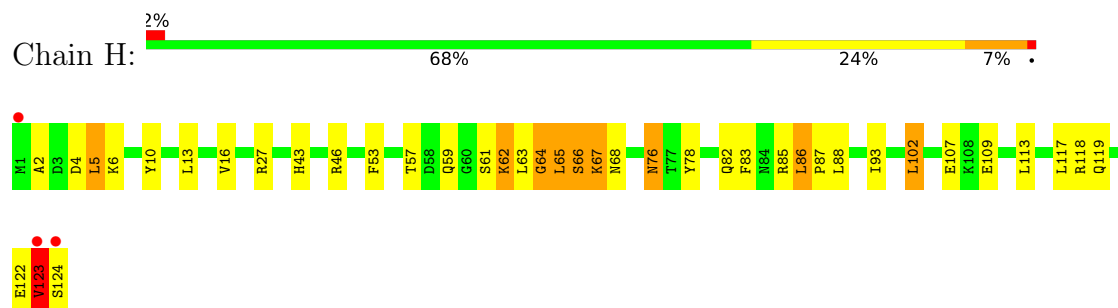
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

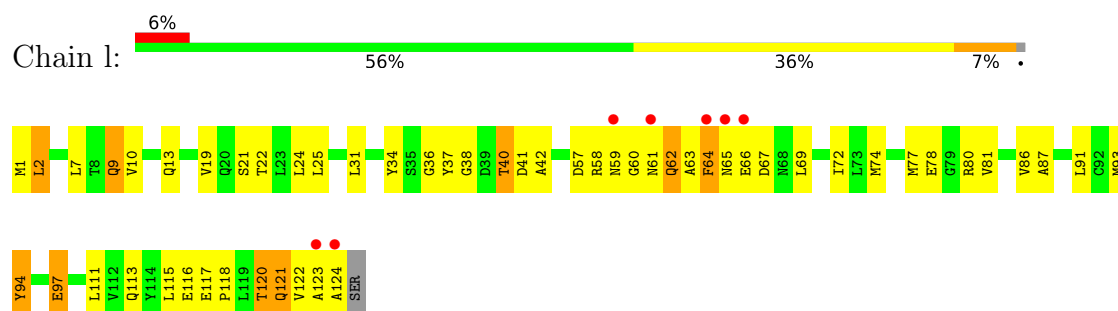
- Molecule 1: Regulator complex protein LAMTOR3



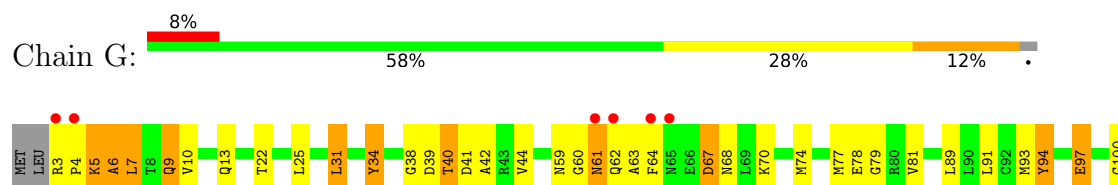
- Molecule 1: Regulator complex protein LAMTOR3



- Molecule 2: Regulator complex protein LAMTOR2

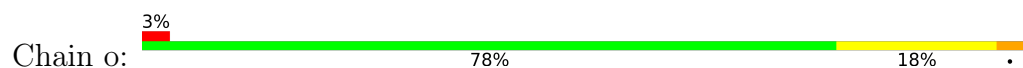


- Molecule 2: Regulator complex protein LAMTOR2

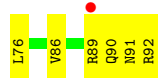
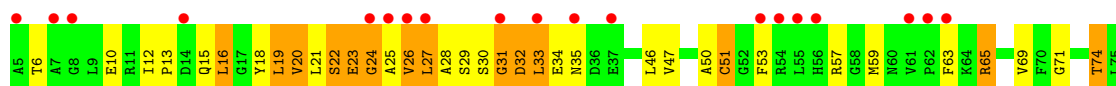




- Molecule 3: Regulator complex protein LAMTOR5



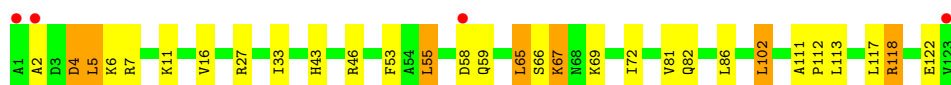
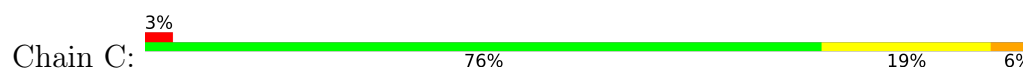
- Molecule 4: Regulator complex protein LAMTOR4



- Molecule 5: Regulator complex protein LAMTOR1



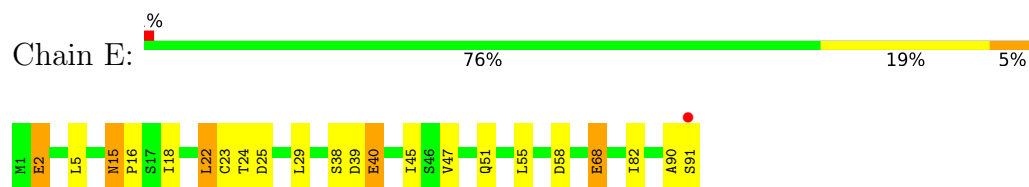
- Molecule 6: Regulator complex protein LAMTOR3



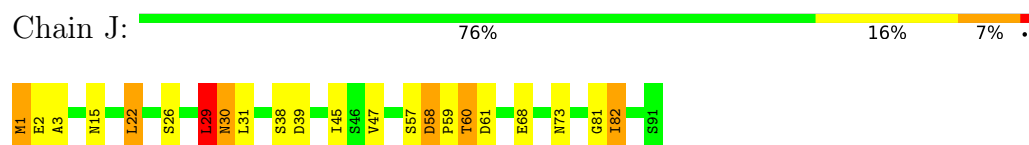
- Molecule 7: Regulator complex protein LAMTOR2



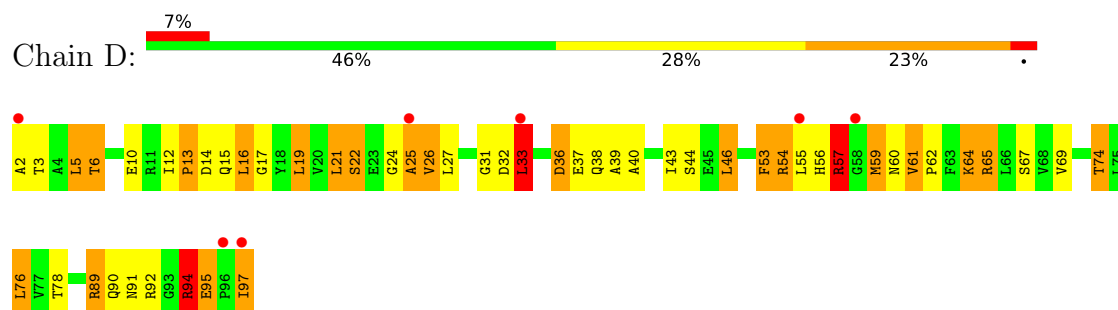
- Molecule 8: Regulator complex protein LAMTOR5



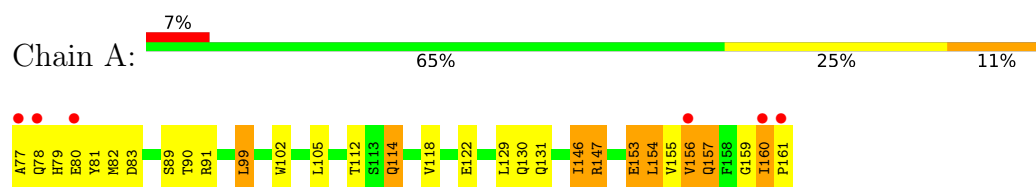
- Molecule 8: Regulator complex protein LAMTOR5



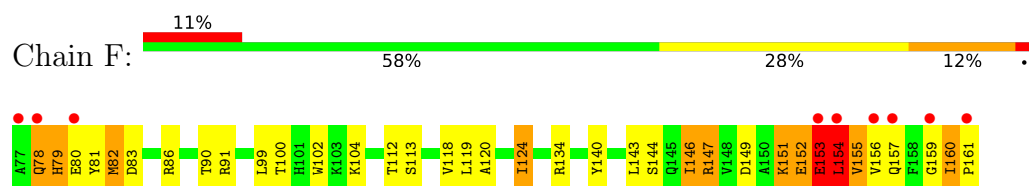
- Molecule 9: Regulator complex protein LAMTOR4



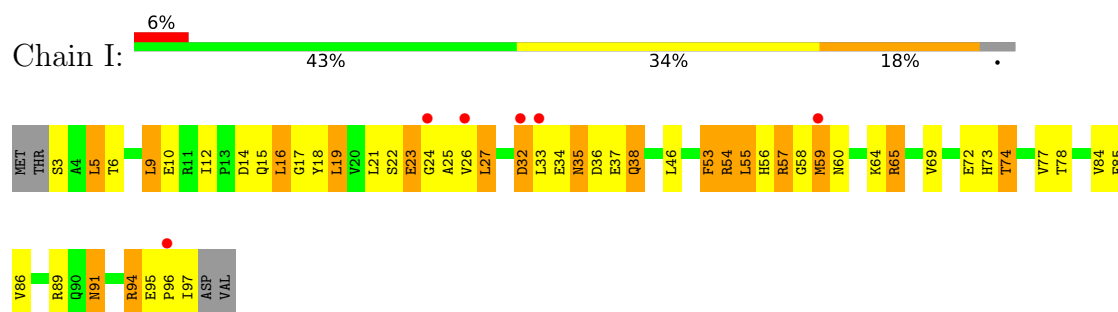
- Molecule 10: Regulator complex protein LAMTOR1



- Molecule 10: Regulator complex protein LAMTOR1



- Molecule 11: Regulator complex protein LAMTOR4



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.64Å 126.64Å 614.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.01 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	86.7 (50.00-3.01) 86.7 (50.00-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.285 (Not available) , 0.304	Depositor DCC
R_{free} test set	2569 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11608	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.50	0/974	0.86	3/1322 (0.2%)
1	m	0.48	0/958	0.82	1/1304 (0.1%)
2	G	0.44	0/913	0.92	3/1240 (0.2%)
2	l	0.45	0/939	0.79	0/1272
3	o	0.65	0/663	0.89	1/899 (0.1%)
4	n	0.59	0/638	1.06	3/866 (0.3%)
5	k	0.58	0/674	0.99	3/922 (0.3%)
6	C	0.49	0/968	0.82	0/1314
7	B	0.46	0/926	0.90	1/1257 (0.1%)
8	E	0.70	0/672	0.87	0/911
8	J	0.68	0/672	0.84	1/911 (0.1%)
9	D	0.69	0/724	1.09	4/980 (0.4%)
10	A	0.67	0/681	0.84	0/929
10	F	0.64	0/681	0.94	3/929 (0.3%)
11	I	0.61	0/699	1.02	3/947 (0.3%)
All	All	0.57	0/11782	0.91	26/16003 (0.2%)

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	H	0	1
9	D	0	3
10	A	0	1
10	F	0	1
All	All	0	6

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	n	24	GLY	N-CA-C	-12.81	96.38	111.36
2	G	124	ALA	N-CA-C	9.19	120.91	111.07
9	D	25	ALA	N-CA-C	-7.98	97.03	113.31
4	n	31	GLY	N-CA-C	-7.40	101.19	112.51
7	B	58	ARG	N-CA-C	-7.04	100.03	110.23
8	J	29	LEU	N-CA-C	6.67	118.44	110.44
5	k	104	LYS	N-CA-C	6.59	118.12	111.07
10	F	154	LEU	N-CA-C	6.29	119.17	108.67
9	D	61	VAL	CA-C-N	6.26	126.17	119.28
9	D	61	VAL	C-N-CA	6.26	126.17	119.28
1	H	65	LEU	N-CA-C	-6.20	99.08	109.07
11	I	91	ASN	N-CA-C	6.15	117.86	111.03
5	k	122	GLU	CA-C-N	6.00	126.84	120.11
5	k	122	GLU	C-N-CA	6.00	126.84	120.11
2	G	6	ALA	N-CA-C	-5.99	104.75	111.28
9	D	53	PHE	CB-CA-C	-5.97	102.83	111.91
4	n	23	GLU	CB-CA-C	-5.83	109.84	116.54
3	o	82	ILE	N-CA-C	5.66	116.00	107.80
10	F	154	LEU	CB-CA-C	-5.62	109.59	117.23
1	H	123	VAL	N-CA-C	5.49	120.76	109.34
1	H	64	GLY	N-CA-C	-5.33	107.96	115.32
11	I	34	GLU	N-CA-C	5.30	118.06	109.79
11	I	53	PHE	N-CA-C	5.29	117.52	108.90
2	G	39	ASP	N-CA-C	-5.24	105.68	111.71
1	m	65	LEU	N-CA-C	-5.12	101.35	109.59
10	F	80	GLU	N-CA-C	-5.06	105.76	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	156	VAL	Peptide
9	D	33	LEU	Peptide
9	D	57	ARG	Peptide
9	D	94	ARG	Peptide
10	F	153	GLU	Peptide
1	H	122	GLU	Peptide

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	H	957	0	982	47	0
1	m	941	0	949	33	0
2	G	903	0	893	65	0
2	l	928	0	938	58	0
3	o	657	0	659	19	0
4	n	630	0	607	51	0
5	k	658	0	648	72	0
6	C	951	0	980	30	0
7	B	916	0	916	40	0
8	E	666	0	666	21	0
8	J	666	0	666	36	0
9	D	715	0	720	73	0
10	A	665	0	665	53	0
10	F	665	0	665	51	0
11	I	690	0	672	90	0
All	All	11608	0	11626	668	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 29.

All (668) 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)
10:F:154:LEU:CD1	10:F:157:GLN:H	1.31	1.40
10:F:154:LEU:CD1	10:F:157:GLN:N	1.90	1.24
10:A:160:ILE:HG23	10:A:161:PRO:CD	1.68	1.22
2:G:40:THR:HB	2:G:41:ASP:CA	1.68	1.21
5:k:158:PHE:C	5:k:160:ILE:HD12	1.69	1.18
5:k:155:VAL:HG12	5:k:157:GLN:NE2	1.58	1.16
10:A:160:ILE:HG23	10:A:161:PRO:HD2	1.18	1.16
11:I:54:ARG:HB2	11:I:59:MET:HA	1.26	1.16
4:n:21:LEU:HA	4:n:26:VAL:O	1.44	1.16
11:I:23:GLU:C	11:I:25:ALA:HA	1.71	1.16
10:F:154:LEU:HD11	10:F:157:GLN:N	1.57	1.15
11:I:54:ARG:CB	11:I:59:MET:HA	1.77	1.13
11:I:56:HIS:C	11:I:57:ARG:HD3	1.73	1.12
9:D:54:ARG:HD2	9:D:55:LEU:N	1.63	1.11
2:G:40:THR:CB	2:G:41:ASP:HA	1.80	1.11
11:I:56:HIS:O	11:I:57:ARG:HD3	1.51	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:145:GLN:NE2	5:k:147:ARG:HH12	1.48	1.11
4:n:27:LEU:HD23	4:n:27:LEU:H	1.10	1.09
8:E:38:SER:OG	8:E:40:GLU:OE2	1.66	1.09
7:B:2:ALA:HB2	10:A:156:VAL:HA	1.35	1.09
11:I:95:GLU:OE1	11:I:96:PRO:HD2	1.52	1.08
2:G:5:LYS:HB3	2:G:5:LYS:HZ2	0.96	1.07
9:D:24:GLY:CA	9:D:26:VAL:HG12	1.85	1.06
9:D:17:GLY:HA2	9:D:32:ASP:HB2	1.36	1.06
11:I:22:SER:O	11:I:25:ALA:HB1	1.53	1.06
9:D:54:ARG:CD	9:D:55:LEU:N	2.19	1.05
10:A:160:ILE:CG2	10:A:161:PRO:HD2	1.85	1.05
10:F:154:LEU:HD13	10:F:157:GLN:H	0.94	1.04
11:I:59:MET:SD	11:I:59:MET:C	2.41	1.04
2:G:5:LYS:HB3	2:G:5:LYS:NZ	1.60	1.02
4:n:27:LEU:HD23	4:n:27:LEU:N	1.72	1.02
1:H:66:SER:HB2	2:G:77:MET:HB2	1.42	1.02
2:l:9:GLN:HE22	2:l:13:GLN:HE21	1.07	1.02
9:D:24:GLY:HA3	9:D:26:VAL:CG1	1.89	1.02
11:I:5:LEU:HD12	11:I:5:LEU:H	1.25	1.02
5:k:145:GLN:NE2	5:k:147:ARG:NH1	2.08	1.01
6:C:118:ARG:HH11	6:C:118:ARG:HB3	1.20	1.00
9:D:60:ASN:O	9:D:62:PRO:HD3	1.62	1.00
4:n:22:SER:O	4:n:24:GLY:O	1.80	1.00
9:D:24:GLY:HA3	9:D:26:VAL:HG12	1.03	0.99
2:G:117:GLU:HB3	2:G:118:PRO:HD3	1.45	0.98
7:B:60:GLY:HA2	7:B:61:ASN:C	1.88	0.98
6:C:58:ASP:OD1	6:C:59:GLN:N	1.97	0.98
11:I:17:GLY:HA2	11:I:32:ASP:HB2	1.47	0.97
10:F:78:GLN:HA	10:F:82:MET:HG2	1.47	0.97
11:I:53:PHE:O	11:I:59:MET:O	1.83	0.96
4:n:33:LEU:N	4:n:33:LEU:HD23	1.80	0.96
1:H:86:LEU:HD22	1:H:87:PRO:N	1.80	0.96
11:I:22:SER:C	11:I:25:ALA:HB1	1.90	0.96
5:k:158:PHE:HD2	5:k:158:PHE:O	1.51	0.93
4:n:32:ASP:C	4:n:33:LEU:HD23	1.92	0.93
9:D:54:ARG:CD	9:D:54:ARG:C	2.41	0.93
1:m:66:SER:HB3	2:l:77:MET:HB2	1.46	0.93
11:I:23:GLU:O	11:I:25:ALA:HA	1.68	0.93
8:E:90:ALA:HA	8:E:91:SER:HB3	1.50	0.92
6:C:118:ARG:HH11	6:C:118:ARG:CB	1.83	0.92
8:J:29:LEU:HA	8:J:30:ASN:ND2	1.85	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:94:ARG:HH11	11:I:94:ARG:CG	1.82	0.92
4:n:6:THR:O	4:n:18:TYR:OH	1.89	0.91
11:I:16:LEU:O	11:I:33:LEU:CD1	2.17	0.91
9:D:54:ARG:C	9:D:54:ARG:HD3	1.96	0.90
9:D:33:LEU:HD23	9:D:33:LEU:N	1.84	0.90
2:G:102:GLY:HA3	8:J:29:LEU:O	1.72	0.90
2:l:121:GLN:HE21	2:l:121:GLN:N	1.70	0.90
4:n:19:LEU:HD12	4:n:20:VAL:N	1.87	0.90
9:D:94:ARG:HD2	10:A:122:GLU:HG2	1.52	0.89
7:B:3:ALA:N	7:B:4:PRO:HA	1.86	0.89
5:k:145:GLN:HE22	5:k:147:ARG:HH12	0.89	0.89
6:C:4:ASP:OD2	6:C:7:ARG:NH1	2.04	0.89
5:k:79:HIS:C	5:k:79:HIS:CD2	2.51	0.89
2:G:4:PRO:O	10:F:155:VAL:CG1	2.20	0.88
5:k:155:VAL:HG12	5:k:157:GLN:HE22	1.36	0.88
5:k:158:PHE:C	5:k:160:ILE:CD1	2.47	0.88
8:J:30:ASN:N	8:J:30:ASN:HD22	1.72	0.87
2:l:9:GLN:NE2	2:l:13:GLN:HE21	1.71	0.87
2:G:40:THR:HB	2:G:41:ASP:HA	0.90	0.87
4:n:32:ASP:O	4:n:34:GLU:O	1.93	0.86
7:B:2:ALA:HB2	10:A:156:VAL:CA	2.04	0.86
10:A:159:GLY:O	10:A:160:ILE:HD12	1.74	0.86
10:A:160:ILE:HG23	10:A:161:PRO:CG	2.06	0.86
11:I:5:LEU:H	11:I:5:LEU:CD1	1.88	0.85
11:I:94:ARG:HH11	11:I:94:ARG:HG3	1.41	0.85
1:H:64:GLY:C	1:H:65:LEU:HD23	2.01	0.85
11:I:22:SER:O	11:I:26:VAL:N	2.10	0.85
2:G:117:GLU:HB3	2:G:118:PRO:CD	2.06	0.85
5:k:145:GLN:HE22	5:k:147:ARG:NH1	1.70	0.84
5:k:119:LEU:HD23	5:k:119:LEU:O	1.75	0.84
2:G:117:GLU:OE2	2:G:117:GLU:HA	1.75	0.84
7:B:3:ALA:H	7:B:4:PRO:HA	1.40	0.84
1:H:86:LEU:HD22	1:H:86:LEU:C	2.02	0.84
2:l:58:ARG:HG2	2:l:59:ASN:OD1	1.77	0.83
9:D:57:ARG:HA	9:D:59:MET:H	1.44	0.83
4:n:23:GLU:HG3	4:n:24:GLY:N	1.94	0.82
6:C:118:ARG:HB3	6:C:118:ARG:NH1	1.93	0.82
5:k:105:LEU:HD22	5:k:105:LEU:C	2.05	0.82
9:D:2:ALA:O	9:D:5:LEU:HG	1.79	0.82
2:G:78:GLU:HA	2:G:97:GLU:OE2	1.78	0.82
5:k:158:PHE:CA	5:k:160:ILE:HD11	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:5:LEU:HD12	11:I:5:LEU:N	1.93	0.82
10:F:154:LEU:HD13	10:F:157:GLN:N	1.76	0.82
7:B:38:GLY:HA3	7:B:94:TYR:OH	1.79	0.82
9:D:54:ARG:CD	9:D:55:LEU:CA	2.57	0.82
10:F:155:VAL:O	10:F:155:VAL:HG12	1.78	0.82
4:n:53:PHE:HD1	4:n:53:PHE:O	1.62	0.81
9:D:54:ARG:CD	9:D:55:LEU:HA	2.10	0.81
5:k:160:ILE:HG23	5:k:161:PRO:HA	1.62	0.81
1:H:123:VAL:HG13	1:H:123:VAL:O	1.77	0.81
11:I:16:LEU:O	11:I:33:LEU:HD12	1.81	0.81
11:I:22:SER:O	11:I:25:ALA:CB	2.27	0.81
4:n:47:VAL:O	4:n:51:CYS:SG	2.38	0.81
1:H:86:LEU:HD13	1:H:86:LEU:O	1.79	0.81
4:n:23:GLU:HG3	4:n:24:GLY:O	1.81	0.80
1:H:65:LEU:HD13	2:G:79:GLY:HA3	1.63	0.80
10:F:154:LEU:HD13	10:F:156:VAL:H	1.47	0.80
4:n:18:TYR:O	4:n:31:GLY:N	2.12	0.80
8:J:29:LEU:C	8:J:30:ASN:ND2	2.39	0.80
11:I:74:THR:CG2	11:I:91:ASN:OD1	2.30	0.80
11:I:95:GLU:HG3	11:I:97:ILE:H	1.45	0.80
11:I:54:ARG:HA	11:I:59:MET:O	1.82	0.79
11:I:59:MET:SD	11:I:59:MET:O	2.41	0.79
10:A:112:THR:HG21	10:A:118:VAL:HG21	1.65	0.79
10:F:79:HIS:HB3	10:F:81:TYR:H	1.48	0.79
5:k:158:PHE:O	5:k:158:PHE:CD2	2.36	0.78
7:B:34:TYR:CD1	7:B:34:TYR:C	2.61	0.78
3:o:56:THR:OG1	3:o:58:ASP:HB3	1.84	0.78
10:F:155:VAL:CG1	10:F:155:VAL:O	2.31	0.78
9:D:5:LEU:HD12	9:D:6:THR:N	1.97	0.78
9:D:24:GLY:O	9:D:25:ALA:HB3	1.83	0.78
2:G:5:LYS:NZ	2:G:5:LYS:CB	2.41	0.78
8:J:1:MET:HE3	8:J:1:MET:C	2.09	0.78
1:m:86:LEU:CD2	1:m:86:LEU:H	1.96	0.78
5:k:105:LEU:HD22	5:k:105:LEU:O	1.83	0.78
6:C:55:LEU:O	6:C:58:ASP:OD1	2.02	0.77
5:k:105:LEU:O	5:k:105:LEU:HD13	1.85	0.77
4:n:34:GLU:CB	4:n:35:ASN:C	2.58	0.77
5:k:90:THR:HG22	10:A:91:ARG:HD3	1.65	0.77
9:D:54:ARG:HD3	9:D:55:LEU:CA	2.13	0.77
10:A:160:ILE:CB	10:A:161:PRO:HD2	2.13	0.77
3:o:58:ASP:N	3:o:59:PRO:HD3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:158:PHE:CA	5:k:160:ILE:CD1	2.63	0.77
2:G:4:PRO:O	10:F:155:VAL:HG11	1.83	0.77
2:l:117:GLU:CG	2:l:118:PRO:HD3	2.15	0.77
5:k:155:VAL:CG1	5:k:157:GLN:NE2	2.46	0.76
10:A:90:THR:HG22	10:F:91:ARG:HD3	1.67	0.76
2:l:64:PHE:CD1	2:l:64:PHE:C	2.64	0.76
10:A:160:ILE:CG2	10:A:161:PRO:CD	2.54	0.76
10:F:82:MET:SD	10:F:82:MET:N	2.57	0.76
10:F:99:LEU:HD21	10:F:102:TRP:HE3	1.51	0.76
9:D:14:ASP:HB2	9:D:92:ARG:NH2	2.00	0.76
11:I:23:GLU:HB2	11:I:26:VAL:HG23	1.68	0.76
10:F:112:THR:HG21	10:F:118:VAL:HG21	1.68	0.75
4:n:19:LEU:CD1	4:n:20:VAL:H	2.00	0.75
4:n:19:LEU:CD1	4:n:20:VAL:N	2.50	0.75
4:n:53:PHE:O	4:n:53:PHE:CD1	2.40	0.74
4:n:71:GLY:O	4:n:91:ASN:ND2	2.21	0.74
8:J:31:LEU:HD13	10:F:143:LEU:HD21	1.68	0.74
6:C:118:ARG:HH11	6:C:118:ARG:CG	2.00	0.74
2:G:5:LYS:H	10:F:155:VAL:HG21	1.52	0.74
5:k:91:ARG:HD3	10:F:90:THR:HG22	1.69	0.74
5:k:158:PHE:CB	5:k:160:ILE:HD11	2.18	0.74
1:m:85:ARG:O	1:m:88:LEU:O	2.06	0.74
10:A:153:GLU:OE2	10:A:154:LEU:N	2.21	0.74
7:B:62:GLN:CB	7:B:65:ASN:O	2.36	0.73
2:G:4:PRO:O	10:F:155:VAL:HG13	1.89	0.73
1:H:16:VAL:HG22	1:H:102:LEU:HD13	1.70	0.73
4:n:27:LEU:N	4:n:27:LEU:CD2	2.47	0.73
10:A:78:GLN:O	10:A:81:TYR:HB2	1.89	0.73
2:l:117:GLU:HG3	2:l:118:PRO:HD3	1.70	0.72
7:B:60:GLY:CA	7:B:61:ASN:C	2.58	0.72
9:D:94:ARG:CG	9:D:95:GLU:O	2.37	0.72
2:G:62:GLN:N	2:G:63:ALA:HA	2.04	0.72
2:G:102:GLY:CA	8:J:29:LEU:O	2.37	0.72
5:k:158:PHE:HB2	5:k:160:ILE:HD11	1.69	0.72
5:k:155:VAL:HG12	5:k:157:GLN:HE21	1.54	0.72
5:k:159:GLY:N	5:k:160:ILE:HD12	2.03	0.72
1:H:64:GLY:O	1:H:65:LEU:HD23	1.89	0.72
1:H:65:LEU:HD11	2:G:94:TYR:CD1	2.24	0.72
5:k:78:ALA:O	5:k:81:TYR:CD2	2.43	0.72
2:l:61:ASN:C	2:l:63:ALA:HB2	2.15	0.72
9:D:21:LEU:HD23	9:D:27:LEU:HD23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:160:ILE:HG23	5:k:161:PRO:CA	2.19	0.72
10:A:147:ARG:HG3	10:A:147:ARG:HH11	1.55	0.72
9:D:17:GLY:CA	9:D:32:ASP:HB2	2.16	0.71
11:I:56:HIS:C	11:I:57:ARG:CD	2.59	0.71
5:k:157:GLN:O	5:k:158:PHE:CD2	2.42	0.71
5:k:158:PHE:HA	5:k:160:ILE:HD11	1.72	0.71
1:H:2:ALA:O	1:H:6:LYS:HG3	1.91	0.71
10:A:147:ARG:HH11	10:A:147:ARG:CG	2.04	0.71
10:F:154:LEU:HD11	10:F:157:GLN:CB	2.10	0.71
10:F:151:LYS:HG2	10:F:152:GLU:N	2.05	0.71
6:C:66:SER:HB3	7:B:77:MET:HB2	1.73	0.70
9:D:94:ARG:HG3	9:D:95:GLU:O	1.91	0.70
11:I:54:ARG:O	11:I:54:ARG:HG2	1.89	0.70
4:n:19:LEU:HD13	4:n:29:SER:O	1.92	0.70
8:J:29:LEU:CA	8:J:30:ASN:ND2	2.54	0.70
8:J:57:SER:O	8:J:59:PRO:HD3	1.91	0.70
4:n:23:GLU:HG2	4:n:26:VAL:HG22	1.74	0.70
1:m:86:LEU:H	1:m:86:LEU:HD22	1.57	0.70
10:F:159:GLY:O	10:F:161:PRO:HD3	1.92	0.70
1:H:65:LEU:HD23	1:H:65:LEU:N	2.04	0.70
11:I:74:THR:HG22	11:I:91:ASN:OD1	1.92	0.70
8:J:29:LEU:C	8:J:30:ASN:HD22	1.98	0.69
10:A:90:THR:CG2	10:F:91:ARG:HD3	2.22	0.69
11:I:23:GLU:N	11:I:23:GLU:CD	2.49	0.69
3:o:56:THR:OG1	3:o:58:ASP:N	2.25	0.69
11:I:54:ARG:HB3	11:I:59:MET:HA	1.69	0.69
4:n:34:GLU:CB	4:n:35:ASN:O	2.40	0.69
9:D:54:ARG:HD3	9:D:55:LEU:N	1.96	0.69
9:D:54:ARG:HD3	9:D:55:LEU:HA	1.71	0.69
2:G:34:TYR:CD1	2:G:34:TYR:C	2.70	0.69
1:m:65:LEU:HD21	2:l:94:TYR:CE1	2.28	0.69
8:E:90:ALA:CA	8:E:91:SER:HB3	2.23	0.69
4:n:18:TYR:C	4:n:31:GLY:H	2.02	0.68
11:I:24:GLY:N	11:I:25:ALA:HA	2.04	0.68
2:l:121:GLN:HE21	2:l:121:GLN:CA	2.06	0.68
4:n:18:TYR:HD1	4:n:30:SER:O	1.75	0.68
11:I:35:ASN:O	11:I:36:ASP:C	2.37	0.68
9:D:24:GLY:O	9:D:25:ALA:CB	2.40	0.67
1:m:85:ARG:O	1:m:88:LEU:N	2.28	0.67
9:D:64:LYS:O	9:D:78:THR:HG22	1.93	0.67
10:A:160:ILE:O	10:A:161:PRO:C	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:17:GLY:HA2	9:D:32:ASP:CB	2.18	0.67
9:D:60:ASN:O	9:D:62:PRO:CD	2.42	0.67
7:B:34:TYR:OH	7:B:37:TYR:CZ	2.47	0.67
10:A:159:GLY:O	10:A:160:ILE:CD1	2.42	0.67
11:I:17:GLY:HA2	11:I:32:ASP:CB	2.24	0.67
11:I:27:LEU:HD11	11:I:37:GLU:HG3	1.77	0.67
5:k:160:ILE:CG2	5:k:161:PRO:HB3	2.25	0.66
4:n:19:LEU:HD12	4:n:20:VAL:H	1.58	0.66
2:l:34:TYR:OH	2:l:37:TYR:OH	2.10	0.66
1:m:5:LEU:HD11	1:m:113:LEU:HD11	1.77	0.66
10:F:160:ILE:O	10:F:160:ILE:HG22	1.94	0.66
11:I:74:THR:HG23	11:I:91:ASN:OD1	1.95	0.66
9:D:97:ILE:C	9:D:97:ILE:HD12	2.20	0.66
1:H:86:LEU:HA	1:H:88:LEU:N	2.10	0.66
5:k:160:ILE:CG2	5:k:161:PRO:CA	2.73	0.65
8:E:2:GLU:O	8:E:2:GLU:HG2	1.94	0.65
9:D:32:ASP:C	9:D:33:LEU:HD23	2.21	0.65
2:G:3:ARG:O	10:F:155:VAL:HG11	1.96	0.65
4:n:18:TYR:C	4:n:31:GLY:N	2.54	0.65
6:C:65:LEU:HG	7:B:79:GLY:HA3	1.76	0.65
9:D:22:SER:O	9:D:24:GLY:N	2.28	0.65
1:H:59:GLN:O	1:H:62:LYS:CG	2.45	0.65
2:G:124:ALA:O	2:G:125:SER:C	2.39	0.65
9:D:59:MET:SD	9:D:59:MET:N	2.67	0.65
9:D:90:GLN:H	9:D:90:GLN:CD	2.05	0.65
10:F:154:LEU:HD13	10:F:156:VAL:N	2.12	0.65
2:l:9:GLN:NE2	2:l:13:GLN:NE2	2.45	0.65
3:o:56:THR:OG1	3:o:58:ASP:CB	2.45	0.65
11:I:72:GLU:C	11:I:91:ASN:ND2	2.55	0.65
7:B:59:ASN:OD1	7:B:59:ASN:N	2.29	0.64
7:B:3:ALA:N	7:B:4:PRO:CA	2.60	0.64
1:H:59:GLN:O	1:H:62:LYS:HG2	1.97	0.64
1:H:86:LEU:HD22	1:H:87:PRO:CA	2.27	0.64
10:F:99:LEU:HD21	10:F:102:TRP:CE3	2.33	0.64
8:J:1:MET:HB2	8:J:2:GLU:OE1	1.97	0.64
2:l:36:GLY:O	2:l:37:TYR:CG	2.51	0.64
2:G:38:GLY:HA3	2:G:94:TYR:OH	1.97	0.64
7:B:60:GLY:HA2	7:B:61:ASN:O	1.97	0.64
2:G:61:ASN:OD1	2:G:68:ASN:OD1	2.16	0.64
8:J:59:PRO:O	8:J:60:THR:HG22	1.98	0.64
2:G:89:LEU:HD12	2:G:119:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:24:GLY:N	11:I:25:ALA:CA	2.60	0.63
8:J:58:ASP:OD2	8:J:61:ASP:N	2.32	0.63
2:G:74:MET:HB2	2:G:81:VAL:HB	1.78	0.63
11:I:36:ASP:CG	11:I:36:ASP:O	2.40	0.63
11:I:94:ARG:HD3	11:I:94:ARG:H	1.63	0.63
5:k:79:HIS:CD2	5:k:79:HIS:O	2.52	0.63
8:J:26:SER:OG	8:J:81:GLY:O	2.15	0.63
11:I:17:GLY:CA	11:I:32:ASP:HB2	2.27	0.63
10:A:160:ILE:HG23	10:A:161:PRO:HG2	1.80	0.63
8:J:82:ILE:HG12	8:J:82:ILE:O	1.98	0.63
4:n:19:LEU:HB3	4:n:86:VAL:HB	1.80	0.63
2:G:89:LEU:HD21	2:G:124:ALA:HB2	1.81	0.63
5:k:78:ALA:O	5:k:81:TYR:HD2	1.82	0.62
2:G:41:ASP:HB3	2:G:44:VAL:HG23	1.81	0.62
8:J:29:LEU:HA	8:J:30:ASN:HD22	1.64	0.62
9:D:14:ASP:HB2	9:D:92:ARG:HH22	1.63	0.62
10:A:153:GLU:OE2	10:A:153:GLU:CA	2.47	0.62
8:J:30:ASN:HB3	8:J:39:ASP:OD2	1.99	0.62
1:m:61:SER:CB	1:m:67:LYS:HE3	2.30	0.62
5:k:158:PHE:HA	5:k:160:ILE:CD1	2.29	0.61
11:I:10:GLU:HG3	11:I:18:TYR:HE2	1.63	0.61
11:I:22:SER:O	11:I:25:ALA:CA	2.47	0.61
11:I:24:GLY:N	11:I:25:ALA:HB2	2.15	0.61
2:l:38:GLY:HA3	2:l:94:TYR:OH	2.00	0.61
10:A:153:GLU:OE2	10:A:153:GLU:HA	2.00	0.61
2:l:63:ALA:H	2:l:64:PHE:HA	1.65	0.61
1:m:61:SER:OG	1:m:67:LYS:HD3	2.01	0.61
7:B:124:ALA:O	7:B:125:ALA:C	2.44	0.61
9:D:36:ASP:O	9:D:38:GLN:N	2.32	0.61
6:C:58:ASP:OD1	6:C:59:GLN:HG2	2.00	0.61
11:I:53:PHE:C	11:I:59:MET:O	2.44	0.61
5:k:155:VAL:CG1	5:k:157:GLN:HE22	2.10	0.60
9:D:67:SER:HB3	9:D:76:LEU:HD23	1.83	0.60
11:I:94:ARG:HH11	11:I:94:ARG:HG2	1.64	0.60
8:J:30:ASN:CB	8:J:39:ASP:OD2	2.49	0.60
7:B:2:ALA:CB	10:A:156:VAL:HA	2.23	0.60
2:G:115:LEU:O	2:G:119:LEU:HB2	2.02	0.59
2:G:41:ASP:OD2	2:G:42:ALA:N	2.35	0.59
2:G:9:GLN:HE21	2:G:9:GLN:C	2.09	0.59
1:m:86:LEU:HD23	1:m:86:LEU:O	2.01	0.59
2:G:10:VAL:HG11	2:G:115:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:GLN:C	2:G:9:GLN:NE2	2.60	0.59
7:B:7:LEU:HD23	10:A:154:LEU:HD11	1.85	0.59
8:J:29:LEU:HA	8:J:30:ASN:HD21	1.66	0.59
6:C:16:VAL:HG22	6:C:102:LEU:HD13	1.85	0.58
9:D:54:ARG:O	9:D:55:LEU:C	2.45	0.58
2:G:63:ALA:H	2:G:64:PHE:HA	1.68	0.58
2:l:69:LEU:HD21	2:l:72:ILE:HD11	1.85	0.58
8:E:2:GLU:O	8:E:2:GLU:CG	2.51	0.58
7:B:22:THR:HG23	7:B:93:MET:HG2	1.86	0.58
9:D:19:LEU:HD12	9:D:21:LEU:HD21	1.84	0.58
10:A:89:SER:CB	1:H:124:SER:HA	2.34	0.58
11:I:56:HIS:HB3	11:I:57:ARG:HH11	1.69	0.58
11:I:3:SER:CB	11:I:6:THR:HG23	2.34	0.58
4:n:16:LEU:HD21	4:n:90:GLN:HE21	1.67	0.58
6:C:67:LYS:HB3	7:B:77:MET:HG3	1.86	0.58
11:I:73:HIS:N	11:I:91:ASN:ND2	2.52	0.58
11:I:94:ARG:HG3	11:I:94:ARG:NH1	2.15	0.58
4:n:24:GLY:O	4:n:25:ALA:C	2.47	0.58
2:l:121:GLN:CA	2:l:121:GLN:NE2	2.67	0.57
10:A:78:GLN:CD	10:A:81:TYR:CE2	2.82	0.57
9:D:54:ARG:HD2	9:D:55:LEU:CA	2.30	0.57
11:I:94:ARG:CG	11:I:94:ARG:NH1	2.53	0.57
1:m:123:VAL:O	1:m:124:SER:C	2.47	0.57
3:o:58:ASP:HA	3:o:61:ASP:HB3	1.87	0.57
5:k:160:ILE:CG2	5:k:161:PRO:HA	2.31	0.57
9:D:69:VAL:HA	9:D:74:THR:HB	1.85	0.57
8:J:30:ASN:ND2	8:J:30:ASN:N	2.35	0.57
1:m:85:ARG:O	1:m:88:LEU:CA	2.53	0.57
10:A:156:VAL:O	10:A:157:GLN:O	2.23	0.57
11:I:59:MET:SD	11:I:60:ASN:N	2.77	0.57
4:n:30:SER:HB2	4:n:35:ASN:CB	2.35	0.57
2:G:89:LEU:CD2	2:G:124:ALA:HB2	2.35	0.57
4:n:23:GLU:CG	4:n:24:GLY:O	2.52	0.57
5:k:77:ALA:C	5:k:81:TYR:HE2	2.13	0.57
5:k:121:SER:O	5:k:123:PRO:HD3	2.05	0.57
8:J:29:LEU:CA	8:J:30:ASN:HD22	2.15	0.57
11:I:54:ARG:CA	11:I:59:MET:O	2.53	0.57
4:n:12:ILE:HG23	4:n:13:PRO:HD2	1.87	0.56
1:H:86:LEU:CD2	1:H:87:PRO:HA	2.35	0.56
9:D:24:GLY:C	9:D:26:VAL:H	2.10	0.56
1:H:86:LEU:C	1:H:86:LEU:HD13	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:72:ILE:HG23	6:C:81:VAL:HG22	1.88	0.56
7:B:117:GLU:HB3	7:B:118:PRO:HD3	1.86	0.56
10:A:160:ILE:CG1	10:A:161:PRO:HD2	2.34	0.56
2:l:117:GLU:HG2	2:l:118:PRO:HD3	1.87	0.56
3:o:58:ASP:N	3:o:59:PRO:CD	2.68	0.56
8:J:22:LEU:HD22	8:J:45:ILE:HD13	1.88	0.56
4:n:30:SER:OG	4:n:31:GLY:O	2.21	0.56
11:I:95:GLU:OE1	11:I:96:PRO:CD	2.40	0.56
2:G:6:ALA:O	2:G:7:LEU:C	2.46	0.56
11:I:19:LEU:HD12	11:I:21:LEU:HD21	1.87	0.56
3:o:62:ILE:HG13	3:o:62:ILE:O	2.04	0.56
10:A:78:GLN:OE1	10:A:81:TYR:CE2	2.58	0.56
1:H:27:ARG:NH2	1:H:57:THR:HG21	2.21	0.56
2:G:4:PRO:C	10:F:155:VAL:HG11	2.30	0.56
10:A:78:GLN:O	10:A:81:TYR:N	2.37	0.55
11:I:56:HIS:O	11:I:57:ARG:CD	2.42	0.55
5:k:79:HIS:C	5:k:79:HIS:HD2	2.10	0.55
1:H:123:VAL:O	1:H:123:VAL:CG1	2.51	0.55
1:m:16:VAL:HG22	1:m:102:LEU:HD13	1.89	0.55
1:H:102:LEU:HG	8:J:47:VAL:HG21	1.88	0.55
11:I:16:LEU:O	11:I:33:LEU:HD13	2.05	0.55
11:I:35:ASN:N	11:I:35:ASN:OD1	2.36	0.55
3:o:56:THR:OG1	3:o:58:ASP:CA	2.55	0.55
3:o:58:ASP:CG	3:o:58:ASP:O	2.49	0.55
10:A:146:ILE:HG13	10:A:146:ILE:O	2.06	0.55
2:G:122:VAL:CG1	10:F:156:VAL:HG11	2.37	0.55
6:C:43:HIS:HB2	6:C:46:ARG:HH21	1.71	0.55
1:H:61:SER:HB3	1:H:67:LYS:HD2	1.89	0.55
1:m:123:VAL:O	1:m:123:VAL:HG12	2.07	0.55
3:o:60:THR:HG23	3:o:60:THR:O	2.06	0.55
3:o:22:LEU:HD21	3:o:24:THR:HG23	1.88	0.55
11:I:24:GLY:N	11:I:25:ALA:CB	2.70	0.55
4:n:27:LEU:H	4:n:27:LEU:CD2	1.88	0.55
1:H:27:ARG:HH22	1:H:57:THR:CG2	2.19	0.55
1:H:85:ARG:NH1	1:H:107:GLU:OE2	2.40	0.55
4:n:18:TYR:CD1	4:n:30:SER:O	2.59	0.54
11:I:59:MET:SD	11:I:60:ASN:CB	2.95	0.54
11:I:9:LEU:N	11:I:9:LEU:HD23	2.22	0.54
5:k:105:LEU:O	5:k:105:LEU:CD2	2.55	0.54
1:H:86:LEU:C	1:H:86:LEU:CD2	2.74	0.54
11:I:33:LEU:HD12	11:I:33:LEU:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:41:PRO:HG3	1:m:78:TYR:CZ	2.42	0.54
6:C:102:LEU:HD12	8:E:47:VAL:HG21	1.90	0.54
11:I:3:SER:CB	11:I:6:THR:CG2	2.86	0.54
7:B:62:GLN:H	7:B:66:GLU:HG3	1.72	0.54
3:o:57:SER:C	3:o:59:PRO:HD3	2.33	0.54
11:I:14:ASP:OD2	11:I:14:ASP:N	2.41	0.54
4:n:19:LEU:HD13	4:n:20:VAL:H	1.71	0.54
1:m:85:ARG:O	1:m:88:LEU:C	2.51	0.53
2:l:58:ARG:CG	2:l:59:ASN:OD1	2.52	0.53
2:l:62:GLN:N	2:l:63:ALA:HA	2.24	0.53
5:k:80:GLU:O	5:k:83:ASP:HB3	2.08	0.53
8:E:68:GLU:HG3	9:D:65:ARG:O	2.09	0.53
2:l:86:VAL:HG13	2:l:86:VAL:O	2.07	0.53
5:k:105:LEU:C	5:k:105:LEU:CD2	2.77	0.53
8:J:1:MET:HE1	8:J:3:ALA:HB3	1.90	0.53
2:G:9:GLN:HE21	2:G:10:VAL:N	2.06	0.53
1:m:63:LEU:O	2:l:40:THR:OG1	2.26	0.53
2:l:2:LEU:HG	2:l:122:VAL:HG21	1.89	0.53
10:F:153:GLU:HB2	10:F:154:LEU:HB2	1.89	0.53
9:D:54:ARG:HD2	9:D:55:LEU:H	1.65	0.53
5:k:105:LEU:O	5:k:105:LEU:CD1	2.55	0.53
10:A:153:GLU:OE2	10:A:153:GLU:C	2.52	0.53
5:k:160:ILE:CG2	5:k:161:PRO:CB	2.86	0.52
9:D:5:LEU:HD12	9:D:5:LEU:C	2.33	0.52
11:I:32:ASP:N	11:I:32:ASP:OD2	2.42	0.52
5:k:160:ILE:HD12	5:k:160:ILE:N	2.24	0.52
5:k:160:ILE:HG22	5:k:161:PRO:HB3	1.91	0.52
2:l:19:VAL:HG11	2:l:93:MET:HE3	1.91	0.52
6:C:58:ASP:OD1	6:C:58:ASP:C	2.50	0.52
11:I:95:GLU:CD	11:I:96:PRO:HD2	2.31	0.52
2:G:5:LYS:N	10:F:155:VAL:HG21	2.21	0.52
11:I:12:ILE:HG12	10:F:120:ALA:HB2	1.92	0.52
2:l:64:PHE:HD1	2:l:65:ASN:N	2.08	0.52
7:B:41:ASP:HB3	7:B:44:VAL:HG23	1.92	0.52
5:k:160:ILE:HG23	5:k:161:PRO:CB	2.40	0.52
7:B:47:ALA:O	7:B:50:SER:OG	2.27	0.52
1:H:63:LEU:HD13	2:G:81:VAL:HG21	1.92	0.52
4:n:69:VAL:HA	4:n:74:THR:HB	1.92	0.51
9:D:31:GLY:C	9:D:32:ASP:OD2	2.53	0.51
1:m:66:SER:HB3	2:l:77:MET:CB	2.29	0.51
1:H:5:LEU:HD11	1:H:113:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:22:SER:C	11:I:25:ALA:CB	2.74	0.51
2:l:64:PHE:C	2:l:64:PHE:HD1	2.15	0.51
5:k:81:TYR:O	5:k:84:ARG:N	2.43	0.51
1:m:86:LEU:CD2	1:m:86:LEU:N	2.63	0.51
11:I:85:PHE:HB3	10:F:119:LEU:HD11	1.92	0.51
10:A:147:ARG:CG	10:A:147:ARG:NH1	2.68	0.51
8:J:68:GLU:HG2	10:F:124:ILE:HD11	1.91	0.51
2:l:34:TYR:OH	2:l:37:TYR:CZ	2.49	0.51
7:B:10:VAL:HG11	7:B:115:LEU:HD21	1.92	0.51
1:H:43:HIS:HB2	1:H:46:ARG:HH21	1.75	0.51
1:H:86:LEU:HD23	1:H:87:PRO:HA	1.92	0.51
1:m:66:SER:H	2:l:78:GLU:HB2	1.76	0.51
6:C:118:ARG:NH1	6:C:118:ARG:CG	2.67	0.51
2:G:115:LEU:N	2:G:115:LEU:HD23	2.27	0.50
6:C:111:ALA:N	6:C:112:PRO:HD2	2.26	0.50
8:E:58:ASP:OD2	8:E:58:ASP:C	2.54	0.50
9:D:54:ARG:NE	9:D:55:LEU:HA	2.26	0.50
2:G:22:THR:HG23	2:G:93:MET:HG2	1.93	0.50
7:B:74:MET:HB2	7:B:81:VAL:HB	1.93	0.50
9:D:36:ASP:HB3	9:D:39:ALA:HB3	1.93	0.50
10:A:99:LEU:HD21	10:A:102:TRP:CZ3	2.47	0.50
2:l:120:THR:C	2:l:121:GLN:HE21	2.18	0.50
6:C:118:ARG:HH11	6:C:118:ARG:HG2	1.75	0.50
2:G:40:THR:HB	2:G:41:ASP:C	2.33	0.50
5:k:160:ILE:HG23	5:k:161:PRO:HB3	1.92	0.50
1:m:53:PHE:O	1:m:57:THR:HG22	2.11	0.50
2:G:122:VAL:CG1	10:F:156:VAL:CG1	2.89	0.50
4:n:23:GLU:CG	4:n:24:GLY:N	2.63	0.50
7:B:2:ALA:HB1	7:B:3:ALA:HB2	1.94	0.50
9:D:16:LEU:O	9:D:33:LEU:HG	2.12	0.50
9:D:56:HIS:C	9:D:57:ARG:HD3	2.37	0.50
8:J:82:ILE:HG21	10:F:143:LEU:CD1	2.41	0.50
11:I:23:GLU:C	11:I:25:ALA:CA	2.62	0.49
7:B:19:VAL:HG11	7:B:93:MET:CE	2.42	0.49
10:A:78:GLN:HB3	10:A:81:TYR:CD2	2.47	0.49
8:E:22:LEU:HD22	8:E:45:ILE:HD13	1.93	0.49
1:m:76:ASN:HD22	1:m:77:THR:HG23	1.76	0.49
4:n:65:ARG:HD3	4:n:76:LEU:HB3	1.94	0.49
11:I:64:LYS:HG3	10:F:112:THR:HG22	1.94	0.49
10:F:160:ILE:O	10:F:160:ILE:CG2	2.57	0.49
9:D:94:ARG:HG2	9:D:95:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:36:ASP:OD2	11:I:38:GLN:HG3	2.12	0.49
11:I:94:ARG:HD3	11:I:94:ARG:N	2.27	0.49
1:H:86:LEU:CD2	1:H:87:PRO:CA	2.91	0.49
11:I:19:LEU:HG	11:I:86:VAL:HB	1.95	0.49
11:I:21:LEU:HB2	11:I:84:VAL:HB	1.95	0.49
2:l:10:VAL:HG11	2:l:115:LEU:HD21	1.93	0.49
4:n:22:SER:N	4:n:26:VAL:H	2.10	0.49
4:n:26:VAL:C	4:n:28:ALA:H	2.20	0.49
5:k:77:ALA:CB	5:k:81:TYR:OH	2.61	0.49
5:k:157:GLN:O	5:k:158:PHE:C	2.55	0.49
7:B:117:GLU:HB3	7:B:118:PRO:CD	2.43	0.49
1:H:85:ARG:O	1:H:86:LEU:C	2.55	0.49
2:l:19:VAL:HG11	2:l:93:MET:CE	2.43	0.48
4:n:10:GLU:HG3	4:n:18:TYR:CE2	2.47	0.48
2:G:62:GLN:N	2:G:63:ALA:CA	2.76	0.48
1:m:87:PRO:HD2	1:m:118:ARG:HD3	1.95	0.48
11:I:22:SER:O	11:I:25:ALA:C	2.56	0.48
5:k:140:TYR:O	5:k:143:LEU:HB2	2.13	0.48
2:l:121:GLN:N	2:l:121:GLN:NE2	2.51	0.48
9:D:90:GLN:HG2	9:D:92:ARG:HE	1.79	0.48
8:E:47:VAL:O	8:E:51:GLN:HG3	2.13	0.48
10:F:144:SER:O	10:F:147:ARG:HD3	2.12	0.48
9:D:37:GLU:HA	9:D:40:ALA:HB3	1.96	0.48
8:E:22:LEU:HG	8:E:23:CYS:N	2.28	0.48
1:H:27:ARG:HH22	1:H:57:THR:HG21	1.78	0.48
10:A:99:LEU:HD21	10:A:102:TRP:HZ3	1.78	0.48
2:l:21:SER:HB2	2:l:36:GLY:HA3	1.95	0.47
2:l:58:ARG:HA	2:l:59:ASN:HA	1.56	0.47
4:n:6:THR:C	4:n:18:TYR:OH	2.54	0.47
5:k:143:LEU:C	5:k:145:GLN:H	2.22	0.47
7:B:2:ALA:CB	10:A:156:VAL:CA	2.86	0.47
1:m:71:ILE:HG12	2:l:74:MET:HG2	1.95	0.47
2:l:62:GLN:HB3	2:l:63:ALA:HA	1.96	0.47
9:D:22:SER:O	9:D:26:VAL:HG13	2.14	0.47
9:D:69:VAL:HG11	10:A:129:LEU:HD11	1.95	0.47
1:H:102:LEU:HD23	1:H:102:LEU:HA	1.76	0.47
1:m:116:GLU:OE2	1:m:116:GLU:HA	2.13	0.47
1:m:86:LEU:HD23	1:m:86:LEU:N	2.28	0.47
5:k:158:PHE:HB2	5:k:160:ILE:CD1	2.40	0.47
8:E:51:GLN:HB2	9:D:46:LEU:HD23	1.96	0.47
1:H:53:PHE:HB2	1:H:82:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:55:LEU:HD13	11:I:55:LEU:N	2.29	0.47
8:E:25:ASP:OD1	8:E:25:ASP:C	2.58	0.47
1:H:86:LEU:HA	1:H:87:PRO:C	2.40	0.47
1:H:87:PRO:HD2	1:H:118:ARG:HD3	1.96	0.47
2:G:40:THR:CB	2:G:41:ASP:CA	2.56	0.47
2:G:59:ASN:OD1	2:G:59:ASN:O	2.33	0.47
5:k:91:ARG:HH11	10:F:86:ARG:HG3	1.80	0.47
9:D:56:HIS:HB3	9:D:57:ARG:HH21	1.80	0.47
11:I:56:HIS:O	11:I:58:GLY:N	2.48	0.47
2:l:34:TYR:OH	2:l:37:TYR:CE2	2.64	0.47
9:D:65:ARG:NH2	9:D:76:LEU:HD22	2.30	0.47
2:G:3:ARG:CB	2:G:4:PRO:CD	2.93	0.47
8:E:90:ALA:CA	8:E:91:SER:CB	2.91	0.46
2:G:62:GLN:CB	2:G:63:ALA:HA	2.41	0.46
4:n:22:SER:O	4:n:26:VAL:N	2.48	0.46
5:k:105:LEU:O	5:k:105:LEU:CG	2.63	0.46
11:I:10:GLU:HG3	11:I:18:TYR:CE2	2.47	0.46
7:B:2:ALA:HA	7:B:3:ALA:HA	1.79	0.46
9:D:22:SER:O	9:D:22:SER:OG	2.32	0.46
2:G:122:VAL:HG12	10:F:156:VAL:HG11	1.96	0.46
1:m:60:GLY:HA3	2:l:74:MET:HE1	1.97	0.46
2:l:36:GLY:O	2:l:37:TYR:CD1	2.68	0.46
3:o:82:ILE:O	3:o:82:ILE:HG13	2.15	0.46
8:J:82:ILE:HG21	10:F:143:LEU:HD12	1.97	0.46
2:l:123:ALA:O	2:l:124:ALA:C	2.59	0.46
8:E:22:LEU:HD21	8:E:24:THR:HG23	1.98	0.46
2:l:80:ARG:HG3	2:l:97:GLU:HA	1.97	0.46
3:o:22:LEU:HD21	3:o:24:THR:CG2	2.45	0.46
7:B:34:TYR:CD1	7:B:35:SER:N	2.84	0.46
9:D:24:GLY:CA	9:D:26:VAL:CG1	2.70	0.46
5:k:101:HIS:CB	5:k:102:TRP:CE3	2.98	0.46
9:D:12:ILE:HG23	9:D:13:PRO:HD2	1.98	0.46
10:A:160:ILE:HG13	10:A:161:PRO:HD2	1.98	0.46
2:G:89:LEU:CD2	2:G:124:ALA:CB	2.94	0.46
2:l:74:MET:HB2	2:l:81:VAL:HB	1.97	0.46
2:l:86:VAL:O	2:l:87:ALA:C	2.58	0.46
3:o:15:ASN:HB3	3:o:18:ILE:HB	1.98	0.46
10:A:78:GLN:O	10:A:81:TYR:CB	2.62	0.46
7:B:2:ALA:CB	10:A:156:VAL:N	2.78	0.45
7:B:62:GLN:H	7:B:66:GLU:HA	1.81	0.45
1:H:76:ASN:HA	2:G:70:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:151:LYS:HG2	10:F:152:GLU:HG2	1.98	0.45
4:n:26:VAL:HG12	4:n:28:ALA:HB2	1.98	0.45
5:k:77:ALA:C	5:k:81:TYR:CE2	2.94	0.45
7:B:57:ASP:O	7:B:60:GLY:O	2.34	0.45
1:H:59:GLN:O	1:H:62:LYS:HG3	2.16	0.45
2:G:102:GLY:N	8:J:29:LEU:O	2.48	0.45
10:F:79:HIS:HB3	10:F:81:TYR:N	2.23	0.45
8:E:90:ALA:HA	8:E:91:SER:CB	2.23	0.45
10:A:77:ALA:HA	10:A:78:GLN:HA	1.52	0.45
1:H:10:TYR:CD2	1:H:13:LEU:HD12	2.51	0.45
10:F:146:ILE:O	10:F:146:ILE:HG22	2.16	0.45
6:C:102:LEU:CD1	8:E:47:VAL:HG21	2.47	0.45
9:D:57:ARG:CA	9:D:59:MET:H	2.23	0.45
8:J:1:MET:HB2	8:J:2:GLU:H	1.67	0.45
11:I:69:VAL:HG13	11:I:74:THR:HG22	1.99	0.45
2:l:63:ALA:CB	2:l:66:GLU:HA	2.46	0.45
11:I:54:ARG:HA	11:I:59:MET:C	2.41	0.45
2:l:41:ASP:OD2	2:l:41:ASP:C	2.60	0.45
2:l:121:GLN:NE2	2:l:121:GLN:HA	2.30	0.45
7:B:34:TYR:HD1	7:B:35:SER:N	2.15	0.45
10:A:155:VAL:O	10:A:156:VAL:C	2.59	0.45
2:G:31:LEU:HD21	2:G:34:TYR:HB3	1.98	0.45
8:J:60:THR:O	8:J:60:THR:HG23	2.16	0.45
9:D:24:GLY:C	9:D:26:VAL:N	2.66	0.44
2:l:117:GLU:HG3	2:l:118:PRO:CD	2.44	0.44
5:k:143:LEU:C	5:k:145:GLN:N	2.75	0.44
9:D:53:PHE:O	9:D:54:ARG:C	2.60	0.44
2:G:122:VAL:HG11	10:F:156:VAL:HG13	2.00	0.44
4:n:18:TYR:O	4:n:31:GLY:CA	2.66	0.44
2:l:117:GLU:O	2:l:121:GLN:HG2	2.17	0.44
8:J:57:SER:O	8:J:59:PRO:CD	2.64	0.44
11:I:22:SER:C	11:I:23:GLU:OE1	2.60	0.44
10:F:140:TYR:O	10:F:143:LEU:HB2	2.17	0.44
6:C:4:ASP:O	6:C:7:ARG:HB2	2.18	0.44
2:G:114:TYR:HD2	2:G:115:LEU:CD2	2.31	0.44
2:G:60:GLY:HA2	2:G:67:ASP:O	2.18	0.44
2:l:62:GLN:CB	2:l:63:ALA:HA	2.47	0.44
6:C:11:LYS:HB3	10:A:105:LEU:HD11	2.00	0.43
5:k:86:ARG:HG3	10:A:91:ARG:HH11	1.82	0.43
6:C:2:ALA:O	6:C:6:LYS:HG3	2.18	0.43
9:D:94:ARG:HG3	9:D:97:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:95:GLU:CG	11:I:97:ILE:H	2.24	0.43
1:m:2:ALA:O	1:m:6:LYS:HG3	2.19	0.43
7:B:60:GLY:HA2	7:B:62:GLN:N	2.29	0.43
4:n:21:LEU:C	4:n:26:VAL:HB	2.39	0.43
5:k:160:ILE:HG22	5:k:161:PRO:CB	2.47	0.43
9:D:61:VAL:HA	9:D:62:PRO:HD2	1.81	0.43
11:I:73:HIS:N	11:I:91:ASN:HD21	2.14	0.43
2:l:57:ASP:O	2:l:60:GLY:N	2.52	0.43
2:l:61:ASN:CA	2:l:63:ALA:HB2	2.48	0.43
5:k:119:LEU:HD23	5:k:119:LEU:C	2.39	0.43
8:E:15:ASN:HA	8:E:16:PRO:HD3	1.87	0.43
2:l:121:GLN:HE21	2:l:121:GLN:HA	1.84	0.43
4:n:22:SER:HB3	4:n:26:VAL:HG11	1.99	0.43
6:C:53:PHE:HB2	6:C:82:GLN:OE1	2.18	0.43
6:C:118:ARG:NH1	6:C:118:ARG:HG2	2.34	0.43
1:H:83:PHE:CD2	1:H:107:GLU:HG3	2.53	0.43
2:G:9:GLN:HE22	2:G:13:GLN:HE21	1.67	0.43
2:G:13:GLN:NE2	10:F:149:ASP:O	2.51	0.43
10:F:152:GLU:HG2	10:F:152:GLU:H	1.50	0.43
5:k:117:GLN:HE22	5:k:118:VAL:HG23	1.84	0.42
10:A:114:GLN:O	10:A:118:VAL:HG23	2.18	0.42
8:J:22:LEU:HD22	8:J:45:ILE:CD1	2.49	0.42
5:k:160:ILE:CD1	5:k:160:ILE:N	2.81	0.42
9:D:74:THR:HG22	9:D:91:ASN:OD1	2.19	0.42
11:I:54:ARG:CB	11:I:59:MET:CA	2.72	0.42
2:l:86:VAL:O	2:l:86:VAL:CG1	2.67	0.42
5:k:79:HIS:O	5:k:82:MET:N	2.51	0.42
1:H:57:THR:OG1	1:H:68:ASN:HB3	2.20	0.42
1:m:85:ARG:O	1:m:88:LEU:HB2	2.20	0.42
5:k:78:ALA:C	5:k:80:GLU:N	2.77	0.42
10:A:114:GLN:HE21	10:A:114:GLN:HB3	1.65	0.42
6:C:55:LEU:O	6:C:59:GLN:HG2	2.20	0.42
6:C:67:LYS:CB	7:B:77:MET:HG3	2.48	0.42
1:H:102:LEU:HD21	11:I:53:PHE:CE2	2.55	0.42
1:m:102:LEU:HD23	1:m:102:LEU:HA	1.92	0.42
6:C:5:LEU:HD11	6:C:113:LEU:HD11	2.01	0.42
6:C:6:LYS:HE3	6:C:33:ILE:HG13	2.02	0.42
11:I:69:VAL:HA	11:I:74:THR:HB	2.02	0.42
5:k:158:PHE:O	5:k:159:GLY:C	2.63	0.42
2:G:89:LEU:HD21	2:G:124:ALA:CB	2.50	0.41
4:n:50:ALA:O	4:n:53:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:3:THR:HA	9:D:6:THR:HG23	2.02	0.41
9:D:89:ARG:HD3	9:D:90:GLN:NE2	2.35	0.41
11:I:95:GLU:CD	11:I:96:PRO:CD	2.92	0.41
7:B:61:ASN:CA	7:B:68:ASN:OD1	2.68	0.41
9:D:14:ASP:O	9:D:16:LEU:HD23	2.21	0.41
10:A:146:ILE:O	10:A:146:ILE:CG1	2.69	0.41
1:H:119:GLN:O	10:F:91:ARG:NH2	2.53	0.41
1:H:123:VAL:O	1:H:124:SER:CB	2.68	0.41
3:o:46:SER:O	3:o:50:GLN:HG2	2.20	0.41
3:o:82:ILE:HG21	5:k:143:LEU:CD1	2.50	0.41
8:E:15:ASN:HB3	8:E:18:ILE:HB	2.03	0.41
8:J:1:MET:H3	8:J:1:MET:HG3	1.64	0.41
5:k:77:ALA:HA	5:k:81:TYR:CE2	2.56	0.41
8:E:55:LEU:HD21	9:D:43:ILE:HG13	2.03	0.41
2:G:100:GLY:HA3	8:J:30:ASN:O	2.20	0.41
8:J:30:ASN:HB2	8:J:39:ASP:OD2	2.20	0.41
11:I:65:ARG:HA	11:I:78:THR:HG22	2.03	0.41
2:l:62:GLN:N	2:l:63:ALA:CA	2.83	0.41
3:o:6:GLU:HG3	3:o:34:ARG:HH22	1.86	0.41
6:C:102:LEU:HG	8:E:47:VAL:HG21	2.03	0.41
1:H:65:LEU:HD11	2:G:94:TYR:HD1	1.82	0.41
8:J:1:MET:HE3	8:J:1:MET:CA	2.51	0.40
11:I:77:VAL:HA	11:I:85:PHE:O	2.22	0.40
3:o:22:LEU:HD22	3:o:45:ILE:CD1	2.51	0.40
5:k:79:HIS:HD2	5:k:80:GLU:N	2.19	0.40
2:l:22:THR:HG23	2:l:93:MET:HG2	2.03	0.40
2:l:41:ASP:OD2	2:l:42:ALA:N	2.55	0.40
7:B:106:ALA:O	10:A:146:ILE:HD11	2.20	0.40
10:A:78:GLN:HB3	10:A:81:TYR:CG	2.57	0.40
10:A:89:SER:HB2	1:H:124:SER:HA	2.03	0.40
1:m:33:ILE:HD12	5:k:92:LEU:HD21	2.03	0.40
1:m:112:PRO:HB2	5:k:102:TRP:HZ2	1.86	0.40
9:D:69:VAL:HG11	10:A:129:LEU:CD1	2.50	0.40
1:m:61:SER:HB3	1:m:67:LYS:HE3	2.02	0.40
4:n:6:THR:HB	4:n:18:TYR:OH	2.21	0.40
9:D:36:ASP:C	9:D:38:GLN:N	2.78	0.40
2:G:117:GLU:CB	2:G:118:PRO:CD	2.82	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	H	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
1	m	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
2	G	121/125 (97%)	108 (89%)	13 (11%)	0	100	100
2	l	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
3	o	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
4	n	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
5	k	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
6	C	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
7	B	123/125 (98%)	118 (96%)	4 (3%)	1 (1%)	16	48
8	E	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
8	J	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
9	D	94/96 (98%)	81 (86%)	12 (13%)	1 (1%)	11	41
10	A	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	38
10	F	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	10	38
11	I	93/99 (94%)	84 (90%)	9 (10%)	0	100	100
All	All	1519/1556 (98%)	1428 (94%)	87 (6%)	4 (0%)	36	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	A	157	GLN
10	F	155	VAL
7	B	3	ALA
9	D	13	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	H	107/108 (99%)	94 (88%)	13 (12%)	5	20
1	m	104/108 (96%)	98 (94%)	6 (6%)	18	49
2	G	91/98 (93%)	73 (80%)	18 (20%)	1	7
2	l	94/98 (96%)	75 (80%)	19 (20%)	1	7
3	o	75/76 (99%)	68 (91%)	7 (9%)	8	31
4	n	63/72 (88%)	45 (71%)	18 (29%)	0	2
5	k	71/74 (96%)	59 (83%)	12 (17%)	2	10
6	C	106/106 (100%)	94 (89%)	12 (11%)	5	23
7	B	90/93 (97%)	73 (81%)	17 (19%)	1	8
8	E	77/77 (100%)	68 (88%)	9 (12%)	5	21
8	J	77/77 (100%)	67 (87%)	10 (13%)	4	18
9	D	76/79 (96%)	52 (68%)	24 (32%)	0	1
10	A	73/75 (97%)	60 (82%)	13 (18%)	2	9
10	F	73/75 (97%)	57 (78%)	16 (22%)	1	5
11	I	70/83 (84%)	51 (73%)	19 (27%)	0	2
All	All	1247/1299 (96%)	1034 (83%)	213 (17%)	2	10

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	m	4	ASP
1	m	5	LEU
1	m	58	ASP
1	m	86	LEU
1	m	102	LEU
1	m	117	LEU
2	l	1	MET
2	l	2	LEU
2	l	7	LEU
2	l	9	GLN

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Mol	Chain	Res	Type
2	l	24	LEU
2	l	25	LEU
2	l	31	LEU
2	l	40	THR
2	l	62	GLN
2	l	64	PHE
2	l	67	ASP
2	l	91	LEU
2	l	94	TYR
2	l	97	GLU
2	l	111	LEU
2	l	113	GLN
2	l	116	GLU
2	l	120	THR
2	l	121	GLN
3	o	23	CYS
3	o	29	LEU
3	o	39	ASP
3	o	56	THR
3	o	58	ASP
3	o	60	THR
3	o	82	ILE
4	n	15	GLN
4	n	16	LEU
4	n	19	LEU
4	n	20	VAL
4	n	22	SER
4	n	26	VAL
4	n	27	LEU
4	n	32	ASP
4	n	33	LEU
4	n	46	LEU
4	n	51	CYS
4	n	57	ARG
4	n	59	MET
4	n	63	PHE
4	n	65	ARG
4	n	74	THR
4	n	89	ARG
4	n	92	ARG
5	k	79	HIS
5	k	80	GLU

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Mol	Chain	Res	Type
5	k	98	SER
5	k	105	LEU
5	k	116	HIS
5	k	118	VAL
5	k	130	GLN
5	k	149	ASP
5	k	152	GLU
5	k	155	VAL
5	k	156	VAL
5	k	158	PHE
6	C	4	ASP
6	C	5	LEU
6	C	27	ARG
6	C	55	LEU
6	C	65	LEU
6	C	67	LYS
6	C	69	LYS
6	C	86	LEU
6	C	102	LEU
6	C	117	LEU
6	C	118	ARG
6	C	122	GLU
7	B	7	LEU
7	B	9	GLN
7	B	24	LEU
7	B	25	LEU
7	B	30	SER
7	B	31	LEU
7	B	34	TYR
7	B	40	THR
7	B	59	ASN
7	B	66	GLU
7	B	67	ASP
7	B	91	LEU
7	B	97	GLU
7	B	98	THR
7	B	111	LEU
7	B	120	THR
7	B	121	GLN
8	E	2	GLU
8	E	5	LEU
8	E	15	ASN

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Mol	Chain	Res	Type
8	E	22	LEU
8	E	29	LEU
8	E	39	ASP
8	E	40	GLU
8	E	68	GLU
8	E	82	ILE
9	D	5	LEU
9	D	6	THR
9	D	10	GLU
9	D	15	GLN
9	D	16	LEU
9	D	19	LEU
9	D	21	LEU
9	D	22	SER
9	D	26	VAL
9	D	33	LEU
9	D	36	ASP
9	D	44	SER
9	D	46	LEU
9	D	54	ARG
9	D	57	ARG
9	D	59	MET
9	D	64	LYS
9	D	65	ARG
9	D	74	THR
9	D	76	LEU
9	D	89	ARG
9	D	94	ARG
9	D	95	GLU
9	D	97	ILE
10	A	79	HIS
10	A	80	GLU
10	A	82	MET
10	A	83	ASP
10	A	99	LEU
10	A	114	GLN
10	A	130	GLN
10	A	131	GLN
10	A	146	ILE
10	A	147	ARG
10	A	153	GLU
10	A	154	LEU

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Mol	Chain	Res	Type
10	A	160	ILE
1	H	4	ASP
1	H	5	LEU
1	H	62	LYS
1	H	66	SER
1	H	67	LYS
1	H	76	ASN
1	H	78	TYR
1	H	86	LEU
1	H	93	ILE
1	H	102	LEU
1	H	109	GLU
1	H	117	LEU
1	H	123	VAL
2	G	5	LYS
2	G	7	LEU
2	G	9	GLN
2	G	25	LEU
2	G	31	LEU
2	G	34	TYR
2	G	40	THR
2	G	61	ASN
2	G	67	ASP
2	G	91	LEU
2	G	94	TYR
2	G	97	GLU
2	G	111	LEU
2	G	115	LEU
2	G	117	GLU
2	G	120	THR
2	G	121	GLN
2	G	122	VAL
8	J	1	MET
8	J	15	ASN
8	J	22	LEU
8	J	29	LEU
8	J	30	ASN
8	J	38	SER
8	J	58	ASP
8	J	60	THR
8	J	73	ASN
8	J	82	ILE

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Mol	Chain	Res	Type
11	I	5	LEU
11	I	9	LEU
11	I	15	GLN
11	I	16	LEU
11	I	19	LEU
11	I	23	GLU
11	I	27	LEU
11	I	32	ASP
11	I	35	ASN
11	I	38	GLN
11	I	46	LEU
11	I	54	ARG
11	I	55	LEU
11	I	57	ARG
11	I	59	MET
11	I	65	ARG
11	I	74	THR
11	I	89	ARG
11	I	94	ARG
10	F	78	GLN
10	F	79	HIS
10	F	82	MET
10	F	83	ASP
10	F	100	THR
10	F	104	LYS
10	F	113	SER
10	F	124	ILE
10	F	134	ARG
10	F	146	ILE
10	F	147	ARG
10	F	151	LYS
10	F	152	GLU
10	F	153	GLU
10	F	154	LEU
10	F	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	m	37	ASN
2	l	9	GLN
2	l	113	GLN

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Mol	Chain	Res	Type
2	l	121	GLN
3	o	73	ASN
3	o	77	GLN
4	n	90	GLN
5	k	79	HIS
5	k	117	GLN
5	k	145	GLN
5	k	157	GLN
7	B	121	GLN
9	D	82	GLN
10	A	78	GLN
10	A	114	GLN
10	A	130	GLN
1	H	43	HIS
2	G	9	GLN
2	G	20	GLN
2	G	59	ASN
2	G	121	GLN
8	J	27	GLN
8	J	30	ASN
8	J	51	GLN
11	I	56	HIS
10	F	114	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	124/124 (100%)	-0.14	3 (2%) 59 36	37, 53, 81, 99	0
1	m	124/124 (100%)	-0.21	2 (1%) 70 47	28, 54, 74, 115	0
2	G	123/125 (98%)	0.13	10 (8%) 18 9	39, 57, 103, 143	0
2	l	124/125 (99%)	-0.15	7 (5%) 30 15	25, 42, 91, 148	0
3	o	90/90 (100%)	-0.02	3 (3%) 49 28	37, 59, 97, 108	0
4	n	88/88 (100%)	1.22	20 (22%) 2 1	65, 109, 134, 154	0
5	k	85/85 (100%)	0.68	15 (17%) 4 2	38, 69, 115, 124	0
6	C	123/123 (100%)	-0.35	4 (3%) 49 28	21, 46, 66, 102	0
7	B	125/125 (100%)	-0.01	6 (4%) 35 18	21, 49, 87, 138	0
8	E	91/91 (100%)	-0.27	1 (1%) 78 57	25, 35, 55, 65	0
8	J	91/91 (100%)	-0.21	0 100 100	30, 47, 78, 99	0
9	D	96/96 (100%)	0.24	7 (7%) 21 10	23, 47, 75, 86	0
10	A	85/85 (100%)	0.12	6 (7%) 22 11	32, 49, 74, 88	0
10	F	85/85 (100%)	0.42	9 (10%) 11 6	37, 58, 79, 96	0
11	I	95/99 (95%)	0.44	6 (6%) 26 13	41, 68, 101, 107	0
All	All	1549/1556 (99%)	0.09	99 (6%) 25 13	21, 53, 108, 154	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	B	63	ALA	5.5
4	n	54	ARG	5.5
8	E	91	SER	5.0
7	B	64	PHE	4.6
2	l	61	ASN	4.5
3	o	58	ASP	4.4
1	H	124	SER	4.3

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Mol	Chain	Res	Type	RSRZ
10	F	80	GLU	4.1
2	l	123	ALA	4.1
5	k	106	PRO	4.0
10	F	156	VAL	4.0
2	G	123	ALA	3.9
4	n	27	LEU	3.9
2	l	64	PHE	3.9
11	I	59	MET	3.8
2	G	65	ASN	3.7
2	G	64	PHE	3.7
1	H	1	MET	3.7
7	B	65	ASN	3.7
10	F	78	GLN	3.7
2	l	124	ALA	3.7
10	A	156	VAL	3.6
5	k	161	PRO	3.6
9	D	96	PRO	3.5
5	k	104	LYS	3.5
5	k	103	LYS	3.4
2	G	61	ASN	3.4
10	F	154	LEU	3.4
4	n	14	ASP	3.4
10	A	160	ILE	3.4
4	n	33	LEU	3.4
4	n	7	ALA	3.3
11	I	33	LEU	3.3
4	n	25	ALA	3.3
2	G	122	VAL	3.2
5	k	120	ALA	3.2
1	H	123	VAL	3.2
5	k	160	ILE	3.2
9	D	97	ILE	3.2
10	A	161	PRO	3.1
2	l	66	GLU	3.1
10	F	157	GLN	3.0
4	n	89	ARG	3.0
5	k	105	LEU	3.0
7	B	1	ALA	2.9
9	D	55	LEU	2.9
2	l	65	ASN	2.9
4	n	56	HIS	2.9
3	o	70	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	62	GLN	2.8
4	n	61	VAL	2.8
2	G	4	PRO	2.8
5	k	108	LEU	2.8
9	D	2	ALA	2.8
4	n	8	GLY	2.7
5	k	122	GLU	2.7
5	k	117	GLN	2.7
10	F	77	ALA	2.7
4	n	24	GLY	2.6
2	G	124	ALA	2.6
6	C	1	ALA	2.6
7	B	122	ALA	2.6
10	A	78	GLN	2.5
4	n	5	ALA	2.5
2	G	121	GLN	2.5
4	n	35	ASN	2.5
7	B	2	ALA	2.5
11	I	24	GLY	2.5
4	n	55	LEU	2.4
4	n	26	VAL	2.4
10	A	80	GLU	2.4
5	k	102	TRP	2.4
4	n	62	PRO	2.3
10	A	77	ALA	2.3
4	n	37	GLU	2.3
4	n	63	PHE	2.3
2	G	3	ARG	2.3
4	n	31	GLY	2.3
6	C	2	ALA	2.3
6	C	123	VAL	2.3
10	F	159	GLY	2.2
2	l	59	ASN	2.2
3	o	80	ASP	2.2
1	m	1	MET	2.2
9	D	25	ALA	2.2
4	n	53	PHE	2.2
5	k	101	HIS	2.2
11	I	26	VAL	2.2
9	D	58	GLY	2.2
11	I	32	ASP	2.2
5	k	109	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
11	I	96	PRO	2.1
10	F	161	PRO	2.1
5	k	126	PHE	2.1
10	F	153	GLU	2.1
1	m	124	SER	2.1
5	k	112	THR	2.0
6	C	58	ASP	2.0
9	D	33	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.