Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 PM GMT

PDB ID	:	4U7U
Title	:	Crystal structure of RNA-guided immune Cascade complex from E.coli
Authors	:	Zhao, H.; Sheng, G.; Wang, J.; Wang, M.; Bunkoczi, G.; Gong, W.; Wei, Z.; Wang, Y.
Deposited on	:	2014-07-31
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

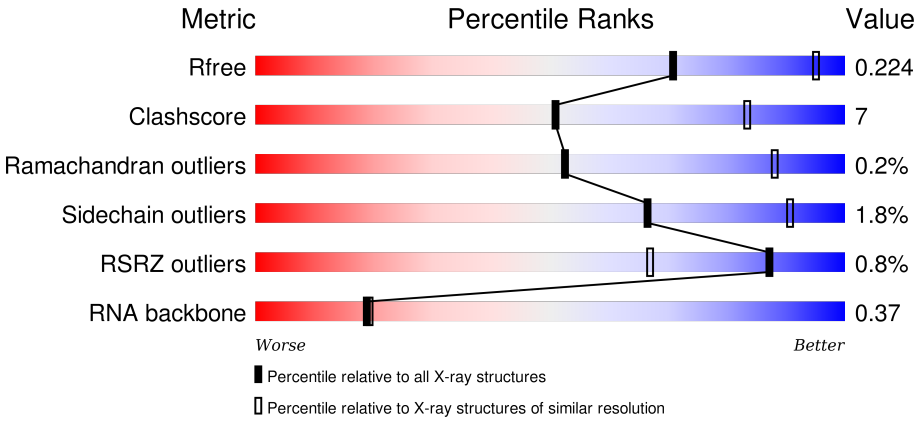
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	76% 18%
1	M	502	82% 14%
2	B	160	2% 84% 14%
2	C	160	% 86% 11%

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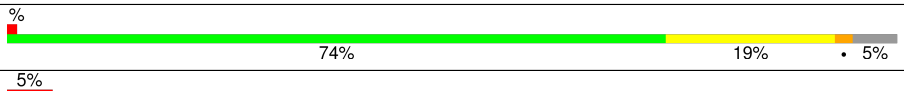
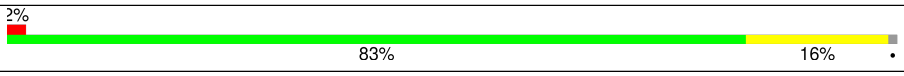
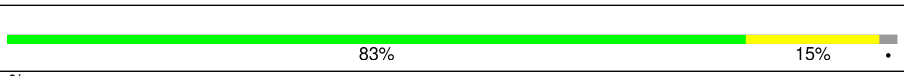
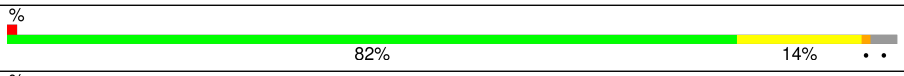
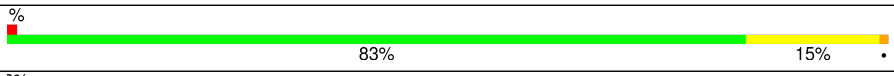
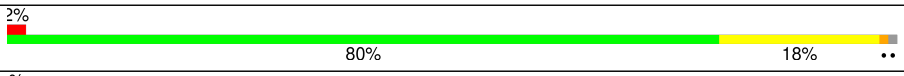
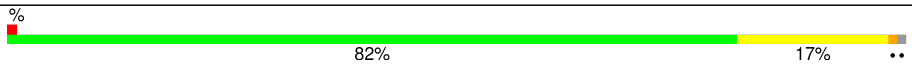
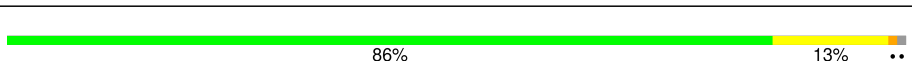
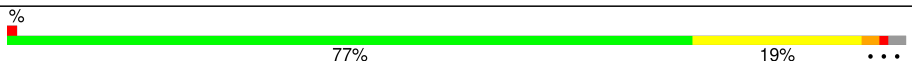
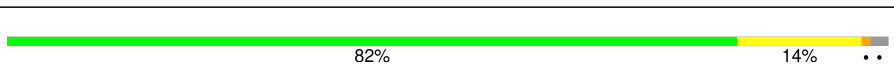
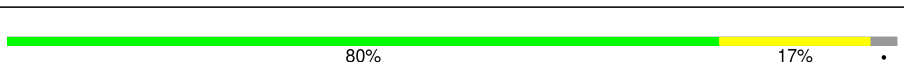
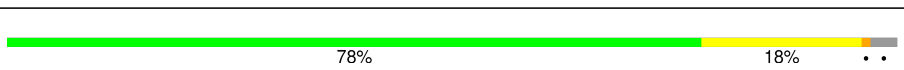
Mol	Chain	Length	Quality of chain
2	N	160	
2	O	160	
3	D	201	
3	P	201	
4	E	363	
4	F	363	
4	G	363	
4	H	363	
4	I	363	
4	J	363	
4	Q	363	
4	R	363	
4	S	363	
4	T	363	
4	U	363	
4	V	363	
5	K	224	
5	W	224	
6	L	61	
6	X	61	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54555 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 CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2386	659	674	20			
1	M	489	Total	C	N	O	S	0	0	0
			3812	2428	673	691	20			

- Molecule 2 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	157	Total	C	N	O	S	0	0	0
			1291	808	249	227	7			
2	C	157	Total	C	N	O	S	0	0	0
			1292	809	249	227	7			
2	N	152	Total	C	N	O	S	0	0	0
			1246	784	240	215	7			
2	O	156	Total	C	N	O	S	0	0	0
			1247	785	234	221	7			

- Molecule 3 is a protein called CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	191	Total	C	N	O	S	0	0	0
			1451	931	255	258	7			
3	P	191	Total	C	N	O	S	0	0	0
			1459	936	258	258	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP Q46897
D	0	TRP	-	expression tag	UNP Q46897
P	-1	ALA	-	expression tag	UNP Q46897
P	0	TRP	-	expression tag	UNP Q46897

- Molecule 4 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	357	Total	C	N	O	S	0	0	0
			2752	1721	490	525	16			
4	F	359	Total	C	N	O	S	0	0	0
			2760	1727	489	528	16			
4	G	356	Total	C	N	O	S	0	0	0
			2753	1720	490	527	16			
4	H	363	Total	C	N	O	S	0	0	0
			2774	1736	493	529	16			
4	I	355	Total	C	N	O	S	0	0	0
			2731	1711	485	519	16			
4	J	351	Total	C	N	O	S	0	0	0
			2680	1678	473	513	16			
4	Q	362	Total	C	N	O	S	0	0	0
			2790	1744	495	535	16			
4	R	359	Total	C	N	O	S	0	0	0
			2736	1712	484	524	16			
4	S	361	Total	C	N	O	S	0	0	0
			2773	1734	494	529	16			
4	T	360	Total	C	N	O	S	0	0	0
			2777	1738	494	529	16			
4	U	354	Total	C	N	O	S	0	0	0
			2723	1704	482	521	16			
4	V	355	Total	C	N	O	S	0	0	0
			2725	1704	482	523	16			

- Molecule 5 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	218	Total	C	N	O	S	0	0	0
			1722	1090	305	318	9			
5	W	218	Total	C	N	O	S	0	0	0
			1726	1093	306	318	9			

- Molecule 6 is a RNA chain called crRNA.

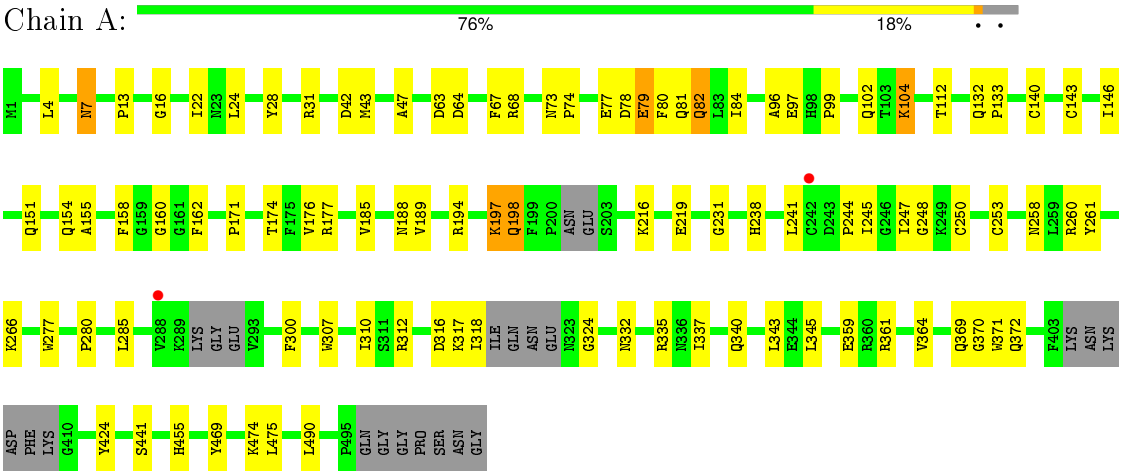
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	61	Total	C	N	O	P	0	0	0
			1298	580	230	428	60			
6	X	61	Total	C	N	O	P	0	0	0
			1298	580	230	428	60			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

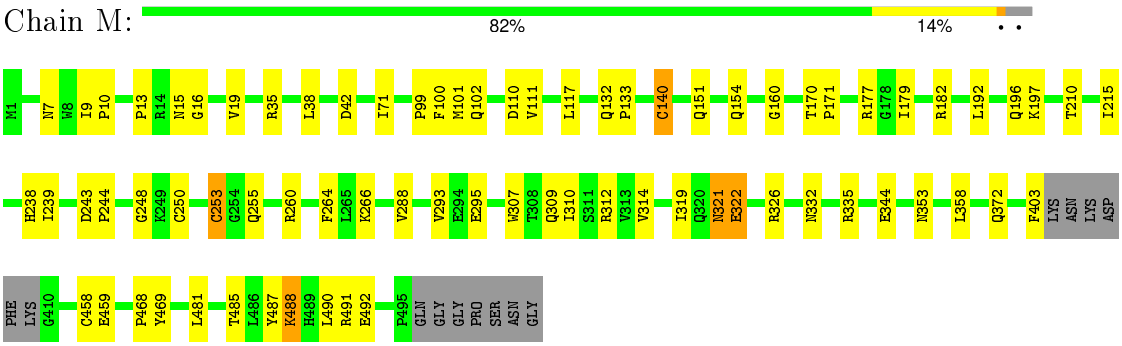
- Molecule 1: CRISPR system Cascade subunit CasA

Chain A:



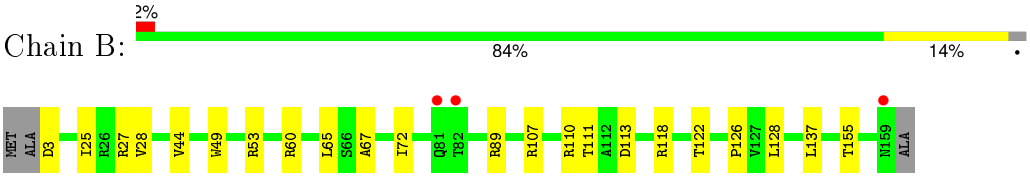
- Molecule 1: CRISPR system Cascade subunit CasA

Chain M:



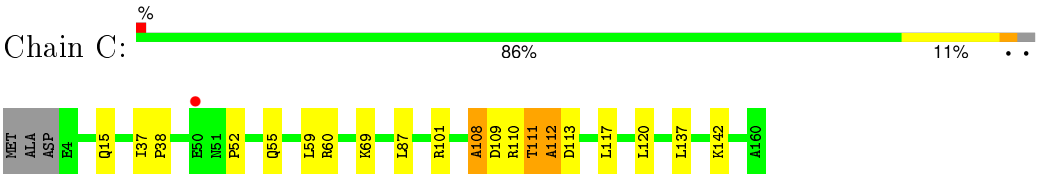
- Molecule 2: CRISPR system Cascade subunit CasB

Chain B:



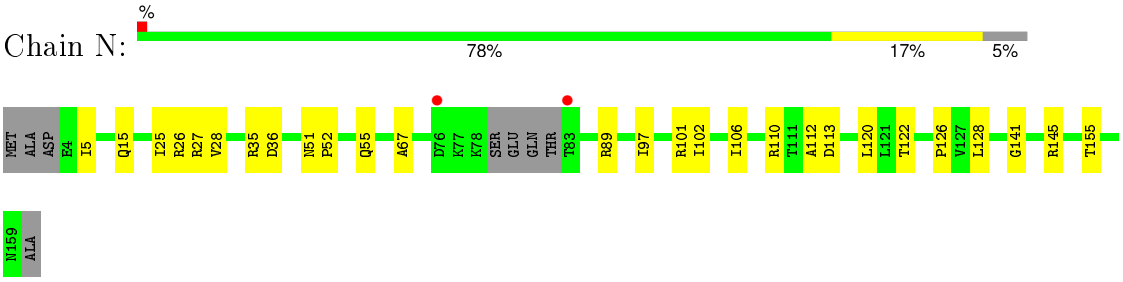
- Molecule 2: CRISPR system Cascade subunit CasB

Chain C:



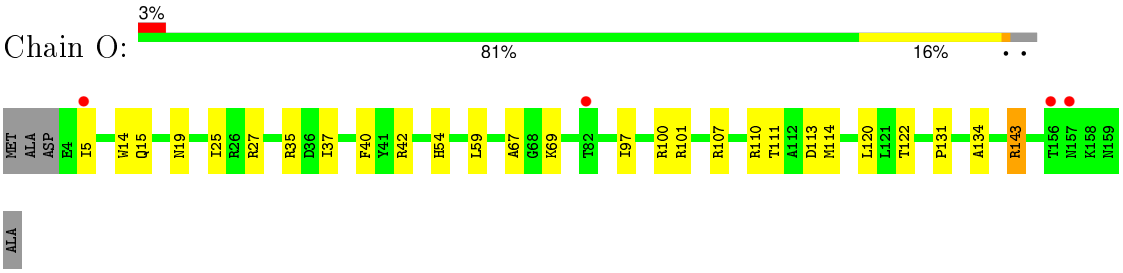
• Molecule 2: CRISPR system Cascade subunit CasB

Chain N:



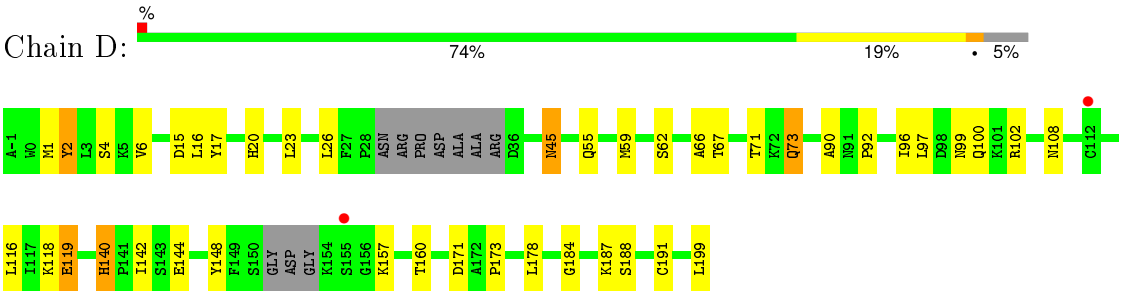
• Molecule 2: CRISPR system Cascade subunit CasB

Chain O:



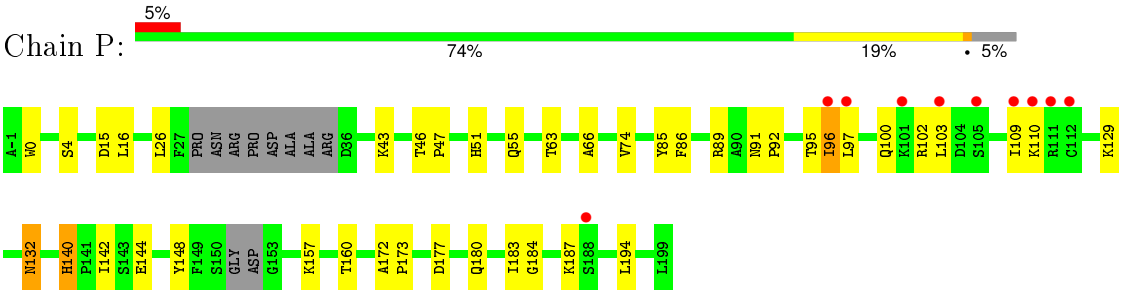
• Molecule 3: CRISPR system Cascade subunit CasE

Chain D:



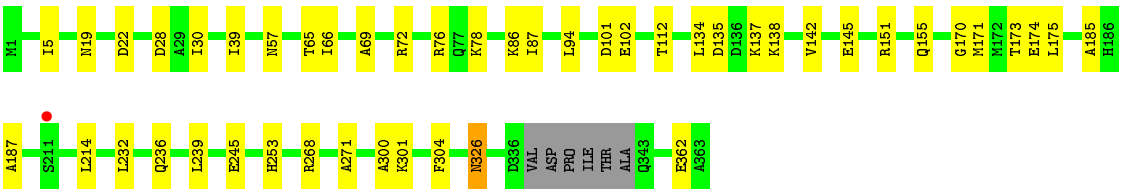
• Molecule 3: CRISPR system Cascade subunit CasE

Chain P:



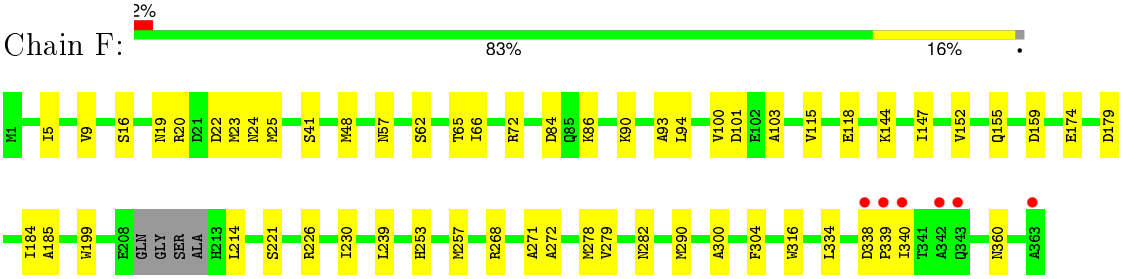
• Molecule 4: CRISPR system Cascade subunit CasC

Chain E:



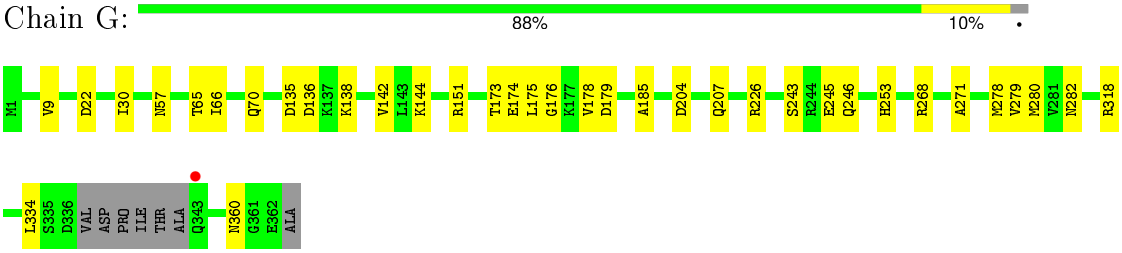
• Molecule 4: CRISPR system Cascade subunit CasC

Chain F:



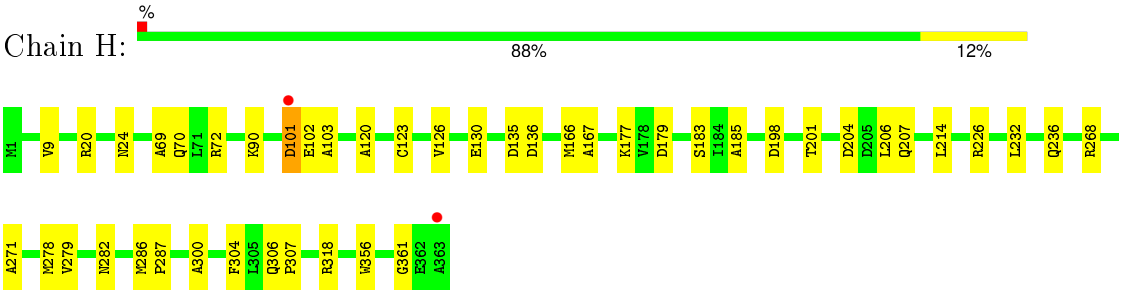
• Molecule 4: CRISPR system Cascade subunit CasC

Chain G:



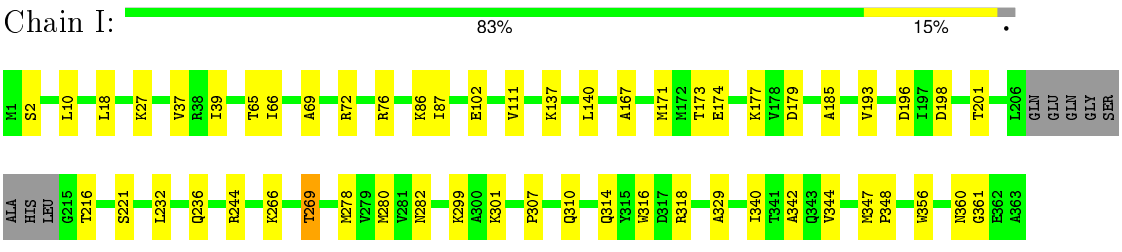
• Molecule 4: CRISPR system Cascade subunit CasC

Chain H:



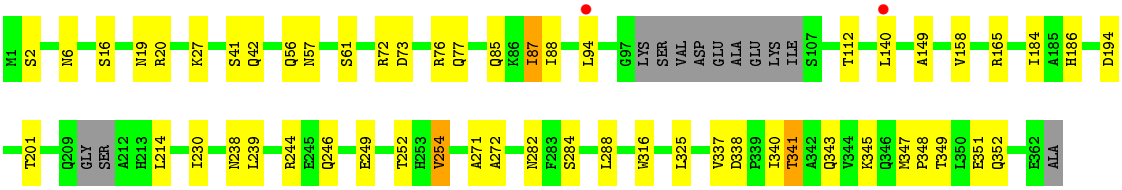
• Molecule 4: CRISPR system Cascade subunit CasC

Chain I:

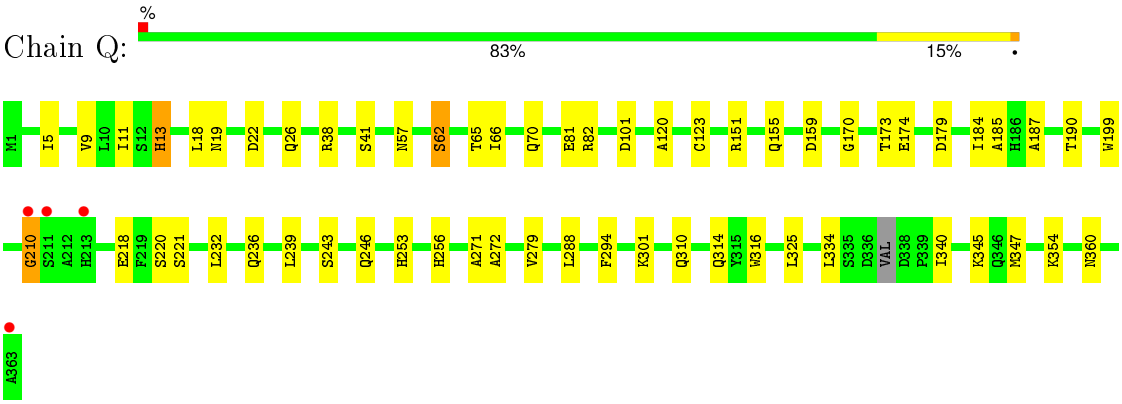


• Molecule 4: CRISPR system Cascade subunit CasC

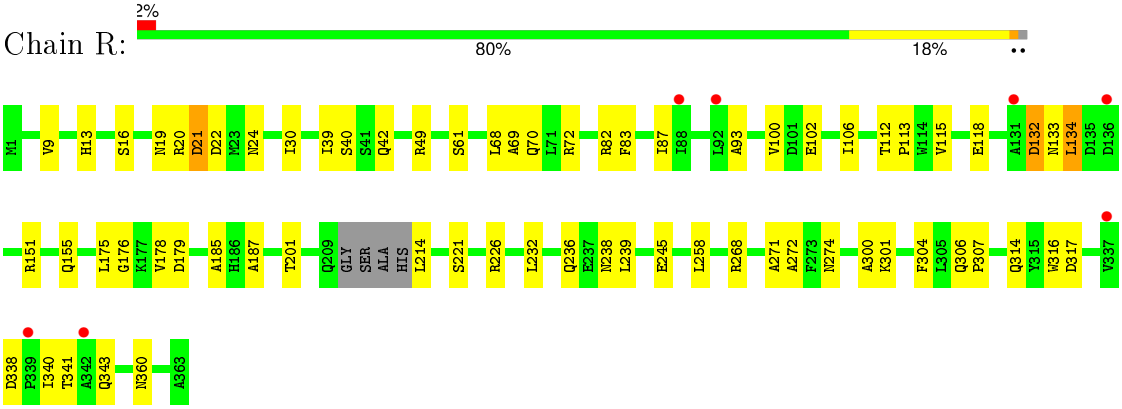
Chain J:



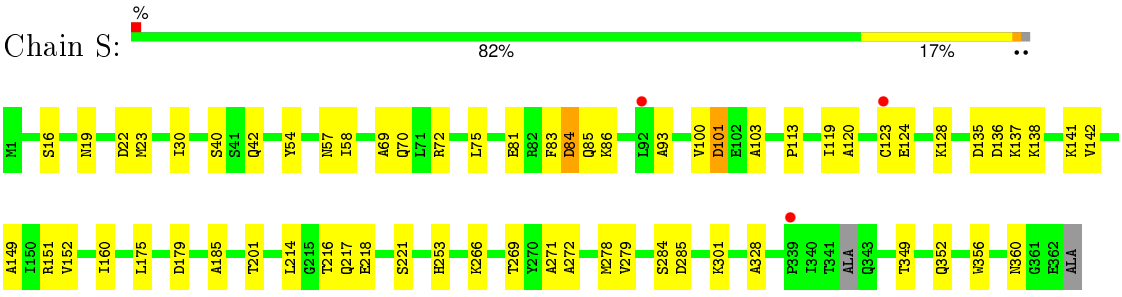
• Molecule 4: CRISPR system Cascade subunit CasC



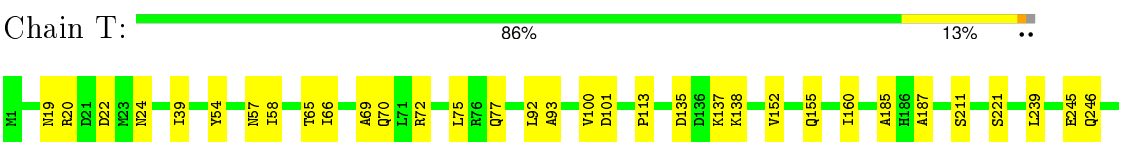
• Molecule 4: CRISPR system Cascade subunit CasC

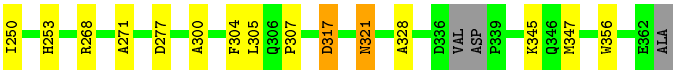


• Molecule 4: CRISPR system Cascade subunit CasC



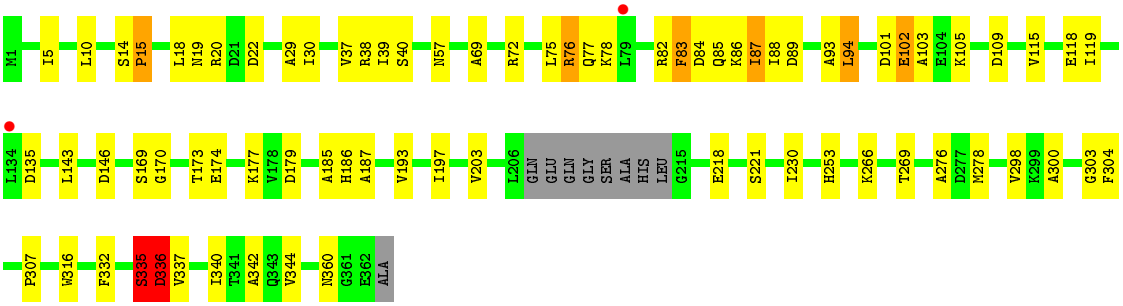
• Molecule 4: CRISPR system Cascade subunit CasC





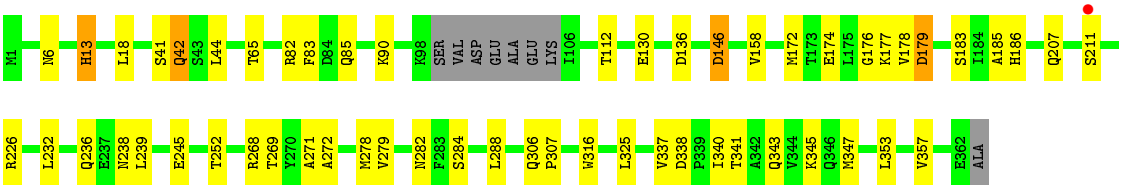
• Molecule 4: CRISPR system Cascade subunit CasC

Chain U:



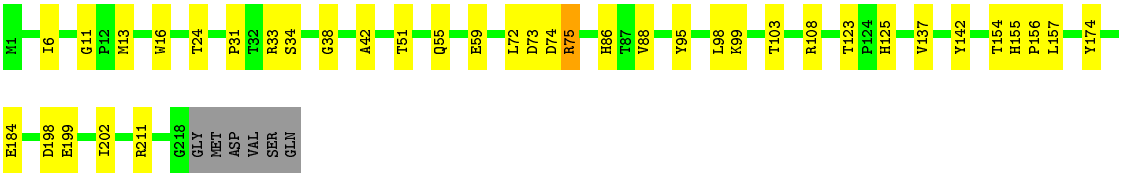
• Molecule 4: CRISPR system Cascade subunit CasC

Chain V:



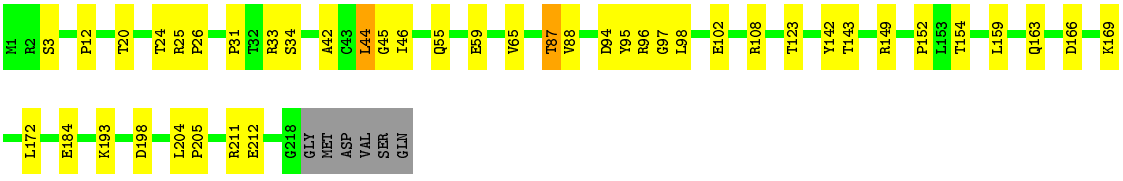
• Molecule 5: CRISPR system Cascade subunit CasD

Chain K:



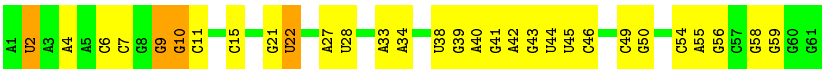
• Molecule 5: CRISPR system Cascade subunit CasD

Chain W:



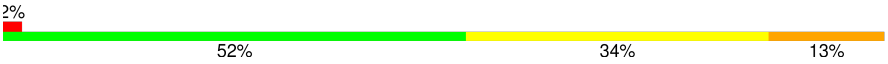
• Molecule 6: crRNA

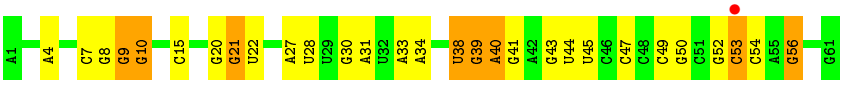
Chain L:



- Molecule 6: crRNA

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	111.41Å 118.14Å 225.87Å 92.23° 93.55° 106.06°	Depositor
Resolution (Å)	43.80 – 3.00 50.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (43.80-3.00) 87.4 (50.05-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.179 , 0.218 0.194 , 0.224	Depositor DCC
R_{free} test set	9791 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 195336 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	54555	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/3825	0.55	0/5197
1	M	0.65	1/3901 (0.0%)	0.57	1/5303 (0.0%)
2	B	0.58	0/1316	0.53	0/1777
2	C	0.55	0/1317	0.60	2/1778 (0.1%)
2	N	0.50	0/1270	0.52	0/1714
2	O	0.42	0/1272	0.57	0/1724
3	D	0.50	0/1480	0.65	0/2011
3	P	0.40	0/1488	0.60	0/2019
4	E	0.60	0/2795	0.53	0/3768
4	F	0.60	0/2803	0.52	0/3785
4	G	0.64	0/2796	0.52	0/3771
4	H	0.63	0/2819	0.54	0/3809
4	I	0.61	0/2774	0.55	0/3744
4	J	0.53	0/2722	0.55	0/3681
4	Q	0.70	0/2834	0.56	0/3823
4	R	0.59	0/2779	0.57	2/3758 (0.1%)
4	S	0.59	0/2817	0.56	0/3802
4	T	0.60	0/2821	0.55	0/3805
4	U	0.51	0/2766	0.59	0/3737
4	V	0.72	0/2768	0.62	1/3741 (0.0%)
5	K	0.47	0/1764	0.54	0/2398
5	W	0.69	0/1768	0.61	1/2402 (0.0%)
6	L	1.04	0/1450	1.06	1/2259 (0.0%)
6	X	1.04	0/1450	0.99	0/2259
All	All	0.62	1/55795 (0.0%)	0.60	8/76065 (0.0%)

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
4	R	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	U	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	458	CYS	CB-SG	-5.56	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	112	ALA	N-CA-C	-6.88	92.42	111.00
5	W	44	LEU	CA-CB-CG	5.83	128.71	115.30
1	M	250	CYS	CA-CB-SG	5.62	124.11	114.00
6	L	22	U	O4'-C1'-N1	5.32	112.46	108.20
4	R	21	ASP	CB-CG-OD1	-5.32	113.51	118.30
4	R	133	ASN	CB-CA-C	-5.20	99.99	110.40
2	C	108	ALA	N-CA-C	5.08	124.72	111.00
4	V	186	HIS	N-CA-CB	5.05	119.70	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	132	ASP	Peptide
4	R	338	ASP	Peptide
4	U	335	SER	Peptide
4	U	94	LEU	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	3739	0	3705	64	0
1	M	3812	0	3775	47	0
2	B	1291	0	1295	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1292	0	1300	25	0
2	N	1246	0	1253	15	0
2	O	1247	0	1226	17	0
3	D	1451	0	1447	37	0
3	P	1459	0	1466	31	0
4	E	2752	0	2729	31	0
4	F	2760	0	2730	36	0
4	G	2753	0	2727	27	0
4	H	2774	0	2731	30	0
4	I	2731	0	2714	38	0
4	J	2680	0	2624	36	0
4	Q	2790	0	2764	39	0
4	R	2736	0	2672	41	0
4	S	2773	0	2734	42	0
4	T	2777	0	2761	32	0
4	U	2723	0	2690	84	0
4	V	2725	0	2682	37	0
5	K	1722	0	1700	29	0
5	W	1726	0	1711	31	0
6	L	1298	0	658	13	0
6	X	1298	0	658	16	0
All	All	54555	0	52752	738	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 7.

All (738) 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)
4:U:82:ARG:CG	4:U:83:PHE:CE2	1.79	1.60
4:U:82:ARG:CG	4:U:83:PHE:HE2	1.03	1.58
4:U:82:ARG:CB	4:U:83:PHE:CE2	1.92	1.50
4:U:82:ARG:C	4:U:83:PHE:CD2	1.88	1.47
4:U:82:ARG:HB3	4:U:83:PHE:CE2	1.50	1.40
4:U:82:ARG:C	4:U:83:PHE:HD2	1.23	1.40
4:U:82:ARG:CB	4:U:83:PHE:HE2	1.24	1.38
4:U:101:ASP:OD1	4:U:103:ALA:N	1.57	1.37
4:U:82:ARG:HG2	4:U:83:PHE:CE2	1.51	1.33
4:Q:62:SER:OG	4:Q:159:ASP:OD2	1.53	1.26
4:U:84:ASP:O	4:U:87:ILE:HD13	1.33	1.26
2:C:108:ALA:O	2:C:112:ALA:HB3	1.39	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:82:ARG:CD	4:U:83:PHE:CE2	2.24	1.20
4:U:82:ARG:HB3	4:U:83:PHE:CD2	1.81	1.14
4:U:82:ARG:CB	4:U:83:PHE:CD2	2.33	1.12
4:U:82:ARG:CD	4:U:83:PHE:HE2	1.62	1.09
4:U:82:ARG:O	4:U:83:PHE:CD2	2.10	1.05
4:I:196:ASP:OD2	4:I:299:LYS:NZ	1.91	1.04
4:U:82:ARG:HD3	4:U:83:PHE:CE2	1.94	1.00
4:U:82:ARG:CD	4:U:83:PHE:CZ	2.45	0.98
4:U:83:PHE:N	4:U:83:PHE:HD2	1.57	0.98
4:U:82:ARG:HD3	4:U:83:PHE:CZ	1.99	0.98
4:E:271:ALA:HB3	4:F:185:ALA:HB2	1.46	0.95
2:C:108:ALA:O	2:C:109:ASP:HB2	1.69	0.93
4:U:82:ARG:CA	4:U:83:PHE:CD2	2.52	0.92
4:U:82:ARG:CA	4:U:83:PHE:HD2	1.81	0.91
3:P:132:ASN:HD22	3:P:132:ASN:N	1.64	0.91
4:S:86:LYS:N	4:S:86:LYS:HD3	1.89	0.87
1:A:7:ASN:N	1:A:7:ASN:HD22	1.70	0.86
4:T:93:ALA:HB2	4:T:100:VAL:HG23	1.56	0.86
3:D:2:TYR:HB3	3:D:73:GLN:HA	1.57	0.85
1:M:295:GLU:OE2	1:M:326:ARG:NH2	2.10	0.85
4:U:76:ARG:HH11	4:U:85:GLN:HG3	1.43	0.83
4:S:138:LYS:HG3	4:S:141:LYS:HE3	1.60	0.82
3:P:132:ASN:H	3:P:132:ASN:HD22	1.23	0.81
5:W:166:ASP:HB2	5:W:169:LYS:HG2	1.63	0.80
4:R:93:ALA:HB2	4:R:100:VAL:HG12	1.62	0.80
4:U:84:ASP:O	4:U:87:ILE:CD1	2.24	0.80
3:D:140:HIS:HE2	3:D:142:ILE:HG12	1.46	0.79
4:Q:271:ALA:HB3	4:R:185:ALA:HB2	1.62	0.79
3:P:140:HIS:CE1	3:P:142:ILE:HG12	2.18	0.79
4:U:76:ARG:HD3	4:U:85:GLN:HG3	1.64	0.78
4:E:101:ASP:OD1	4:E:102:GLU:N	2.17	0.78
4:J:186:HIS:HB2	5:K:13:MET:HE1	1.66	0.77
5:K:33:ARG:HB3	5:K:198:ASP:HB3	1.66	0.77
1:A:96:ALA:O	1:A:104:LYS:NZ	2.15	0.77
2:C:108:ALA:O	2:C:109:ASP:CB	2.33	0.77
4:J:20:ARG:NH1	6:L:11:C:OP2	2.18	0.76
3:P:96:ILE:HG22	3:P:97:LEU:H	1.51	0.76
4:T:345:LYS:HG2	4:T:347:MET:HE2	1.68	0.75
5:W:87:THR:HG21	6:X:8:G:H21	1.51	0.75
4:U:82:ARG:CG	4:U:83:PHE:CZ	2.65	0.75
4:I:221:SER:HB2	4:I:269:THR:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:341:THR:OG1	4:V:343:GLN:OE1	2.03	0.75
3:P:140:HIS:HE1	3:P:142:ILE:HG12	1.51	0.75
1:A:140:CYS:HB2	1:A:143:CYS:H	1.51	0.75
4:I:86:LYS:HD2	4:I:86:LYS:H	1.51	0.75
4:R:151:ARG:NH2	4:R:175:LEU:O	2.20	0.74
5:K:33:ARG:NH1	5:K:184:GLU:OE2	2.21	0.74
4:U:170:GLY:O	4:U:173:THR:HG22	1.88	0.73
5:K:199:GLU:HG2	5:K:211:ARG:HD2	1.70	0.73
4:I:173:THR:HG23	4:I:174:GLU:HG3	1.71	0.73
4:Q:13:HIS:CD2	4:Q:18:LEU:HD11	2.24	0.73
4:V:345:LYS:NZ	4:V:347:MET:SD	2.61	0.73
5:K:198:ASP:HB2	5:K:211:ARG:HD3	1.71	0.72
3:D:184:GLY:O	3:D:187:LYS:NZ	2.22	0.72
4:Q:173:THR:HG23	4:Q:174:GLU:HG2	1.72	0.72
3:D:2:TYR:HE1	3:D:59:MET:HA	1.54	0.71
3:P:0:TRP:O	3:P:180:GLN:NE2	2.24	0.71
3:D:20:HIS:CD2	3:D:188:SER:HB2	2.25	0.71
3:P:132:ASN:ND2	3:P:132:ASN:N	2.39	0.71
4:I:37:VAL:HG23	4:I:193:VAL:HG21	1.73	0.70
6:L:49:C:H2'	6:L:50:G:H8	1.56	0.70
4:T:155:GLN:HG2	4:T:239:LEU:HD22	1.73	0.70
3:D:140:HIS:NE2	3:D:142:ILE:HG12	2.07	0.70
4:S:86:LYS:H	4:S:86:LYS:HD3	1.57	0.69
3:P:140:HIS:CD2	4:U:15:PRO:HG2	2.28	0.69
4:U:82:ARG:HG2	4:U:83:PHE:CZ	2.22	0.69
4:V:174:GLU:OE2	4:V:177:LYS:NZ	2.25	0.69
2:N:89:ARG:NE	2:N:155:THR:OG1	2.25	0.69
4:T:135:ASP:HB3	4:T:138:LYS:HG3	1.74	0.69
1:A:247:ILE:HG13	1:A:258:ASN:HA	1.74	0.69
4:R:268:ARG:NH1	4:S:179:ASP:OD1	2.26	0.69
5:W:198:ASP:HB2	5:W:211:ARG:HD3	1.75	0.68
2:C:108:ALA:O	2:C:112:ALA:CB	2.30	0.68
4:U:173:THR:HG23	4:U:174:GLU:OE1	1.92	0.68
3:D:102:ARG:NH2	6:L:46:C:OP2	2.27	0.68
5:W:44:LEU:O	5:W:46:ILE:HG13	1.93	0.68
4:Q:210:GLY:O	6:X:21:G:N2	2.21	0.67
3:P:15:ASP:OD1	3:P:16:LEU:N	2.27	0.67
4:V:85:GLN:OE1	4:V:85:GLN:N	2.27	0.67
1:A:63:ASP:OD1	1:A:64:ASP:N	2.26	0.67
4:E:185:ALA:HB2	4:J:271:ALA:HB3	1.76	0.67
3:D:119:GLU:OE1	4:I:266:LYS:NZ	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:62:SER:OG	4:Q:159:ASP:CG	2.33	0.67
4:I:316:TRP:CD1	4:I:340:ILE:HD11	2.30	0.67
4:S:271:ALA:HB3	4:T:185:ALA:HB2	1.76	0.67
4:R:271:ALA:HB3	4:S:185:ALA:HB2	1.76	0.66
4:J:112:THR:HG23	4:J:238:ASN:HA	1.76	0.66
5:K:108:ARG:NH2	6:L:7:C:O2	2.29	0.66
2:C:110:ARG:O	2:C:112:ALA:N	2.27	0.66
1:A:7:ASN:HB3	1:A:22:ILE:C	2.17	0.66
2:C:111:THR:HG22	2:C:112:ALA:N	2.09	0.66
5:W:55:GLN:O	5:W:59:GLU:HG3	1.96	0.66
4:Q:185:ALA:HB2	4:V:271:ALA:HB3	1.77	0.66
2:O:113:ASP:OD1	2:O:114:MET:N	2.28	0.66
4:T:271:ALA:HB3	4:U:185:ALA:HB2	1.77	0.66
4:T:317:ASP:O	4:T:321:ASN:HB2	1.96	0.65
4:E:268:ARG:NH1	4:F:179:ASP:OD1	2.29	0.65
1:M:321:ASN:OD1	1:M:322:GLU:HB2	1.97	0.65
4:U:102:GLU:CA	4:U:102:GLU:OE1	2.45	0.64
4:G:151:ARG:NH2	4:G:175:LEU:O	2.28	0.64
4:J:94:LEU:HD22	4:J:140:LEU:HD11	1.79	0.64
4:Q:11:ILE:HG12	4:Q:13:HIS:CE1	2.33	0.64
1:A:99:PRO:HB2	1:A:102:GLN:HB2	1.80	0.64
3:D:199:LEU:HD21	4:I:216:THR:HG22	1.79	0.64
4:H:167:ALA:H	4:H:177:LYS:HE3	1.62	0.64
4:E:142:VAL:O	4:E:145:GLU:HB2	1.97	0.64
4:U:101:ASP:OD1	4:U:102:GLU:N	2.30	0.63
4:U:76:ARG:HH11	4:U:85:GLN:CG	2.10	0.63
5:W:94:ASP:OD1	5:W:95:TYR:N	2.30	0.63
5:W:87:THR:HG21	6:X:8:G:N2	2.13	0.63
4:S:84:ASP:OD1	4:S:84:ASP:N	2.29	0.63
1:A:250:CYS:SG	1:A:253:CYS:N	2.71	0.63
4:S:217:GLN:OE1	4:S:266:LYS:HE3	1.99	0.62
2:C:111:THR:O	2:C:112:ALA:C	2.30	0.62
1:A:332:ASN:OD1	1:A:335:ARG:NH1	2.30	0.62
2:B:107:ARG:NH2	4:E:28:ASP:OD2	2.32	0.62
3:D:20:HIS:HD2	3:D:188:SER:HB2	1.63	0.62
3:D:4:SER:HB3	3:D:71:THR:HG23	1.82	0.62
1:A:31:ARG:HG3	1:A:74:PRO:HG2	1.82	0.62
4:R:21:ASP:OD1	4:R:21:ASP:C	2.35	0.62
4:G:334:LEU:O	4:H:318:ARG:NH1	2.32	0.62
4:U:316:TRP:CD1	4:U:340:ILE:HD11	2.35	0.62
4:H:271:ALA:HB3	4:I:185:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:44:LEU:O	5:W:46:ILE:N	2.32	0.61
4:F:271:ALA:HB3	4:G:185:ALA:HB2	1.82	0.61
4:F:300:ALA:HB2	4:F:304:PHE:CE1	2.35	0.61
4:R:201:THR:HG22	4:R:214:LEU:HG	1.80	0.61
4:U:82:ARG:NE	4:U:83:PHE:HZ	1.98	0.61
1:M:10:PRO:HG2	1:M:38:LEU:HD11	1.81	0.61
4:E:65:THR:OG1	4:E:66:ILE:N	2.33	0.61
4:I:167:ALA:O	4:I:177:LYS:NZ	2.19	0.60
5:W:34:SER:HB3	5:W:198:ASP:O	2.01	0.60
1:A:151:GLN:HA	1:A:155:ALA:HB3	1.83	0.60
4:U:87:ILE:HG12	4:U:88:ILE:N	2.11	0.60
4:U:82:ARG:CD	4:U:83:PHE:HZ	2.08	0.60
1:A:7:ASN:N	1:A:7:ASN:ND2	2.42	0.60
4:G:271:ALA:HB3	4:H:185:ALA:HB2	1.82	0.60
3:D:100:GLN:OE1	3:D:102:ARG:NH1	2.35	0.60
1:A:245:ILE:HG22	1:A:260:ARG:HB2	1.82	0.60
4:U:83:PHE:CB	4:U:87:ILE:HD11	2.32	0.60
5:K:33:ARG:NE	5:K:199:GLU:OE1	2.32	0.60
4:T:113:PRO:HB2	4:T:160:ILE:HD11	1.83	0.60
3:P:129:LYS:HD2	3:P:183:ILE:HG23	1.84	0.60
1:A:469:TYR:HB3	1:A:475:LEU:HD13	1.84	0.59
4:E:76:ARG:NH2	4:E:102:GLU:OE1	2.32	0.59
4:R:221:SER:OG	4:S:30:ILE:O	2.20	0.59
2:O:15:GLN:NE2	2:O:69:LYS:O	2.32	0.59
4:H:278:MET:HG2	4:H:279:VAL:N	2.17	0.59
3:P:140:HIS:HD2	4:U:15:PRO:HG2	1.67	0.59
4:S:86:LYS:CD	4:S:86:LYS:H	2.12	0.59
4:S:217:GLN:HG3	4:S:218:GLU:N	2.16	0.59
4:I:2:SER:O	4:I:244:ARG:NH2	2.34	0.59
4:G:204:ASP:HB3	4:G:207:GLN:HB3	1.83	0.59
4:F:155:GLN:HG2	4:F:239:LEU:HD22	1.85	0.59
4:I:10:LEU:HB2	4:I:278:MET:HB3	1.85	0.59
2:C:110:ARG:HG3	2:C:111:THR:HB	1.85	0.59
4:R:132:ASP:O	4:R:134:LEU:N	2.36	0.59
4:G:135:ASP:OD1	4:G:136:ASP:N	2.36	0.59
4:U:102:GLU:OE1	4:U:102:GLU:HA	2.03	0.58
2:C:109:ASP:C	2:C:110:ARG:O	2.37	0.58
4:R:83:PHE:HB3	4:R:87:ILE:HD11	1.84	0.58
1:A:300:PHE:CZ	1:A:361:ARG:HD2	2.38	0.58
4:U:82:ARG:NE	4:U:83:PHE:CZ	2.70	0.58
4:H:268:ARG:NH1	4:I:179:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:ARG:NH1	3:P:144:GLU:OE2	2.36	0.58
4:J:165:ARG:O	6:L:6:C:O2'	2.16	0.58
1:M:117:LEU:HD23	1:M:151:GLN:HG3	1.86	0.58
4:J:345:LYS:HD3	4:J:347:MET:HE2	1.84	0.58
4:Q:316:TRP:CD1	4:Q:340:ILE:HD11	2.39	0.58
4:T:268:ARG:NH1	4:U:179:ASP:OD1	2.37	0.57
1:A:194:ARG:HA	1:A:197:LYS:HG3	1.84	0.57
1:A:335:ARG:HG3	1:A:372:GLN:HB3	1.86	0.57
4:I:198:ASP:OD2	4:I:201:THR:HG23	2.04	0.57
4:R:316:TRP:CD1	4:R:340:ILE:HD11	2.39	0.57
4:G:278:MET:HG2	4:G:279:VAL:N	2.19	0.57
4:H:204:ASP:HB3	4:H:207:GLN:HG2	1.86	0.57
1:A:285:LEU:HD21	1:A:312:ARG:HD3	1.87	0.57
5:W:31:PRO:HD2	5:W:65:VAL:HG11	1.87	0.57
4:U:221:SER:HB2	4:U:269:THR:HG21	1.87	0.57
4:J:341:THR:HG22	4:J:343:GLN:H	1.70	0.57
4:R:245:GLU:N	4:R:245:GLU:OE1	2.38	0.57
3:D:45:ASN:N	3:D:45:ASN:OD1	2.38	0.57
3:P:132:ASN:ND2	3:P:132:ASN:H	2.00	0.56
4:U:335:SER:O	4:U:337:VAL:N	2.38	0.56
4:Q:288:LEU:HD21	4:Q:325:LEU:HD11	1.86	0.56
3:D:140:HIS:O	3:D:140:HIS:HD2	1.88	0.56
1:M:133:PRO:HG3	5:W:95:TYR:CE1	2.40	0.56
1:M:307:TRP:HA	1:M:310:ILE:HG13	1.86	0.56
1:A:307:TRP:HA	1:A:310:ILE:HG13	1.87	0.56
1:A:79:GLU:HA	1:A:82:GLN:HB2	1.87	0.56
5:W:193:LYS:HE2	5:W:212:GLU:HB3	1.87	0.56
4:J:72:ARG:NH1	4:J:73:ASP:OD1	2.39	0.56
4:F:199:TRP:HB3	4:F:214:LEU:HD23	1.88	0.56
4:S:135:ASP:OD1	4:S:136:ASP:N	2.39	0.56
2:B:67:ALA:HB1	2:B:122:THR:HG22	1.85	0.56
2:C:52:PRO:HA	2:C:55:GLN:HG3	1.88	0.56
4:H:101:ASP:HB2	4:H:103:ALA:H	1.70	0.55
4:H:135:ASP:OD1	4:H:136:ASP:N	2.40	0.55
5:W:88:VAL:HG22	6:X:7:C:H1'	1.88	0.55
4:U:109:ASP:OD1	4:U:109:ASP:N	2.27	0.55
4:I:86:LYS:H	4:I:86:LYS:CD	2.19	0.55
4:U:83:PHE:N	4:U:83:PHE:CD2	2.29	0.55
1:M:332:ASN:OD1	1:M:335:ARG:NH1	2.40	0.55
4:I:360:ASN:ND2	4:I:360:ASN:O	2.39	0.55
3:D:140:HIS:CD2	3:D:140:HIS:C	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:243:SER:H	4:G:246:GLN:NE2	2.05	0.55
4:S:151:ARG:NH2	4:S:175:LEU:O	2.38	0.55
4:J:349:THR:HG22	4:J:351:GLU:H	1.71	0.55
4:U:10:LEU:HB2	4:U:278:MET:HB3	1.89	0.55
1:M:492:GLU:N	1:M:492:GLU:OE1	2.40	0.55
4:F:62:SER:OG	4:F:159:ASP:OD2	2.25	0.55
4:F:9:VAL:HB	4:F:226:ARG:HB2	1.89	0.55
5:W:3:SER:HB3	5:W:163:GLN:HE21	1.70	0.54
6:L:9:G:HO2'	6:L:10:G:H8	1.56	0.54
4:T:77:GLN:O	4:T:77:GLN:NE2	2.40	0.54
1:A:174:THR:HB	1:A:345:LEU:HD11	1.88	0.54
4:J:337:VAL:HG12	4:J:338:ASP:H	1.72	0.54
4:F:316:TRP:HD1	4:F:340:ILE:HG21	1.72	0.54
2:B:27:ARG:NH2	4:G:22:ASP:OD1	2.41	0.54
1:M:100:PHE:O	1:M:102:GLN:HG3	2.07	0.54
1:A:340:GLN:HA	1:A:369:GLN:HE21	1.72	0.54
4:S:124:GLU:O	4:S:128:LYS:HG3	2.07	0.54
4:V:179:ASP:N	4:V:179:ASP:OD1	2.41	0.54
4:J:19:ASN:OD1	4:J:27:LYS:HD2	2.08	0.54
1:A:316:ASP:OD2	1:A:332:ASN:ND2	2.31	0.54
4:R:214:LEU:HD22	4:S:22:ASP:HB3	1.90	0.54
4:I:76:ARG:NH2	4:I:102:GLU:OE2	2.39	0.54
4:T:101:ASP:C	4:T:101:ASP:OD1	2.46	0.53
4:I:86:LYS:N	4:I:86:LYS:HD2	2.22	0.53
4:F:48:MET:HG2	4:F:257:MET:HB3	1.90	0.53
4:Q:179:ASP:OD1	4:V:268:ARG:NH1	2.41	0.53
1:A:97:GLU:HA	1:A:104:LYS:NZ	2.24	0.53
2:N:67:ALA:HB1	2:N:122:THR:HG22	1.90	0.53
4:R:179:ASP:O	4:R:238:ASN:ND2	2.38	0.53
4:U:83:PHE:HB2	4:U:87:ILE:HD11	1.89	0.53
3:P:140:HIS:CE1	3:P:142:ILE:CG1	2.91	0.53
6:L:49:C:H2'	6:L:50:G:C8	2.41	0.53
1:A:248:GLY:HA3	1:A:260:ARG:CZ	2.38	0.53
5:W:3:SER:HA	5:W:163:GLN:HG3	1.91	0.53
4:V:245:GLU:OE2	4:V:245:GLU:N	2.40	0.53
4:E:214:LEU:HD13	4:F:22:ASP:HB3	1.90	0.52
4:E:173:THR:HG23	4:E:174:GLU:HG2	1.91	0.52
2:B:89:ARG:NE	2:B:155:THR:OG1	2.43	0.52
4:V:13:HIS:CD2	4:V:18:LEU:HD11	2.43	0.52
5:W:204:LEU:HD12	5:W:205:PRO:HD2	1.91	0.52
2:N:35:ARG:NH2	2:N:55:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:90:LYS:NZ	4:V:130:GLU:OE1	2.39	0.52
4:V:136:ASP:N	4:V:136:ASP:OD1	2.41	0.52
4:I:69:ALA:O	4:I:72:ARG:HB3	2.10	0.52
4:S:113:PRO:HB2	4:S:160:ILE:HD11	1.91	0.52
2:C:110:ARG:CG	2:C:111:THR:HB	2.38	0.52
4:Q:170:GLY:O	4:Q:173:THR:HG22	2.10	0.52
1:A:154:GLN:HA	1:A:171:PRO:HD2	1.92	0.52
1:A:359:GLU:OE2	1:A:361:ARG:NH2	2.42	0.52
2:B:60:ARG:NH1	2:B:137:LEU:O	2.41	0.52
4:F:93:ALA:HB2	4:F:100:VAL:HG23	1.91	0.52
4:S:360:ASN:ND2	4:S:360:ASN:O	2.43	0.52
4:T:39:ILE:HB	4:T:187:ALA:HB3	1.91	0.52
4:J:42:GLN:HG2	5:K:86:HIS:CE1	2.45	0.51
2:B:3:ASP:OD1	2:B:53:ARG:NH2	2.43	0.51
2:C:111:THR:C	2:C:113:ASP:N	2.52	0.51
2:C:111:THR:N	2:C:113:ASP:OD1	2.44	0.51
3:D:2:TYR:HE1	3:D:59:MET:CA	2.23	0.51
5:K:88:VAL:HG22	6:L:7:C:H1'	1.91	0.51
4:Q:345:LYS:HG2	4:Q:347:MET:HE2	1.91	0.51
2:N:27:ARG:HD2	4:S:23:MET:SD	2.51	0.51
4:Q:232:LEU:O	4:Q:236:GLN:HG3	2.11	0.51
4:R:72:ARG:NH1	4:R:102:GLU:HA	2.26	0.51
4:S:75:LEU:HD11	4:S:119:ILE:HD13	1.92	0.51
2:B:126:PRO:HB2	2:B:128:LEU:HD23	1.92	0.51
3:P:43:LYS:HB2	3:P:51:HIS:HB2	1.92	0.51
5:K:74:ASP:O	5:K:74:ASP:OD1	2.29	0.51
1:M:110:ASP:OD1	1:M:111:VAL:N	2.43	0.51
4:H:300:ALA:HB2	4:H:304:PHE:CE1	2.46	0.51
5:K:73:ASP:O	5:K:74:ASP:OD1	2.29	0.51
5:K:55:GLN:O	5:K:59:GLU:HG3	2.10	0.51
1:A:112:THR:HG21	1:A:266:LYS:HE3	1.93	0.51
2:N:36:ASP:OD2	2:O:107:ARG:NH2	2.44	0.51
2:O:110:ARG:O	2:O:113:ASP:OD1	2.29	0.50
5:K:38:GLY:HA3	6:L:2:U:O4'	2.12	0.50
3:P:100:GLN:OE1	3:P:102:ARG:NH1	2.44	0.50
3:P:85:TYR:CD2	4:U:197:ILE:HD11	2.47	0.50
4:U:75:LEU:HD11	4:U:119:ILE:HD13	1.92	0.50
6:X:49:C:H2'	6:X:50:G:H8	1.75	0.50
3:P:144:GLU:OE1	3:P:160:THR:OG1	2.28	0.50
4:G:57:ASN:HB3	4:G:253:HIS:CE1	2.46	0.50
4:V:207:GLN:OE1	4:V:207:GLN:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:41:G:H2'	6:L:42:A:O4'	2.11	0.50
4:Q:120:ALA:O	4:Q:123:CYS:HB2	2.11	0.50
2:C:109:ASP:O	2:C:110:ARG:O	2.30	0.50
4:H:198:ASP:OD1	4:I:27:LYS:NZ	2.36	0.50
4:J:316:TRP:HB3	4:J:340:ILE:HD11	1.94	0.50
1:A:285:LEU:HD11	1:A:312:ARG:HD3	1.93	0.50
4:J:345:LYS:HD3	4:J:347:MET:CE	2.41	0.50
2:B:65:LEU:HD23	2:B:72:ILE:HD12	1.93	0.50
1:A:133:PRO:HG3	5:K:95:TYR:CD1	2.46	0.50
4:F:144:LYS:HD2	4:F:174:GLU:HG2	1.93	0.49
4:V:112:THR:HG23	4:V:238:ASN:HA	1.94	0.49
3:D:23:LEU:O	3:D:26:LEU:HG	2.12	0.49
4:H:20:ARG:HD2	4:H:24:ASN:HA	1.94	0.49
4:U:83:PHE:HB3	4:U:87:ILE:HD11	1.94	0.49
1:M:13:PRO:HB2	1:M:16:GLY:H	1.77	0.49
4:G:176:GLY:O	4:G:178:VAL:HG23	2.12	0.49
4:V:288:LEU:HD12	4:V:325:LEU:HD21	1.94	0.49
2:C:108:ALA:O	2:C:109:ASP:O	2.30	0.49
3:D:2:TYR:HB3	3:D:73:GLN:CA	2.36	0.49
4:J:76:ARG:HD2	4:J:85:GLN:HG2	1.93	0.49
1:M:71:ILE:O	1:M:182:ARG:NH2	2.46	0.49
1:M:15:ASN:OD1	1:M:15:ASN:N	2.41	0.49
4:V:13:HIS:HB3	4:V:272:ALA:HB1	1.93	0.49
4:G:173:THR:HG23	4:G:174:GLU:HG2	1.95	0.49
4:T:69:ALA:O	4:T:72:ARG:HB3	2.12	0.49
4:G:268:ARG:NH1	4:H:179:ASP:OD1	2.45	0.49
2:O:27:ARG:NH2	4:U:22:ASP:OD1	2.36	0.49
4:T:137:LYS:HD3	4:T:137:LYS:N	2.27	0.49
4:T:93:ALA:CB	4:T:100:VAL:HG23	2.36	0.49
4:E:301:LYS:HG3	4:E:301:LYS:O	2.12	0.49
4:G:9:VAL:HB	4:G:226:ARG:HB2	1.94	0.49
4:U:72:ARG:HG3	4:U:76:ARG:NH2	2.27	0.49
4:H:306:GLN:HB2	4:H:307:PRO:HD3	1.94	0.49
4:T:300:ALA:HB2	4:T:304:PHE:CE1	2.47	0.49
2:C:15:GLN:NE2	2:C:69:LYS:O	2.42	0.49
4:Q:155:GLN:HG2	4:Q:239:LEU:HD22	1.95	0.49
4:H:72:ARG:NH1	4:H:102:GLU:HA	2.27	0.49
2:C:109:ASP:O	2:C:110:ARG:C	2.49	0.49
4:F:90:LYS:HE2	4:F:94:LEU:HD11	1.95	0.49
4:U:304:PHE:O	4:U:307:PRO:HD2	2.12	0.49
4:H:9:VAL:HB	4:H:226:ARG:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:74:ASP:C	5:K:74:ASP:OD1	2.49	0.48
4:H:201:THR:HG23	4:H:214:LEU:HG	1.95	0.48
4:J:61:SER:HB3	4:J:158:VAL:HG21	1.94	0.48
4:S:201:THR:HG22	4:S:214:LEU:HG	1.95	0.48
4:J:2:SER:O	4:J:244:ARG:NH2	2.34	0.48
4:H:90:LYS:HE2	4:H:126:VAL:HB	1.96	0.48
1:M:253:CYS:HB2	1:M:255:GLN:H	1.78	0.48
4:I:65:THR:OG1	4:I:66:ILE:N	2.45	0.48
6:X:38:U:H2'	6:X:39:G:H4'	1.96	0.48
4:U:360:ASN:ND2	4:U:360:ASN:O	2.46	0.48
4:I:342:ALA:O	4:I:344:VAL:N	2.47	0.48
4:T:57:ASN:HB3	4:T:253:HIS:CE1	2.49	0.48
4:E:326:ASN:OD1	4:E:326:ASN:N	2.37	0.48
5:K:72:LEU:O	5:K:73:ASP:C	2.51	0.47
1:A:97:GLU:HA	1:A:104:LYS:HZ1	1.79	0.47
5:W:33:ARG:HB3	5:W:198:ASP:HB3	1.95	0.47
4:Q:81:GLU:HG3	4:Q:82:ARG:HG3	1.95	0.47
4:I:137:LYS:CD	4:I:137:LYS:N	2.78	0.47
4:J:87:ILE:HD12	4:J:87:ILE:C	2.34	0.47
4:V:207:GLN:O	4:V:207:GLN:CG	2.61	0.47
4:R:20:ARG:HD2	4:R:24:ASN:HA	1.96	0.47
4:J:149:ALA:HB2	5:K:98:LEU:HD11	1.95	0.47
4:E:155:GLN:HG2	4:E:239:LEU:HD22	1.95	0.47
4:R:360:ASN:ND2	4:R:360:ASN:O	2.47	0.47
3:P:46:THR:HB	3:P:47:PRO:HD2	1.96	0.47
4:T:246:GLN:O	4:T:250:ILE:HG13	2.15	0.47
4:F:65:THR:OG1	4:F:66:ILE:N	2.48	0.47
4:V:176:GLY:O	4:V:178:VAL:HG23	2.14	0.47
5:K:155:HIS:ND1	5:K:156:PRO:O	2.45	0.47
4:E:22:ASP:N	4:E:22:ASP:OD1	2.48	0.47
4:U:69:ALA:HA	4:U:72:ARG:NH1	2.29	0.47
1:A:216:LYS:N	1:A:219:GLU:OE1	2.48	0.47
4:E:232:LEU:O	4:E:236:GLN:HG3	2.15	0.47
4:S:120:ALA:O	4:S:123:CYS:HB2	2.14	0.47
5:K:6:ILE:HG13	5:K:174:TYR:CE1	2.49	0.47
4:Q:57:ASN:HB3	4:Q:253:HIS:CE1	2.50	0.47
2:N:141:GLY:O	2:N:145:ARG:HG3	2.15	0.47
4:U:336:ASP:N	4:U:336:ASP:OD1	2.44	0.47
4:R:232:LEU:O	4:R:236:GLN:HG3	2.15	0.47
4:G:138:LYS:O	4:G:142:VAL:HG23	2.14	0.47
1:M:133:PRO:HG3	5:W:95:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:206:LEU:HD12	4:I:65:THR:HG21	1.96	0.47
3:D:15:ASP:OD1	3:D:16:LEU:N	2.48	0.47
4:F:316:TRP:CD1	4:F:340:ILE:HG21	2.49	0.47
4:U:14:SER:HB3	4:U:266:LYS:HD3	1.97	0.47
4:I:356:TRP:CE2	4:I:361:GLY:HA2	2.50	0.47
4:H:70:GLN:OE1	4:H:70:GLN:N	2.40	0.47
1:A:132:GLN:HA	1:A:133:PRO:HD3	1.82	0.46
2:O:101:ARG:NH2	4:T:22:ASP:OD1	2.37	0.46
1:A:24:LEU:HB3	1:A:80:PHE:HZ	1.80	0.46
6:X:52:G:O3'	6:X:53:C:H6	1.97	0.46
2:B:25:ILE:O	2:B:28:VAL:HG22	2.15	0.46
4:S:54:TYR:CD2	4:S:58:ILE:HD12	2.51	0.46
1:M:488:LYS:O	1:M:491:ARG:N	2.47	0.46
1:A:31:ARG:NH2	1:A:73:ASN:OD1	2.48	0.46
2:O:67:ALA:HB1	2:O:122:THR:HG22	1.98	0.46
2:C:60:ARG:NH1	2:C:137:LEU:O	2.48	0.46
2:N:25:ILE:O	2:N:28:VAL:HG22	2.15	0.46
3:D:90:ALA:HA	3:D:191:CYS:HB3	1.97	0.46
2:N:110:ARG:O	2:N:112:ALA:N	2.44	0.46
4:U:115:VAL:HB	4:U:118:GLU:HB2	1.97	0.46
3:D:2:TYR:HB3	3:D:73:GLN:HB2	1.97	0.46
4:F:278:MET:HG2	4:F:279:VAL:N	2.30	0.46
4:J:249:GLU:O	4:J:252:THR:HB	2.15	0.46
2:N:97:ILE:HD12	2:N:120:LEU:HD22	1.96	0.46
4:J:341:THR:CG2	4:J:343:GLN:H	2.28	0.46
4:U:276:ALA:HB3	4:U:332:PHE:HE2	1.80	0.46
4:G:65:THR:OG1	4:G:66:ILE:N	2.49	0.46
5:K:11:GLY:HA2	5:K:154:THR:HG23	1.97	0.46
4:S:85:GLN:HE21	4:S:85:GLN:HB3	1.46	0.46
2:O:35:ARG:NH1	2:O:59:LEU:HD11	2.30	0.46
1:M:42:ASP:OD1	1:M:42:ASP:N	2.49	0.46
5:K:34:SER:HB3	5:K:198:ASP:O	2.15	0.46
3:D:96:ILE:HG22	3:D:97:LEU:N	2.30	0.46
4:S:137:LYS:HE2	4:S:137:LYS:HB3	1.63	0.46
4:R:82:ARG:HB3	4:R:83:PHE:CD2	2.51	0.46
2:B:118:ARG:O	2:B:122:THR:HG23	2.16	0.46
4:J:76:ARG:HG2	4:J:88:ILE:HG21	1.98	0.46
3:P:110:LYS:HD3	6:X:47:C:OP2	2.15	0.46
4:S:93:ALA:HB2	4:S:100:VAL:HG23	1.97	0.46
2:C:37:ILE:HA	2:C:38:PRO:HD3	1.77	0.46
1:M:321:ASN:OD1	1:M:322:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:PHE:CE2	1:M:101:MET:HG3	2.51	0.46
5:K:16:TRP:CG	5:K:31:PRO:HA	2.50	0.46
1:M:154:GLN:HA	1:M:171:PRO:HD2	1.98	0.46
1:A:68:ARG:NH1	1:A:337:ILE:O	2.42	0.46
3:P:91:ASN:HA	3:P:92:PRO:HD2	1.79	0.46
4:S:328:ALA:HB1	4:S:356:TRP:CZ2	2.50	0.46
2:B:110:ARG:O	2:B:111:THR:HB	2.15	0.46
4:J:288:LEU:HD12	4:J:325:LEU:HD21	1.97	0.46
3:D:199:LEU:O	3:D:199:LEU:HD23	2.16	0.45
4:R:13:HIS:HA	4:R:274:ASN:OD1	2.16	0.45
1:A:13:PRO:HB2	1:A:16:GLY:H	1.81	0.45
4:E:69:ALA:O	4:E:72:ARG:HB3	2.16	0.45
4:E:78:LYS:O	4:E:78:LYS:HD2	2.16	0.45
4:S:138:LYS:O	4:S:142:VAL:HG23	2.17	0.45
4:U:135:ASP:OD1	4:U:135:ASP:N	2.49	0.45
4:F:334:LEU:O	4:G:318:ARG:HD3	2.17	0.45
1:A:102:GLN:OE1	1:A:241:LEU:N	2.31	0.45
1:A:455:HIS:CE1	1:A:490:LEU:HD13	2.52	0.45
4:S:349:THR:OG1	4:S:352:GLN:HG3	2.16	0.45
4:R:16:SER:HB3	4:R:272:ALA:HB2	1.98	0.45
4:V:172:MET:HE1	5:W:96:ARG:HD2	1.99	0.45
4:V:42:GLN:HG3	4:V:42:GLN:H	1.05	0.45
2:C:59:LEU:HD23	2:C:59:LEU:HA	1.81	0.45
4:H:120:ALA:O	4:H:123:CYS:HB2	2.16	0.45
3:D:2:TYR:HB3	3:D:73:GLN:CB	2.47	0.45
4:J:230:ILE:HD11	4:J:254:VAL:HG11	1.99	0.45
4:U:37:VAL:HG23	4:U:193:VAL:HG21	1.97	0.45
4:Q:243:SER:OG	4:Q:246:GLN:HG3	2.15	0.45
4:H:166:MET:HG3	4:H:166:MET:O	2.16	0.45
4:V:146:ASP:N	4:V:146:ASP:OD1	2.46	0.45
4:E:39:ILE:HB	4:E:187:ALA:HB3	1.99	0.45
4:S:284:SER:OG	4:S:285:ASP:N	2.50	0.45
3:D:178:LEU:HA	3:D:178:LEU:HD23	1.84	0.45
4:T:70:GLN:N	4:T:70:GLN:OE1	2.48	0.45
4:F:338:ASP:HA	4:F:339:PRO:HD3	1.56	0.45
5:W:87:THR:HB	6:X:9:G:H5"	1.98	0.45
4:U:40:SER:HA	4:U:186:HIS:ND1	2.32	0.45
4:V:6:ASN:HD21	4:V:284:SER:HB3	1.82	0.45
2:C:113:ASP:N	2:C:113:ASP:OD1	2.47	0.45
3:D:140:HIS:CD2	3:D:140:HIS:O	2.68	0.45
4:R:69:ALA:O	4:R:72:ARG:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:90:LYS:HE3	4:H:130:GLU:OE2	2.16	0.45
4:Q:26:GLN:N	4:Q:218:GLU:OE1	2.47	0.45
4:U:39:ILE:HB	4:U:187:ALA:HB3	1.98	0.45
4:U:115:VAL:HG12	4:U:118:GLU:H	1.81	0.45
2:O:14:TRP:HZ3	2:O:25:ILE:HD12	1.81	0.45
4:R:115:VAL:HG12	4:R:118:GLU:H	1.81	0.45
4:V:337:VAL:HG12	4:V:338:ASP:H	1.82	0.45
4:U:14:SER:O	4:U:18:LEU:HD11	2.17	0.45
1:M:288:VAL:HB	1:M:293:VAL:HG12	1.99	0.45
4:U:173:THR:HA	4:U:177:LYS:NZ	2.33	0.44
1:M:314:VAL:O	1:M:335:ARG:NH2	2.49	0.44
4:G:243:SER:OG	4:G:246:GLN:HG3	2.17	0.44
4:J:42:GLN:HG2	5:K:86:HIS:NE2	2.32	0.44
1:A:24:LEU:HB3	1:A:80:PHE:CZ	2.53	0.44
4:U:29:ALA:HB2	4:U:38:ARG:HD3	1.99	0.44
4:V:239:LEU:HD23	4:V:239:LEU:HA	1.78	0.44
4:E:300:ALA:HB2	4:E:304:PHE:CE1	2.52	0.44
4:H:356:TRP:CE2	4:H:361:GLY:HA2	2.53	0.44
4:T:245:GLU:N	4:T:245:GLU:OE1	2.49	0.44
4:U:82:ARG:O	4:U:83:PHE:CE2	2.68	0.44
4:U:218:GLU:CG	4:U:303:GLY:HA2	2.47	0.44
4:F:268:ARG:NH1	4:G:179:ASP:OD1	2.51	0.44
1:M:248:GLY:HA3	1:M:260:ARG:CZ	2.47	0.44
1:A:198:GLN:O	1:A:198:GLN:HG3	2.17	0.44
3:D:144:GLU:OE1	3:D:160:THR:OG1	2.33	0.44
4:R:300:ALA:HB2	4:R:304:PHE:CE1	2.52	0.44
4:F:360:ASN:ND2	4:F:360:ASN:O	2.50	0.44
4:Q:70:GLN:OE1	4:Q:70:GLN:N	2.45	0.44
4:S:70:GLN:N	4:S:70:GLN:OE1	2.46	0.44
1:M:238:HIS:O	1:M:266:LYS:HA	2.17	0.44
4:T:304:PHE:C	4:T:307:PRO:HD2	2.37	0.44
3:D:96:ILE:HG22	3:D:97:LEU:H	1.83	0.44
4:V:278:MET:HG2	4:V:279:VAL:N	2.28	0.44
4:U:143:LEU:HD23	4:U:143:LEU:HA	1.85	0.44
1:M:7:ASN:OD1	1:M:7:ASN:N	2.51	0.44
4:F:290:MET:SD	4:F:316:TRP:HE3	2.41	0.44
1:A:244:PRO:HG3	1:A:261:TYR:CE2	2.53	0.44
2:C:87:LEU:HD21	2:C:117:LEU:HD11	2.00	0.44
4:J:246:GLN:O	4:J:249:GLU:HB3	2.18	0.44
5:W:42:ALA:O	5:W:142:TYR:HB2	2.18	0.44
3:P:86:PHE:HB2	3:P:194:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:5:ILE:HD11	2:O:54:HIS:HB3	2.00	0.44
3:D:17:TYR:O	3:D:20:HIS:HB3	2.17	0.44
1:A:332:ASN:OD1	1:A:335:ARG:HD2	2.17	0.44
4:T:75:LEU:HD12	4:T:92:LEU:HD22	1.99	0.44
1:M:353:ASN:HB2	1:M:358:LEU:HD11	1.99	0.44
4:S:57:ASN:HB3	4:S:253:HIS:CE1	2.53	0.44
2:N:113:ASP:OD1	2:N:113:ASP:N	2.51	0.44
4:G:70:GLN:N	4:G:70:GLN:OE1	2.47	0.44
1:A:24:LEU:HD22	1:A:28:TYR:HD2	1.83	0.44
1:A:4:LEU:HD23	1:A:84:ILE:HB	1.99	0.44
3:D:171:ASP:OD1	3:D:173:PRO:HD2	2.17	0.44
4:J:27:LYS:NZ	6:L:9:G:OP1	2.44	0.43
3:P:26:LEU:HD21	3:P:66:ALA:HB3	1.99	0.43
1:A:176:VAL:N	1:A:188:ASN:OD1	2.49	0.43
4:R:317:ASP:OD1	4:R:341:THR:HG22	2.17	0.43
1:M:177:ARG:NH1	1:M:344:GLU:OE2	2.51	0.43
4:Q:301:LYS:HG3	4:Q:301:LYS:O	2.18	0.43
1:A:250:CYS:HB3	1:A:253:CYS:HB2	1.75	0.43
1:M:9:ILE:HA	1:M:10:PRO:HD3	1.86	0.43
4:J:201:THR:HG22	4:J:214:LEU:HG	1.99	0.43
3:D:62:SER:OG	3:D:67:THR:HA	2.18	0.43
4:V:82:ARG:HB2	4:V:83:PHE:CD2	2.52	0.43
4:U:57:ASN:HB3	4:U:253:HIS:CE1	2.53	0.43
4:I:66:ILE:HB	4:I:111:VAL:HG22	2.00	0.43
4:U:89:ASP:O	4:U:93:ALA:HB2	2.19	0.43
4:E:134:LEU:HD12	4:E:135:ASP:H	1.84	0.43
4:R:70:GLN:N	4:R:70:GLN:OE1	2.43	0.43
4:G:360:ASN:ND2	4:G:360:ASN:O	2.51	0.43
4:F:23:MET:O	4:F:25:MET:HG2	2.17	0.43
4:V:306:GLN:HB2	4:V:307:PRO:HD3	2.01	0.43
4:F:5:ILE:CG2	4:F:230:ILE:HB	2.49	0.43
1:A:238:HIS:O	1:A:266:LYS:HA	2.19	0.43
1:M:13:PRO:HB2	1:M:16:GLY:HA3	2.00	0.43
4:Q:256:HIS:HB2	4:Q:354:LYS:HD3	2.00	0.43
4:I:310:GLN:O	4:I:314:GLN:HG3	2.19	0.43
4:V:13:HIS:N	4:V:13:HIS:ND1	2.67	0.43
4:H:232:LEU:O	4:H:236:GLN:HG3	2.19	0.43
4:V:44:LEU:HD21	4:V:226:ARG:HD3	2.01	0.43
5:W:97:GLY:O	5:W:98:LEU:HD23	2.19	0.43
1:M:309:GLN:OE1	1:M:312:ARG:HD2	2.18	0.43
2:N:101:ARG:HG3	4:Q:199:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:13:HIS:CD2	4:Q:18:LEU:CD1	3.00	0.43
5:K:137:VAL:HG13	5:K:157:LEU:HB3	2.01	0.43
4:V:316:TRP:CG	4:V:340:ILE:HD11	2.54	0.43
3:D:148:TYR:CE2	3:D:157:LYS:HD2	2.54	0.43
4:U:83:PHE:HB3	4:U:87:ILE:CD1	2.49	0.43
1:M:132:GLN:HA	1:M:133:PRO:HD3	1.83	0.43
3:D:1:MET:SD	3:D:55:GLN:NE2	2.88	0.43
3:D:92:PRO:HB2	3:D:116:LEU:HD12	2.00	0.43
4:F:221:SER:OG	4:G:30:ILE:O	2.36	0.43
4:Q:221:SER:OG	4:R:30:ILE:O	2.37	0.43
2:N:102:ILE:O	2:N:106:ILE:HG23	2.18	0.43
5:W:172:LEU:O	5:W:172:LEU:HD23	2.19	0.43
3:P:103:LEU:HA	3:P:109:ILE:HA	2.01	0.42
1:A:158:PHE:HB2	1:A:162:PHE:CD1	2.53	0.42
1:M:35:ARG:NH2	1:M:179:ILE:O	2.52	0.42
4:Q:310:GLN:O	4:Q:314:GLN:HG3	2.19	0.42
4:V:347:MET:HG3	4:V:353:LEU:HA	2.02	0.42
4:R:22:ASP:HA	6:X:21:G:N7	2.35	0.42
4:U:298:VAL:CG1	4:U:307:PRO:HB2	2.48	0.42
4:S:101:ASP:HB2	4:S:103:ALA:H	1.83	0.42
4:S:83:PHE:HE1	4:S:124:GLU:HB3	1.83	0.42
4:I:301:LYS:HE2	4:I:307:PRO:HG3	2.00	0.42
3:D:99:ASN:N	6:L:44:U:O4	2.29	0.42
4:F:101:ASP:HB2	4:F:103:ALA:H	1.83	0.42
4:S:69:ALA:O	4:S:72:ARG:HB3	2.19	0.42
4:T:152:VAL:O	4:T:155:GLN:HG3	2.18	0.42
2:B:65:LEU:C	2:B:67:ALA:H	2.21	0.42
4:I:140:LEU:HD13	4:I:171:MET:HE3	2.01	0.42
4:U:146:ASP:OD1	4:U:146:ASP:O	2.38	0.42
6:X:9:G:HO2'	6:X:10:G:H8	1.65	0.42
1:A:177:ARG:HH11	1:A:364:VAL:HG11	1.84	0.42
4:R:9:VAL:HB	4:R:226:ARG:HB2	2.02	0.42
1:A:47:ALA:HB2	1:A:146:ILE:HD13	2.02	0.42
4:J:348:PRO:HD2	4:J:352:GLN:OE1	2.20	0.42
1:A:317:LYS:O	1:A:324:GLY:HA3	2.20	0.42
4:E:170:GLY:O	4:E:173:THR:HG22	2.19	0.42
4:U:300:ALA:HB2	4:U:304:PHE:CE1	2.53	0.42
4:U:342:ALA:O	4:U:344:VAL:N	2.53	0.42
4:Q:9:VAL:HG22	4:Q:279:VAL:HG22	2.01	0.42
4:E:138:LYS:O	4:E:142:VAL:HG23	2.18	0.42
4:U:38:ARG:HA	4:U:187:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:314:GLN:O	4:I:318:ARG:HG3	2.20	0.42
4:U:77:GLN:HG3	4:U:78:LYS:HD2	2.01	0.42
4:V:185:ALA:HB2	5:W:152:PRO:HG3	2.00	0.42
4:F:147:ILE:HD13	4:F:147:ILE:HA	1.78	0.42
4:Q:360:ASN:O	4:Q:360:ASN:ND2	2.53	0.42
4:E:86:LYS:HE2	4:E:86:LYS:HB2	1.87	0.42
4:U:20:ARG:HH11	4:U:20:ARG:HG3	1.85	0.42
3:D:26:LEU:HD23	3:D:66:ALA:HB1	2.02	0.42
4:R:341:THR:O	4:R:343:GLN:N	2.52	0.42
5:K:42:ALA:O	5:K:142:TYR:HB2	2.19	0.42
6:L:58:G:C2	6:L:59:G:C8	3.07	0.42
1:M:468:PRO:HG2	1:M:469:TYR:CE2	2.55	0.42
1:M:210:THR:HG23	1:M:215:ILE:HG13	2.01	0.42
4:S:301:LYS:O	4:S:301:LYS:HG3	2.19	0.42
4:T:277:ASP:CG	4:T:305:LEU:HD21	2.40	0.42
4:I:10:LEU:HD23	4:I:10:LEU:HA	1.91	0.42
2:B:65:LEU:O	2:B:67:ALA:N	2.53	0.42
1:M:99:PRO:HB2	1:M:102:GLN:HB2	2.02	0.42
1:A:216:LYS:O	1:A:219:GLU:HB2	2.20	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.84	0.42
6:X:40:A:H2'	6:X:41:G:O4'	2.20	0.42
4:S:278:MET:HG3	4:S:279:VAL:N	2.34	0.42
4:S:40:SER:HB2	4:S:42:GLN:NE2	2.35	0.42
4:R:306:GLN:HB2	4:R:307:PRO:HD3	2.02	0.42
4:J:41:SER:OG	4:J:184:ILE:O	2.26	0.42
5:K:202:ILE:HD12	5:K:202:ILE:H	1.85	0.42
4:I:280:MET:HE3	4:I:329:ALA:HB1	2.01	0.42
4:E:30:ILE:HD12	4:J:194:ASP:CB	2.50	0.42
4:H:69:ALA:O	4:H:72:ARG:HB3	2.19	0.42
4:J:56:GLN:HG2	4:J:57:ASN:ND2	2.35	0.42
4:R:39:ILE:HB	4:R:187:ALA:HB3	2.02	0.42
4:Q:65:THR:OG1	4:Q:66:ILE:N	2.53	0.42
4:R:68:LEU:HB2	4:R:106:ILE:HG13	2.02	0.42
5:W:12:PRO:HD3	5:W:154:THR:HG23	2.01	0.42
2:N:51:ASN:HA	2:N:52:PRO:HD3	1.93	0.42
2:B:113:ASP:N	2:B:113:ASP:OD1	2.53	0.42
4:R:155:GLN:HG2	4:R:239:LEU:HD22	2.02	0.42
4:T:93:ALA:HB2	4:T:100:VAL:CG2	2.40	0.41
4:G:144:LYS:HB3	4:G:144:LYS:HE2	1.77	0.41
4:Q:5:ILE:HD13	4:Q:5:ILE:HG21	1.83	0.41
4:E:151:ARG:NH2	4:E:175:LEU:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:239:ILE:HG23	1:M:264:PHE:CD2	2.55	0.41
3:D:118:LYS:HE2	3:D:118:LYS:HB3	1.84	0.41
4:G:268:ARG:HG3	4:G:268:ARG:HH11	1.85	0.41
4:F:20:ARG:HD2	4:F:24:ASN:HA	2.02	0.41
6:X:30:G:C6	6:X:31:A:N6	2.88	0.41
4:V:232:LEU:O	4:V:236:GLN:HG3	2.21	0.41
5:W:25:ARG:HA	5:W:26:PRO:HD3	1.77	0.41
4:Q:13:HIS:N	4:Q:13:HIS:ND1	2.68	0.41
4:H:167:ALA:H	4:H:177:LYS:CE	2.28	0.41
4:F:214:LEU:HD22	4:G:22:ASP:HB3	2.01	0.41
4:F:115:VAL:HG12	4:F:118:GLU:H	1.84	0.41
4:T:65:THR:OG1	4:T:66:ILE:N	2.52	0.41
1:A:64:ASP:O	1:A:67:PHE:HB3	2.20	0.41
4:E:214:LEU:CD1	4:F:22:ASP:HB3	2.50	0.41
1:M:170:THR:N	1:M:171:PRO:HD3	2.36	0.41
4:I:18:LEU:HD13	4:I:39:ILE:HD11	2.01	0.41
4:I:37:VAL:CG2	4:I:193:VAL:HG21	2.47	0.41
5:W:184:GLU:HG2	5:W:211:ARG:NH2	2.36	0.41
1:M:335:ARG:HG3	1:M:372:GLN:HB3	2.01	0.41
1:A:231:GLY:HA3	1:A:277:TRP:CZ2	2.56	0.41
4:G:280:MET:HE2	4:G:282:ASN:HB2	2.02	0.41
2:O:37:ILE:O	2:O:40:PHE:HB3	2.21	0.41
4:T:54:TYR:CD2	4:T:58:ILE:HD12	2.55	0.41
4:G:245:GLU:OE1	4:G:245:GLU:N	2.52	0.41
2:N:35:ARG:NH1	2:O:143:ARG:HD2	2.35	0.41
1:A:24:LEU:HD22	1:A:28:TYR:CD2	2.56	0.41
4:I:301:LYS:HG3	4:I:307:PRO:HG3	2.03	0.41
2:O:131:PRO:O	2:O:134:ALA:HB3	2.21	0.41
1:A:343:LEU:HB2	1:A:371:TRP:NE1	2.36	0.41
3:P:184:GLY:O	3:P:187:LYS:NZ	2.51	0.41
2:B:44:VAL:HG23	2:B:49:TRP:HB2	2.03	0.41
2:C:111:THR:CG2	2:C:112:ALA:N	2.73	0.41
4:V:6:ASN:ND2	4:V:284:SER:HB3	2.36	0.41
4:Q:41:SER:HB2	4:Q:184:ILE:HG23	2.02	0.41
4:R:49:ARG:NH2	6:X:20:G:OP2	2.44	0.41
4:I:87:ILE:HD13	4:I:87:ILE:HA	1.96	0.41
4:J:239:LEU:HD23	4:J:239:LEU:HA	1.74	0.41
4:E:87:ILE:HA	4:E:87:ILE:HD13	1.91	0.41
4:F:86:LYS:HD2	4:F:86:LYS:HA	1.92	0.41
4:V:345:LYS:HB3	4:V:345:LYS:HE3	1.68	0.41
2:O:113:ASP:C	2:O:113:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:319:ILE:HG22	1:M:321:ASN:OD1	2.21	0.41
1:M:9:ILE:HG21	1:M:9:ILE:HD13	1.80	0.41
5:K:73:ASP:O	5:K:74:ASP:CG	2.58	0.41
4:H:304:PHE:C	4:H:307:PRO:HD2	2.42	0.41
1:A:343:LEU:HB2	1:A:371:TRP:CE2	2.56	0.41
4:R:49:ARG:HG2	4:R:61:SER:HB2	2.03	0.41
4:S:16:SER:HB3	4:S:272:ALA:HB2	2.01	0.41
4:I:347:MET:HA	4:I:348:PRO:HD3	1.81	0.41
4:E:57:ASN:HB3	4:E:253:HIS:CE1	2.56	0.41
4:Q:22:ASP:N	4:Q:22:ASP:OD1	2.48	0.41
4:E:5:ILE:HG21	4:E:5:ILE:HD13	1.85	0.41
5:W:159:LEU:HD12	5:W:159:LEU:HA	1.83	0.41
2:O:19:ASN:ND2	4:T:211:SER:HB3	2.36	0.41
4:Q:190:THR:HG22	4:Q:294:PHE:CD2	2.55	0.41
4:F:41:SER:HB2	4:F:184:ILE:HG23	2.03	0.41
3:P:95:THR:O	6:X:56:G:H5"	2.21	0.41
4:R:112:THR:HA	4:R:113:PRO:HD3	1.85	0.41
1:A:42:ASP:OD1	1:A:43:MET:N	2.54	0.41
4:H:286:MET:HG3	4:H:287:PRO:HD2	2.02	0.41
4:H:177:LYS:HD2	4:H:177:LYS:HA	1.78	0.41
1:M:488:LYS:O	1:M:490:LEU:N	2.54	0.41
4:F:72:ARG:NH1	4:F:101:ASP:O	2.52	0.41
1:A:317:LYS:O	1:A:318:ILE:HD13	2.21	0.41
4:V:183:SER:HB3	5:W:149:ARG:HG2	2.02	0.41
2:O:97:ILE:HD12	2:O:120:LEU:HD22	2.03	0.41
1:M:459:GLU:OE2	1:M:487:TYR:OH	2.35	0.41
4:T:20:ARG:HD2	4:T:24:ASN:HA	2.02	0.41
4:U:5:ILE:HG23	4:U:230:ILE:HB	2.03	0.41
4:E:94:LEU:HD13	4:E:171:MET:HE1	2.03	0.41
3:P:172:ALA:HB3	3:P:173:PRO:HD3	2.03	0.41
4:R:301:LYS:O	4:R:301:LYS:HG3	2.21	0.41
2:C:101:ARG:HB3	2:C:120:LEU:HD21	2.02	0.41
3:P:96:ILE:HG22	3:P:97:LEU:N	2.29	0.40
3:P:26:LEU:HD23	3:P:63:THR:HG23	2.04	0.40
1:M:243:ASP:HA	1:M:244:PRO:HD3	1.76	0.40
4:R:176:GLY:O	4:R:178:VAL:HG23	2.21	0.40
1:A:185:VAL:O	1:A:189:VAL:HG23	2.21	0.40
1:M:192:LEU:O	1:M:196:GLN:HG2	2.21	0.40
3:P:148:TYR:CD2	3:P:157:LYS:HB2	2.56	0.40
2:N:126:PRO:HB2	2:N:128:LEU:HD23	2.03	0.40
5:W:108:ARG:NH2	6:X:7:C:O2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:16:SER:HB3	4:F:272:ALA:HB2	2.03	0.40
4:R:19:ASN:ND2	4:R:40:SER:H	2.19	0.40
4:J:16:SER:HB3	4:J:272:ALA:HB2	2.04	0.40
2:O:100:ARG:HD3	4:S:216:THR:HG21	2.02	0.40
4:S:201:THR:CG2	4:S:214:LEU:HG	2.51	0.40
4:S:149:ALA:O	4:S:152:VAL:HG12	2.22	0.40
4:R:258:LEU:HA	4:R:258:LEU:HD12	1.89	0.40
2:C:142:LYS:HA	2:C:142:LYS:HD2	1.67	0.40
4:S:22:ASP:OD1	4:S:22:ASP:N	2.55	0.40
1:M:485:THR:O	1:M:488:LYS:HB3	2.22	0.40
4:V:172:MET:CE	5:W:96:ARG:HD2	2.52	0.40
1:A:198:GLN:NE2	1:A:280:PRO:HB3	2.36	0.40
1:A:77:GLU:O	1:A:81:GLN:HG2	2.22	0.40
4:T:328:ALA:HB1	4:T:356:TRP:CZ2	2.56	0.40
1:M:403:PHE:HZ	1:M:481:LEU:HB3	1.86	0.40
4:V:252:THR:HG22	4:V:357:VAL:HB	2.03	0.40
4:T:221:SER:OG	4:U:30:ILE:O	2.38	0.40
1:M:197:LYS:HB2	1:M:197:LYS:HE3	1.89	0.40
4:Q:334:LEU:HD23	4:Q:334:LEU:HA	1.86	0.40
3:P:74:VAL:HG21	4:U:203:VAL:HG11	2.04	0.40
4:Q:13:HIS:HB3	4:Q:272:ALA:HB1	2.03	0.40
5:K:74:ASP:C	5:K:75:ARG:HG2	2.42	0.40
4:Q:38:ARG:HA	4:Q:187:ALA:O	2.22	0.40
4:J:6:ASN:HD21	4:J:284:SER:HB3	1.85	0.40
4:I:232:LEU:O	4:I:236:GLN:HG3	2.20	0.40
4:F:57:ASN:HB3	4:F:253:HIS:CE1	2.57	0.40
4:E:137:LYS:HE3	4:E:137:LYS:HB3	1.83	0.40
5:K:99:LYS:HG2	5:K:99:LYS:H	1.71	0.40
4:Q:151:ARG:HA	4:Q:151:ARG:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/502 (94%)	432 (92%)	36 (8%)	2 (0%)	39	80
1	M	485/502 (97%)	457 (94%)	24 (5%)	4 (1%)	24	66
2	B	155/160 (97%)	149 (96%)	6 (4%)	0	100	100
2	C	155/160 (97%)	147 (95%)	8 (5%)	0	100	100
2	N	148/160 (92%)	140 (95%)	7 (5%)	1 (1%)	26	70
2	O	154/160 (96%)	147 (96%)	7 (4%)	0	100	100
3	D	185/201 (92%)	178 (96%)	7 (4%)	0	100	100
3	P	185/201 (92%)	176 (95%)	9 (5%)	0	100	100
4	E	353/363 (97%)	333 (94%)	20 (6%)	0	100	100
4	F	355/363 (98%)	335 (94%)	20 (6%)	0	100	100
4	G	352/363 (97%)	335 (95%)	17 (5%)	0	100	100
4	H	361/363 (99%)	348 (96%)	12 (3%)	1 (0%)	46	84
4	I	351/363 (97%)	335 (95%)	16 (5%)	0	100	100
4	J	345/363 (95%)	324 (94%)	21 (6%)	0	100	100
4	Q	358/363 (99%)	347 (97%)	10 (3%)	1 (0%)	46	84
4	R	355/363 (98%)	335 (94%)	20 (6%)	0	100	100
4	S	357/363 (98%)	343 (96%)	13 (4%)	1 (0%)	46	84
4	T	356/363 (98%)	343 (96%)	13 (4%)	0	100	100
4	U	350/363 (96%)	325 (93%)	23 (7%)	2 (1%)	30	72
4	V	351/363 (97%)	331 (94%)	20 (6%)	0	100	100
5	K	216/224 (96%)	211 (98%)	5 (2%)	0	100	100
5	W	216/224 (96%)	210 (97%)	5 (2%)	1 (0%)	34	76
All	All	6613/6850 (96%)	6281 (95%)	319 (5%)	13 (0%)	52	88

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	U	336	ASP
5	W	45	GLY
1	M	160	GLY
1	M	321	ASN
1	M	488	LYS
4	Q	210	GLY
4	U	15	PRO
4	H	101	ASP

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Mol	Chain	Res	Type
1	M	140	CYS
4	S	101	ASP
2	N	26	ARG
1	A	160	GLY
1	A	370	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	401/426 (94%)	391 (98%)	10 (2%)	55 86
1	M	409/426 (96%)	405 (99%)	4 (1%)	82 95
2	B	136/138 (99%)	136 (100%)	0	100 100
2	C	136/138 (99%)	135 (99%)	1 (1%)	88 96
2	N	130/138 (94%)	128 (98%)	2 (2%)	72 92
2	O	128/138 (93%)	125 (98%)	3 (2%)	58 87
3	D	151/171 (88%)	144 (95%)	7 (5%)	33 73
3	P	152/171 (89%)	146 (96%)	6 (4%)	39 77
4	E	289/298 (97%)	284 (98%)	5 (2%)	68 91
4	F	290/298 (97%)	286 (99%)	4 (1%)	74 93
4	G	291/298 (98%)	291 (100%)	0	100 100
4	H	288/298 (97%)	286 (99%)	2 (1%)	88 96
4	I	287/298 (96%)	285 (99%)	2 (1%)	88 96
4	J	279/298 (94%)	274 (98%)	5 (2%)	66 91
4	Q	294/298 (99%)	289 (98%)	5 (2%)	68 91
4	R	282/298 (95%)	279 (99%)	3 (1%)	80 94
4	S	290/298 (97%)	285 (98%)	5 (2%)	68 91
4	T	293/298 (98%)	290 (99%)	3 (1%)	82 95
4	U	287/298 (96%)	276 (96%)	11 (4%)	40 78
4	V	286/298 (96%)	276 (96%)	10 (4%)	43 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	K	185/192 (96%)	179 (97%)	6 (3%)	46 82
5	W	186/192 (97%)	180 (97%)	6 (3%)	46 82
All	All	5470/5706 (96%)	5370 (98%)	100 (2%)	66 91

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	78	ASP
1	A	79	GLU
1	A	82	GLN
1	A	104	LYS
1	A	197	LYS
1	A	198	GLN
1	A	424	TYR
1	A	441	SER
1	A	474	LYS
2	C	111	THR
3	D	2	TYR
3	D	6	VAL
3	D	45	ASN
3	D	73	GLN
3	D	108	ASN
3	D	119	GLU
3	D	140	HIS
4	E	19	ASN
4	E	112	THR
4	E	245	GLU
4	E	326	ASN
4	E	362	GLU
4	F	19	ASN
4	F	84	ASP
4	F	152	VAL
4	F	282	ASN
4	H	183	SER
4	H	282	ASN
4	I	269	THR
4	I	282	ASN
4	J	77	GLN
4	J	87	ILE
4	J	254	VAL

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Mol	Chain	Res	Type
4	J	282	ASN
4	J	341	THR
5	K	24	THR
5	K	51	THR
5	K	75	ARG
5	K	103	THR
5	K	123	THR
5	K	125	HIS
1	M	19	VAL
1	M	140	CYS
1	M	253	CYS
1	M	322	GLU
2	N	5	ILE
2	N	15	GLN
2	O	42	ARG
2	O	111	THR
2	O	143	ARG
3	P	4	SER
3	P	55	GLN
3	P	96	ILE
3	P	132	ASN
3	P	140	HIS
3	P	177	ASP
4	Q	13	HIS
4	Q	19	ASN
4	Q	62	SER
4	Q	101	ASP
4	Q	220	SER
4	R	42	GLN
4	R	134	LEU
4	R	314	GLN
4	S	19	ASN
4	S	81	GLU
4	S	84	ASP
4	S	221	SER
4	S	269	THR
4	T	19	ASN
4	T	317	ASP
4	T	321	ASN
4	U	19	ASN
4	U	76	ARG
4	U	83	PHE

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Mol	Chain	Res	Type
4	U	86	LYS
4	U	87	ILE
4	U	94	LEU
4	U	102	GLU
4	U	105	LYS
4	U	169	SER
4	U	335	SER
4	U	336	ASP
4	V	13	HIS
4	V	41	SER
4	V	42	GLN
4	V	65	THR
4	V	146	ASP
4	V	158	VAL
4	V	179	ASP
4	V	211	SER
4	V	269	THR
4	V	282	ASN
5	W	20	THR
5	W	24	THR
5	W	87	THR
5	W	102	GLU
5	W	123	THR
5	W	143	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	ASN
3	D	20	HIS
3	D	73	GLN
3	D	140	HIS
4	E	236	GLN
4	F	282	ASN
4	G	246	GLN
4	G	306	GLN
4	J	13	HIS
2	N	15	GLN
3	P	45	ASN
3	P	132	ASN
3	P	140	HIS

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Mol	Chain	Res	Type
4	Q	13	HIS
4	Q	352	GLN
4	R	19	ASN
4	R	314	GLN
4	S	85	GLN
4	U	24	ASN
4	V	207	GLN
5	W	163	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	L	60/61 (98%)	19 (31%)	2 (3%)
6	X	60/61 (98%)	19 (31%)	2 (3%)
All	All	120/122 (98%)	38 (31%)	4 (3%)

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	L	2	U
6	L	4	A
6	L	9	G
6	L	10	G
6	L	15	C
6	L	21	G
6	L	22	U
6	L	27	A
6	L	28	U
6	L	33	A
6	L	34	A
6	L	38	U
6	L	39	G
6	L	40	A
6	L	43	G
6	L	45	U
6	L	54	C
6	L	55	A
6	L	56	G
6	X	4	A
6	X	9	G
6	X	10	G

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Mol	Chain	Res	Type
6	X	15	C
6	X	21	G
6	X	22	U
6	X	27	A
6	X	28	U
6	X	33	A
6	X	34	A
6	X	38	U
6	X	39	G
6	X	40	A
6	X	43	G
6	X	44	U
6	X	45	U
6	X	53	C
6	X	54	C
6	X	56	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L	27	A
6	L	45	U
6	X	15	C
6	X	45	U

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	480/502 (95%)	-0.31	2 (0%) 93 80	37, 80, 111, 135	0
1	M	489/502 (97%)	-0.50	0 100 100	26, 42, 68, 122	0
2	B	157/160 (98%)	-0.22	3 (1%) 70 41	30, 44, 84, 120	0
2	C	157/160 (98%)	-0.20	1 (0%) 90 73	32, 52, 85, 115	0
2	N	152/160 (95%)	-0.04	2 (1%) 79 53	40, 56, 85, 114	0
2	O	156/160 (97%)	0.30	4 (2%) 59 29	53, 84, 124, 146	0
3	D	191/201 (95%)	-0.20	2 (1%) 84 60	41, 70, 112, 122	0
3	P	191/201 (95%)	0.19	10 (5%) 31 12	52, 78, 111, 127	0
4	E	357/363 (98%)	-0.34	1 (0%) 94 84	30, 48, 78, 104	0
4	F	359/363 (98%)	-0.27	6 (1%) 73 45	28, 48, 86, 121	0
4	G	356/363 (98%)	-0.43	1 (0%) 94 84	24, 44, 76, 101	0
4	H	363/363 (100%)	-0.30	2 (0%) 90 73	25, 47, 93, 116	0
4	I	355/363 (97%)	-0.48	0 100 100	26, 47, 79, 104	0
4	J	351/363 (96%)	-0.29	2 (0%) 90 73	35, 62, 110, 129	0
4	Q	362/363 (99%)	-0.38	4 (1%) 82 58	23, 39, 72, 114	0
4	R	359/363 (98%)	-0.14	7 (1%) 70 41	27, 50, 119, 155	0
4	S	361/363 (99%)	-0.16	3 (0%) 87 67	30, 52, 99, 118	0
4	T	360/363 (99%)	-0.34	0 100 100	32, 50, 75, 121	0
4	U	354/363 (97%)	-0.17	2 (0%) 90 73	41, 68, 129, 146	0
4	V	355/363 (97%)	-0.42	1 (0%) 94 84	21, 38, 85, 120	0
5	K	218/224 (97%)	-0.49	0 100 100	44, 67, 90, 106	0
5	W	218/224 (97%)	-0.57	0 100 100	22, 35, 53, 81	0
6	L	61/61 (100%)	-0.23	0 100 100	31, 47, 101, 118	0
6	X	61/61 (100%)	0.08	1 (1%) 74 47	25, 50, 120, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6823/6972 (97%)	-0.29	54 (0%)	87	67	21, 52, 103, 155	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	112	CYS	4.9
2	B	82	THR	4.5
3	P	97	LEU	4.0
3	P	103	LEU	4.0
2	O	82	THR	3.9
4	R	131	ALA	3.6
4	F	340	ILE	3.6
4	Q	210	GLY	3.6
4	F	363	ALA	3.4
3	P	111	ARG	3.4
3	P	110	LYS	3.3
2	O	157	ASN	3.3
4	E	211	SER	3.3
4	R	337	VAL	3.1
4	F	342	ALA	3.0
4	Q	211	SER	3.0
4	H	363	ALA	3.0
4	S	123	CYS	2.9
2	O	156	THR	2.9
4	R	339	PRO	2.9
3	P	109	ILE	2.8
4	V	211	SER	2.8
3	D	155	SER	2.7
4	F	338	ASP	2.7
2	B	81	GLN	2.5
3	P	188	SER	2.5
4	U	134	LEU	2.4
4	Q	213	HIS	2.4
6	X	53	C	2.3
3	P	105	SER	2.3
3	P	96	ILE	2.3
4	J	140	LEU	2.3
4	R	88	ILE	2.3
4	F	339	PRO	2.3
4	F	343	GLN	2.2
4	J	94	LEU	2.2
4	S	92	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	76	ASP	2.2
2	B	159	ASN	2.2
2	C	50	GLU	2.2
4	R	92	LEU	2.2
4	S	339	PRO	2.1
4	R	136	ASP	2.1
1	A	242	CYS	2.1
4	G	343	GLN	2.1
4	Q	363	ALA	2.1
4	R	342	ALA	2.1
2	O	5	ILE	2.1
1	A	288	VAL	2.1
2	N	83	THR	2.1
3	P	101	LYS	2.1
3	D	112	CYS	2.0
4	H	101	ASP	2.0
4	U	79	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.