



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:27 PM UTC

PDB ID : 5WKO / pdb_00005wko
Title : Crystal structure of antibody 27F3 recognizing the HA from
A/California/04/2009 (H1N1) influenza virus
Authors : Wilson, I.A.; Lang, S.; Zhu, X.
Deposited on : 2017-07-25
Resolution : 3.49 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:

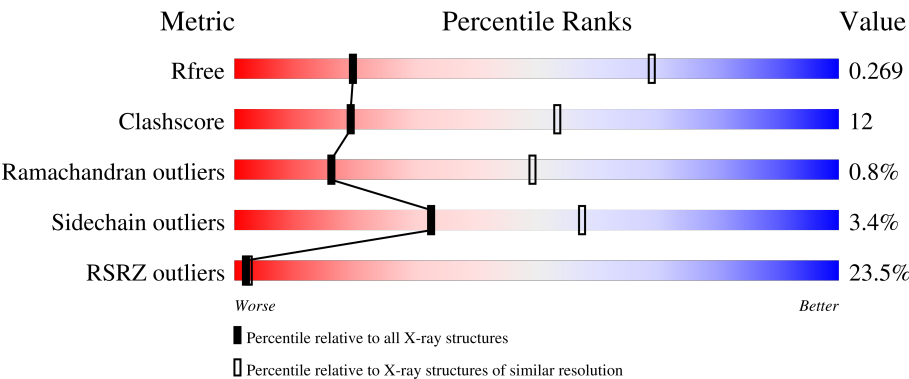
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	225	6% 75% 20% ..
1	C	225	6% 71% 26% ..
1	E	225	6% 76% 23% .
1	G	225	7% 71% 24% .
1	I	225	12% 71% 26% .

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Mol	Chain	Length	Quality of chain
1	K	225	
2	B	213	
2	D	213	
2	F	213	
2	H	213	
2	J	213	
2	L	213	
3	M	331	
3	N	331	
3	O	331	
3	S	331	
3	T	331	
3	U	331	
4	P	177	
4	Q	177	
4	R	177	
4	V	177	
4	W	177	
4	X	177	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43322 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 Antibody 27F3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	C	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	E	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	G	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	I	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	K	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			

- Molecule 2 is a protein called Antibody 27F3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	D	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	F	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	H	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	J	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	L	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	THR	SER	conflict	UNP Q9UL78

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Chain	Residue	Modelled	Actual	Comment	Reference
B	83	PHE	CYS	conflict	UNP Q9UL78
B	92	VAL	GLY	conflict	UNP Q9UL78
B	94	THR	SER	conflict	UNP Q9UL78
D	76	THR	SER	conflict	UNP Q9UL78
D	83	PHE	CYS	conflict	UNP Q9UL78
D	92	VAL	GLY	conflict	UNP Q9UL78
D	94	THR	SER	conflict	UNP Q9UL78
F	76	THR	SER	conflict	UNP Q9UL78
F	83	PHE	CYS	conflict	UNP Q9UL78
F	92	VAL	GLY	conflict	UNP Q9UL78
F	94	THR	SER	conflict	UNP Q9UL78
H	76	THR	SER	conflict	UNP Q9UL78
H	83	PHE	CYS	conflict	UNP Q9UL78
H	92	VAL	GLY	conflict	UNP Q9UL78
H	94	THR	SER	conflict	UNP Q9UL78
J	76	THR	SER	conflict	UNP Q9UL78
J	83	PHE	CYS	conflict	UNP Q9UL78
J	92	VAL	GLY	conflict	UNP Q9UL78
J	94	THR	SER	conflict	UNP Q9UL78
L	76	THR	SER	conflict	UNP Q9UL78
L	83	PHE	CYS	conflict	UNP Q9UL78
L	92	VAL	GLY	conflict	UNP Q9UL78
L	94	THR	SER	conflict	UNP Q9UL78

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	N	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	O	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			
3	S	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	T	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	U	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	7	ALA	-	expression tag	UNP C3W5S1
M	8	ASP	-	expression tag	UNP C3W5S1
M	9	PRO	-	expression tag	UNP C3W5S1
M	10	GLY	-	expression tag	UNP C3W5S1
N	7	ALA	-	expression tag	UNP C3W5S1
N	8	ASP	-	expression tag	UNP C3W5S1
N	9	PRO	-	expression tag	UNP C3W5S1
N	10	GLY	-	expression tag	UNP C3W5S1
O	7	ALA	-	expression tag	UNP C3W5S1
O	8	ASP	-	expression tag	UNP C3W5S1
O	9	PRO	-	expression tag	UNP C3W5S1
O	10	GLY	-	expression tag	UNP C3W5S1
S	7	ALA	-	expression tag	UNP C3W5S1
S	8	ASP	-	expression tag	UNP C3W5S1
S	9	PRO	-	expression tag	UNP C3W5S1
S	10	GLY	-	expression tag	UNP C3W5S1
T	7	ALA	-	expression tag	UNP C3W5S1
T	8	ASP	-	expression tag	UNP C3W5S1
T	9	PRO	-	expression tag	UNP C3W5S1
T	10	GLY	-	expression tag	UNP C3W5S1
U	7	ALA	-	expression tag	UNP C3W5S1
U	8	ASP	-	expression tag	UNP C3W5S1
U	9	PRO	-	expression tag	UNP C3W5S1
U	10	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	Q	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	R	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	V	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	W	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	X	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			

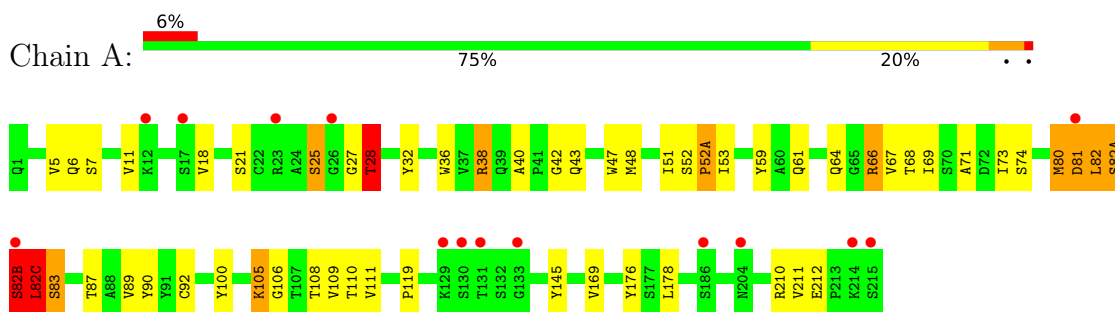
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
P	175	SER	-	expression tag	UNP A0A023ZYH9
P	176	GLY	-	expression tag	UNP A0A023ZYH9
P	177	ARG	-	expression tag	UNP A0A023ZYH9
Q	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
Q	175	SER	-	expression tag	UNP A0A023ZYH9
Q	176	GLY	-	expression tag	UNP A0A023ZYH9
Q	177	ARG	-	expression tag	UNP A0A023ZYH9
R	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
R	175	SER	-	expression tag	UNP A0A023ZYH9
R	176	GLY	-	expression tag	UNP A0A023ZYH9
R	177	ARG	-	expression tag	UNP A0A023ZYH9
V	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
V	175	SER	-	expression tag	UNP A0A023ZYH9
V	176	GLY	-	expression tag	UNP A0A023ZYH9
V	177	ARG	-	expression tag	UNP A0A023ZYH9
W	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
W	175	SER	-	expression tag	UNP A0A023ZYH9
W	176	GLY	-	expression tag	UNP A0A023ZYH9
W	177	ARG	-	expression tag	UNP A0A023ZYH9
X	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
X	175	SER	-	expression tag	UNP A0A023ZYH9
X	176	GLY	-	expression tag	UNP A0A023ZYH9
X	177	ARG	-	expression tag	UNP A0A023ZYH9

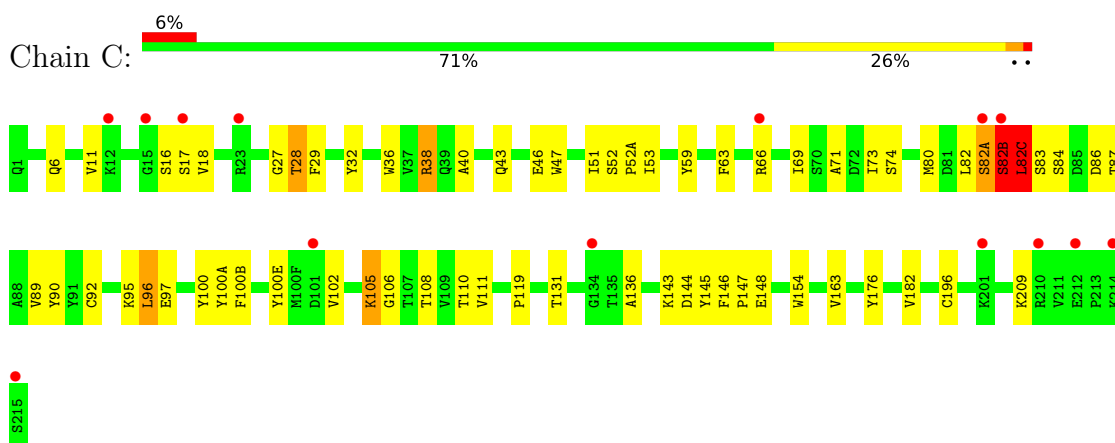
3 Residue-property plots [i](#)

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.

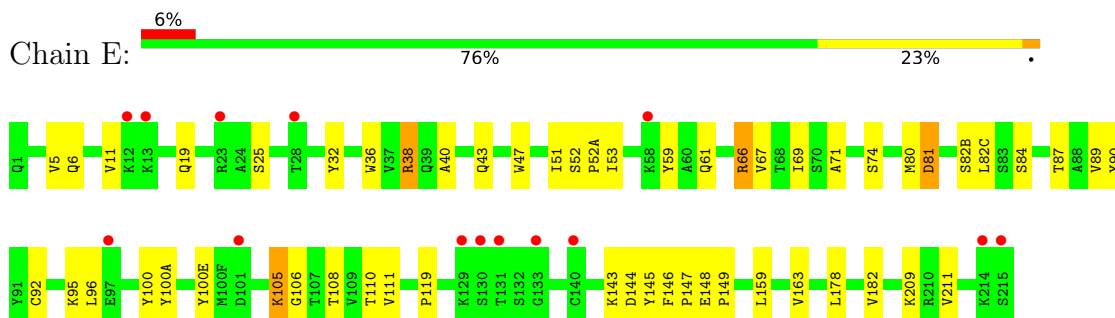
- Molecule 1: Antibody 27F3 heavy chain



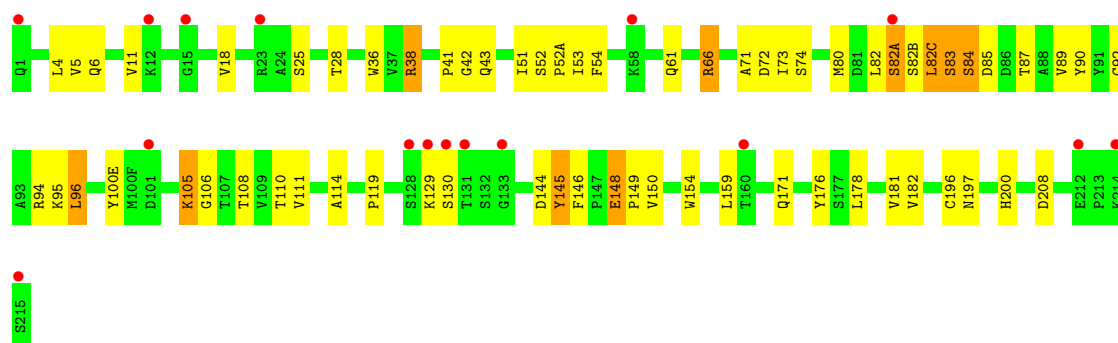
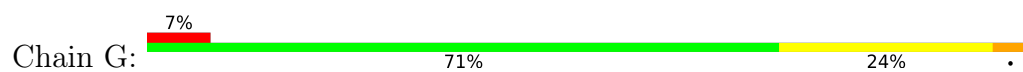
- Molecule 1: Antibody 27F3 heavy chain



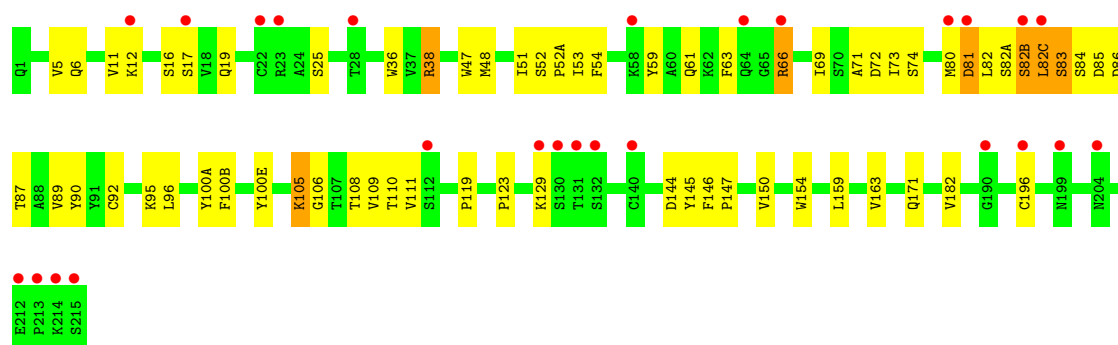
- Molecule 1: Antibody 27F3 heavy chain



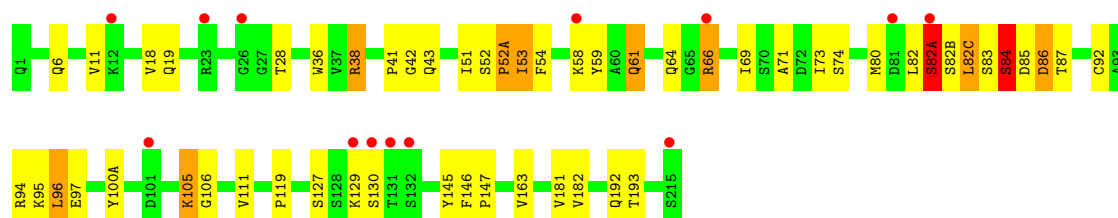
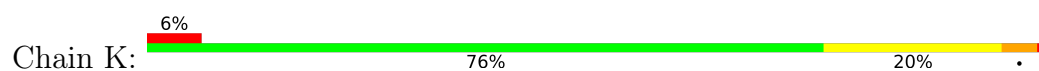
- Molecule 1: Antibody 27F3 heavy chain



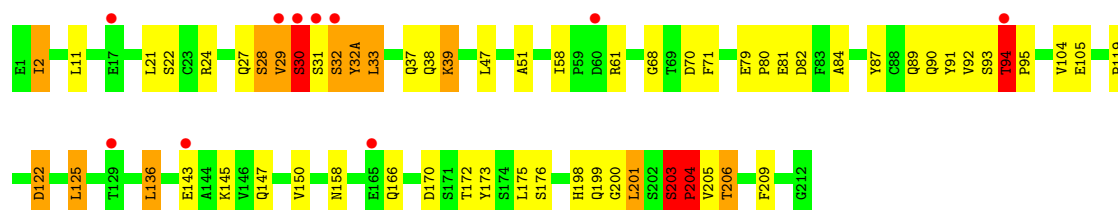
• Molecule 1: Antibody 27F3 heavy chain



• Molecule 1: Antibody 27F3 heavy chain

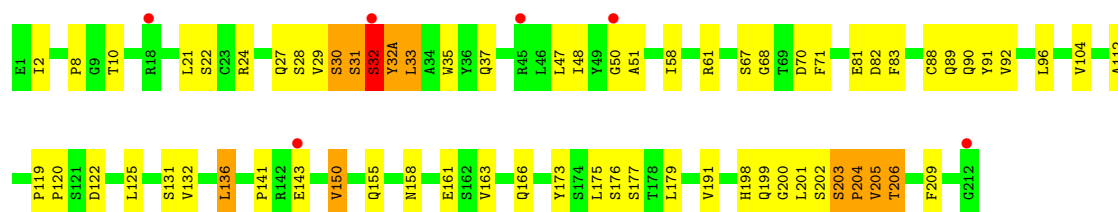


• Molecule 2: Antibody 27F3 light chain



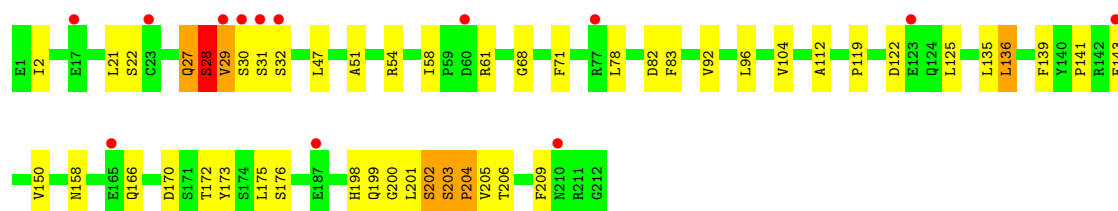
- Molecule 2: Antibody 27F3 light chain

Chain D: 



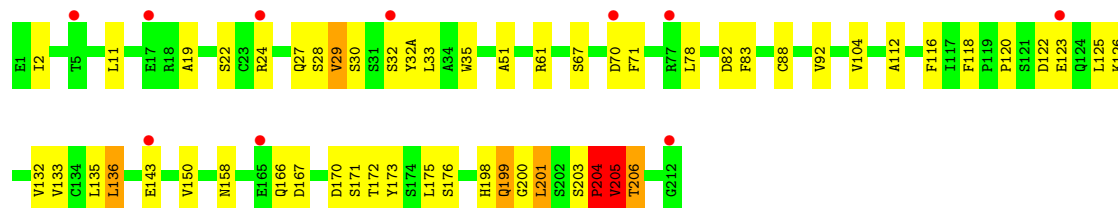
- Molecule 2: Antibody 27F3 light chain

Chain F: 



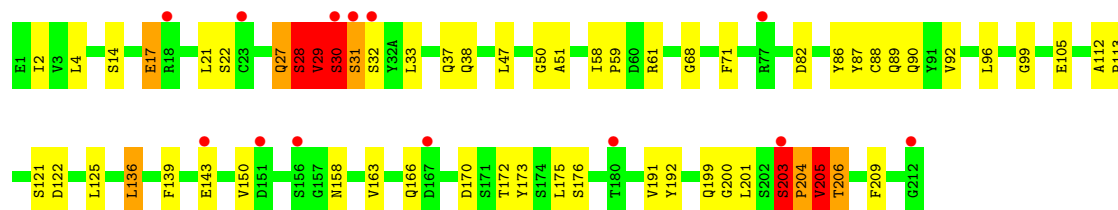
- Molecule 2: Antibody 27F3 light chain

Chain H: 



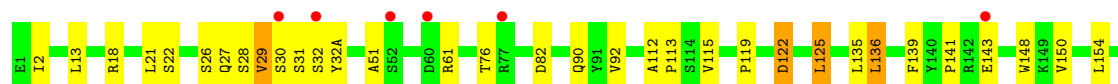
- Molecule 2: Antibody 27F3 light chain

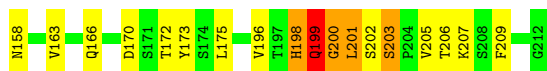
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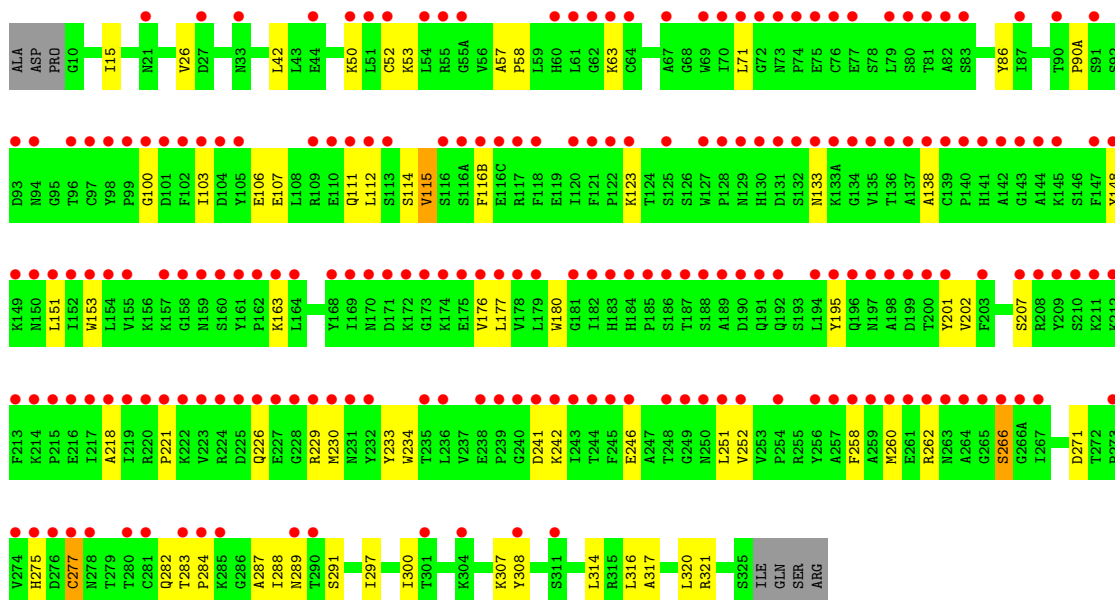
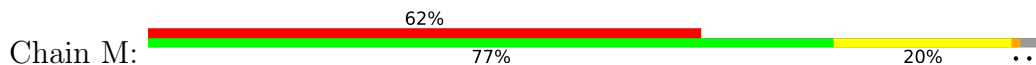
- Molecule 2: Antibody 27F3 light chain

Chain L: 

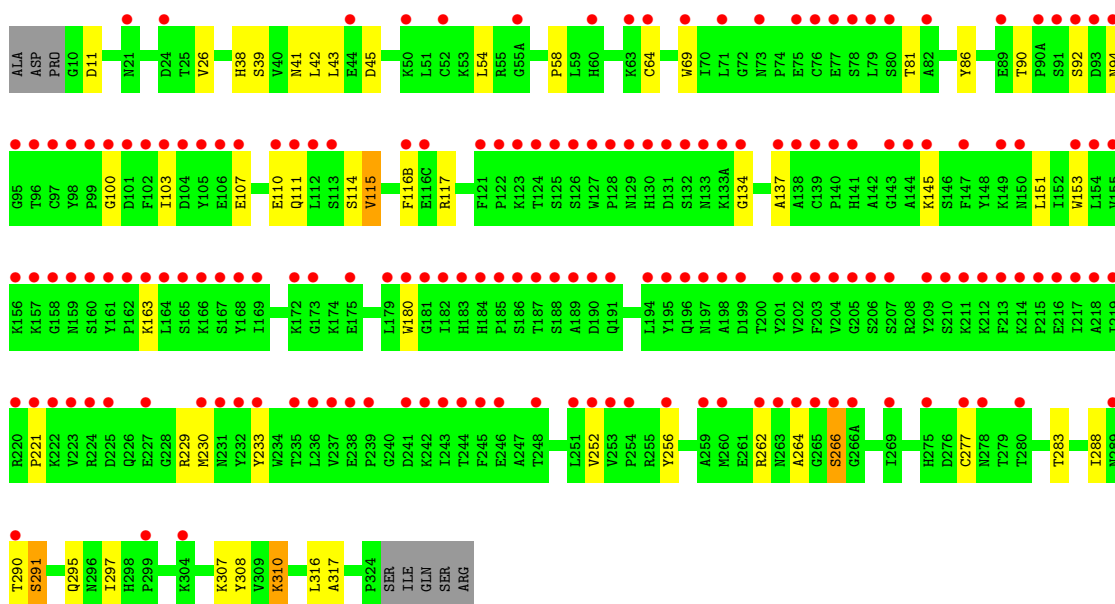
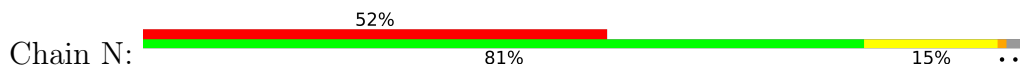




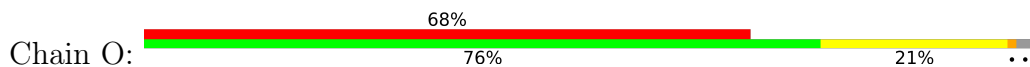
• Molecule 3: Hemagglutinin

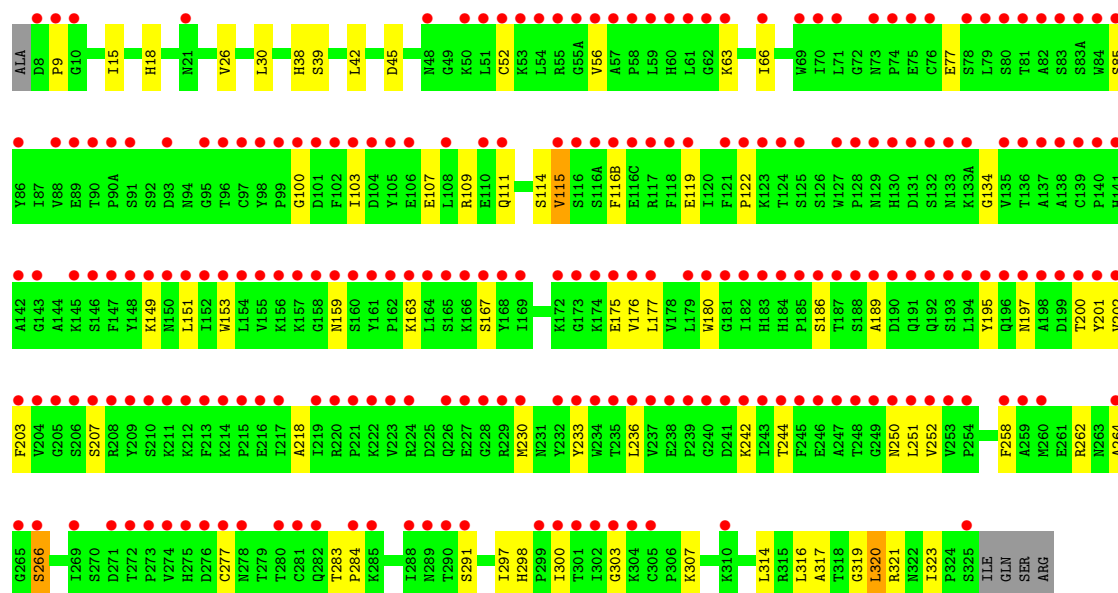


• Molecule 3: Hemagglutinin



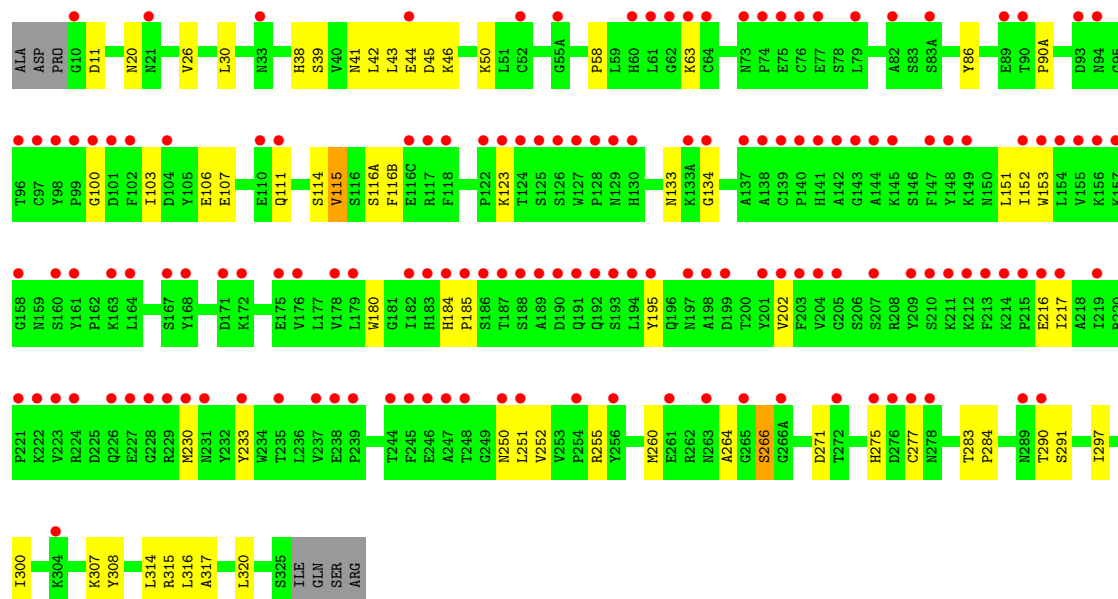
• Molecule 3: Hemagglutinin





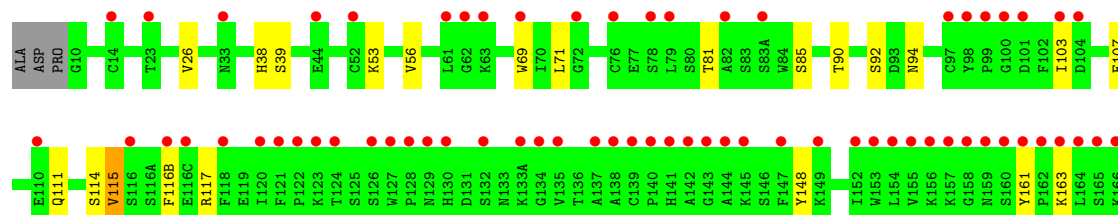
• Molecule 3: Hemagglutinin

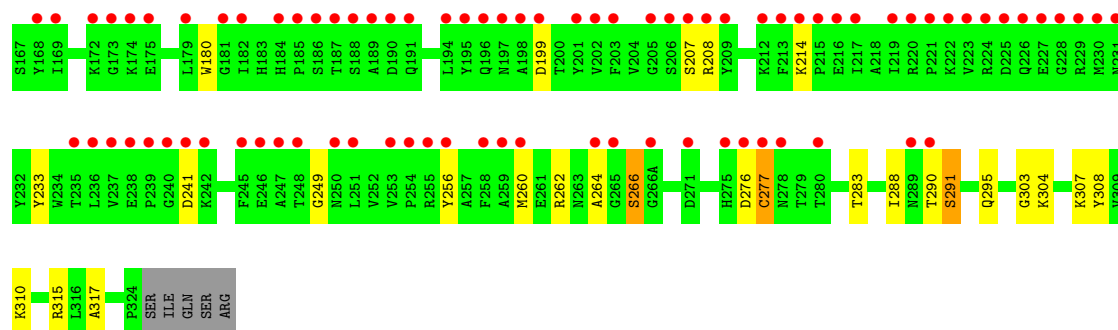
Chain S:



• Molecule 3: Hemagglutinin

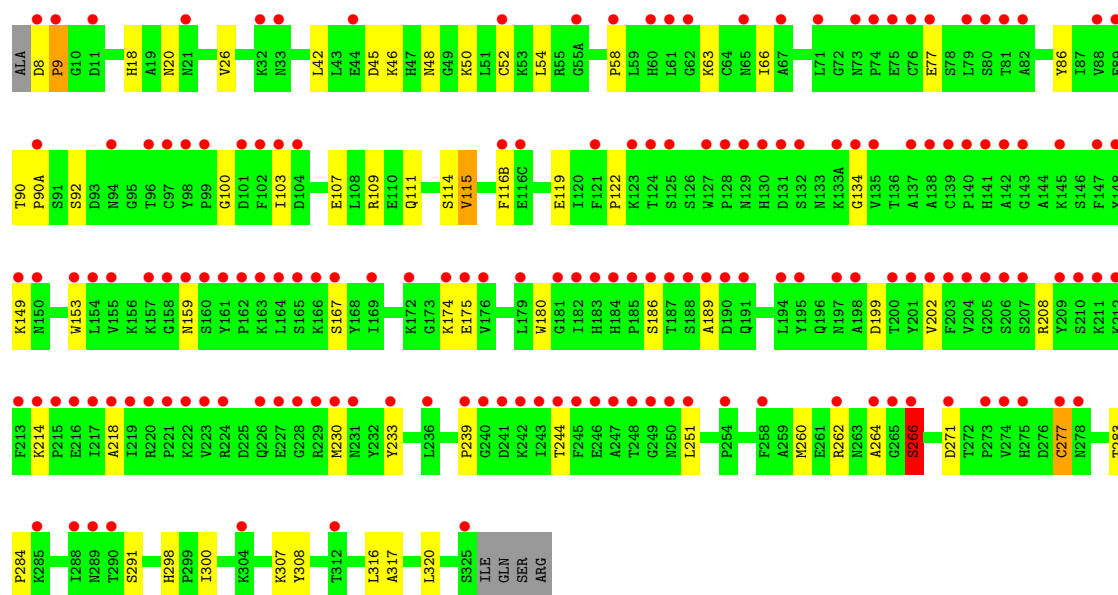
Chain T:





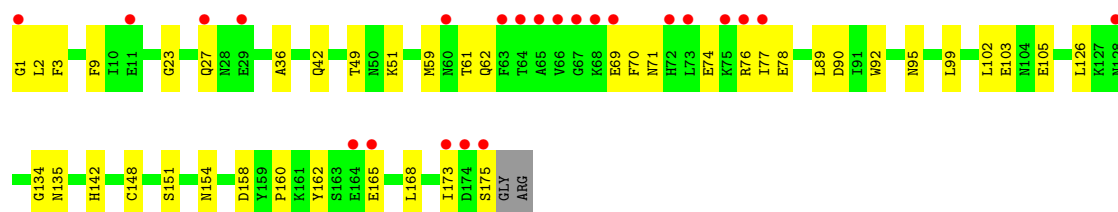
• Molecule 3: Hemagglutinin

Chain U: 49% 79% 19% ..



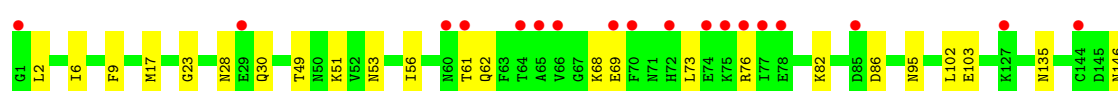
• Molecule 4: Hemagglutinin

Chain P: 13% 75% 24% .



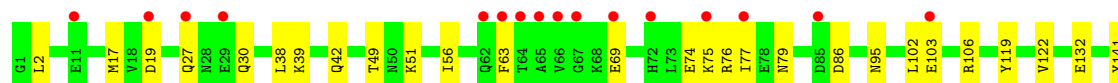
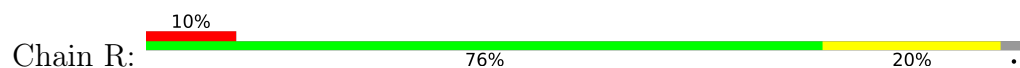
• Molecule 4: Hemagglutinin

Chain Q: 11% 81% 15% .

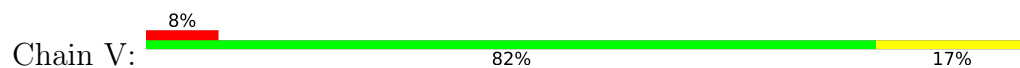




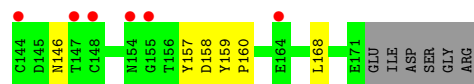
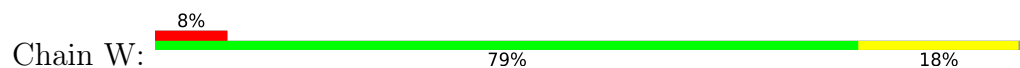
• Molecule 4: Hemagglutinin



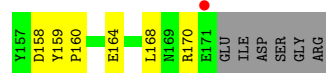
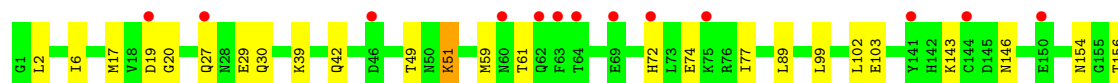
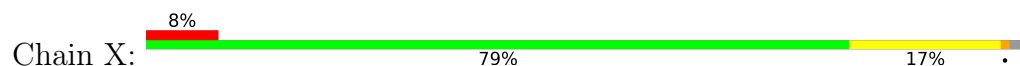
• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	190.58Å 191.49Å 391.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.49 49.45 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.45-3.49) 98.0 (49.45-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.246 , 0.268 0.247 , 0.269	Depositor DCC
R_{free} test set	8912 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	43322	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.01	2/1719 (0.1%)	0.94	3/2344 (0.1%)
1	C	0.88	0/1719	0.90	2/2344 (0.1%)
1	E	0.89	1/1719 (0.1%)	0.91	0/2344
1	G	0.87	1/1719 (0.1%)	0.90	0/2344
1	I	0.79	0/1719	0.88	2/2344 (0.1%)
1	K	0.96	1/1719 (0.1%)	0.95	4/2344 (0.2%)
2	B	1.22	5/1663 (0.3%)	1.21	16/2260 (0.7%)
2	D	0.99	2/1663 (0.1%)	1.01	5/2260 (0.2%)
2	F	0.98	0/1663	0.97	3/2260 (0.1%)
2	H	0.99	1/1663 (0.1%)	0.94	2/2260 (0.1%)
2	J	0.99	1/1663 (0.1%)	1.02	7/2260 (0.3%)
2	L	1.14	1/1663 (0.1%)	1.01	5/2260 (0.2%)
3	M	0.58	0/2593	0.76	0/3524
3	N	0.62	0/2587	0.83	1/3516 (0.0%)
3	O	0.53	0/2609	0.77	2/3547 (0.1%)
3	S	0.57	0/2593	0.73	1/3524 (0.0%)
3	T	0.63	1/2587 (0.0%)	0.87	3/3516 (0.1%)
3	U	0.58	0/2609	0.81	2/3547 (0.1%)
4	P	0.95	0/1434	0.94	1/1932 (0.1%)
4	Q	0.97	0/1403	0.90	0/1890
4	R	0.89	0/1403	0.86	0/1890
4	V	0.94	0/1434	0.93	0/1932
4	W	0.94	0/1403	0.89	0/1890
4	X	0.87	0/1403	0.91	1/1890 (0.1%)
All	All	0.85	16/44350 (0.0%)	0.90	60/60222 (0.1%)

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	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	211	VAL	C-N	8.74	1.51	1.33
1	A	80	MET	CA-C	-8.30	1.42	1.52
2	H	205	VAL	C-O	-6.42	1.17	1.24
2	L	199	GLN	CA-C	-6.33	1.45	1.52
2	J	205	VAL	C-O	-6.14	1.17	1.24
2	B	30	SER	N-CA	5.69	1.53	1.46
2	B	93	SER	C-O	-5.58	1.19	1.24
1	A	211	VAL	C-N	5.56	1.45	1.33
1	K	96	LEU	C-N	-5.50	1.22	1.33
1	G	96	LEU	C-N	-5.42	1.22	1.33
2	B	33	LEU	C-O	-5.35	1.17	1.23
2	B	32	SER	CA-CB	-5.31	1.46	1.53
2	D	205	VAL	C-O	-5.19	1.17	1.24
2	B	205	VAL	C-O	-5.05	1.18	1.24
2	D	33	LEU	C-O	-5.04	1.18	1.23
3	T	277	CYS	CA-CB	5.00	1.64	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	82(B)	SER	N-CA-C	-14.12	88.63	108.54
2	B	203	SER	CA-C-N	12.73	135.75	119.84
2	B	203	SER	C-N-CA	12.73	135.75	119.84
3	T	277	CYS	CA-CB-SG	-12.45	85.77	114.40
2	B	94	THR	CA-C-N	11.72	134.49	119.84
2	B	94	THR	C-N-CA	11.72	134.49	119.84
2	J	203	SER	CA-C-N	10.67	133.18	119.84
2	J	203	SER	C-N-CA	10.67	133.18	119.84
1	K	86	ASP	N-CA-C	-10.48	98.16	112.94
2	F	203	SER	CA-C-N	9.45	131.66	119.84
2	F	203	SER	C-N-CA	9.45	131.66	119.84
2	D	203	SER	CA-C-N	8.81	130.85	119.84
2	D	203	SER	C-N-CA	8.81	130.85	119.84
2	B	93	SER	N-CA-C	8.73	119.45	108.19
3	U	266	SER	CB-CA-C	-8.54	103.73	114.40
2	L	203	SER	CA-C-N	8.36	130.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	203	SER	C-N-CA	8.36	130.29	119.84
2	B	32	SER	N-CA-C	-8.01	92.85	107.75
1	C	82(B)	SER	N-CA-C	-7.99	102.66	111.36
2	L	201	LEU	N-CA-C	-7.87	94.04	110.80
3	T	304	LYS	CG-CD-CE	7.26	128.00	111.30
3	S	277	CYS	CA-CB-SG	-7.20	97.85	114.40
1	C	82(C)	LEU	N-CA-C	7.00	125.71	110.80
2	L	200	GLY	N-CA-C	-6.79	97.08	113.18
2	J	17	GLU	N-CA-CB	-6.73	100.08	110.85
2	B	30	SER	N-CA-CB	6.67	121.75	110.49
2	B	32(A)	TYR	N-CA-C	-6.41	95.27	108.53
2	F	27	GLN	O-C-N	-6.34	115.44	123.24
2	D	32	SER	N-CA-C	-6.34	95.27	107.57
2	B	29	VAL	CA-C-N	6.08	133.15	121.54
2	B	29	VAL	C-N-CA	6.08	133.15	121.54
2	B	201	LEU	N-CA-C	5.83	123.22	110.80
2	J	30	SER	N-CA-C	5.83	123.22	110.80
2	D	30	SER	CB-CA-C	-5.75	109.93	116.54
2	J	27	GLN	O-C-N	-5.74	115.68	123.15
2	B	29	VAL	O-C-N	5.67	127.37	121.87
2	H	203	SER	CA-C-N	5.66	126.92	119.84
2	H	203	SER	C-N-CA	5.66	126.92	119.84
3	T	310	LYS	CB-CG-CD	5.65	124.30	111.30
1	A	28	THR	N-CA-C	-5.65	98.89	108.26
2	L	202	SER	N-CA-C	-5.60	98.86	110.80
1	A	82(C)	LEU	N-CA-C	5.57	122.67	110.80
2	J	29	VAL	N-CA-C	5.55	120.88	109.34
3	N	277	CYS	CA-CB-SG	-5.51	101.72	114.40
3	U	277	CYS	N-CA-CB	-5.39	101.56	111.37
2	B	201	LEU	CA-C-N	5.32	131.71	121.54
2	B	201	LEU	C-N-CA	5.32	131.71	121.54
1	I	82(C)	LEU	N-CA-C	5.32	117.92	109.24
4	X	51	LYS	CB-CG-CD	-5.31	99.09	111.30
2	B	29	VAL	CA-C-O	-5.30	115.44	120.95
2	D	206	THR	CB-CA-C	-5.29	102.90	110.62
2	B	29	VAL	N-CA-CB	5.20	117.61	110.54
1	K	58	LYS	CB-CG-CD	5.16	123.17	111.30
2	J	205	VAL	CB-CA-C	-5.16	104.72	110.96
1	K	84	SER	N-CA-C	5.14	121.74	110.80
1	K	53	ILE	CA-CB-CG1	-5.13	101.67	110.40
3	O	319	GLY	CA-C-N	-5.08	113.76	123.32
3	O	319	GLY	C-N-CA	-5.08	113.76	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82(A)	SER	C-N-CA	5.01	134.23	121.70
4	P	27	GLN	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	148	GLU	Peptide
2	L	198	HIS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1675	0	1642	66	0
1	C	1675	0	1642	68	0
1	E	1675	0	1643	45	0
1	G	1675	0	1643	76	0
1	I	1675	0	1643	73	0
1	K	1675	0	1642	47	0
2	B	1628	0	1592	62	0
2	D	1628	0	1591	66	0
2	F	1628	0	1592	32	0
2	H	1628	0	1592	36	0
2	J	1628	0	1590	64	0
2	L	1628	0	1592	37	0
3	M	2529	0	2479	49	0
3	N	2523	0	2474	37	0
3	O	2544	0	2490	54	0
3	S	2529	0	2479	44	0
3	T	2523	0	2474	33	0
3	U	2544	0	2490	48	0
4	P	1406	0	1326	35	0
4	Q	1375	0	1300	28	0
4	R	1375	0	1300	33	0
4	V	1406	0	1326	34	0
4	W	1375	0	1300	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	1375	0	1300	29	0
All	All	43322	0	42142	1003	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1003) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:SER:OG	2:J:92:VAL:CG1	1.64	1.44
2:B:94:THR:CB	2:B:95:PRO:HD3	1.33	1.34
1:I:66:ARG:HB3	1:I:82(B):SER:CB	1.59	1.33
2:B:94:THR:CB	2:B:95:PRO:CD	2.07	1.32
1:I:17:SER:CB	1:I:82(A):SER:OG	1.76	1.31
1:A:68:THR:O	1:A:81:ASP:CB	1.78	1.29
1:I:17:SER:CA	1:I:82(A):SER:OG	1.83	1.25
1:I:83:SER:O	1:I:111:VAL:HG11	1.33	1.24
1:C:83:SER:O	1:C:111:VAL:HG11	1.27	1.24
2:D:29:VAL:HG11	2:D:71:PHE:CZ	1.71	1.24
1:A:83:SER:O	1:A:111:VAL:HG11	1.38	1.23
1:A:68:THR:O	1:A:81:ASP:HB2	1.08	1.23
2:D:112:ALA:HB2	2:D:200:GLY:O	1.36	1.23
1:G:145:TYR:CE2	1:G:150:VAL:CG2	2.22	1.21
2:J:30:SER:OG	2:J:92:VAL:HG11	1.17	1.19
2:F:29:VAL:HG23	2:F:68:GLY:O	1.38	1.19
1:G:145:TYR:CE1	1:G:176:TYR:HB2	1.78	1.18
1:G:145:TYR:HE2	1:G:150:VAL:CG2	1.56	1.16
1:G:145:TYR:HE1	1:G:176:TYR:CB	1.56	1.16
1:G:83:SER:O	1:G:111:VAL:HG11	1.46	1.15
1:I:66:ARG:HB3	1:I:82(B):SER:HB2	1.20	1.14
1:I:66:ARG:CB	1:I:82(B):SER:HB3	1.76	1.14
1:I:17:SER:HA	1:I:82(A):SER:OG	1.42	1.14
1:G:145:TYR:CE2	1:G:150:VAL:HG23	1.80	1.13
2:B:94:THR:HB	2:B:95:PRO:CD	1.71	1.13
2:B:94:THR:OG1	2:B:95:PRO:CD	2.00	1.10
1:A:67:VAL:HG23	1:A:81:ASP:O	1.51	1.08
2:J:29:VAL:CG2	2:J:68:GLY:O	2.01	1.08
1:I:66:ARG:CB	1:I:82(B):SER:CB	2.29	1.07
2:D:29:VAL:HG11	2:D:71:PHE:CE2	1.89	1.06
2:J:29:VAL:HG23	2:J:68:GLY:O	1.54	1.05
1:G:145:TYR:CE1	1:G:176:TYR:CB	2.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:H	1:A:81:ASP:HB3	1.20	1.04
2:B:31:SER:OG	2:B:32(A):TYR:HD2	1.41	1.03
2:J:32:SER:O	2:J:50:GLY:O	1.76	1.03
1:A:18:VAL:HG23	1:A:82(C):LEU:HD21	1.38	1.02
1:A:68:THR:OG1	1:A:81:ASP:CG	2.03	1.02
1:K:66:ARG:O	1:K:82(A):SER:N	1.86	1.02
1:G:145:TYR:CE2	1:G:150:VAL:HG21	1.90	1.02
1:I:83:SER:O	1:I:111:VAL:CG1	2.09	1.01
1:E:66:ARG:NH1	1:E:82(B):SER:OG	1.90	1.01
2:B:94:THR:OG1	2:B:95:PRO:HD2	1.61	1.01
1:G:145:TYR:HE1	1:G:176:TYR:HB3	1.22	1.00
1:I:66:ARG:HB3	1:I:82(B):SER:HB3	1.37	1.00
1:I:17:SER:HA	1:I:82(A):SER:HG	1.16	0.99
1:G:28:THR:HG22	4:V:53:ASN:ND2	1.78	0.98
1:C:83:SER:O	1:C:111:VAL:CG1	2.11	0.98
3:M:221:PRO:HG3	3:O:242:LYS:HB3	1.46	0.97
1:A:74:SER:HB3	3:N:291:SER:HB3	1.43	0.97
2:D:29:VAL:CG1	2:D:71:PHE:CZ	2.48	0.97
1:I:66:ARG:HB2	1:I:82(B):SER:HB3	1.47	0.97
1:C:27:GLY:O	1:C:28:THR:HG23	1.65	0.96
1:A:68:THR:C	1:A:81:ASP:HB2	1.90	0.96
1:A:68:THR:OG1	1:A:81:ASP:CB	2.14	0.96
1:I:17:SER:HB3	1:I:82(A):SER:OG	1.64	0.96
2:B:31:SER:OG	2:B:32(A):TYR:CD2	2.16	0.95
2:D:33:LEU:HD12	2:D:89:GLN:O	1.67	0.95
1:C:27:GLY:C	1:C:28:THR:HG23	1.92	0.94
1:A:18:VAL:CG2	1:A:82(C):LEU:HD21	1.97	0.94
2:B:29:VAL:HG11	2:B:71:PHE:CZ	2.02	0.94
3:M:229:ARG:HH21	3:O:207:SER:HA	1.33	0.94
1:G:83:SER:O	1:G:111:VAL:CG1	2.16	0.93
2:D:29:VAL:CG1	2:D:71:PHE:HZ	1.80	0.93
2:B:94:THR:OG1	2:B:95:PRO:HD3	1.64	0.93
1:K:18:VAL:HG23	1:K:82(C):LEU:HD11	1.49	0.93
1:C:66:ARG:HB2	1:C:82(B):SER:HB2	1.48	0.93
1:I:17:SER:CA	1:I:82(A):SER:HG	1.73	0.92
1:G:28:THR:HG22	4:V:53:ASN:HD21	1.35	0.91
1:G:145:TYR:CD2	1:G:150:VAL:CG2	2.52	0.91
1:A:68:THR:N	1:A:81:ASP:HB3	1.85	0.91
1:G:28:THR:CG2	4:V:53:ASN:ND2	2.34	0.90
1:A:83:SER:O	1:A:111:VAL:CG1	2.20	0.90
1:G:145:TYR:CD2	1:G:150:VAL:HG21	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLY:O	1:C:28:THR:CB	2.20	0.89
2:D:29:VAL:HG11	2:D:71:PHE:HZ	1.34	0.89
2:D:32:SER:CB	2:D:51:ALA:HB2	2.02	0.88
2:J:30:SER:OG	2:J:92:VAL:CB	2.20	0.88
1:A:67:VAL:CG2	1:A:81:ASP:O	2.22	0.88
1:G:145:TYR:CD1	1:G:176:TYR:HB2	2.08	0.88
1:C:27:GLY:O	1:C:28:THR:OG1	1.91	0.88
2:J:30:SER:OG	2:J:92:VAL:HG12	1.74	0.88
1:C:27:GLY:O	1:C:28:THR:CG2	2.22	0.87
4:X:51:LYS:HE3	4:X:103:GLU:OE1	1.75	0.87
1:A:28:THR:HG22	4:Q:53:ASN:HD22	1.41	0.86
1:A:28:THR:HG22	4:Q:53:ASN:ND2	1.90	0.86
1:A:18:VAL:HG23	1:A:82(C):LEU:CD2	2.06	0.85
2:D:112:ALA:CB	2:D:200:GLY:O	2.24	0.85
2:J:112:ALA:HB2	2:J:200:GLY:O	1.76	0.85
2:B:94:THR:HB	2:B:95:PRO:HD3	0.85	0.84
1:I:96:LEU:HD12	1:I:96:LEU:O	1.77	0.84
1:I:17:SER:HB2	1:I:82(A):SER:OG	1.77	0.82
2:D:29:VAL:HG12	2:D:68:GLY:O	1.80	0.82
4:R:51:LYS:HE3	4:R:103:GLU:OE1	1.80	0.82
3:N:114:SER:HB2	3:N:266:SER:HB2	1.62	0.81
1:K:38:ARG:NH2	1:K:86:ASP:OD1	2.13	0.81
1:G:28:THR:CG2	4:V:53:ASN:HD22	1.93	0.81
1:A:47:TRP:CZ3	2:B:95:PRO:HA	2.14	0.81
1:C:66:ARG:HB2	1:C:82(B):SER:CB	2.11	0.80
2:B:29:VAL:HG11	2:B:71:PHE:HZ	1.46	0.80
2:B:39:LYS:NZ	2:B:81:GLU:O	2.14	0.80
3:M:242:LYS:HB3	3:N:221:PRO:HG3	1.63	0.80
2:J:112:ALA:HB1	2:J:201:LEU:HD13	1.63	0.80
1:I:66:ARG:CB	1:I:82(B):SER:HB2	2.02	0.78
3:O:298:HIS:HE1	3:O:300:ILE:HD12	1.47	0.78
2:J:29:VAL:HG22	2:J:68:GLY:O	1.84	0.77
1:E:6:GLN:NE2	1:E:92:CYS:SG	2.58	0.77
2:J:61:ARG:NH1	2:J:82:ASP:OD2	2.18	0.77
2:L:112:ALA:HB2	2:L:200:GLY:O	1.85	0.77
1:A:6:GLN:NE2	1:A:92:CYS:SG	2.58	0.77
3:T:114:SER:HB2	3:T:266:SER:HB2	1.67	0.76
4:P:51:LYS:HE3	4:P:103:GLU:OE1	1.84	0.76
1:I:83:SER:OG	1:I:85:ASP:OD1	2.02	0.76
2:B:198:HIS:CD2	2:B:200:GLY:H	2.04	0.75
1:G:74:SER:HB3	3:S:291:SER:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD22	2:B:71:PHE:CD2	2.22	0.74
1:G:18:VAL:HG23	1:G:82(C):LEU:CD2	2.17	0.74
2:J:31:SER:OG	2:J:32:SER:N	2.18	0.74
4:R:119:TYR:OH	4:R:132:GLU:OE2	2.04	0.74
1:A:68:THR:O	1:A:81:ASP:N	2.20	0.74
1:G:18:VAL:HG23	1:G:82(C):LEU:HD21	1.69	0.74
2:J:29:VAL:HG21	2:J:71:PHE:HE2	1.52	0.73
2:D:32:SER:OG	2:D:51:ALA:CB	2.36	0.73
1:E:6:GLN:HG3	1:E:106:GLY:H	1.54	0.73
1:I:89:VAL:HG22	1:I:108:THR:HG22	1.70	0.73
2:B:27:GLN:O	2:B:28:SER:C	2.30	0.73
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.21	0.73
1:G:74:SER:HB3	3:S:291:SER:OG	1.89	0.73
1:C:74:SER:HB3	3:U:291:SER:HB2	1.69	0.72
3:T:117:ARG:HD3	3:T:256:TYR:CD1	2.23	0.72
1:G:83:SER:OG	1:G:85:ASP:OD1	2.06	0.72
1:I:6:GLN:NE2	1:I:92:CYS:SG	2.62	0.72
1:C:6:GLN:HG3	1:C:106:GLY:H	1.54	0.72
1:G:6:GLN:NE2	1:G:92:CYS:SG	2.63	0.72
1:A:66:ARG:HD2	1:A:82(B):SER:OG	1.90	0.72
2:B:38:GLN:HE21	2:B:87:TYR:HE2	1.38	0.72
2:L:32:SER:HB2	2:L:51:ALA:HB2	1.70	0.71
2:B:198:HIS:HD2	2:B:200:GLY:H	1.36	0.71
2:F:29:VAL:HG21	2:F:71:PHE:HE2	1.54	0.70
1:G:5:VAL:HA	1:G:105:LYS:HZ1	1.55	0.70
1:G:145:TYR:CE1	1:G:176:TYR:HB3	2.15	0.70
2:H:204:PRO:O	2:H:206:THR:HG22	1.91	0.70
2:D:32:SER:HB2	2:D:51:ALA:HB2	1.71	0.70
1:K:18:VAL:CG2	1:K:82(C):LEU:HD11	2.21	0.70
2:F:31:SER:OG	2:F:32:SER:N	2.16	0.70
3:M:114:SER:HB2	3:M:266:SER:HB2	1.73	0.70
1:C:18:VAL:HG23	1:C:82(C):LEU:HD21	1.74	0.70
2:D:32:SER:CB	2:D:51:ALA:CB	2.70	0.70
2:B:29:VAL:HG11	2:B:71:PHE:CE2	2.26	0.69
1:E:66:ARG:NH1	1:E:82(B):SER:HG	1.88	0.69
1:G:74:SER:HB3	3:S:291:SER:HB2	1.73	0.69
2:J:27:GLN:O	2:J:28:SER:O	2.09	0.69
1:A:89:VAL:HG22	1:A:108:THR:HG22	1.75	0.68
3:N:117:ARG:HD3	3:N:256:TYR:CD1	2.28	0.68
1:I:74:SER:HB2	4:R:56:ILE:HG21	1.75	0.68
3:U:298:HIS:HE1	3:U:300:ILE:HD12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:103:GLU:OE2	4:X:102:LEU:HD21	1.93	0.68
2:D:32:SER:HB2	2:D:51:ALA:CB	2.24	0.68
2:L:31:SER:OG	2:L:32:SER:N	2.24	0.68
1:I:82(B):SER:O	1:I:86:ASP:OD2	2.11	0.68
3:N:107:GLU:O	3:N:111:GLN:HG2	1.93	0.68
1:E:82(B):SER:HB2	1:E:82(C):LEU:HA	1.75	0.68
1:G:6:GLN:HG3	1:G:106:GLY:H	1.58	0.68
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.76	0.68
2:J:112:ALA:HB1	2:J:201:LEU:CD1	2.23	0.68
1:A:68:THR:O	1:A:81:ASP:CA	2.42	0.67
2:J:30:SER:O	2:J:31:SER:CB	2.41	0.67
1:I:163:VAL:HG22	1:I:182:VAL:HG22	1.76	0.67
1:K:74:SER:HB3	3:T:291:SER:HB3	1.75	0.67
1:C:66:ARG:CB	1:C:82(B):SER:HB2	2.23	0.67
3:T:107:GLU:O	3:T:111:GLN:HG2	1.95	0.67
2:B:38:GLN:NE2	2:B:87:TYR:HE2	1.91	0.66
1:C:18:VAL:HG23	1:C:82(C):LEU:CD2	2.25	0.66
2:D:32:SER:OG	2:D:51:ALA:HB2	1.93	0.66
3:O:134:GLY:HA3	3:O:153:TRP:HB3	1.77	0.66
1:K:119:PRO:HB3	1:K:145:TYR:HB3	1.77	0.66
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.78	0.66
1:A:68:THR:OG1	1:A:81:ASP:OD2	2.13	0.66
2:J:29:VAL:HG21	2:J:71:PHE:CE2	2.30	0.66
3:N:111:GLN:HE22	3:N:262:ARG:NH1	1.92	0.66
4:W:51:LYS:HE3	4:W:103:GLU:OE1	1.95	0.66
2:J:30:SER:OG	2:J:92:VAL:HB	1.96	0.66
4:Q:51:LYS:HE3	4:Q:103:GLU:OE1	1.96	0.66
1:C:16:SER:O	1:C:82(C):LEU:HB2	1.97	0.65
2:J:201:LEU:HD21	2:J:205:VAL:HG12	1.79	0.65
2:B:29:VAL:CG1	2:B:71:PHE:HZ	2.10	0.65
1:A:67:VAL:HA	1:A:81:ASP:O	1.96	0.65
1:C:27:GLY:C	1:C:28:THR:CG2	2.61	0.65
1:C:53:ILE:HD13	4:X:49:THR:HA	1.79	0.65
2:D:141:PRO:HG3	2:D:199:GLN:NE2	2.12	0.65
2:D:27:GLN:O	2:D:28:SER:C	2.35	0.64
2:B:29:VAL:CG1	2:B:71:PHE:CZ	2.78	0.64
3:O:26:VAL:HG21	3:O:317:ALA:HB2	1.78	0.64
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.78	0.64
1:I:82(B):SER:O	1:I:82(B):SER:OG	2.09	0.64
3:N:163:LYS:HB3	3:U:159:ASN:ND2	2.13	0.64
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:69:GLU:O	4:R:76:ARG:NH1	2.28	0.64
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.32	0.64
1:I:66:ARG:O	1:I:82:LEU:HD12	1.98	0.64
4:P:69:GLU:O	4:Q:76:ARG:NH1	2.31	0.64
2:H:112:ALA:HB2	2:H:200:GLY:O	1.98	0.64
2:F:170:ASP:OD1	2:F:172:THR:HG22	1.98	0.63
2:H:61:ARG:NH1	2:H:82:ASP:OD2	2.32	0.63
3:S:115:VAL:HG11	3:S:116(B):PHE:HB2	1.80	0.63
2:F:29:VAL:HG21	2:F:71:PHE:CE2	2.34	0.63
2:H:27:GLN:O	2:H:28:SER:C	2.41	0.63
1:G:18:VAL:CG2	1:G:82(C):LEU:HD21	2.28	0.63
2:J:32:SER:O	2:J:50:GLY:C	2.40	0.63
2:J:61:ARG:NH1	2:J:82:ASP:CG	2.57	0.63
4:X:154:ASN:OD1	4:X:156:THR:OG1	2.06	0.63
2:L:158:ASN:OD1	2:L:158:ASN:N	2.28	0.63
4:Q:30:GLN:OE1	4:Q:146:ASN:N	2.29	0.63
3:S:307:LYS:HE2	4:V:61:THR:HG22	1.81	0.63
1:I:52:SER:OG	1:I:54:PHE:HB3	1.99	0.63
3:U:115:VAL:HG11	3:U:116(B):PHE:HB2	1.79	0.63
2:B:170:ASP:OD1	2:B:172:THR:HG22	1.99	0.63
1:G:145:TYR:CD2	1:G:150:VAL:HG23	2.26	0.62
2:J:32:SER:HB2	2:J:51:ALA:HB2	1.80	0.62
2:B:32:SER:HB2	2:B:51:ALA:HB2	1.81	0.62
3:N:90:THR:OG1	3:N:92:SER:OG	2.10	0.62
1:G:83:SER:O	1:G:111:VAL:CB	2.48	0.62
1:I:48:MET:HE1	1:I:82:LEU:HD22	1.80	0.62
3:M:115:VAL:HG11	3:M:116(B):PHE:HB2	1.80	0.62
1:A:68:THR:C	1:A:81:ASP:CB	2.59	0.62
1:K:6:GLN:NE2	1:K:92:CYS:SG	2.73	0.62
1:A:87:THR:OG1	1:A:110:THR:HA	1.99	0.62
3:O:202:VAL:HG11	3:O:251:LEU:HD13	1.80	0.62
2:L:141:PRO:HG3	2:L:199:GLN:NE2	2.15	0.61
3:O:114:SER:HB2	3:O:266:SER:HB2	1.82	0.61
4:R:30:GLN:OE1	4:R:146:ASN:N	2.31	0.61
1:A:74:SER:HB2	4:Q:56:ILE:HG21	1.81	0.61
3:O:38:HIS:CD2	3:O:39:SER:N	2.68	0.61
1:K:6:GLN:HG3	1:K:106:GLY:H	1.63	0.61
3:N:111:GLN:NE2	3:N:262:ARG:NH1	2.48	0.61
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.82	0.61
2:D:61:ARG:NH1	2:D:82:ASP:OD1	2.33	0.61
2:F:166:GLN:HG3	2:F:173:TYR:CZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.36	0.60
1:I:74:SER:HB3	3:O:291:SER:CB	2.31	0.60
3:M:229:ARG:NH2	3:O:207:SER:HA	2.10	0.60
3:O:42:LEU:HD11	3:O:316:LEU:HD22	1.82	0.60
1:I:74:SER:HB3	3:O:291:SER:HB2	1.83	0.60
4:V:158:ASP:OD1	4:V:160:PRO:HD2	2.01	0.60
1:E:74:SER:HB3	3:M:291:SER:OG	2.01	0.60
1:A:74:SER:HB3	3:N:291:SER:CB	2.25	0.60
2:H:32:SER:HB2	2:H:51:ALA:HB2	1.84	0.60
1:G:89:VAL:HG22	1:G:108:THR:HG22	1.83	0.60
3:U:90:THR:OG1	3:U:92:SER:OG	2.08	0.60
4:W:30:GLN:OE1	4:W:146:ASN:N	2.32	0.60
1:A:68:THR:CA	1:A:81:ASP:HB3	2.30	0.60
1:E:36:TRP:CZ3	1:E:92:CYS:HB3	2.37	0.60
3:M:201:TYR:OH	3:M:246:GLU:OE2	2.15	0.60
3:T:90:THR:HG1	3:T:92:SER:HG	1.49	0.60
1:K:42:GLY:O	1:K:43:GLN:NE2	2.30	0.60
4:P:103:GLU:OE2	4:Q:102:LEU:HD21	2.01	0.60
2:D:30:SER:OG	2:D:92:VAL:CG1	2.50	0.60
1:A:61:GLN:N	1:A:61:GLN:OE1	2.35	0.60
1:E:66:ARG:HH11	1:E:82(B):SER:HG	1.42	0.60
1:E:36:TRP:CE2	1:E:80:MET:HB2	2.36	0.59
2:F:27:GLN:O	2:F:28:SER:C	2.41	0.59
2:J:205:VAL:HG13	2:J:205:VAL:O	2.02	0.59
1:A:6:GLN:HG3	1:A:106:GLY:H	1.67	0.59
2:B:158:ASN:OD1	2:B:158:ASN:N	2.33	0.59
3:U:308:TYR:CD2	4:X:89:LEU:HD13	2.38	0.59
3:U:116(B):PHE:CE1	3:U:260:MET:HE2	2.37	0.59
2:L:29:VAL:O	2:L:29:VAL:HG12	2.02	0.59
4:V:51:LYS:HE3	4:V:103:GLU:OE1	2.03	0.59
1:E:40:ALA:HB3	1:E:43:GLN:HG3	1.85	0.58
1:G:36:TRP:CZ3	1:G:92:CYS:HB3	2.37	0.58
1:I:25:SER:O	1:I:25:SER:OG	2.15	0.58
2:J:30:SER:O	2:J:31:SER:OG	2.20	0.58
4:V:9:PHE:O	4:V:135:ASN:HA	2.03	0.58
1:G:87:THR:OG1	1:G:110:THR:HA	2.02	0.58
1:I:5:VAL:HA	1:I:105:LYS:NZ	2.19	0.58
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.38	0.58
3:M:153:TRP:HE1	3:M:195:TYR:HH	1.49	0.58
2:F:158:ASN:OD1	2:F:158:ASN:N	2.35	0.58
1:G:53:ILE:HD13	4:V:49:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:ASN:OD1	2:H:158:ASN:N	2.36	0.58
1:I:74:SER:HB3	3:O:291:SER:OG	2.03	0.58
3:S:42:LEU:HD11	3:S:316:LEU:HD22	1.86	0.58
1:C:63:PHE:HD2	1:C:66:ARG:HD2	1.68	0.58
1:C:95:LYS:HE3	1:C:100(E):TYR:CZ	2.39	0.58
3:S:44:GLU:OE2	3:S:46:LYS:HG2	2.02	0.58
1:A:28:THR:CG2	4:Q:53:ASN:HD22	2.13	0.58
1:A:68:THR:OG1	1:A:81:ASP:HB2	2.02	0.58
2:D:32(A):TYR:HD1	2:D:91:TYR:CE2	2.22	0.58
2:D:158:ASN:OD1	2:D:158:ASN:N	2.37	0.58
2:D:112:ALA:HB1	2:D:201:LEU:CD2	2.34	0.58
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.86	0.58
2:J:201:LEU:HD21	2:J:205:VAL:CG1	2.33	0.58
4:Q:95:ASN:ND2	4:R:95:ASN:HD21	2.01	0.58
4:P:134:GLY:O	4:P:135:ASN:OD1	2.23	0.57
1:I:96:LEU:HD12	1:I:96:LEU:C	2.22	0.57
3:S:39:SER:OG	3:S:315:ARG:NE	2.32	0.57
1:G:83:SER:OG	1:G:84:SER:N	2.35	0.57
2:J:61:ARG:NH1	2:J:82:ASP:OD1	2.37	0.57
3:U:199:ASP:OD1	3:U:214:LYS:NZ	2.37	0.57
1:K:83:SER:O	1:K:83:SER:OG	2.17	0.57
2:D:29:VAL:HG22	2:D:29:VAL:O	2.03	0.57
3:U:114:SER:HB2	3:U:266:SER:HB2	1.86	0.57
4:V:62:GLN:H	4:V:62:GLN:CD	2.13	0.57
4:W:82:LYS:NZ	4:W:86:ASP:OD2	2.34	0.57
1:C:96:LEU:CD1	1:C:102:VAL:HG21	2.35	0.57
1:E:25:SER:O	1:E:25:SER:OG	2.22	0.57
2:L:198:HIS:CG	2:L:199:GLN:H	2.23	0.57
3:T:115:VAL:HG11	3:T:116(B):PHE:HB2	1.87	0.57
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.39	0.57
3:S:103:ILE:HG13	3:S:233:TYR:CE2	2.40	0.57
3:O:163:LYS:NZ	3:O:201:TYR:OH	2.38	0.57
3:S:114:SER:HB2	3:S:266:SER:HB2	1.86	0.56
3:S:180:TRP:CE2	3:S:233:TYR:HB2	2.40	0.56
1:G:5:VAL:HA	1:G:105:LYS:NZ	2.20	0.56
3:N:42:LEU:HD11	3:N:316:LEU:HD22	1.87	0.56
3:S:307:LYS:HE2	4:V:61:THR:CG2	2.36	0.56
3:N:180:TRP:CE2	3:N:233:TYR:HB2	2.40	0.56
1:I:159:LEU:HD21	1:I:182:VAL:HG11	1.88	0.56
2:J:27:GLN:O	2:J:28:SER:C	2.44	0.56
2:H:166:GLN:HG3	2:H:173:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:TRP:CE2	1:I:80:MET:HB2	2.40	0.56
3:N:26:VAL:HG21	3:N:317:ALA:HB2	1.88	0.56
1:A:105:LYS:HE2	1:A:105:LYS:H	1.69	0.56
1:E:87:THR:OG1	1:E:110:THR:HA	2.05	0.56
3:M:207:SER:HA	3:N:229:ARG:HH21	1.71	0.56
3:M:221:PRO:HG2	3:O:242:LYS:O	2.06	0.56
1:C:66:ARG:HB3	1:C:82(B):SER:OG	2.06	0.56
3:S:151:LEU:HB3	3:S:252:VAL:HG12	1.87	0.56
3:T:180:TRP:CE2	3:T:233:TYR:HB2	2.41	0.56
3:O:175:GLU:OE1	3:O:262:ARG:NH1	2.39	0.55
4:P:76:ARG:NH1	4:R:69:GLU:O	2.39	0.55
1:C:73:ILE:HD12	1:C:73:ILE:H	1.71	0.55
3:N:288:ILE:HG22	3:N:290:THR:HG22	1.88	0.55
1:I:105:LYS:H	1:I:105:LYS:HE2	1.71	0.55
3:U:42:LEU:HD11	3:U:316:LEU:HD22	1.87	0.55
3:M:221:PRO:CG	3:O:242:LYS:HB3	2.28	0.55
4:P:148:CYS:O	4:P:151:SER:OG	2.23	0.55
2:B:136:LEU:N	2:B:136:LEU:HD23	2.22	0.55
1:K:83:SER:O	1:K:85:ASP:N	2.36	0.55
2:F:29:VAL:CG2	2:F:68:GLY:O	2.33	0.55
2:L:170:ASP:OD1	2:L:172:THR:HG22	2.06	0.55
2:D:206:THR:O	2:D:206:THR:OG1	2.22	0.55
2:J:14:SER:N	2:J:17:GLU:OE2	2.39	0.55
2:H:24:ARG:NH1	2:H:70:ASP:OD1	2.40	0.55
3:S:26:VAL:HG21	3:S:317:ALA:HB2	1.89	0.55
1:E:52:SER:O	1:E:53:ILE:N	2.40	0.54
2:D:33:LEU:HD12	2:D:89:GLN:C	2.33	0.54
1:E:67:VAL:HA	1:E:81:ASP:O	2.08	0.54
1:I:19:GLN:HG3	1:I:81:ASP:OD2	2.08	0.54
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.88	0.54
1:C:66:ARG:CB	1:C:82(B):SER:CB	2.82	0.54
2:F:136:LEU:HD23	2:F:136:LEU:N	2.22	0.54
1:E:19:GLN:HG3	1:E:81:ASP:OD2	2.06	0.54
2:H:204:PRO:O	2:H:206:THR:CG2	2.56	0.54
1:I:5:VAL:HA	1:I:105:LYS:HZ1	1.73	0.54
3:M:52:CYS:HB3	3:M:277:CYS:O	2.07	0.54
4:W:62:GLN:CD	4:W:62:GLN:H	2.14	0.54
3:O:18:HIS:O	3:O:320:LEU:HD11	2.07	0.54
3:U:175:GLU:OE1	3:U:262:ARG:NH1	2.41	0.54
2:B:38:GLN:NE2	2:B:87:TYR:CE2	2.75	0.54
1:I:38:ARG:HG3	1:I:90:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:115:VAL:HG11	3:N:116(B):PHE:HB2	1.90	0.54
3:T:277:CYS:O	3:T:277:CYS:SG	2.55	0.53
1:K:163:VAL:HG22	1:K:182:VAL:HG22	1.90	0.53
3:N:295:GLN:O	3:N:308:TYR:HA	2.08	0.53
3:O:77:GLU:HG3	3:O:149:LYS:HE3	1.90	0.53
4:Q:82:LYS:NZ	4:Q:86:ASP:OD2	2.36	0.53
1:C:66:ARG:HD3	1:C:82(B):SER:HB2	1.89	0.53
1:K:59:TYR:HE1	1:K:69:ILE:HG13	1.74	0.53
3:U:202:VAL:HG11	3:U:251:LEU:HD13	1.90	0.53
1:E:84:SER:HA	1:E:111:VAL:HB	1.90	0.53
3:N:103:ILE:HG13	3:N:233:TYR:CE2	2.44	0.53
2:J:201:LEU:CD2	2:J:205:VAL:HG12	2.38	0.53
3:O:111:GLN:OE1	3:O:262:ARG:NE	2.42	0.53
3:O:307:LYS:NZ	4:P:90:ASP:OD2	2.41	0.53
4:X:27:GLN:O	4:X:27:GLN:HG3	2.08	0.53
1:C:74:SER:CB	3:U:291:SER:HB2	2.37	0.53
2:D:29:VAL:CG1	2:D:71:PHE:CE2	2.76	0.53
2:H:136:LEU:N	2:H:136:LEU:HD23	2.24	0.53
1:I:105:LYS:H	1:I:105:LYS:CE	2.21	0.53
2:F:27:GLN:O	2:F:28:SER:O	2.27	0.53
1:G:114:ALA:HB3	1:G:146:PHE:CE2	2.43	0.53
3:N:58:PRO:HB3	3:N:86:TYR:CZ	2.44	0.53
2:D:30:SER:OG	2:D:92:VAL:HG12	2.09	0.53
2:D:32:SER:C	2:D:50:GLY:O	2.52	0.53
2:L:32(A):TYR:HB2	2:L:92:VAL:HG12	1.91	0.53
4:V:103:GLU:OE2	4:W:102:LEU:HD21	2.09	0.53
2:B:32:SER:HB2	2:B:51:ALA:CB	2.39	0.52
1:I:6:GLN:HG3	1:I:106:GLY:H	1.74	0.52
2:J:158:ASN:OD1	2:J:158:ASN:N	2.40	0.52
3:U:180:TRP:CE2	3:U:233:TYR:HB2	2.44	0.52
3:O:115:VAL:HG11	3:O:116(B):PHE:HB2	1.91	0.52
2:L:136:LEU:HD21	2:L:196:VAL:HG21	1.90	0.52
3:T:307:LYS:HE2	4:W:61:THR:HG22	1.90	0.52
2:D:30:SER:OG	2:D:92:VAL:HG11	2.10	0.52
2:F:119:PRO:HB3	2:F:209:PHE:CE2	2.44	0.52
3:T:307:LYS:HE2	4:W:61:THR:CG2	2.40	0.52
3:M:26:VAL:HG21	3:M:317:ALA:HB2	1.92	0.52
4:P:62:GLN:NE2	4:Q:86:ASP:HB3	2.24	0.52
4:V:134:GLY:O	4:V:135:ASN:OD1	2.27	0.52
1:K:84:SER:H	1:K:111:VAL:HG11	1.75	0.52
3:O:38:HIS:CD2	3:O:39:SER:H	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:H	1:A:81:ASP:CB	2.08	0.52
1:A:210:ARG:HH12	1:A:212:GLU:HB3	1.75	0.52
2:J:37:GLN:HG3	2:J:86:TYR:CE2	2.45	0.52
3:N:134:GLY:HA3	3:N:153:TRP:HB3	1.92	0.52
1:C:96:LEU:HD13	1:C:102:VAL:CG2	2.40	0.51
2:H:170:ASP:OD1	2:H:172:THR:HG22	2.09	0.51
1:G:52:SER:O	1:G:53:ILE:N	2.43	0.51
3:M:284:PRO:HD3	3:M:300:ILE:O	2.09	0.51
3:N:163:LYS:HB3	3:U:159:ASN:HD21	1.74	0.51
1:I:154:TRP:CH2	1:I:196:CYS:HB3	2.45	0.51
1:A:52:SER:O	1:A:53:ILE:N	2.44	0.51
1:C:52:SER:O	1:C:53:ILE:N	2.43	0.51
1:E:5:VAL:HA	1:E:105:LYS:NZ	2.24	0.51
1:C:163:VAL:HG22	1:C:182:VAL:HG22	1.93	0.51
1:I:87:THR:OG1	1:I:110:THR:HA	2.11	0.51
3:M:288:ILE:HG21	3:M:297:ILE:HG13	1.93	0.51
3:S:123:LYS:HZ1	3:S:133:ASN:ND2	2.08	0.51
2:B:166:GLN:HG3	2:B:173:TYR:CZ	2.46	0.51
2:D:141:PRO:O	2:D:198:HIS:HE1	1.93	0.51
1:G:145:TYR:CD1	1:G:145:TYR:C	2.85	0.51
4:V:142:HIS:HB2	4:V:165:GLU:CD	2.36	0.51
1:E:148:GLU:OE1	1:E:149:PRO:HA	2.11	0.51
3:N:100:GLY:HA3	3:N:230:MET:O	2.10	0.51
2:B:32:SER:O	2:B:32:SER:OG	2.21	0.51
2:D:112:ALA:HB1	2:D:201:LEU:HD23	1.93	0.51
1:G:38:ARG:HG3	1:G:90:TYR:CE1	2.46	0.50
1:C:38:ARG:HG3	1:C:90:TYR:CE1	2.46	0.50
1:K:100(A):TYR:HD2	4:W:42:GLN:OE1	1.93	0.50
1:A:59:TYR:HE1	1:A:69:ILE:HG13	1.77	0.50
1:C:74:SER:HB3	3:U:291:SER:CB	2.38	0.50
2:H:175:LEU:HD12	2:H:176:SER:H	1.77	0.50
3:M:103:ILE:HG13	3:M:233:TYR:CE2	2.47	0.50
1:E:32:TYR:HB3	1:E:100:TYR:CD1	2.46	0.50
1:G:28:THR:HG21	4:V:53:ASN:HD22	1.71	0.50
3:T:69:TRP:HE1	3:T:81:THR:HG21	1.77	0.50
1:A:68:THR:CA	1:A:81:ASP:CB	2.89	0.50
2:D:29:VAL:HG11	2:D:71:PHE:HE2	1.69	0.50
2:F:47:LEU:HD23	2:F:58:ILE:HD12	1.94	0.50
2:J:32:SER:HB2	2:J:51:ALA:CB	2.42	0.50
2:L:115:VAL:HG22	2:L:136:LEU:HD22	1.93	0.50
3:O:100:GLY:HA3	3:O:230:MET:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:95:ASN:HD21	4:R:95:ASN:HD21	1.58	0.50
4:V:98:LEU:O	4:V:102:LEU:HG	2.11	0.50
1:A:105:LYS:H	1:A:105:LYS:CE	2.25	0.50
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.46	0.50
3:M:151:LEU:HB3	3:M:252:VAL:HG12	1.94	0.50
3:U:77:GLU:HG3	3:U:149:LYS:HE3	1.94	0.50
1:E:59:TYR:HE1	1:E:69:ILE:HG13	1.76	0.49
4:P:158:ASP:OD1	4:P:160:PRO:HD2	2.12	0.49
1:K:74:SER:HB2	4:W:56:ILE:HG21	1.93	0.49
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.47	0.49
3:N:11:ASP:OD1	4:Q:28:ASN:HA	2.11	0.49
4:P:70:PHE:CE2	4:P:78:GLU:HA	2.47	0.49
3:S:134:GLY:HA3	3:S:153:TRP:HB3	1.93	0.49
3:O:45:ASP:C	3:O:297:ILE:HD11	2.36	0.49
3:O:189:ALA:HA	3:U:189:ALA:CB	2.42	0.49
3:M:111:GLN:OE1	3:M:262:ARG:NH1	2.41	0.49
2:B:32(A):TYR:HD1	2:B:91:TYR:CE2	2.30	0.49
2:J:170:ASP:OD1	2:J:172:THR:HG22	2.12	0.49
2:D:24:ARG:NH1	2:D:70:ASP:OD1	2.45	0.49
1:K:74:SER:HB3	3:T:291:SER:CB	2.40	0.49
4:P:9:PHE:O	4:P:135:ASN:HA	2.12	0.49
1:E:36:TRP:CH2	1:E:92:CYS:HB3	2.47	0.49
1:G:145:TYR:HD2	1:G:150:VAL:CG2	2.19	0.49
3:S:50:LYS:HD2	3:S:275:HIS:HB2	1.94	0.49
1:I:83:SER:O	1:I:111:VAL:CB	2.59	0.49
3:U:284:PRO:HD3	3:U:300:ILE:O	2.13	0.49
1:C:66:ARG:CB	1:C:82(B):SER:OG	2.61	0.49
1:I:52:SER:O	1:I:53:ILE:N	2.46	0.49
3:T:103:ILE:HG13	3:T:233:TYR:CE2	2.47	0.49
2:B:30:SER:OG	2:B:92:VAL:HG11	2.12	0.48
2:D:67:SER:HA	2:D:71:PHE:CE1	2.47	0.48
1:G:178:LEU:C	1:G:178:LEU:HD12	2.38	0.48
2:B:29:VAL:CG1	2:B:71:PHE:CE2	2.95	0.48
1:C:47:TRP:CG	2:D:96:LEU:HB2	2.48	0.48
2:F:32:SER:HB2	2:F:51:ALA:HB2	1.95	0.48
1:K:84:SER:O	1:K:87:THR:HG22	2.13	0.48
3:M:207:SER:OG	3:M:241:ASP:OD1	2.27	0.48
1:E:95:LYS:HE3	1:E:100(E):TYR:CZ	2.48	0.48
1:G:42:GLY:O	1:G:43:GLN:NE2	2.43	0.48
1:G:145:TYR:HD1	1:G:145:TYR:O	1.97	0.48
3:O:284:PRO:HD3	3:O:300:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:GLU:OE1	2:B:173:TYR:OH	2.26	0.48
1:C:87:THR:OG1	1:C:110:THR:HA	2.13	0.48
1:G:25:SER:O	1:G:25:SER:OG	2.19	0.48
2:J:4:LEU:HD11	2:J:90:GLN:HB3	1.96	0.48
2:L:141:PRO:O	2:L:198:HIS:HE1	1.97	0.48
3:S:123:LYS:NZ	3:S:133:ASN:HD21	2.10	0.48
4:V:1:GLY:O	4:V:2:LEU:C	2.56	0.48
1:E:74:SER:HB3	3:M:291:SER:CB	2.43	0.48
1:K:52:SER:O	1:K:53:ILE:N	2.46	0.48
3:N:45:ASP:C	3:N:297:ILE:HD11	2.39	0.48
3:O:186:SER:HA	3:O:218:ALA:O	2.12	0.48
2:F:83:PHE:HA	2:F:104:VAL:HG23	1.96	0.48
1:G:73:ILE:H	1:G:73:ILE:HD12	1.79	0.48
1:I:123:PRO:HD2	2:J:121:SER:HB3	1.94	0.48
3:T:199:ASP:OD1	3:T:214:LYS:NZ	2.42	0.48
4:X:158:ASP:OD1	4:X:160:PRO:HD2	2.13	0.48
4:X:159:TYR:HB3	4:X:160:PRO:HD3	1.95	0.48
2:D:61:ARG:NH1	2:D:82:ASP:OD2	2.47	0.48
1:E:38:ARG:HG3	1:E:90:TYR:CE1	2.48	0.48
2:L:198:HIS:CG	2:L:199:GLN:N	2.81	0.48
3:O:66:ILE:HD12	3:O:109:ARG:CZ	2.44	0.48
4:V:148:CYS:O	4:V:151:SER:OG	2.29	0.48
4:W:17:MET:HE3	4:W:20:GLY:O	2.14	0.48
2:D:30:SER:OG	2:D:31:SER:N	2.46	0.48
1:E:36:TRP:CG	1:E:80:MET:HG3	2.48	0.48
1:E:53:ILE:HD13	4:P:49:THR:HA	1.96	0.48
1:K:129:LYS:HZ3	2:L:207:LYS:HD3	1.79	0.48
1:C:40:ALA:HB3	1:C:43:GLN:HB2	1.95	0.48
2:D:61:ARG:NH1	2:D:82:ASP:CG	2.72	0.48
2:D:163:VAL:HG22	2:D:175:LEU:HD13	1.96	0.48
1:E:178:LEU:C	1:E:178:LEU:HD12	2.39	0.48
1:I:47:TRP:CG	2:J:96:LEU:HB2	2.49	0.48
1:I:82(C):LEU:HD12	1:I:82(C):LEU:HA	1.53	0.48
4:P:62:GLN:CD	4:P:62:GLN:H	2.22	0.48
1:I:95:LYS:HE3	1:I:100(E):TYR:CZ	2.49	0.48
4:R:164:GLU:O	4:R:168:LEU:HD13	2.13	0.48
1:A:7:SER:HB3	1:A:21:SER:OG	2.14	0.47
1:C:6:GLN:NE2	1:C:92:CYS:SG	2.87	0.47
1:I:47:TRP:CD2	2:J:96:LEU:HB2	2.49	0.47
3:U:100:GLY:HA3	3:U:230:MET:O	2.14	0.47
1:C:100(B):PHE:CE1	4:X:19:ASP:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:ILE:HD11	1:K:71:ALA:HB2	1.96	0.47
3:O:159:ASN:ND2	3:T:163:LYS:NZ	2.62	0.47
3:T:288:ILE:HG22	3:T:290:THR:HG22	1.96	0.47
1:C:47:TRP:NE1	2:D:96:LEU:HD12	2.29	0.47
1:E:143:LYS:HE3	1:E:144:ASP:OD1	2.14	0.47
1:K:105:LYS:HE2	1:K:105:LYS:H	1.80	0.47
2:L:141:PRO:CG	2:L:199:GLN:NE2	2.77	0.47
3:S:44:GLU:HG2	3:S:290:THR:HG21	1.97	0.47
4:V:102:LEU:CD2	4:X:103:GLU:OE2	2.62	0.47
1:I:100(B):PHE:CE1	4:R:19:ASP:HA	2.49	0.47
3:M:307:LYS:HE2	4:P:61:THR:HG22	1.97	0.47
3:T:111:GLN:HE22	3:T:262:ARG:NH1	2.11	0.47
3:U:48:ASN:O	3:U:50:LYS:HG2	2.14	0.47
2:D:8:PRO:HG2	2:D:10:THR:O	2.14	0.47
1:G:129:LYS:HE2	1:G:129:LYS:HA	1.96	0.47
2:L:136:LEU:N	2:L:136:LEU:HD23	2.28	0.47
1:C:59:TYR:HE1	1:C:69:ILE:HG13	1.80	0.47
2:D:47:LEU:O	2:D:48:ILE:HD13	2.15	0.47
2:H:204:PRO:O	2:H:205:VAL:C	2.55	0.47
1:A:32:TYR:HB3	1:A:100:TYR:CD1	2.50	0.47
1:A:38:ARG:HG3	1:A:90:TYR:CE1	2.50	0.47
1:G:159:LEU:HD21	1:G:182:VAL:HG11	1.96	0.47
3:M:100:GLY:HA3	3:M:230:MET:O	2.15	0.47
3:S:185:PRO:O	3:S:217:ILE:HA	2.15	0.47
3:U:262:ARG:HG3	3:U:262:ARG:HH11	1.78	0.47
3:U:307:LYS:HE2	4:X:61:THR:HG22	1.96	0.47
1:I:47:TRP:NE1	2:J:96:LEU:HD12	2.30	0.47
3:N:307:LYS:HE2	4:Q:61:THR:CG2	2.45	0.47
3:O:195:TYR:CZ	3:O:250:ASN:HA	2.49	0.47
3:T:38:HIS:CD2	3:T:39:SER:N	2.83	0.47
2:B:175:LEU:HD12	2:B:176:SER:H	1.79	0.47
1:C:38:ARG:NH2	1:C:86:ASP:OD1	2.48	0.47
3:S:202:VAL:HG11	3:S:251:LEU:HD13	1.97	0.47
1:I:144:ASP:OD1	1:I:171:GLN:NE2	2.43	0.46
3:M:106:GLU:CD	4:P:71:ASN:HB3	2.39	0.46
3:O:56:VAL:HB	3:O:85:SER:HB3	1.98	0.46
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.97	0.46
3:S:45:ASP:C	3:S:297:ILE:HD11	2.40	0.46
3:S:100:GLY:HA3	3:S:230:MET:O	2.15	0.46
1:A:61:GLN:HA	1:A:64:GLN:HB2	1.98	0.46
3:M:50:LYS:HD2	3:M:275:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:58:PRO:HB3	3:M:86:TYR:CZ	2.51	0.46
1:C:105:LYS:HE2	1:C:105:LYS:H	1.80	0.46
1:G:105:LYS:H	1:G:105:LYS:HE2	1.80	0.46
1:K:94:ARG:NE	1:K:95:LYS:O	2.41	0.46
3:U:119:GLU:CD	3:U:122:PRO:HA	2.39	0.46
4:X:30:GLN:OE1	4:X:146:ASN:N	2.42	0.46
2:B:21:LEU:N	2:B:21:LEU:HD12	2.31	0.46
1:K:129:LYS:HE2	1:K:129:LYS:HA	1.96	0.46
3:M:114:SER:HB2	3:M:266:SER:CB	2.44	0.46
3:N:110:GLU:HG3	4:R:75:LYS:HE3	1.96	0.46
3:U:58:PRO:HB3	3:U:86:TYR:CZ	2.50	0.46
2:F:30:SER:HB2	2:F:92:VAL:CG1	2.46	0.46
2:H:67:SER:HA	2:H:71:PHE:CE1	2.51	0.46
3:N:163:LYS:CB	3:U:159:ASN:ND2	2.78	0.46
4:P:102:LEU:HD23	4:P:102:LEU:HA	1.77	0.46
3:S:107:GLU:O	3:S:111:GLN:HG2	2.15	0.46
3:S:123:LYS:NZ	3:S:133:ASN:ND2	2.64	0.46
3:T:111:GLN:NE2	3:T:262:ARG:NH1	2.63	0.46
1:A:67:VAL:CA	1:A:81:ASP:O	2.63	0.46
2:B:89:GLN:HG2	2:B:90:GLN:N	2.31	0.46
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.50	0.46
2:J:47:LEU:HD11	2:J:86:TYR:HE2	1.81	0.46
2:J:89:GLN:HG2	2:J:90:GLN:N	2.31	0.46
2:J:192:TYR:HB2	2:J:209:PHE:CE1	2.51	0.46
1:K:84:SER:H	1:K:111:VAL:CG1	2.29	0.46
3:U:208:ARG:NH1	4:V:72:HIS:CD2	2.83	0.46
2:B:206:THR:O	2:B:206:THR:OG1	2.26	0.46
1:G:52:SER:OG	1:G:54:PHE:HB3	2.15	0.46
3:M:202:VAL:HG11	3:M:251:LEU:HD13	1.96	0.46
4:R:158:ASP:OD1	4:R:160:PRO:HD2	2.16	0.46
1:C:53:ILE:CD1	4:X:49:THR:HA	2.46	0.46
2:F:119:PRO:HB3	2:F:209:PHE:CZ	2.51	0.46
1:I:59:TYR:HE1	1:I:69:ILE:HG13	1.81	0.46
2:L:21:LEU:HD12	2:L:21:LEU:N	2.30	0.46
3:O:107:GLU:O	3:O:111:GLN:HG2	2.16	0.46
3:O:303:GLY:HA2	4:R:63:PHE:CE2	2.50	0.46
4:W:4:GLY:O	4:W:8:GLY:HA3	2.15	0.46
2:D:141:PRO:CG	2:D:199:GLN:NE2	2.77	0.46
1:E:47:TRP:CG	2:F:96:LEU:HB2	2.51	0.46
2:H:198:HIS:CD2	2:H:199:GLN:O	2.68	0.46
3:O:167:SER:OG	3:O:244:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:1:GLY:O	4:P:2:LEU:C	2.57	0.46
3:S:284:PRO:HD3	3:S:300:ILE:O	2.15	0.46
1:A:48:MET:HE1	1:A:82:LEU:HD13	1.98	0.45
2:D:136:LEU:N	2:D:136:LEU:HD23	2.31	0.45
2:D:150:VAL:HG13	2:D:155:GLN:HG2	1.98	0.45
2:H:200:GLY:O	2:H:201:LEU:HD23	2.16	0.45
2:L:90:GLN:CD	2:L:90:GLN:C	2.83	0.45
3:S:38:HIS:CD2	3:S:39:SER:N	2.84	0.45
1:A:36:TRP:CD2	1:A:80:MET:HG3	2.52	0.45
3:N:38:HIS:CD2	3:N:39:SER:N	2.84	0.45
4:V:59:MET:HE2	4:V:59:MET:HB2	1.86	0.45
1:A:47:TRP:HZ3	2:B:95:PRO:HA	1.75	0.45
1:E:96:LEU:HD12	1:E:96:LEU:HA	1.75	0.45
1:G:4:LEU:HD11	1:G:94:ARG:HG2	1.99	0.45
1:G:145:TYR:CD1	1:G:145:TYR:O	2.70	0.45
3:U:107:GLU:O	3:U:111:GLN:HG2	2.17	0.45
4:V:102:LEU:HD21	4:X:103:GLU:OE2	2.16	0.45
2:D:175:LEU:HD12	2:D:176:SER:H	1.81	0.45
2:J:136:LEU:N	2:J:136:LEU:HD23	2.31	0.45
4:Q:62:GLN:H	4:Q:62:GLN:CD	2.24	0.45
4:W:9:PHE:O	4:W:135:ASN:HA	2.16	0.45
1:G:95:LYS:HE3	1:G:100(E):TYR:CZ	2.51	0.45
1:I:72:ASP:OD1	3:O:291:SER:OG	2.30	0.45
2:J:33:LEU:HD22	2:J:71:PHE:CG	2.52	0.45
3:N:69:TRP:HE1	3:N:81:THR:HG21	1.81	0.45
4:R:74:GLU:HB3	4:R:77:ILE:HD11	1.98	0.45
3:U:134:GLY:HA3	3:U:153:TRP:HB3	1.98	0.45
2:F:141:PRO:HG3	2:F:199:GLN:NE2	2.31	0.45
2:H:32(A):TYR:HB2	2:H:92:VAL:HG12	1.99	0.45
2:J:38:GLN:NE2	2:J:87:TYR:HE2	2.14	0.45
2:L:112:ALA:CB	2:L:200:GLY:O	2.60	0.45
3:U:116(B):PHE:HE1	3:U:260:MET:HE2	1.81	0.45
4:X:39:LYS:HB2	4:X:39:LYS:HE3	1.69	0.45
1:A:5:VAL:HA	1:A:105:LYS:NZ	2.32	0.45
1:C:83:SER:O	1:C:111:VAL:CB	2.64	0.45
2:J:21:LEU:HD12	2:J:21:LEU:N	2.32	0.45
4:X:17:MET:HE2	4:X:17:MET:HB3	1.75	0.45
1:C:131:THR:HA	1:C:136:ALA:HA	1.97	0.45
2:F:139:PHE:HD2	2:F:198:HIS:CE1	2.34	0.45
1:G:83:SER:O	1:G:111:VAL:HB	2.17	0.45
2:J:105:GLU:OE1	2:J:173:TYR:OH	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:321:ARG:HD2	3:O:323:ILE:HD11	1.98	0.45
2:L:148:TRP:O	2:L:154:LEU:HD12	2.17	0.45
3:M:282:GLN:OE1	3:M:287:ALA:HB2	2.17	0.45
4:W:158:ASP:OD1	4:W:160:PRO:HD2	2.17	0.45
4:X:6:ILE:HD13	4:X:6:ILE:HG21	1.73	0.45
2:J:113:PRO:HB3	2:J:139:PHE:HB3	1.99	0.45
2:L:32(A):TYR:HB2	2:L:92:VAL:CG1	2.47	0.45
3:M:221:PRO:HG3	3:O:242:LYS:CB	2.32	0.45
4:V:4:GLY:O	4:V:8:GLY:HA3	2.17	0.45
4:V:38:LEU:HA	4:V:38:LEU:HD23	1.77	0.45
1:C:96:LEU:CD1	1:C:102:VAL:CG2	2.95	0.44
4:V:2:LEU:HD12	4:V:2:LEU:HA	1.69	0.44
1:G:66:ARG:HB3	1:G:82(A):SER:O	2.18	0.44
2:J:166:GLN:HG3	2:J:173:TYR:CZ	2.52	0.44
2:J:203:SER:O	2:J:203:SER:OG	2.34	0.44
1:K:66:ARG:HB3	1:K:82(A):SER:HB2	1.03	0.44
3:N:137:ALA:HA	3:N:145:LYS:HG2	1.99	0.44
4:Q:9:PHE:O	4:Q:135:ASN:HA	2.18	0.44
3:U:90(A):PRO:HD2	3:U:271:ASP:OD1	2.17	0.44
4:V:3:PHE:CZ	4:W:2:LEU:HG	2.52	0.44
1:C:209:LYS:HD2	1:C:209:LYS:HA	1.86	0.44
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.98	0.44
1:G:53:ILE:CD1	4:V:49:THR:HA	2.47	0.44
1:G:197:ASN:ND2	1:G:208:ASP:OD2	2.45	0.44
3:M:314:LEU:HD23	3:M:314:LEU:HA	1.85	0.44
3:T:69:TRP:HE1	3:T:81:THR:CG2	2.31	0.44
3:T:295:GLN:O	3:T:308:TYR:HA	2.17	0.44
2:B:145:LYS:HE2	2:B:147:GLN:NE2	2.32	0.44
1:C:66:ARG:CD	1:C:82(B):SER:HB2	2.47	0.44
2:D:47:LEU:HD23	2:D:58:ILE:HD12	1.98	0.44
2:D:161:GLU:HA	2:D:177:SER:HA	1.99	0.44
2:J:33:LEU:HD22	2:J:71:PHE:CD2	2.52	0.44
3:T:90:THR:OG1	3:T:92:SER:OG	2.21	0.44
3:U:111:GLN:OE1	3:U:262:ARG:NE	2.50	0.44
1:A:53:ILE:HD13	4:Q:49:THR:HA	1.98	0.44
1:A:66:ARG:HB3	1:A:82(B):SER:OG	2.18	0.44
2:D:33:LEU:HD12	2:D:33:LEU:HA	1.70	0.44
2:J:163:VAL:HG22	2:J:175:LEU:HD13	1.99	0.44
2:J:175:LEU:HD12	2:J:176:SER:H	1.82	0.44
1:K:73:ILE:HD12	1:K:73:ILE:H	1.81	0.44
3:M:90(A):PRO:HD2	3:M:271:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:180:TRP:CE2	3:O:233:TYR:HB2	2.52	0.44
3:S:30:LEU:HD23	3:S:30:LEU:HA	1.61	0.44
3:T:56:VAL:HB	3:T:85:SER:HB3	1.99	0.44
4:X:2:LEU:HD12	4:X:2:LEU:HA	1.75	0.44
1:A:178:LEU:HD12	1:A:178:LEU:C	2.43	0.44
1:C:32:TYR:HB3	1:C:100:TYR:CD1	2.53	0.44
1:C:63:PHE:CD2	1:C:66:ARG:HD2	2.51	0.44
1:C:154:TRP:CZ3	1:C:196:CYS:HB3	2.52	0.44
2:F:78:LEU:HD23	2:F:78:LEU:HA	1.73	0.44
2:F:175:LEU:HD12	2:F:176:SER:H	1.83	0.44
2:H:118:PHE:HB2	2:H:133:VAL:HB	2.00	0.44
2:L:18:ARG:HG2	2:L:76:THR:HA	1.99	0.44
3:O:52:CYS:HB3	3:O:277:CYS:O	2.16	0.44
4:P:59:MET:HE1	4:P:92:TRP:CZ3	2.53	0.44
3:S:20:ASN:OD1	3:S:20:ASN:C	2.60	0.44
2:B:11:LEU:O	2:B:104:VAL:HA	2.18	0.44
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.98	0.44
2:F:21:LEU:N	2:F:21:LEU:HD12	2.33	0.44
1:G:36:TRP:CH2	1:G:92:CYS:HB3	2.52	0.44
3:M:71:LEU:O	3:M:148:TYR:HB3	2.18	0.44
3:M:112:LEU:HD23	3:M:260:MET:HE1	1.99	0.44
3:S:314:LEU:HD23	3:S:314:LEU:HA	1.71	0.44
3:T:116(B):PHE:CE1	3:T:260:MET:HE2	2.53	0.44
3:U:45:ASP:O	3:U:46:LYS:HD2	2.18	0.44
1:A:51:ILE:HD11	1:A:71:ALA:HB2	2.00	0.44
1:A:73:ILE:HD12	1:A:73:ILE:H	1.82	0.44
2:B:31:SER:HB2	2:B:32:SER:H	1.63	0.44
2:B:33:LEU:HD12	2:B:89:GLN:O	2.18	0.44
2:D:81:GLU:CD	2:D:81:GLU:H	2.25	0.44
4:R:102:LEU:HD23	4:R:102:LEU:HA	1.73	0.44
3:T:53:LYS:HE3	3:T:276:ASP:OD1	2.18	0.44
2:B:90:GLN:C	2:B:90:GLN:CD	2.86	0.44
2:H:175:LEU:HD12	2:H:176:SER:N	2.32	0.44
1:I:53:ILE:HD13	4:R:49:THR:HA	2.00	0.44
1:I:100(A):TYR:HD2	4:R:42:GLN:OE1	2.01	0.44
3:M:107:GLU:O	3:M:111:GLN:HG2	2.17	0.44
3:M:138:ALA:HB2	3:M:226:GLN:HE21	1.82	0.44
1:I:16:SER:O	1:I:82(C):LEU:HB2	2.17	0.43
1:I:73:ILE:HD12	1:I:73:ILE:H	1.83	0.43
2:J:14:SER:O	2:J:17:GLU:OE2	2.36	0.43
3:O:15:ILE:HD11	4:R:122:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:151:LEU:HB3	3:O:252:VAL:HG12	1.99	0.43
1:A:51:ILE:CD1	1:A:71:ALA:HB2	2.48	0.43
1:A:80:MET:HE3	1:A:80:MET:HB3	1.56	0.43
2:D:191:VAL:O	2:D:191:VAL:HG13	2.18	0.43
3:M:163:LYS:HE3	3:M:246:GLU:OE2	2.18	0.43
3:O:197:ASN:HB2	3:O:200:THR:HG22	2.00	0.43
4:Q:17:MET:SD	4:Q:23:GLY:HA3	2.58	0.43
1:A:169:VAL:O	1:A:176:TYR:HA	2.18	0.43
2:B:33:LEU:CD2	2:B:71:PHE:CD2	2.97	0.43
1:G:41:PRO:O	1:G:43:GLN:HG2	2.18	0.43
2:J:37:GLN:HG3	2:J:86:TYR:CZ	2.54	0.43
3:M:218:ALA:HB3	3:O:203:PHE:CE2	2.53	0.43
3:N:64:CYS:O	3:N:92:SER:HB3	2.18	0.43
4:Q:6:ILE:HD13	4:Q:6:ILE:HG21	1.79	0.43
4:R:2:LEU:HA	4:R:2:LEU:HD12	1.58	0.43
3:S:195:TYR:CZ	3:S:250:ASN:HA	2.53	0.43
4:W:128:ASN:ND2	4:W:159:TYR:OH	2.47	0.43
4:X:164:GLU:O	4:X:168:LEU:HD13	2.18	0.43
1:K:80:MET:HB3	1:K:80:MET:HE3	1.75	0.43
4:P:126:LEU:HA	4:P:126:LEU:HD23	1.70	0.43
4:X:74:GLU:HB3	4:X:77:ILE:HD11	2.00	0.43
1:C:28:THR:O	1:C:29:PHE:C	2.60	0.43
1:G:51:ILE:HD11	1:G:71:ALA:HB2	1.99	0.43
1:G:130:SER:HA	2:H:116:PHE:HD1	1.83	0.43
4:W:2:LEU:HD12	4:W:2:LEU:HA	1.54	0.43
2:D:32:SER:O	2:D:50:GLY:O	2.36	0.43
1:K:105:LYS:H	1:K:105:LYS:CE	2.32	0.43
1:K:192:GLN:OE1	1:K:193:THR:N	2.51	0.43
2:L:61:ARG:NH1	2:L:82:ASP:CG	2.76	0.43
3:M:176:VAL:HA	3:M:258:PHE:O	2.18	0.43
3:O:189:ALA:HA	3:U:189:ALA:HB1	2.00	0.43
3:T:208:ARG:HH11	4:X:72:HIS:CE1	2.37	0.43
2:B:31:SER:OG	2:B:32(A):TYR:CE2	2.69	0.43
1:C:18:VAL:CG2	1:C:82(C):LEU:HD21	2.44	0.43
1:E:82(B):SER:CB	1:E:82(C):LEU:HA	2.46	0.43
1:G:145:TYR:CD1	1:G:176:TYR:O	2.72	0.43
2:J:27:GLN:C	2:J:28:SER:O	2.57	0.43
4:P:102:LEU:HD21	4:R:103:GLU:OE2	2.18	0.43
4:P:105:GLU:CG	4:R:106:ARG:HH12	2.31	0.43
4:P:173:ILE:C	4:P:175:SER:H	2.27	0.43
3:S:315:ARG:HH11	3:S:315:ARG:HD2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:SER:HA	1:C:111:VAL:HB	2.00	0.43
1:E:32:TYR:HB3	1:E:100:TYR:CE1	2.53	0.43
1:K:53:ILE:HD13	4:W:49:THR:HA	2.01	0.43
3:O:119:GLU:CD	3:O:122:PRO:HA	2.44	0.43
3:T:161:TYR:CZ	3:T:249:GLY:HA2	2.54	0.43
3:T:315:ARG:HH11	3:T:315:ARG:HD2	1.60	0.43
2:J:88:CYS:O	2:J:99:GLY:N	2.51	0.43
3:M:53:LYS:HG2	3:M:57:ALA:HA	2.00	0.43
3:O:314:LEU:HD23	3:O:314:LEU:HA	1.76	0.43
4:P:95:ASN:ND2	4:Q:95:ASN:HD21	2.17	0.43
3:U:308:TYR:HD2	4:X:89:LEU:HD13	1.81	0.43
4:W:99:LEU:HD12	4:W:99:LEU:HA	1.78	0.43
2:B:175:LEU:HD12	2:B:176:SER:N	2.33	0.43
1:E:159:LEU:HD21	1:E:182:VAL:HG11	2.01	0.43
2:H:201:LEU:HD23	2:H:201:LEU:HA	1.73	0.43
3:O:177:LEU:HA	3:O:236:LEU:HD23	2.01	0.43
4:Q:68:LYS:HE3	4:R:79:ASN:HB2	2.00	0.43
4:R:27:GLN:O	4:R:27:GLN:HG3	2.18	0.43
3:U:167:SER:OG	3:U:244:THR:HG22	2.18	0.43
1:C:82(C):LEU:HD12	1:C:82(C):LEU:HA	1.55	0.42
1:G:146:PHE:O	1:G:200:HIS:HE1	2.02	0.42
1:G:154:TRP:CZ3	1:G:196:CYS:HB3	2.53	0.42
1:I:83:SER:OG	1:I:84:SER:N	2.51	0.42
4:X:59:MET:HB2	4:X:59:MET:HE2	1.81	0.42
2:B:58:ILE:HD13	2:B:58:ILE:HA	1.83	0.42
1:C:89:VAL:HG22	1:C:108:THR:HG22	2.02	0.42
2:L:136:LEU:CD2	2:L:196:VAL:HG21	2.48	0.42
3:M:123:LYS:HZ2	3:M:133:ASN:HD21	1.66	0.42
4:Q:158:ASP:OD1	4:Q:160:PRO:HD2	2.19	0.42
2:B:122:ASP:O	2:B:125:LEU:N	2.51	0.42
2:B:203:SER:HA	2:B:204:PRO:HD3	1.53	0.42
1:E:80:MET:HE3	1:E:80:MET:HB3	1.84	0.42
2:F:61:ARG:NH1	2:F:82:ASP:OD1	2.52	0.42
4:Q:103:GLU:OE2	4:R:102:LEU:HD21	2.19	0.42
3:U:26:VAL:HG21	3:U:317:ALA:HB2	2.00	0.42
4:W:102:LEU:HD23	4:W:102:LEU:HA	1.60	0.42
2:D:29:VAL:O	2:D:29:VAL:HG13	2.18	0.42
2:F:198:HIS:CD2	2:F:200:GLY:H	2.37	0.42
2:H:205:VAL:O	2:H:205:VAL:HG12	2.18	0.42
1:I:123:PRO:HD2	2:J:121:SER:CB	2.49	0.42
1:I:154:TRP:CZ3	1:I:196:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:SER:OG	1:K:54:PHE:HB3	2.20	0.42
3:O:30:LEU:HA	3:O:30:LEU:HD23	1.82	0.42
4:P:70:PHE:CD2	4:P:78:GLU:HA	2.53	0.42
3:S:116(A):SER:O	3:S:260:MET:HA	2.20	0.42
3:U:103:ILE:N	3:U:103:ILE:HD12	2.34	0.42
1:A:25:SER:O	1:A:25:SER:OG	2.24	0.42
1:A:40:ALA:HB3	1:A:43:GLN:HB2	2.01	0.42
1:A:52:SER:O	1:A:52(A):PRO:C	2.61	0.42
2:B:29:VAL:HG12	2:B:68:GLY:O	2.20	0.42
1:C:143:LYS:HE3	1:C:144:ASP:OD1	2.20	0.42
1:E:100(A):TYR:HD2	4:P:42:GLN:OE1	2.03	0.42
2:F:54:ARG:HG2	2:F:58:ILE:HB	2.02	0.42
2:J:191:VAL:HG13	2:J:191:VAL:O	2.19	0.42
1:K:181:VAL:HG11	2:L:135:LEU:CD2	2.50	0.42
3:M:177:LEU:HD11	3:M:234:TRP:HB2	2.01	0.42
3:O:298:HIS:CE1	3:O:300:ILE:HD12	2.38	0.42
4:W:118:LEU:HA	4:W:118:LEU:HD12	1.75	0.42
2:B:2:ILE:HG12	2:B:27:GLN:HB2	2.02	0.42
1:E:5:VAL:HA	1:E:105:LYS:HZ1	1.83	0.42
1:K:127:SER:H	1:K:130:SER:HB2	1.83	0.42
2:L:32:SER:HB2	2:L:51:ALA:CB	2.46	0.42
2:L:198:HIS:CD2	2:L:199:GLN:O	2.72	0.42
3:N:137:ALA:HB2	3:N:145:LYS:HE3	2.01	0.42
3:O:103:ILE:N	3:O:103:ILE:HD12	2.34	0.42
4:P:168:LEU:HD23	4:P:168:LEU:HA	1.78	0.42
3:T:26:VAL:HG21	3:T:317:ALA:HB2	2.00	0.42
3:U:8:ASP:N	3:U:9:PRO:HD2	2.33	0.42
2:H:32(A):TYR:HB2	2:H:92:VAL:CG1	2.49	0.42
1:I:48:MET:HE3	1:I:63:PHE:CE2	2.54	0.42
1:I:51:ILE:CD1	1:I:71:ALA:HB2	2.50	0.42
2:J:206:THR:O	2:J:206:THR:OG1	2.32	0.42
4:R:17:MET:HE2	4:R:17:MET:HB3	1.87	0.42
3:U:66:ILE:HD12	3:U:109:ARG:HG2	2.00	0.42
1:E:163:VAL:HG22	1:E:182:VAL:HG22	2.01	0.42
2:F:135:LEU:C	2:F:136:LEU:HD23	2.44	0.42
2:F:203:SER:HA	2:F:204:PRO:HD3	1.78	0.42
1:K:51:ILE:HD13	1:K:51:ILE:HG21	1.68	0.42
3:M:123:LYS:NZ	3:M:133:ASN:HD21	2.17	0.42
4:V:168:LEU:HA	4:V:168:LEU:HD23	1.80	0.42
1:A:210:ARG:NH1	1:A:212:GLU:HB3	2.35	0.42
2:F:141:PRO:O	2:F:198:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:198:HIS:HD2	2:F:200:GLY:H	1.68	0.42
1:G:18:VAL:HG23	1:G:82(C):LEU:HD22	1.99	0.42
1:G:181:VAL:HG11	2:H:135:LEU:HD22	2.02	0.42
2:H:120:PRO:HD3	2:H:132:VAL:HG22	2.02	0.42
1:A:82(C):LEU:HD12	1:A:82(C):LEU:HA	1.75	0.42
1:C:146:PHE:HA	1:C:147:PRO:HA	1.79	0.42
1:K:181:VAL:HG11	2:L:135:LEU:HD22	2.02	0.42
2:L:163:VAL:HG22	2:L:175:LEU:HD13	2.02	0.42
2:L:198:HIS:CD2	2:L:199:GLN:H	2.37	0.42
2:B:24:ARG:NH1	2:B:70:ASP:OD1	2.53	0.41
1:C:17:SER:HA	1:C:82(A):SER:HA	1.96	0.41
1:C:51:ILE:HG21	1:C:51:ILE:HD13	1.71	0.41
2:H:29:VAL:O	2:H:29:VAL:CG1	2.68	0.41
1:K:61:GLN:N	1:K:61:GLN:OE1	2.52	0.41
1:K:95:LYS:HE2	1:K:97:GLU:O	2.19	0.41
2:B:32(A):TYR:CD1	2:B:91:TYR:CE2	3.08	0.41
2:D:29:VAL:CG1	2:D:68:GLY:O	2.61	0.41
1:E:61:GLN:OE1	1:E:61:GLN:N	2.54	0.41
2:H:32:SER:HB2	2:H:51:ALA:CB	2.49	0.41
2:H:123:GLU:HA	2:H:126:LYS:HE2	2.03	0.41
2:J:205:VAL:HG12	2:J:205:VAL:H	1.59	0.41
1:K:52:SER:O	1:K:52(A):PRO:C	2.63	0.41
4:P:95:ASN:HD21	4:R:95:ASN:ND2	2.17	0.41
4:P:99:LEU:HA	4:P:99:LEU:HD12	1.86	0.41
3:S:58:PRO:HB3	3:S:86:TYR:CZ	2.55	0.41
3:S:152:ILE:HD11	3:S:255:ARG:HD2	2.02	0.41
4:W:37:ASP:OD2	4:W:40:SER:OG	2.21	0.41
1:E:51:ILE:HG21	1:E:51:ILE:HD13	1.72	0.41
1:E:209:LYS:HD2	1:E:209:LYS:HA	1.77	0.41
2:F:112:ALA:HB2	2:F:200:GLY:HA3	2.02	0.41
1:G:72:ASP:OD1	3:S:291:SER:OG	2.28	0.41
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.55	0.41
2:H:35:TRP:CZ3	2:H:88:CYS:HB3	2.55	0.41
2:H:78:LEU:HD23	2:H:78:LEU:HA	1.83	0.41
1:I:129:LYS:HE2	1:I:129:LYS:HA	2.03	0.41
1:K:18:VAL:HG12	1:K:19:GLN:N	2.35	0.41
3:N:151:LEU:HB3	3:N:252:VAL:HG12	2.02	0.41
4:R:170:ARG:HH11	4:R:170:ARG:HD2	1.72	0.41
3:S:11:ASP:OD1	4:V:28:ASN:HA	2.20	0.41
3:U:8:ASP:N	3:U:9:PRO:CD	2.84	0.41
3:U:174:LYS:CA	3:U:239:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.55	0.41
1:E:105:LYS:HE2	1:E:105:LYS:H	1.84	0.41
3:S:90(A):PRO:HD2	3:S:271:ASP:OD1	2.19	0.41
3:T:207:SER:OG	3:T:241:ASP:OD1	2.36	0.41
3:U:20:ASN:OD1	3:U:20:ASN:C	2.63	0.41
3:U:186:SER:HA	3:U:218:ALA:O	2.20	0.41
4:X:102:LEU:HD23	4:X:102:LEU:HA	1.87	0.41
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.56	0.41
1:C:148:GLU:HG2	1:C:176:TYR:CD2	2.55	0.41
2:H:61:ARG:NH1	2:H:82:ASP:CG	2.79	0.41
1:I:80:MET:HE3	1:I:80:MET:HB3	1.90	0.41
1:K:6:GLN:HG3	1:K:106:GLY:N	2.33	0.41
4:P:3:PHE:CZ	4:Q:2:LEU:HG	2.55	0.41
4:R:159:TYR:HB3	4:R:160:PRO:HD3	2.01	0.41
2:B:79:GLU:HB3	2:B:80:PRO:HD2	2.02	0.41
2:B:95:PRO:O	2:B:95:PRO:CG	2.69	0.41
2:D:120:PRO:HD3	2:D:132:VAL:HG22	2.01	0.41
2:D:201:LEU:HD23	2:D:201:LEU:HA	1.85	0.41
1:G:74:SER:CB	3:S:291:SER:HB2	2.45	0.41
1:G:80:MET:HE3	1:G:80:MET:HB3	1.71	0.41
1:G:144:ASP:OD1	1:G:171:GLN:NE2	2.52	0.41
3:O:195:TYR:O	3:O:197:ASN:N	2.49	0.41
4:R:38:LEU:HA	4:R:38:LEU:HD23	1.61	0.41
3:S:308:TYR:CD2	4:V:89:LEU:HD13	2.56	0.41
4:V:1:GLY:O	4:V:4:GLY:N	2.51	0.41
1:K:100(A):TYR:HB3	4:W:42:GLN:OE1	2.20	0.41
3:M:15:ILE:N	3:M:15:ILE:HD12	2.35	0.41
3:M:180:TRP:CE2	3:M:233:TYR:HB2	2.56	0.41
3:N:94:ASN:HD22	3:N:94:ASN:HA	1.69	0.41
1:A:53:ILE:CD1	4:Q:49:THR:HA	2.50	0.41
2:B:32(A):TYR:CB	2:B:92:VAL:HG12	2.51	0.41
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.54	0.41
1:C:38:ARG:NH1	1:C:46:GLU:OE2	2.48	0.41
1:C:51:ILE:HD11	1:C:71:ALA:HB2	2.03	0.41
1:G:96:LEU:HA	1:G:96:LEU:HD12	1.84	0.41
1:K:146:PHE:CE1	1:K:147:PRO:HB3	2.56	0.41
3:S:41:ASN:ND2	3:S:43:LEU:O	2.54	0.41
3:S:106:GLU:CD	3:S:106:GLU:H	2.29	0.41
3:S:184:HIS:HB3	3:S:216:GLU:O	2.21	0.41
3:U:262:ARG:NH1	3:U:262:ARG:HG3	2.36	0.41
4:W:142:HIS:NE2	4:W:157:TYR:OH	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:CZ2	1:C:80:MET:HB2	2.55	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
2:D:83:PHE:HA	2:D:104:VAL:HG23	2.03	0.41
2:D:131:SER:HA	2:D:179:LEU:O	2.21	0.41
1:E:89:VAL:HG22	1:E:108:THR:HG22	2.03	0.41
2:F:201:LEU:O	2:F:202:SER:C	2.62	0.41
2:H:11:LEU:O	2:H:104:VAL:HA	2.20	0.41
1:I:47:TRP:HB3	2:J:96:LEU:O	2.21	0.41
1:K:61:GLN:HA	1:K:64:GLN:HB2	2.02	0.41
1:K:96:LEU:HA	1:K:96:LEU:HD12	1.82	0.41
2:L:122:ASP:O	2:L:125:LEU:N	2.54	0.41
3:M:308:TYR:CD2	4:P:89:LEU:HD13	2.56	0.41
3:N:54:LEU:HA	3:N:54:LEU:HD12	1.82	0.41
3:O:176:VAL:HA	3:O:258:PHE:O	2.20	0.41
4:P:2:LEU:HD12	4:P:2:LEU:HA	1.62	0.41
4:P:74:GLU:HB3	4:P:77:ILE:HD11	2.03	0.41
4:R:39:LYS:HE3	4:R:39:LYS:HB2	1.79	0.41
3:U:18:HIS:HB2	4:X:20:GLY:O	2.21	0.41
4:V:170:ARG:HH11	4:V:170:ARG:HD2	1.74	0.41
4:X:29:GLU:CD	4:X:143:LYS:HE2	2.46	0.41
4:X:170:ARG:HH11	4:X:170:ARG:HD2	1.72	0.41
3:N:310:LYS:HD3	3:N:310:LYS:HA	1.90	0.41
3:O:262:ARG:HH11	3:O:262:ARG:HG3	1.85	0.41
4:P:142:HIS:CE1	4:P:162:TYR:CG	3.09	0.41
4:Q:62:GLN:NE2	4:R:86:ASP:HB3	2.35	0.41
3:T:303:GLY:HA2	4:W:63:PHE:CE2	2.56	0.41
4:V:101:LEU:HD23	4:V:101:LEU:HA	1.75	0.41
4:X:99:LEU:HA	4:X:99:LEU:HD12	1.87	0.41
1:C:100(A):TYR:HD2	4:X:42:GLN:OE1	2.04	0.40
2:D:89:GLN:HG2	2:D:90:GLN:N	2.35	0.40
2:H:19:ALA:HB2	2:H:78:LEU:HD11	2.03	0.40
1:I:61:GLN:N	1:I:61:GLN:OE1	2.54	0.40
1:I:146:PHE:HA	1:I:147:PRO:HA	1.90	0.40
3:M:42:LEU:HD11	3:M:316:LEU:HD22	2.03	0.40
3:M:321:ARG:HH11	3:M:321:ARG:HD2	1.75	0.40
4:P:23:GLY:HA3	4:P:36:ALA:HA	2.02	0.40
3:U:52:CYS:HB3	3:U:277:CYS:O	2.20	0.40
4:V:28:ASN:OD1	4:V:28:ASN:C	2.65	0.40
1:C:47:TRP:CD1	2:D:96:LEU:HD12	2.57	0.40
1:E:146:PHE:HA	1:E:147:PRO:HA	1.91	0.40
1:G:89:VAL:HA	1:G:108:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ARG:NH2	1:I:86:ASP:OD1	2.55	0.40
1:I:145:TYR:CE1	1:I:150:VAL:HG23	2.57	0.40
2:L:13:LEU:HD23	2:L:13:LEU:HA	1.75	0.40
2:L:141:PRO:HG3	2:L:199:GLN:HE22	1.82	0.40
3:T:71:LEU:O	3:T:148:TYR:HB3	2.21	0.40
2:D:21:LEU:HD12	2:D:21:LEU:N	2.36	0.40
1:I:12:LYS:HD2	1:I:12:LYS:HA	1.94	0.40
2:J:203:SER:HA	2:J:204:PRO:HD3	1.63	0.40
1:K:41:PRO:O	1:K:43:GLN:HG2	2.21	0.40
4:Q:73:LEU:HD23	4:Q:73:LEU:HA	1.84	0.40
4:R:141:TYR:O	4:R:166:ALA:HA	2.21	0.40
4:R:157:TYR:CE2	4:R:159:TYR:HA	2.56	0.40
4:W:38:LEU:HA	4:W:38:LEU:HD23	1.82	0.40
1:E:51:ILE:HD11	1:E:71:ALA:HB2	2.03	0.40
2:H:83:PHE:HA	2:H:104:VAL:HG23	2.04	0.40
3:N:41:ASN:ND2	3:N:43:LEU:O	2.53	0.40
4:P:142:HIS:HB2	4:P:165:GLU:CD	2.46	0.40
3:T:94:ASN:HD22	3:T:94:ASN:HA	1.75	0.40
1:A:42:GLY:O	1:A:43:GLN:NE2	2.44	0.40
1:C:105:LYS:H	1:C:105:LYS:CE	2.35	0.40
2:D:203:SER:HB3	2:D:204:PRO:HD2	2.02	0.40
1:G:82(C):LEU:HD12	1:G:82(C):LEU:HA	1.81	0.40
2:H:167:ASP:O	2:H:171:SER:HA	2.22	0.40
2:J:47:LEU:HD11	2:J:86:TYR:CE2	2.57	0.40
2:J:58:ILE:HA	2:J:59:PRO:HD2	1.89	0.40
3:M:289:ASN:O	3:M:289:ASN:CG	2.65	0.40
3:S:42:LEU:HA	3:S:42:LEU:HD23	1.67	0.40
3:U:54:LEU:HD12	3:U:54:LEU:HA	1.92	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	223/225 (99%)	204 (92%)	16 (7%)	3 (1%)	9	39
1	C	223/225 (99%)	200 (90%)	20 (9%)	3 (1%)	9	39
1	E	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	30	62
1	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	14	47
1	I	223/225 (99%)	205 (92%)	17 (8%)	1 (0%)	30	62
1	K	223/225 (99%)	203 (91%)	17 (8%)	3 (1%)	9	39
2	B	211/213 (99%)	189 (90%)	16 (8%)	6 (3%)	4	26
2	D	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	9	38
2	F	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	9	38
2	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	14	47
2	J	211/213 (99%)	190 (90%)	15 (7%)	6 (3%)	4	26
2	L	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	9	38
3	M	322/331 (97%)	312 (97%)	10 (3%)	0	100	100
3	N	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	O	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	21	54
3	S	322/331 (97%)	312 (97%)	9 (3%)	1 (0%)	36	67
3	T	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	U	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	21	54
4	P	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	Q	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	R	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	V	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	W	169/177 (96%)	166 (98%)	3 (2%)	0	100	100
4	X	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
All	All	5560/5676 (98%)	5246 (94%)	271 (5%)	43 (1%)	16	49

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82(B)	SER
2	B	30	SER
2	B	94	THR
1	C	28	THR
1	G	149	PRO
2	J	30	SER

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Mol	Chain	Res	Type
1	K	82(A)	SER
1	A	27	GLY
2	D	31	SER
2	F	204	PRO
2	H	204	PRO
2	J	28	SER
2	B	204	PRO
1	C	82(C)	LEU
2	J	31	SER
1	K	84	SER
2	B	201	LEU
2	B	203	SER
2	J	203	SER
2	L	203	SER
2	F	28	SER
2	L	201	LEU
3	O	264	ALA
3	U	264	ALA
3	N	264	ALA
3	O	9	PRO
3	S	264	ALA
3	T	264	ALA
3	U	9	PRO
2	D	204	PRO
1	E	52(A)	PRO
1	G	52(A)	PRO
2	J	204	PRO
1	A	52(A)	PRO
2	B	2	ILE
1	C	52(A)	PRO
2	D	2	ILE
2	F	2	ILE
2	H	2	ILE
2	J	2	ILE
1	K	52(A)	PRO
2	L	2	ILE
1	I	52(A)	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	176 (93%)	13 (7%)	14	39
1	C	189/189 (100%)	180 (95%)	9 (5%)	23	49
1	E	189/189 (100%)	184 (97%)	5 (3%)	40	62
1	G	189/189 (100%)	176 (93%)	13 (7%)	14	39
1	I	189/189 (100%)	182 (96%)	7 (4%)	30	56
1	K	189/189 (100%)	178 (94%)	11 (6%)	18	44
2	B	184/184 (100%)	172 (94%)	12 (6%)	15	42
2	D	184/184 (100%)	174 (95%)	10 (5%)	20	46
2	F	184/184 (100%)	173 (94%)	11 (6%)	17	44
2	H	184/184 (100%)	171 (93%)	13 (7%)	13	38
2	J	184/184 (100%)	172 (94%)	12 (6%)	15	42
2	L	184/184 (100%)	170 (92%)	14 (8%)	12	37
3	M	284/290 (98%)	278 (98%)	6 (2%)	47	66
3	N	283/290 (98%)	278 (98%)	5 (2%)	51	69
3	O	286/290 (99%)	281 (98%)	5 (2%)	53	70
3	S	284/290 (98%)	279 (98%)	5 (2%)	51	69
3	T	283/290 (98%)	279 (99%)	4 (1%)	59	71
3	U	286/290 (99%)	281 (98%)	5 (2%)	53	70
4	P	150/151 (99%)	149 (99%)	1 (1%)	76	78
4	Q	146/151 (97%)	145 (99%)	1 (1%)	76	78
4	R	146/151 (97%)	146 (100%)	0	100	100
4	V	150/151 (99%)	150 (100%)	0	100	100
4	W	146/151 (97%)	145 (99%)	1 (1%)	76	78
4	X	146/151 (97%)	146 (100%)	0	100	100
All	All	4828/4884 (99%)	4665 (97%)	163 (3%)	32	57

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL

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Mol	Chain	Res	Type
1	A	25	SER
1	A	28	THR
1	A	38	ARG
1	A	66	ARG
1	A	81	ASP
1	A	82	LEU
1	A	82(A)	SER
1	A	82(B)	SER
1	A	82(C)	LEU
1	A	83	SER
1	A	105	LYS
1	A	109	VAL
2	B	22	SER
2	B	28	SER
2	B	39	LYS
2	B	122	ASP
2	B	125	LEU
2	B	136	LEU
2	B	143	GLU
2	B	150	VAL
2	B	199	GLN
2	B	203	SER
2	B	204	PRO
2	B	206	THR
1	C	11	VAL
1	C	38	ARG
1	C	82	LEU
1	C	82(A)	SER
1	C	82(B)	SER
1	C	82(C)	LEU
1	C	96	LEU
1	C	97	GLU
1	C	105	LYS
2	D	22	SER
2	D	32	SER
2	D	32(A)	TYR
2	D	122	ASP
2	D	125	LEU
2	D	136	LEU
2	D	143	GLU
2	D	150	VAL
2	D	202	SER

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Mol	Chain	Res	Type
2	D	205	VAL
1	E	11	VAL
1	E	38	ARG
1	E	66	ARG
1	E	81	ASP
1	E	105	LYS
2	F	22	SER
2	F	28	SER
2	F	29	VAL
2	F	122	ASP
2	F	125	LEU
2	F	136	LEU
2	F	143	GLU
2	F	150	VAL
2	F	202	SER
2	F	205	VAL
2	F	206	THR
1	G	11	VAL
1	G	38	ARG
1	G	61	GLN
1	G	66	ARG
1	G	82	LEU
1	G	82(A)	SER
1	G	82(B)	SER
1	G	82(C)	LEU
1	G	83	SER
1	G	84	SER
1	G	105	LYS
1	G	145	TYR
1	G	148	GLU
2	H	22	SER
2	H	29	VAL
2	H	30	SER
2	H	122	ASP
2	H	125	LEU
2	H	136	LEU
2	H	143	GLU
2	H	150	VAL
2	H	199	GLN
2	H	201	LEU
2	H	204	PRO
2	H	205	VAL

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Mol	Chain	Res	Type
2	H	206	THR
1	I	11	VAL
1	I	38	ARG
1	I	66	ARG
1	I	81	ASP
1	I	83	SER
1	I	105	LYS
1	I	109	VAL
2	J	22	SER
2	J	28	SER
2	J	29	VAL
2	J	30	SER
2	J	122	ASP
2	J	125	LEU
2	J	136	LEU
2	J	143	GLU
2	J	150	VAL
2	J	199	GLN
2	J	205	VAL
2	J	206	THR
1	K	11	VAL
1	K	28	THR
1	K	38	ARG
1	K	61	GLN
1	K	66	ARG
1	K	82	LEU
1	K	82(A)	SER
1	K	82(B)	SER
1	K	82(C)	LEU
1	K	84	SER
1	K	105	LYS
2	L	22	SER
2	L	26	SER
2	L	27	GLN
2	L	28	SER
2	L	29	VAL
2	L	30	SER
2	L	122	ASP
2	L	125	LEU
2	L	136	LEU
2	L	143	GLU
2	L	150	VAL

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Mol	Chain	Res	Type
2	L	199	GLN
2	L	205	VAL
2	L	206	THR
3	M	63	LYS
3	M	115	VAL
3	M	266	SER
3	M	277	CYS
3	M	283	THR
3	M	320	LEU
3	N	115	VAL
3	N	266	SER
3	N	283	THR
3	N	291	SER
3	N	310	LYS
3	O	63	LYS
3	O	115	VAL
3	O	266	SER
3	O	283	THR
3	O	320	LEU
4	P	154	ASN
4	Q	168	LEU
3	S	63	LYS
3	S	115	VAL
3	S	266	SER
3	S	283	THR
3	S	320	LEU
3	T	115	VAL
3	T	266	SER
3	T	283	THR
3	T	291	SER
3	U	63	LYS
3	U	115	VAL
3	U	266	SER
3	U	283	THR
3	U	320	LEU
4	W	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	B	38	GLN

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Mol	Chain	Res	Type
2	B	198	HIS
2	B	199	GLN
1	C	39	GLN
1	C	164	HIS
1	C	192	GLN
2	D	38	GLN
2	D	198	HIS
2	D	199	GLN
1	E	6	GLN
1	E	39	GLN
1	E	199	ASN
2	F	38	GLN
2	F	189	HIS
2	F	198	HIS
2	H	137	ASN
2	H	189	HIS
2	H	198	HIS
1	I	39	GLN
2	J	37	GLN
2	J	38	GLN
2	J	199	GLN
1	K	6	GLN
2	L	198	HIS
3	M	94	ASN
3	M	133	ASN
3	M	226	GLN
3	N	94	ASN
3	N	111	GLN
3	O	94	ASN
3	O	159	ASN
3	O	226	GLN
3	O	275	HIS
4	P	43	ASN
4	P	95	ASN
4	Q	53	ASN
4	Q	95	ASN
4	Q	154	ASN
4	R	25	HIS
4	R	50	ASN
4	R	72	HIS
4	R	79	ASN
3	S	94	ASN

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Mol	Chain	Res	Type
3	S	133	ASN
3	T	94	ASN
3	T	111	GLN
3	T	226	GLN
3	T	289	ASN
3	U	94	ASN
3	U	159	ASN
3	U	226	GLN
3	U	275	HIS
4	V	26	HIS
4	V	43	ASN
4	V	53	ASN
4	V	95	ASN
4	W	25	HIS
4	W	26	HIS
4	W	95	ASN
4	X	50	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	225/225 (100%)	0.50	14 (6%)	26	16	51, 74, 96, 116	0
1	C	225/225 (100%)	0.60	14 (6%)	26	16	59, 78, 95, 114	0
1	E	225/225 (100%)	0.49	14 (6%)	26	16	55, 79, 99, 111	0
1	G	225/225 (100%)	0.51	16 (7%)	22	14	54, 81, 105, 124	0
1	I	225/225 (100%)	0.90	26 (11%)	9	6	59, 91, 116, 128	0
1	K	225/225 (100%)	0.42	13 (5%)	29	17	51, 72, 98, 114	0
2	B	213/213 (100%)	0.28	10 (4%)	36	20	53, 61, 76, 85	0
2	D	213/213 (100%)	0.43	6 (2%)	55	32	62, 71, 83, 94	0
2	F	213/213 (100%)	0.36	13 (6%)	27	16	58, 68, 83, 92	0
2	H	213/213 (100%)	0.31	10 (4%)	36	20	54, 68, 86, 98	0
2	J	213/213 (100%)	0.49	13 (6%)	27	16	55, 71, 89, 106	0
2	L	213/213 (100%)	0.16	6 (2%)	55	32	51, 61, 76, 88	0
3	M	324/331 (97%)	2.47	204 (62%)	0	0	55, 175, 212, 218	0
3	N	323/331 (97%)	2.20	172 (53%)	0	0	50, 168, 205, 211	0
3	O	326/331 (98%)	2.88	226 (69%)	0	0	54, 196, 228, 232	0
3	S	324/331 (97%)	1.83	147 (45%)	0	1	55, 153, 182, 186	0
3	T	323/331 (97%)	1.88	149 (46%)	0	1	52, 157, 192, 196	0
3	U	326/331 (98%)	2.07	163 (50%)	0	1	55, 159, 190, 197	0
4	P	175/177 (98%)	0.59	23 (13%)	7	6	51, 73, 141, 170	0
4	Q	171/177 (96%)	0.66	20 (11%)	9	6	50, 72, 133, 157	0
4	R	171/177 (96%)	0.61	18 (10%)	11	8	51, 74, 134, 156	0
4	V	175/177 (98%)	0.57	15 (8%)	16	11	52, 77, 128, 147	0
4	W	171/177 (96%)	0.55	14 (8%)	17	11	51, 72, 113, 141	0
4	X	171/177 (96%)	0.57	14 (8%)	17	11	53, 77, 116, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5608/5676 (98%)	1.09	1320 (23%) 2 2	50, 80, 199, 232	0

All (1320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	155	VAL	8.6
3	O	243	ILE	8.4
3	O	179	LEU	8.3
3	M	154	LEU	8.2
3	M	195	TYR	8.1
3	U	55(A)	GLY	7.8
3	M	127	TRP	7.6
3	O	164	LEU	7.4
3	O	245	PHE	7.2
3	S	154	LEU	7.2
3	O	213	PHE	7.1
3	O	250	ASN	7.0
3	M	191	GLN	7.0
3	O	215	PRO	6.9
3	O	229	ARG	6.9
3	N	187	THR	6.8
3	S	183	HIS	6.6
3	O	194	LEU	6.6
3	M	250	ASN	6.6
3	O	155	VAL	6.6
3	M	140	PRO	6.5
3	T	154	LEU	6.4
3	U	139	CYS	6.3
3	M	161	TYR	6.2
3	O	187	THR	6.2
3	O	181	GLY	6.1
3	N	207	SER	6.1
1	I	131	THR	6.1
3	O	153	TRP	6.1
3	O	139	CYS	6.1
3	O	182	ILE	6.1
3	O	198	ALA	6.0
3	M	198	ALA	6.0
3	N	127	TRP	6.0
3	U	154	LEU	6.0
3	M	149	LYS	6.0
3	T	198	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
3	O	251	LEU	5.9
3	O	202	VAL	5.9
3	N	138	ALA	5.9
3	O	247	ALA	5.9
3	M	153	TRP	5.8
3	N	198	ALA	5.8
3	S	140	PRO	5.8
3	U	198	ALA	5.8
3	N	154	LEU	5.8
3	N	97	CYS	5.7
3	M	251	LEU	5.7
3	M	217	ILE	5.7
3	S	155	VAL	5.7
2	J	77	ARG	5.7
3	N	224	ARG	5.6
3	M	144	ALA	5.6
3	O	137	ALA	5.5
3	M	188	SER	5.5
3	N	223	VAL	5.5
3	O	116(B)	PHE	5.5
3	N	184	HIS	5.5
3	U	184	HIS	5.5
3	U	187	THR	5.5
3	M	187	THR	5.5
3	O	154	LEU	5.5
3	M	82	ALA	5.5
3	M	76	CYS	5.4
3	S	277	CYS	5.4
3	O	169	ILE	5.4
3	O	219	ILE	5.4
3	U	182	ILE	5.4
3	M	155	VAL	5.4
3	O	127	TRP	5.4
1	A	81	ASP	5.3
3	N	251	LEU	5.3
3	M	260	MET	5.3
3	N	158	GLY	5.3
3	S	214	LYS	5.3
3	T	208	ARG	5.2
3	M	121	PHE	5.2
3	O	242	LYS	5.2
3	N	290	THR	5.2

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Mol	Chain	Res	Type	RSRZ
3	U	155	VAL	5.1
3	M	240	GLY	5.1
3	O	140	PRO	5.1
3	O	133(A)	LYS	5.1
3	N	99	PRO	5.1
3	O	273	PRO	5.1
3	N	149	LYS	5.1
3	M	139	CYS	5.1
3	O	205	GLY	5.1
3	T	132	SER	5.1
3	O	304	LYS	5.0
4	W	72	HIS	5.0
3	O	82	ALA	5.0
3	O	148	TYR	5.0
3	O	97	CYS	5.0
3	O	174	LYS	5.0
3	U	140	PRO	4.9
3	U	157	LYS	4.9
3	U	290	THR	4.9
3	O	102	PHE	4.9
3	O	55(A)	GLY	4.9
3	N	217	ILE	4.9
3	O	246	GLU	4.9
4	P	72	HIS	4.9
3	O	190	ASP	4.8
3	O	185	PRO	4.8
3	O	214	LYS	4.8
3	M	134	GLY	4.8
3	O	212	LYS	4.8
3	N	186	SER	4.8
3	S	157	LYS	4.8
3	O	244	THR	4.8
3	T	155	VAL	4.8
1	I	82(B)	SER	4.7
3	O	201	TYR	4.7
3	O	138	ALA	4.7
3	M	162	PRO	4.7
1	A	131	THR	4.7
3	U	190	ASP	4.7
3	O	98	TYR	4.7
3	N	197	ASN	4.7
3	M	147	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	4.7
3	U	148	TYR	4.7
3	O	277	CYS	4.7
3	M	157	LYS	4.7
3	O	254	PRO	4.6
3	O	69	TRP	4.6
2	H	143	GLU	4.6
3	U	153	TRP	4.6
3	U	188	SER	4.6
3	M	74	PRO	4.6
3	N	221	PRO	4.6
3	N	189	ALA	4.6
3	O	88	VAL	4.6
3	S	138	ALA	4.6
2	L	30	SER	4.6
3	O	116(A)	SER	4.6
3	O	188	SER	4.6
3	T	122	PRO	4.6
1	A	215	SER	4.6
4	R	69	GLU	4.6
3	S	129	ASN	4.6
3	M	257	ALA	4.6
3	S	198	ALA	4.6
3	T	128	PRO	4.5
3	N	194	LEU	4.5
1	G	129	LYS	4.5
3	O	110	GLU	4.5
4	W	164	GLU	4.5
3	O	145	LYS	4.5
3	U	133(A)	LYS	4.5
3	U	203	PHE	4.5
3	N	96	THR	4.5
3	M	145	LYS	4.5
3	O	62	GLY	4.4
3	O	163	LYS	4.4
3	U	163	LYS	4.4
3	M	116(A)	SER	4.4
3	M	122	PRO	4.4
3	N	153	TRP	4.4
3	O	269	ILE	4.4
3	T	153	TRP	4.4
1	A	214	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	J	32	SER	4.4
3	S	188	SER	4.4
3	M	224	ARG	4.4
3	N	140	PRO	4.4
3	M	223	VAL	4.4
3	O	116(C)	GLU	4.4
3	M	225	ASP	4.4
3	O	76	CYS	4.4
3	M	129	ASN	4.4
3	M	128	PRO	4.4
1	K	130	SER	4.4
3	U	221	PRO	4.4
1	I	214	LYS	4.3
3	O	208	ARG	4.3
3	U	218	ALA	4.3
3	M	214	LYS	4.3
3	M	116(B)	PHE	4.3
3	M	213	PHE	4.3
3	U	245	PHE	4.3
3	O	93	ASP	4.3
3	N	278	ASN	4.3
3	S	160	SER	4.3
3	M	116(C)	GLU	4.3
3	M	192	GLN	4.3
3	M	248	THR	4.3
3	N	219	ILE	4.3
3	O	83(A)	SER	4.3
3	O	132	SER	4.3
3	O	203	PHE	4.2
3	O	73	ASN	4.2
3	O	61	LEU	4.2
3	O	184	HIS	4.2
3	O	162	PRO	4.2
3	M	219	ILE	4.2
3	O	217	ILE	4.2
3	S	124	THR	4.2
3	M	123	LYS	4.2
3	N	160	SER	4.2
3	S	289	ASN	4.2
3	T	129	ASN	4.2
3	T	197	ASN	4.2
3	U	97	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
3	M	111	GLN	4.2
3	S	194	LEU	4.2
3	T	127	TRP	4.2
3	U	138	ALA	4.2
3	O	75	GLU	4.2
3	N	254	PRO	4.2
3	M	100	GLY	4.2
3	U	223	VAL	4.2
3	N	289	ASN	4.2
3	O	101	ASP	4.2
3	M	62	GLY	4.2
3	U	158	GLY	4.2
4	V	11	GLU	4.1
4	X	62	GLN	4.1
3	N	239	PRO	4.1
3	S	153	TRP	4.1
4	P	64	THR	4.1
3	N	179	LEU	4.1
3	O	71	LEU	4.1
3	O	58	PRO	4.1
3	T	290	THR	4.1
3	M	194	LEU	4.1
3	M	197	ASN	4.1
3	N	185	PRO	4.1
3	T	224	ARG	4.1
3	U	186	SER	4.1
4	V	1	GLY	4.1
3	M	98	TYR	4.1
3	M	182	ILE	4.1
3	O	142	ALA	4.1
3	M	71	LEU	4.1
3	T	223	VAL	4.1
3	U	248	THR	4.1
3	O	216	GLU	4.1
3	T	182	ILE	4.1
4	R	171	GLU	4.1
3	T	189	ALA	4.1
3	T	264	ALA	4.1
3	N	215	PRO	4.1
3	T	221	PRO	4.1
3	O	204	VAL	4.0
3	O	252	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
4	V	135	ASN	4.0
3	N	190	ASP	4.0
1	K	129	LYS	4.0
3	M	133(A)	LYS	4.0
2	F	143	GLU	4.0
3	O	60	HIS	4.0
3	M	159	ASN	4.0
3	U	212	LYS	4.0
4	W	60	ASN	4.0
3	M	266	SER	4.0
3	O	104	ASP	4.0
3	U	179	LEU	4.0
3	O	80	SER	4.0
3	O	224	ARG	4.0
3	U	217	ILE	4.0
1	G	131	THR	4.0
3	O	173	GLY	4.0
3	S	141	HIS	4.0
3	M	102	PHE	4.0
3	M	150	ASN	4.0
3	S	217	ILE	4.0
3	N	188	SER	4.0
3	T	158	GLY	4.0
3	M	263	ASN	4.0
3	O	124	THR	4.0
3	O	290	THR	4.0
3	U	185	PRO	3.9
3	T	82	ALA	3.9
3	T	238	GLU	3.9
3	U	205	GLY	3.9
3	U	76	CYS	3.9
3	N	212	LYS	3.9
3	O	57	ALA	3.9
3	T	161	TYR	3.9
3	M	290	THR	3.9
4	Q	60	ASN	3.9
3	O	9	PRO	3.9
3	S	184	HIS	3.9
3	T	78	SER	3.9
3	T	188	SER	3.9
3	O	183	HIS	3.9
3	O	189	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	T	139	CYS	3.9
3	M	222	LYS	3.9
3	M	275	HIS	3.9
3	S	130	HIS	3.9
3	O	220	ARG	3.8
3	N	76	CYS	3.8
3	T	201	TYR	3.8
3	U	222	LYS	3.8
4	P	75	LYS	3.8
3	O	206	SER	3.8
1	K	23	ARG	3.8
3	O	253	VAL	3.8
3	S	76	CYS	3.8
3	M	152	ILE	3.8
3	U	181	GLY	3.8
3	U	228	GLY	3.8
3	S	278	ASN	3.8
3	M	276	ASP	3.8
3	O	165	SER	3.8
3	M	60	HIS	3.8
3	T	142	ALA	3.8
1	I	129	LYS	3.8
3	N	182	ILE	3.8
3	O	106	GLU	3.8
3	M	81	THR	3.8
3	O	228	GLY	3.8
3	S	248	THR	3.8
1	E	23	ARG	3.8
3	M	79	LEU	3.8
3	N	159	ASN	3.8
3	U	224	ARG	3.8
3	U	247	ALA	3.8
1	C	214	LYS	3.8
3	M	143	GLY	3.8
3	T	220	ARG	3.8
3	T	277	CYS	3.8
3	U	141	HIS	3.8
3	N	126	SER	3.8
3	O	266	SER	3.8
3	N	79	LEU	3.8
3	O	128	PRO	3.8
3	O	221	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
3	U	216	GLU	3.8
1	K	131	THR	3.8
2	J	31	SER	3.7
3	O	103	ILE	3.7
3	O	158	GLY	3.7
3	U	214	LYS	3.7
4	Q	70	PHE	3.7
3	N	145	LYS	3.7
3	O	285	LYS	3.7
3	U	124	THR	3.7
3	M	289	ASN	3.7
3	O	197	ASN	3.7
3	S	197	ASN	3.7
3	U	231	ASN	3.7
1	C	101	ASP	3.7
3	T	62	GLY	3.7
3	O	74	PRO	3.7
3	T	97	CYS	3.7
3	T	236	LEU	3.7
3	N	203	PHE	3.7
3	O	157	LYS	3.7
3	M	221	PRO	3.7
3	N	210	SER	3.7
3	O	167	SER	3.7
3	O	175	GLU	3.7
3	T	195	TYR	3.7
3	T	216	GLU	3.7
3	M	55	ARG	3.7
3	M	97	CYS	3.7
3	O	52	CYS	3.7
1	I	204	ASN	3.7
3	S	133(A)	LYS	3.7
3	N	162	PRO	3.6
3	M	175	GLU	3.6
3	N	175	GLU	3.6
3	M	135	VAL	3.6
3	T	251	LEU	3.6
3	O	100	GLY	3.6
3	O	258	PHE	3.6
3	O	129	ASN	3.6
3	O	265	GLY	3.6
3	U	99	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	M	160	SER	3.6
4	P	174	ASP	3.6
3	M	189	ALA	3.6
2	F	165	GLU	3.6
3	N	116(C)	GLU	3.6
3	T	246	GLU	3.6
3	S	195	TYR	3.6
3	T	207	SER	3.6
3	M	172	LYS	3.6
3	U	60	HIS	3.6
4	Q	72	HIS	3.6
4	X	63	PHE	3.6
3	U	134	GLY	3.6
3	N	129	ASN	3.6
3	O	195	TYR	3.6
3	O	211	LYS	3.6
3	T	149	LYS	3.6
1	I	17	SER	3.6
3	S	199	ASP	3.6
3	M	185	PRO	3.6
3	S	142	ALA	3.6
3	U	129	ASN	3.6
3	O	161	TYR	3.6
3	U	160	SER	3.6
3	S	213	PHE	3.5
3	T	215	PRO	3.5
3	O	123	LYS	3.5
3	N	195	TYR	3.5
3	O	150	ASN	3.5
3	U	250	ASN	3.5
1	C	82(B)	SER	3.5
3	M	101	ASP	3.5
3	O	191	GLN	3.5
3	T	100	GLY	3.5
3	U	265	GLY	3.5
3	O	149	LYS	3.5
3	T	166	LYS	3.5
3	T	194	LEU	3.5
1	C	23	ARG	3.5
3	N	104	ASP	3.5
3	N	265	GLY	3.5
3	O	237	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	M	259	ALA	3.5
3	M	179	LEU	3.5
3	U	61	LEU	3.5
3	N	77	GLU	3.5
3	U	102	PHE	3.5
3	S	187	THR	3.5
3	O	78	SER	3.5
3	O	66	ILE	3.5
3	S	96	THR	3.5
3	T	248	THR	3.5
3	O	249	GLY	3.5
3	S	64	CYS	3.5
3	N	236	LEU	3.5
3	S	189	ALA	3.5
3	U	207	SER	3.5
3	U	172	LYS	3.4
3	O	159	ASN	3.4
3	S	21	ASN	3.4
1	G	133	GLY	3.4
3	U	142	ALA	3.4
1	I	132	SER	3.4
3	U	116(C)	GLU	3.4
3	O	233	TYR	3.4
3	T	179	LEU	3.4
3	M	137	ALA	3.4
3	N	124	THR	3.4
3	S	224	ARG	3.4
3	T	191	GLN	3.4
3	U	229	ARG	3.4
3	M	215	PRO	3.4
3	N	128	PRO	3.4
3	O	300	ILE	3.4
1	I	215	SER	3.4
3	N	167	SER	3.4
3	O	186	SER	3.4
3	M	63	LYS	3.4
3	O	166	LYS	3.4
1	I	23	ARG	3.4
1	E	131	THR	3.4
3	T	130	HIS	3.4
3	T	196	GLN	3.4
3	U	9	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
3	S	212	LYS	3.4
3	U	304	LYS	3.4
3	S	193	SER	3.4
3	N	101	ASP	3.4
3	N	201	TYR	3.4
1	C	210	ARG	3.4
3	M	142	ALA	3.4
3	N	137	ALA	3.4
3	T	219	ILE	3.4
3	T	140	PRO	3.4
3	T	121	PHE	3.4
3	U	204	VAL	3.4
4	Q	74	GLU	3.4
3	O	168	TYR	3.4
3	U	137	ALA	3.4
1	C	12	LYS	3.4
3	O	63	LYS	3.4
3	M	141	HIS	3.4
3	T	23	THR	3.4
3	T	187	THR	3.4
3	M	258	PHE	3.3
2	B	29	VAL	3.3
2	D	32	SER	3.3
2	H	32	SER	3.3
3	M	54	LEU	3.3
3	M	151	LEU	3.3
3	O	79	LEU	3.3
3	N	75	GLU	3.3
4	Q	144	CYS	3.3
3	N	100	GLY	3.3
3	N	105	TYR	3.3
3	U	201	TYR	3.3
3	S	182	ILE	3.3
3	M	99	PRO	3.3
3	S	128	PRO	3.3
3	M	94	ASN	3.3
3	S	263	ASN	3.3
3	T	159	ASN	3.3
3	U	197	ASN	3.3
3	U	147	PHE	3.3
3	S	127	TRP	3.3
3	N	204	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	M	132	SER	3.3
3	N	123	LYS	3.3
3	M	230	MET	3.3
3	N	277	CYS	3.3
3	U	52	CYS	3.3
3	U	242	LYS	3.3
3	U	277	CYS	3.3
3	N	134	GLY	3.3
3	O	284	PRO	3.3
3	O	56	VAL	3.3
3	O	135	VAL	3.3
3	N	133(A)	LYS	3.3
3	N	156	LYS	3.3
3	T	175	GLU	3.3
4	V	164	GLU	3.3
4	W	144	CYS	3.3
3	M	226	GLN	3.3
3	M	211	LYS	3.3
2	J	143	GLU	3.3
3	O	160	SER	3.3
3	U	80	SER	3.3
3	U	162	PRO	3.3
3	M	203	PHE	3.3
3	N	63	LYS	3.3
3	N	202	VAL	3.3
3	N	169	ILE	3.3
3	N	227	GLU	3.3
3	O	89	GLU	3.3
3	T	185	PRO	3.2
1	E	101	ASP	3.2
3	O	180	TRP	3.2
3	M	75	GLU	3.2
3	N	216	GLU	3.2
3	N	222	LYS	3.2
3	S	251	LEU	3.2
3	U	116(B)	PHE	3.2
3	U	275	HIS	3.2
3	T	230	MET	3.2
3	U	230	MET	3.2
3	N	144	ALA	3.2
3	S	75	GLU	3.2
3	S	238	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	M	212	LYS	3.2
3	U	145	LYS	3.2
3	N	113	SER	3.2
3	T	126	SER	3.2
3	N	191	GLN	3.2
4	R	64	THR	3.2
3	N	82	ALA	3.2
3	N	264	ALA	3.2
3	M	265	GLY	3.2
3	S	116(C)	GLU	3.2
3	U	227	GLU	3.2
4	Q	164	GLU	3.2
3	U	194	LEU	3.2
3	T	203	PHE	3.2
3	M	184	HIS	3.2
3	N	132	SER	3.2
3	T	260	MET	3.2
2	J	151	ASP	3.2
3	O	241	ASP	3.2
3	M	72	GLY	3.2
3	M	174	LYS	3.2
3	T	123	LYS	3.2
3	T	33	ASN	3.2
3	U	226	GLN	3.2
3	O	96	THR	3.2
3	T	266(A)	GLY	3.1
3	S	98	TYR	3.1
3	S	223	VAL	3.1
3	T	209	TYR	3.1
3	U	202	VAL	3.1
4	R	63	PHE	3.1
3	M	138	ALA	3.1
3	S	145	LYS	3.1
3	M	61	LEU	3.1
3	N	205	GLY	3.1
3	O	8	ASP	3.1
3	T	79	LEU	3.1
3	S	230	MET	3.1
1	E	129	LYS	3.1
3	O	275	HIS	3.1
3	U	123	LYS	3.1
3	M	158	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	S	276	ASP	3.1
3	U	241	ASP	3.1
2	H	123	GLU	3.1
3	O	223	VAL	3.1
3	S	117	ARG	3.1
3	O	99	PRO	3.1
3	M	50	LYS	3.1
3	O	48	ASN	3.1
3	O	226	GLN	3.1
3	O	143	GLY	3.1
3	S	290	THR	3.1
3	T	124	THR	3.1
3	S	210	SER	3.1
3	T	165	SER	3.1
3	U	132	SER	3.1
3	S	216	GLU	3.1
3	T	133(A)	LYS	3.1
3	U	215	PRO	3.1
3	S	161	TYR	3.1
3	N	164	LEU	3.1
3	U	251	LEU	3.1
4	Q	1	GLY	3.1
3	M	208	ARG	3.1
3	T	206	SER	3.1
1	E	214	LYS	3.1
3	U	219	ILE	3.1
1	A	26	GLY	3.0
1	K	66	ARG	3.0
3	O	240	GLY	3.0
3	U	312	THR	3.0
3	S	77	GLU	3.0
3	M	70	ILE	3.0
3	M	87	ILE	3.0
3	S	74	PRO	3.0
3	M	281	CYS	3.0
3	O	51	LEU	3.0
3	S	52	CYS	3.0
1	I	66	ARG	3.0
3	S	94	ASN	3.0
3	S	231	ASN	3.0
3	U	289	ASN	3.0
3	S	228	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	28	THR	3.0
3	M	163	LYS	3.0
3	N	172	LYS	3.0
3	U	244	THR	3.0
2	B	143	GLU	3.0
3	S	227	GLU	3.0
3	U	246	GLU	3.0
4	Q	29	GLU	3.0
3	T	217	ILE	3.0
3	S	215	PRO	3.0
4	V	174	ASP	3.0
3	T	214	LYS	3.0
3	T	265	GLY	3.0
3	U	211	LYS	3.0
4	V	128	ASN	3.0
1	A	17	SER	3.0
3	M	210	SER	3.0
3	N	71	LEU	3.0
3	N	78	SER	3.0
3	U	79	LEU	3.0
3	S	209	TYR	3.0
3	M	93	ASP	3.0
3	T	225	ASP	3.0
3	T	241	ASP	3.0
3	O	141	HIS	3.0
3	S	250	ASN	3.0
3	S	221	PRO	3.0
3	N	266	SER	3.0
3	U	161	TYR	3.0
1	K	26	GLY	3.0
3	M	130	HIS	3.0
3	N	139	CYS	3.0
3	N	245	PHE	3.0
3	O	281	CYS	3.0
3	M	244	THR	3.0
3	T	212	LYS	2.9
4	P	65	ALA	2.9
3	N	91	SER	2.9
3	M	266(A)	GLY	2.9
3	O	199	ASP	2.9
3	S	134	GLY	2.9
3	U	130	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
4	V	70	PHE	2.9
3	M	73	ASN	2.9
4	Q	64	THR	2.9
3	U	149	LYS	2.9
3	N	161	TYR	2.9
3	N	209	TYR	2.9
3	U	240	GLY	2.9
2	J	167	ASP	2.9
3	N	131	ASP	2.9
3	S	149	LYS	2.9
3	O	105	TYR	2.9
3	T	118	PHE	2.9
3	T	245	PHE	2.9
2	D	18	ARG	2.9
3	T	145	LYS	2.9
3	U	271	ASP	2.9
3	M	239	PRO	2.9
3	M	254	PRO	2.9
3	T	250	ASN	2.9
3	N	52	CYS	2.9
3	U	127	TRP	2.9
3	O	274	VAL	2.9
3	S	245	PHE	2.9
1	A	130	SER	2.9
3	S	152	ILE	2.9
3	S	167	SER	2.9
4	V	72	HIS	2.9
1	I	213	PRO	2.9
3	N	107	GLU	2.9
3	O	238	GLU	2.9
3	O	278	ASN	2.9
3	M	277	CYS	2.9
3	M	249	GLY	2.9
3	O	118	PHE	2.9
3	S	118	PHE	2.9
3	N	166	LYS	2.9
3	S	79	LEU	2.9
3	T	157	LYS	2.9
3	T	172	LYS	2.9
3	U	103	ILE	2.9
1	G	130	SER	2.8
3	M	136	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	O	248	THR	2.8
3	M	261	GLU	2.8
4	P	69	GLU	2.8
3	M	278	ASN	2.8
4	X	60	ASN	2.8
3	N	242	LYS	2.8
3	T	173	GLY	2.8
3	M	201	TYR	2.8
3	M	209	TYR	2.8
3	O	302	ILE	2.8
4	P	73	LEU	2.8
3	N	60	HIS	2.8
1	C	215	SER	2.8
3	T	160	SER	2.8
4	R	62	GLN	2.8
4	V	27	GLN	2.8
3	T	254	PRO	2.8
1	G	101	ASP	2.8
3	O	235	THR	2.8
3	O	271	ASP	2.8
3	N	213	PHE	2.8
3	S	179	LEU	2.8
3	N	98	TYR	2.8
4	V	137	CYS	2.8
3	M	183	HIS	2.8
3	O	207	SER	2.8
3	O	210	SER	2.8
4	P	175	SER	2.8
3	M	117	ARG	2.8
3	N	225	ASP	2.8
3	S	163	LYS	2.8
4	R	75	LYS	2.8
3	N	231	ASN	2.8
3	T	152	ILE	2.8
4	V	154	ASN	2.8
3	N	111	GLN	2.8
3	U	264	ALA	2.8
3	S	99	PRO	2.8
3	N	248	THR	2.8
3	O	236	LEU	2.8
3	T	116(C)	GLU	2.8
3	O	147	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
4	V	60	ASN	2.8
3	N	168	TYR	2.8
3	S	137	ALA	2.8
4	P	76	ARG	2.8
1	E	13	LYS	2.8
3	O	176	VAL	2.8
1	A	186	SER	2.8
3	S	261	GLU	2.8
3	M	245	PHE	2.7
3	O	70	ILE	2.8
3	O	152	ILE	2.8
3	O	303	GLY	2.7
3	S	10	GLY	2.7
3	T	190	ASP	2.7
3	U	8	ASP	2.7
1	I	199	ASN	2.7
3	M	33	ASN	2.7
3	M	168	TYR	2.7
3	M	229	ARG	2.7
3	T	242	LYS	2.7
4	X	75	LYS	2.7
3	S	97	CYS	2.7
3	U	164	LEU	2.7
1	E	215	SER	2.7
1	K	82(A)	SER	2.7
3	O	200	THR	2.7
3	O	260	MET	2.7
3	U	167	SER	2.7
4	P	63	PHE	2.7
4	V	69	GLU	2.7
3	S	93	ASP	2.7
2	L	77	ARG	2.7
3	M	262	ARG	2.7
3	S	33	ASN	2.7
3	U	21	ASN	2.7
4	X	141	TYR	2.7
4	X	27	GLN	2.7
1	I	140	CYS	2.7
3	M	64	CYS	2.7
3	O	90(A)	PRO	2.7
3	O	122	PRO	2.7
3	T	52	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	W	63	PHE	2.7
3	N	246	GLU	2.7
1	K	215	SER	2.7
3	O	272	THR	2.7
3	S	125	SER	2.7
3	T	228	GLY	2.7
3	M	109	ARG	2.7
3	N	73	ASN	2.7
3	S	275	HIS	2.7
3	T	247	ALA	2.7
3	O	121	PHE	2.7
3	M	110	GLU	2.7
3	M	238	GLU	2.7
3	T	229	ARG	2.7
4	R	67	GLY	2.7
3	M	80	SER	2.7
3	O	86	TYR	2.7
4	R	72	HIS	2.7
2	F	210	ASN	2.7
3	M	231	ASN	2.7
3	N	122	PRO	2.7
3	N	260	MET	2.7
1	I	58	LYS	2.7
2	B	165	GLU	2.7
2	B	30	SER	2.7
3	T	138	ALA	2.7
3	O	209	TYR	2.7
3	M	104	ASP	2.7
3	U	101	ASP	2.7
3	T	239	PRO	2.6
3	U	169	ILE	2.6
3	U	254	PRO	2.6
1	K	12	LYS	2.6
3	S	63	LYS	2.6
3	S	62	GLY	2.6
2	B	94	THR	2.6
3	S	139	CYS	2.6
2	F	30	SER	2.6
3	O	276	ASP	2.6
3	T	169	ILE	2.6
3	U	131	ASP	2.6
1	E	12	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	196	GLN	2.6
4	P	128	ASN	2.6
3	O	95	GLY	2.6
3	S	205	GLY	2.6
3	O	90	THR	2.6
3	M	164	LEU	2.6
3	O	84	TRP	2.6
3	O	151	LEU	2.6
3	U	135	VAL	2.6
1	I	130	SER	2.6
3	N	206	SER	2.6
3	O	116	SER	2.6
3	O	146	SER	2.6
3	U	266	SER	2.6
3	T	256	TYR	2.6
3	U	209	TYR	2.6
3	O	239	PRO	2.6
3	S	203	PHE	2.6
3	U	258	PHE	2.6
3	S	100	GLY	2.6
1	I	82(C)	LEU	2.6
3	M	67	ALA	2.6
3	O	115	VAL	2.6
3	O	234	TRP	2.6
4	R	144	CYS	2.6
3	N	103	ILE	2.6
3	O	50	LYS	2.6
3	N	183	HIS	2.6
3	O	83	SER	2.6
3	N	121	PHE	2.6
3	N	230	MET	2.6
3	T	116(B)	PHE	2.6
3	T	162	PRO	2.6
2	L	60	ASP	2.6
3	U	104	ASP	2.6
3	M	173	GLY	2.6
3	M	228	GLY	2.6
3	T	134	GLY	2.6
3	N	237	VAL	2.6
3	N	252	VAL	2.6
3	N	253	VAL	2.6
3	S	176	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	96	THR	2.6
3	T	137	ALA	2.6
1	G	214	LYS	2.6
3	N	232	TYR	2.6
3	N	165	SER	2.6
3	U	210	SER	2.6
3	N	199	ASP	2.6
3	N	266(A)	GLY	2.6
3	M	246	GLU	2.6
3	U	75	GLU	2.6
3	S	144	ALA	2.6
3	S	156	LYS	2.6
3	T	280	THR	2.6
4	W	64	THR	2.6
3	T	120	ILE	2.5
3	O	230	MET	2.5
3	T	275	HIS	2.5
3	T	186	SER	2.5
1	G	1	GLN	2.5
3	S	143	GLY	2.5
3	U	71	LEU	2.5
2	H	17	GLU	2.5
3	M	178	VAL	2.5
3	N	157	LYS	2.5
3	S	202	VAL	2.5
3	N	259	ALA	2.5
3	U	189	ALA	2.5
3	M	120	ILE	2.5
3	O	81	THR	2.5
3	S	219	ILE	2.5
3	T	235	THR	2.5
3	M	273	PRO	2.5
3	O	130	HIS	2.5
3	O	232	TYR	2.5
3	T	72	GLY	2.5
3	M	171	ASP	2.5
3	N	238	GLU	2.5
3	U	278	ASN	2.5
3	T	69	TRP	2.5
3	N	116(B)	PHE	2.5
3	N	141	HIS	2.5
3	S	201	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	T	184	HIS	2.5
3	N	181	GLY	2.5
3	T	163	LYS	2.5
3	U	285	LYS	2.5
4	W	155	GLY	2.5
2	F	32	SER	2.5
3	T	202	VAL	2.5
3	M	77	GLU	2.5
3	U	44	GLU	2.5
4	P	165	GLU	2.5
1	G	160	THR	2.5
3	M	69	TRP	2.5
3	U	273	PRO	2.5
1	A	129	LYS	2.5
1	E	58	LYS	2.5
3	M	51	LEU	2.5
3	T	222	LYS	2.5
2	D	50	GLY	2.5
3	S	55(A)	GLY	2.5
3	O	282	GLN	2.5
3	O	264	ALA	2.5
3	S	82	ALA	2.5
3	T	116	SER	2.5
3	M	44	GLU	2.5
3	N	106	GLU	2.5
3	U	175	GLU	2.5
4	Q	69	GLU	2.5
4	X	150	GLU	2.5
3	U	94	ASN	2.5
3	U	159	ASN	2.5
1	I	28	THR	2.5
1	G	23	ARG	2.5
3	N	163	LYS	2.5
1	G	15	GLY	2.5
3	T	240	GLY	2.5
1	I	64	GLN	2.5
2	B	31	SER	2.4
2	F	31	SER	2.4
3	M	311	SER	2.4
2	F	123	GLU	2.4
3	S	89	GLU	2.4
3	S	175	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	U	77	GLU	2.4
3	S	222	LYS	2.4
2	B	129	THR	2.4
3	N	235	THR	2.4
4	X	19	ASP	2.4
3	S	122	PRO	2.4
3	S	168	TYR	2.4
4	X	72	HIS	2.4
3	T	237	VAL	2.4
4	P	67	GLY	2.4
4	R	77	ILE	2.4
1	C	82(A)	SER	2.4
3	O	193	SER	2.4
4	W	70	PHE	2.4
3	O	54	LEU	2.4
2	J	180	THR	2.4
3	T	289	ASN	2.4
3	S	101	ASP	2.4
3	U	200	THR	2.4
4	Q	85	ASP	2.4
3	M	252	VAL	2.4
3	N	233	TYR	2.4
3	S	266(A)	GLY	2.4
3	M	242	LYS	2.4
3	S	123	LYS	2.4
3	T	63	LYS	2.4
3	T	156	LYS	2.4
3	T	147	PHE	2.4
3	M	116	SER	2.4
3	M	207	SER	2.4
3	O	85	SER	2.4
3	U	125	SER	2.4
3	N	112	LEU	2.4
3	O	305	CYS	2.4
3	O	301	THR	2.4
3	T	278	ASN	2.4
1	C	15	GLY	2.4
1	I	190	GLY	2.4
3	M	196	GLN	2.4
1	A	23	ARG	2.4
3	T	174	LYS	2.4
3	U	220	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	17	GLU	2.4
2	L	143	GLU	2.4
4	P	29	GLU	2.4
3	M	83	SER	2.4
2	F	29	VAL	2.4
3	M	200	THR	2.4
4	R	66	VAL	2.4
2	B	60	ASP	2.4
2	H	70	ASP	2.4
3	N	173	GLY	2.4
3	U	73	ASN	2.4
3	N	275	HIS	2.4
3	M	105	TYR	2.4
3	S	190	ASP	2.4
3	O	310	LYS	2.4
3	O	192	GLN	2.4
3	S	226	GLN	2.4
3	S	44	GLU	2.4
3	N	125	SER	2.4
3	N	64	CYS	2.4
4	W	148	CYS	2.4
3	N	214	LYS	2.3
3	N	269	ILE	2.3
3	S	304	LYS	2.3
3	S	229	ARG	2.3
3	T	144	ALA	2.3
3	U	33	ASN	2.3
3	O	131	ASP	2.3
3	T	168	TYR	2.3
3	T	199	ASP	2.3
4	Q	76	ARG	2.3
3	O	196	GLN	2.3
3	O	227	GLU	2.3
4	R	103	GLU	2.3
3	T	135	VAL	2.3
2	J	156	SER	2.3
3	M	186	SER	2.3
3	U	128	PRO	2.3
1	A	133	GLY	2.3
1	G	58	LYS	2.3
3	N	50	LYS	2.3
3	N	304	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	23	CYS	2.3
3	O	55	ARG	2.3
4	P	1	GLY	2.3
3	N	130	HIS	2.3
3	T	141	HIS	2.3
3	U	67	ALA	2.3
3	M	148	TYR	2.3
3	O	289	ASN	2.3
3	T	276	ASP	2.3
4	X	171	GLU	2.3
3	O	222	LYS	2.3
4	W	75	LYS	2.3
3	U	262	ARG	2.3
3	M	280	THR	2.3
3	N	280	THR	2.3
2	J	23	CYS	2.3
3	M	21	ASN	2.3
3	U	65	ASN	2.3
3	T	213	PHE	2.3
3	M	304	LYS	2.3
1	C	66	ARG	2.3
3	O	117	ARG	2.3
3	M	169	ILE	2.3
3	M	181	GLY	2.3
3	O	10	GLY	2.3
3	O	325	SER	2.3
3	M	112	LEU	2.3
3	O	108	LEU	2.3
1	A	204	ASN	2.3
1	K	81	ASP	2.3
3	S	104	ASP	2.3
3	T	104	ASP	2.3
4	P	68	LYS	2.3
2	J	18	ARG	2.3
3	M	176	VAL	2.3
3	N	110	GLU	2.3
3	N	220	ARG	2.3
3	S	110	GLU	2.3
3	S	178	VAL	2.3
3	T	253	VAL	2.3
4	R	29	GLU	2.3
4	X	69	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	U	239	PRO	2.3
3	U	243	ILE	2.3
3	N	95	GLY	2.3
3	U	62	GLY	2.3
3	U	143	GLY	2.3
3	S	83(A)	SER	2.3
3	M	232	TYR	2.3
3	M	256	TYR	2.3
3	S	256	TYR	2.3
3	T	98	TYR	2.3
3	U	195	TYR	2.3
3	M	285	LYS	2.3
3	U	166	LYS	2.3
4	W	154	ASN	2.3
3	S	191	GLN	2.3
4	X	144	CYS	2.3
2	F	60	ASP	2.3
3	N	24	ASP	2.3
3	S	237	VAL	2.3
3	U	88	VAL	2.3
2	H	165	GLU	2.2
4	V	165	GLU	2.2
3	N	55(A)	GLY	2.2
3	S	239	PRO	2.2
3	S	164	LEU	2.2
3	M	301	THR	2.2
3	N	147	PHE	2.2
3	S	244	THR	2.2
3	T	258	PHE	2.2
3	U	96	THR	2.2
1	C	17	SER	2.2
3	O	156	LYS	2.2
3	O	291	SER	2.2
3	U	206	SER	2.2
3	U	233	TYR	2.2
2	F	77	ARG	2.2
2	D	143	GLU	2.2
3	M	227	GLU	2.2
3	N	44	GLU	2.2
3	S	246	GLU	2.2
4	R	11	GLU	2.2
3	O	288	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	T	103	ILE	2.2
3	U	288	ILE	2.2
3	M	55(A)	GLY	2.2
3	M	284	PRO	2.2
3	N	299	PRO	2.2
3	T	99	PRO	2.2
3	O	177	LEU	2.2
3	U	82	ALA	2.2
1	I	12	LYS	2.2
1	K	58	LYS	2.2
3	N	102	PHE	2.2
3	S	147	PHE	2.2
4	Q	61	THR	2.2
4	Q	127	LYS	2.2
1	G	128	SER	2.2
1	I	112	SER	2.2
3	M	113	SER	2.2
3	S	207	SER	2.2
3	O	111	GLN	2.2
3	N	133	ASN	2.2
3	N	263	ASN	2.2
3	O	21	ASN	2.2
1	E	140	CYS	2.2
1	I	196	CYS	2.2
3	M	216	GLU	2.2
3	M	267	ILE	2.2
3	N	89	GLU	2.2
3	M	131	ASP	2.2
3	S	171	ASP	2.2
3	T	101	ASP	2.2
2	H	212	GLY	2.2
3	M	264	ALA	2.2
3	T	205	GLY	2.2
3	U	236	LEU	2.2
4	R	65	ALA	2.2
3	O	172	LYS	2.2
3	S	211	LYS	2.2
3	U	213	PHE	2.2
3	M	220	ARG	2.2
2	H	5	THR	2.2
3	M	90	THR	2.2
3	N	244	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	66	VAL	2.2
1	G	82(A)	SER	2.2
3	M	125	SER	2.2
1	C	212	GLU	2.2
1	I	80	MET	2.2
4	V	73	LEU	2.2
2	J	212	GLY	2.2
3	N	90(A)	PRO	2.2
3	O	299	PRO	2.2
3	M	190	ASP	2.2
3	M	241	ASP	2.2
4	Q	167	LYS	2.2
4	R	19	ASP	2.2
4	R	85	ASP	2.2
3	M	274	VAL	2.2
3	U	176	VAL	2.2
2	L	32	SER	2.2
3	O	91	SER	2.2
3	S	186	SER	2.2
3	U	165	SER	2.2
4	Q	77	ILE	2.2
3	O	59	LEU	2.2
3	N	94	ASN	2.2
3	T	44	GLU	2.2
3	T	231	ASN	2.2
2	H	77	ARG	2.2
3	N	262	ARG	2.2
3	N	241	ASP	2.2
3	U	11	ASP	2.2
3	S	60	HIS	2.2
3	S	204	VAL	2.1
3	S	235	THR	2.1
4	W	147	THR	2.1
3	S	233	TYR	2.1
3	M	236	LEU	2.1
1	A	82(B)	SER	2.1
1	K	132	SER	2.1
3	N	80	SER	2.1
3	S	172	LYS	2.1
3	U	174	LYS	2.1
3	N	218	ALA	2.1
1	E	133	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	45	ARG	2.1
4	P	11	GLU	2.1
2	D	212	GLY	2.1
3	U	249	GLY	2.1
3	M	133	ASN	2.1
3	N	21	ASN	2.1
3	U	121	PHE	2.1
4	X	46	ASP	2.1
3	U	183	HIS	2.1
3	U	98	TYR	2.1
4	P	77	ILE	2.1
1	A	12	LYS	2.1
3	O	53	LYS	2.1
1	G	212	GLU	2.1
2	L	52	SER	2.1
3	M	91	SER	2.1
3	S	265	GLY	2.1
3	T	83(A)	SER	2.1
3	T	227	GLU	2.1
3	S	102	PHE	2.1
3	T	271	ASP	2.1
4	P	66	VAL	2.1
3	M	103	ILE	2.1
3	M	235	THR	2.1
3	M	283	THR	2.1
2	H	24	ARG	2.1
3	S	111	GLN	2.1
3	T	259	ALA	2.1
3	S	254	PRO	2.1
3	U	58	PRO	2.1
2	J	30	SER	2.1
3	U	325	SER	2.1
3	S	73	ASN	2.1
3	S	61	LEU	2.1
4	P	173	ILE	2.1
3	M	308	TYR	2.1
3	S	272	THR	2.1
3	U	191	GLN	2.1
3	N	143	GLY	2.1
3	U	90(A)	PRO	2.1
1	G	215	SER	2.1
2	B	32	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	203	SER	2.1
3	O	125	SER	2.1
3	S	126	SER	2.1
3	U	274	VAL	2.1
1	C	201	LYS	2.1
3	N	150	ASN	2.1
4	Q	75	LYS	2.1
3	M	177	LEU	2.1
3	M	243	ILE	2.1
3	N	69	TRP	2.1
3	T	61	LEU	2.1
3	T	255	ARG	2.1
3	M	199	ASP	2.1
3	M	218	ALA	2.1
3	S	192	GLN	2.1
4	R	27	GLN	2.1
1	I	212	GLU	2.1
3	M	118	PHE	2.1
3	O	119	GLU	2.1
3	S	185	PRO	2.1
3	T	110	GLU	2.1
1	G	12	LYS	2.0
3	N	211	LYS	2.0
3	O	133	ASN	2.0
3	U	150	ASN	2.0
4	P	60	ASN	2.0
3	N	180	TRP	2.0
1	K	101	ASP	2.0
3	M	27	ASP	2.0
3	O	259	ALA	2.0
3	S	90	THR	2.0
3	S	247	ALA	2.0
3	U	81	THR	2.0
3	M	52	CYS	2.0
4	Q	65	ALA	2.0
4	W	137	CYS	2.0
3	S	158	GLY	2.0
3	T	181	GLY	2.0
4	P	27	GLN	2.0
4	W	27	GLN	2.0
2	B	17	GLU	2.0
3	U	32	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	U	89	GLU	2.0
4	P	164	GLU	2.0
3	T	164	LEU	2.0
1	E	130	SER	2.0
3	N	92	SER	2.0
3	M	170	ASN	2.0
3	N	256	TYR	2.0
3	O	136	THR	2.0
3	O	280	THR	2.0
3	S	148	TYR	2.0
4	X	64	THR	2.0
1	I	81	ASP	2.0
3	N	93	ASP	2.0
1	I	22	CYS	2.0
3	T	14	CYS	2.0
3	T	76	CYS	2.0
3	T	143	GLY	2.0
3	T	226	GLN	2.0
3	U	74	PRO	2.0
1	E	97	GLU	2.0
2	F	187	GLU	2.0
4	Q	78	GLU	2.0
3	N	243	ILE	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.