



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2017 – 10:13 PM EST

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

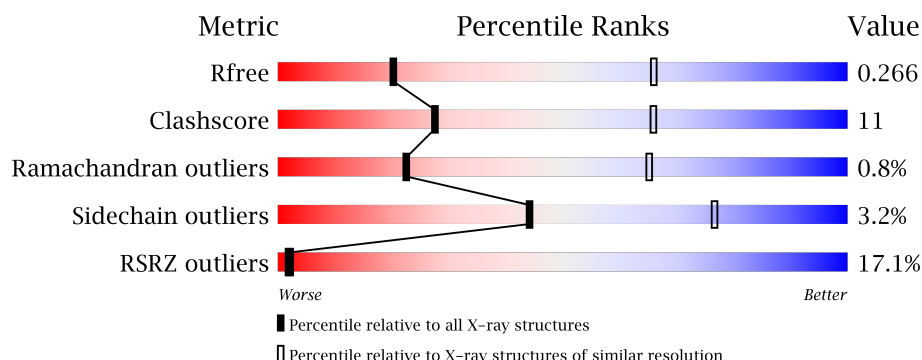
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>5%</div> </div> </div>
1	C	225	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	E	225	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>.</div> </div> </div>
1	G	225	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div>
1	I	225	<div> <div>15%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	225	 5% 74% 23% .
2	B	213	 72% 23% ..
2	D	213	 68% 29% .
2	F	213	 78% 21% .
2	H	213	 75% 23% .
2	J	213	 2% 72% 25% ..
2	L	213	 76% 21% .
3	M	331	 44% 77% 20% ..
3	N	331	 41% 81% 16% ..
3	O	331	 50% 76% 21% ..
3	S	331	 34% 79% 18% ..
3	T	331	 34% 83% 13% ..
3	U	331	 35% 79% 18% ..
4	P	177	 6% 79% 20% .
4	Q	177	 6% 80% 17% .
4	R	177	 5% 76% 19% ..
4	V	177	 7% 80% 19% .
4	W	177	 7% 81% 15% ..
4	X	177	 6% 80% 16% ..

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			

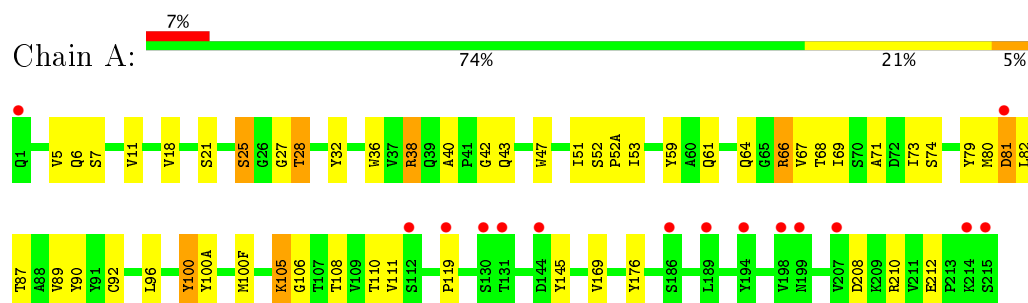
There are 24 discrepancies between the modelled and reference sequences:

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

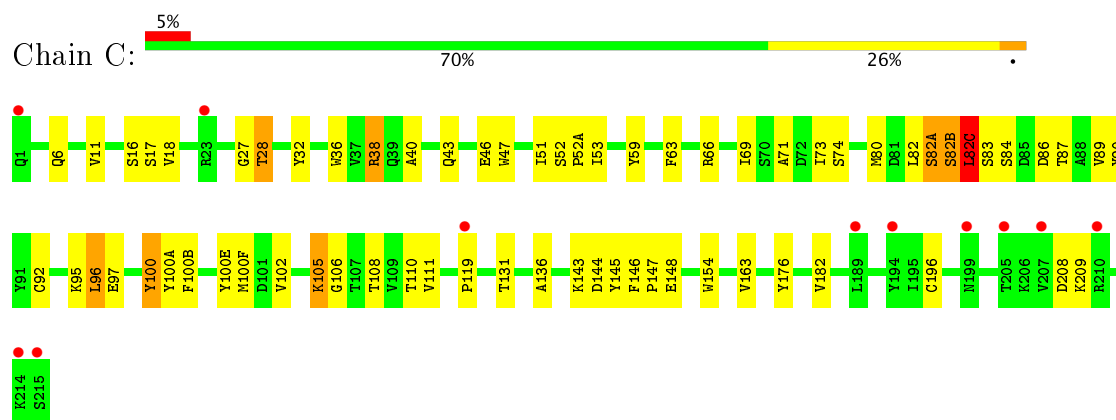
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

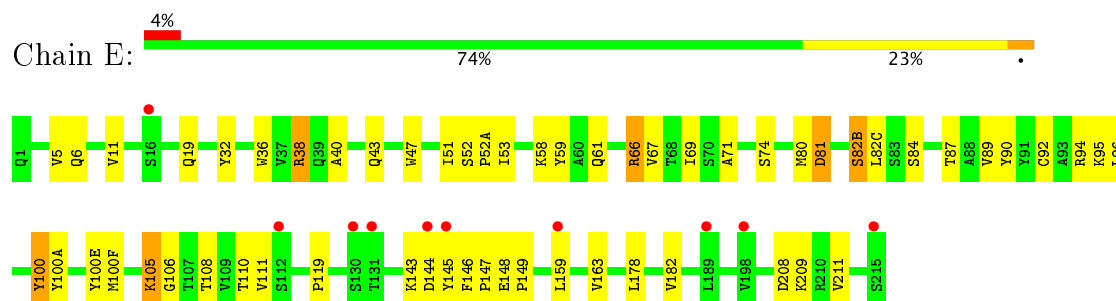
• Molecule 1: Antibody 27F3 heavy chain



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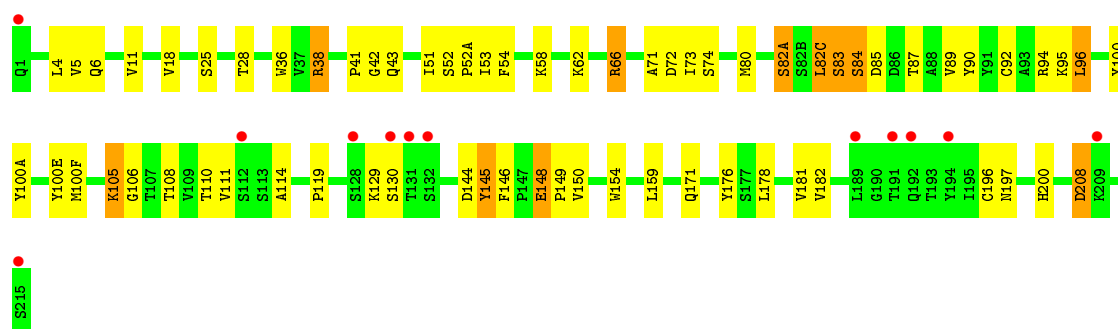


• Molecule 1: Antibody 27F3 heavy chain

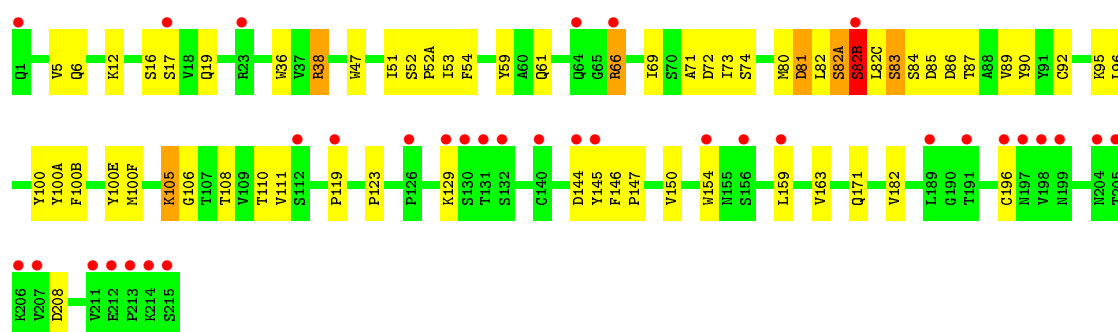


• Molecule 1: Antibody 27F3 heavy chain

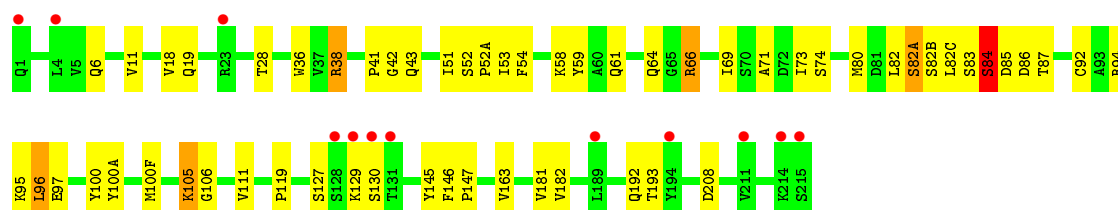
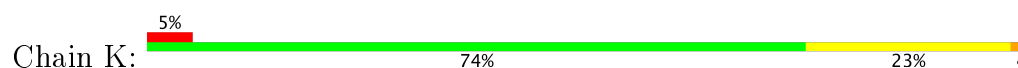




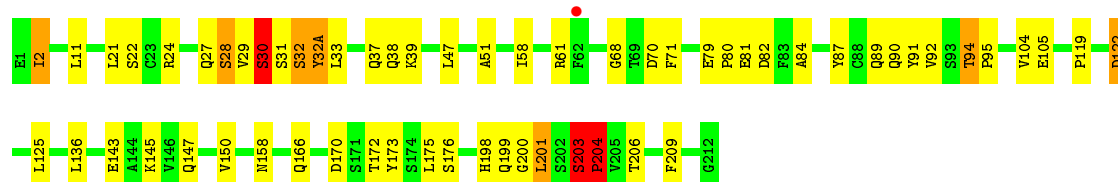
• Molecule 1: Antibody 27F3 heavy chain



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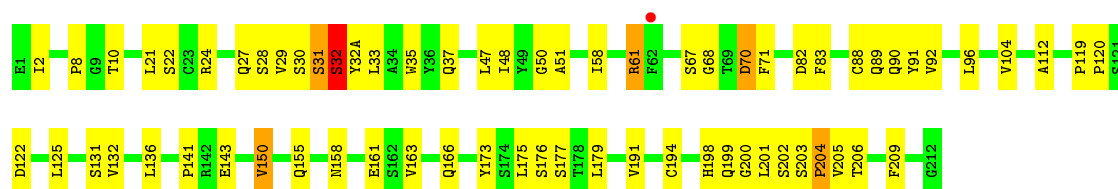


• Molecule 2: Antibody 27F3 light chain

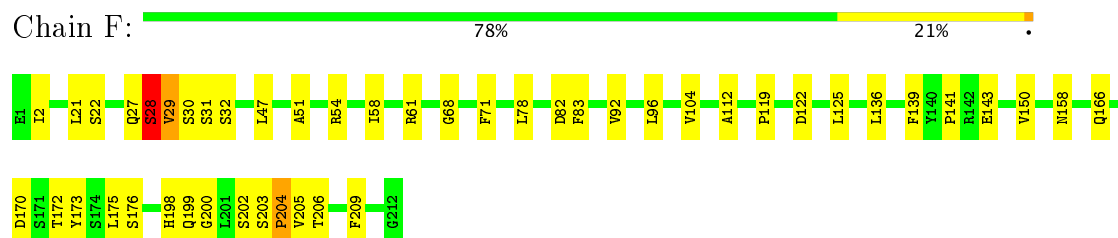


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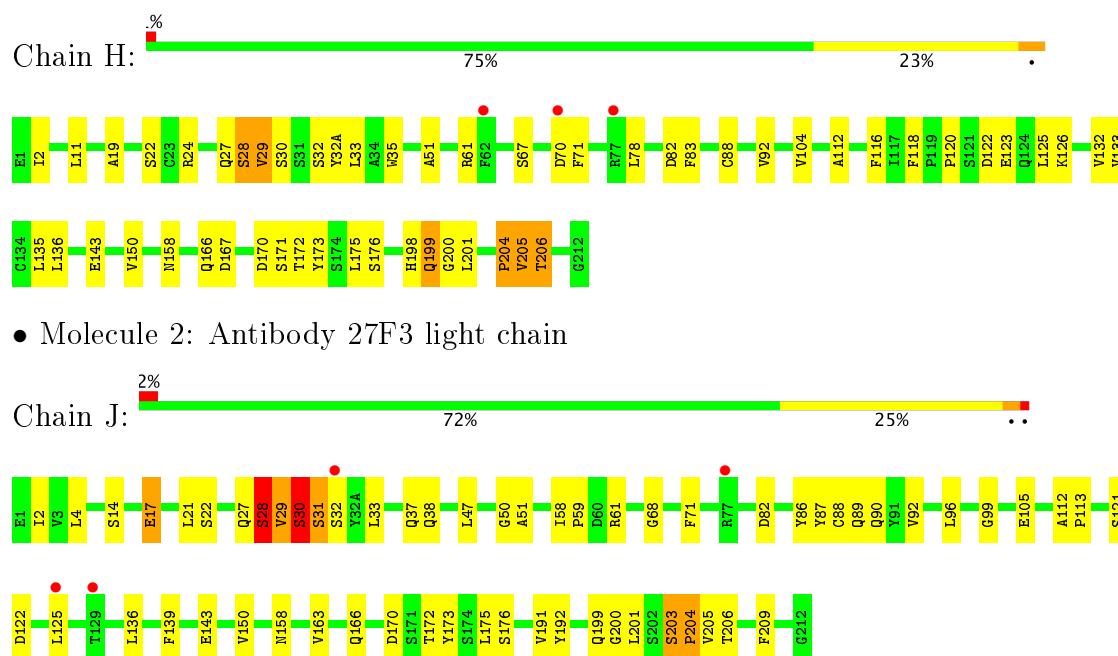




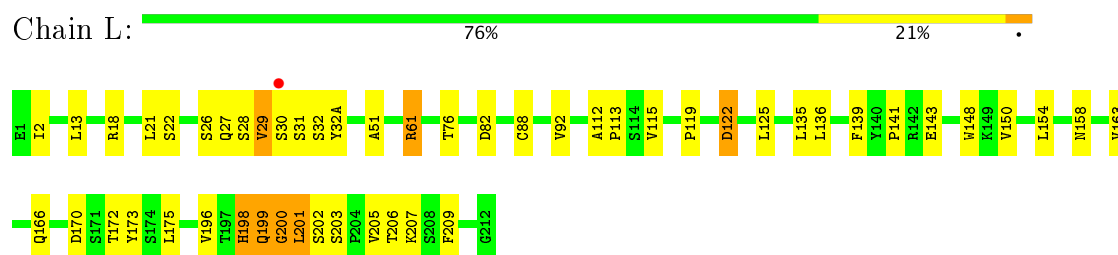
• Molecule 2: Antibody 27F3 light chain



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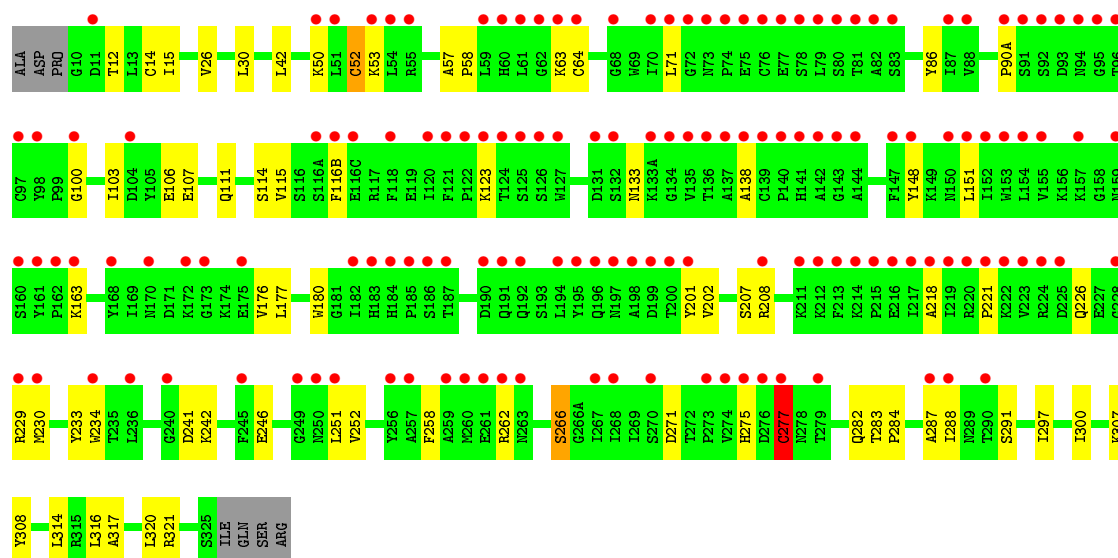


• Molecule 2: Antibody 27F3 light chain

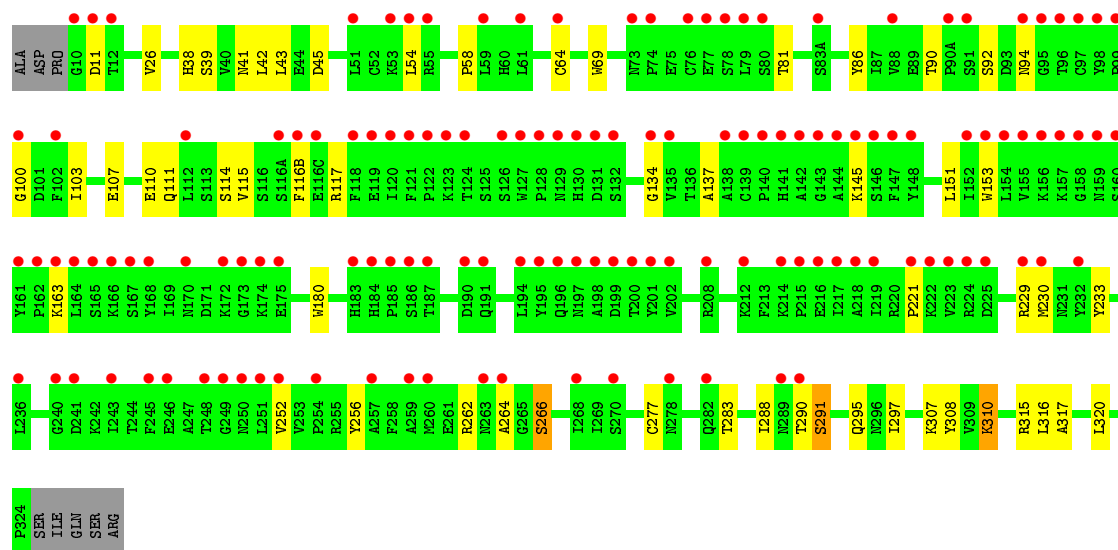
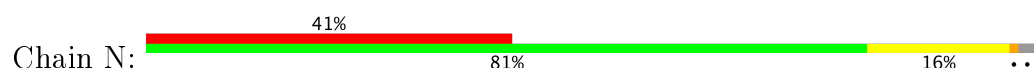


• Molecule 3: Hemagglutinin

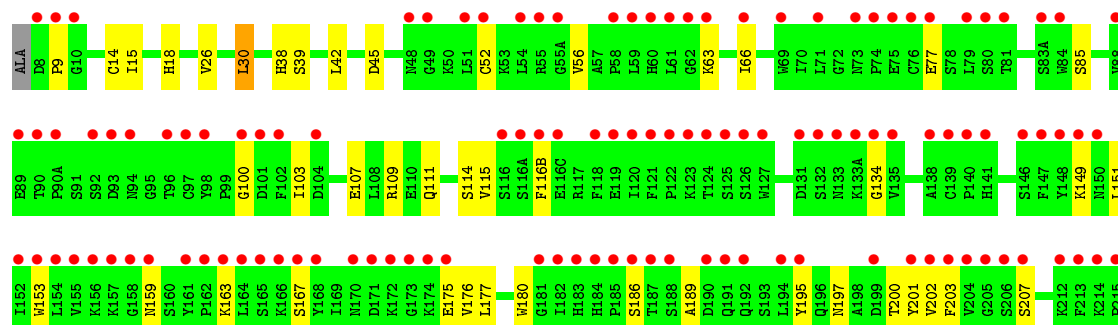
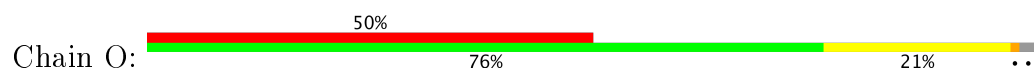


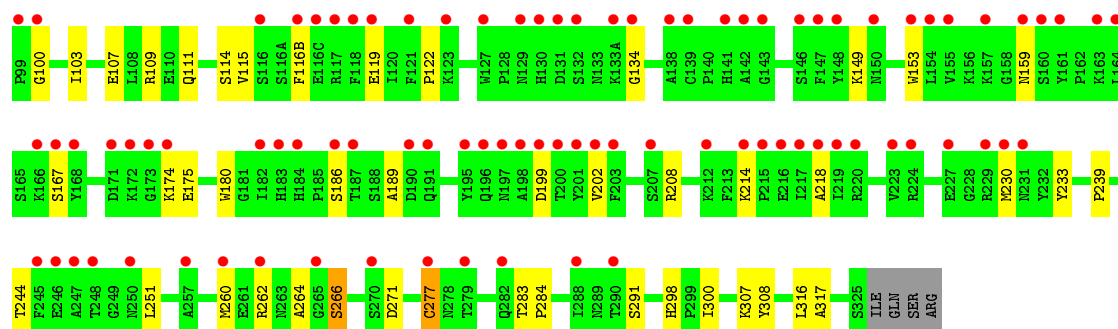


• Molecule 3: Hemagglutinin

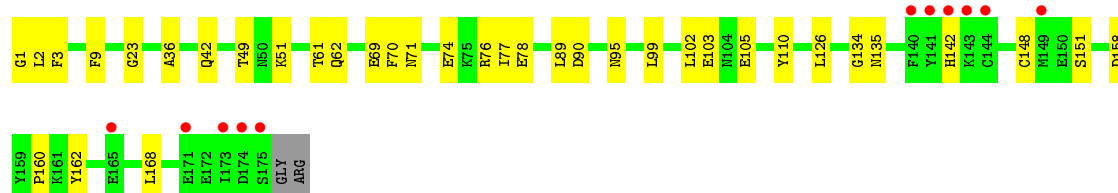
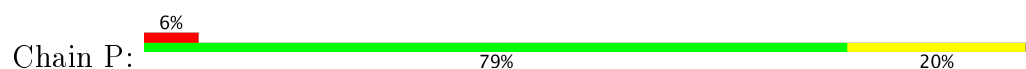


• Molecule 3: Hemagglutinin

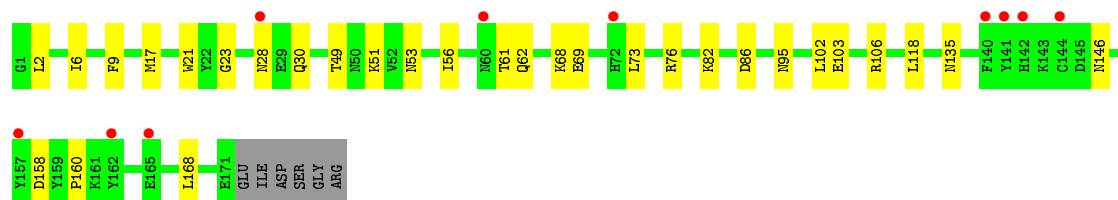
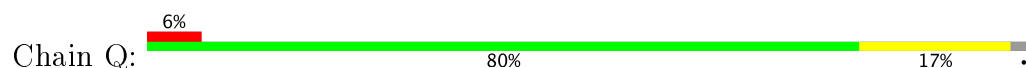




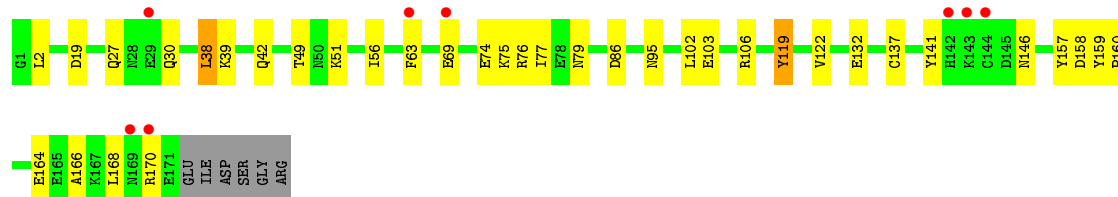
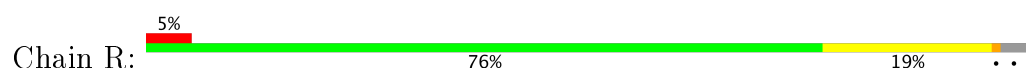
• Molecule 4: Hemagglutinin



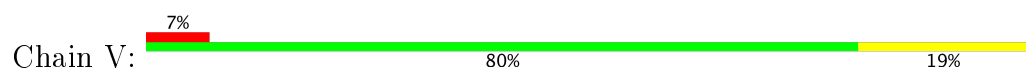
• Molecule 4: Hemagglutinin

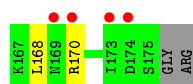


• Molecule 4: Hemagglutinin

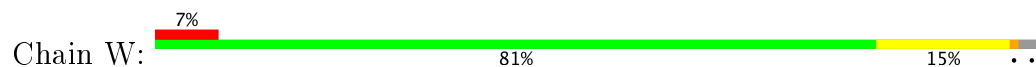


• Molecule 4: Hemagglutinin

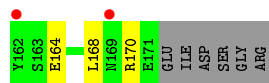
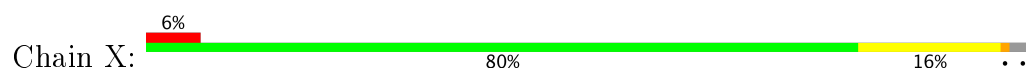




● Molecule 4: Hemagglutinin



● 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) 98.1 (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 0.242 , 0.266	Depositor DCC
R_{free} test set	8902 reflections (5.01%)	DCC
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 , 52.9	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	1.09	3/1719 (0.2%)	0.83	2/2344 (0.1%)
1	C	0.92	0/1719	0.82	1/2344 (0.0%)
1	E	0.96	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	G	0.92	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	I	0.83	0/1719	0.75	1/2344 (0.0%)
1	K	1.05	1/1719 (0.1%)	0.82	1/2344 (0.0%)
2	B	1.19	0/1663	0.93	4/2260 (0.2%)
2	D	0.98	1/1663 (0.1%)	0.85	2/2260 (0.1%)
2	F	0.99	0/1663	0.83	0/2260
2	H	1.00	0/1663	0.84	0/2260
2	J	0.99	1/1663 (0.1%)	0.87	1/2260 (0.0%)
2	L	1.14	1/1663 (0.1%)	0.88	2/2260 (0.1%)
3	M	0.62	3/2593 (0.1%)	0.72	3/3524 (0.1%)
3	N	0.62	0/2587	0.79	3/3516 (0.1%)
3	O	0.57	1/2609 (0.0%)	0.74	2/3547 (0.1%)
3	S	0.62	0/2593	0.73	4/3524 (0.1%)
3	T	0.64	1/2587 (0.0%)	0.83	6/3516 (0.2%)
3	U	0.60	0/2609	0.75	1/3547 (0.0%)
4	P	1.01	1/1434 (0.1%)	0.87	0/1932
4	Q	1.04	1/1403 (0.1%)	0.86	2/1890 (0.1%)
4	R	0.94	2/1403 (0.1%)	0.86	1/1890 (0.1%)
4	V	0.99	0/1434	0.90	3/1932 (0.2%)
4	W	0.96	1/1403 (0.1%)	0.84	3/1890 (0.2%)
4	X	0.90	1/1403 (0.1%)	0.89	3/1890 (0.2%)
All	All	0.88	20/44350 (0.0%)	0.82	49/60222 (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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	TYR	CE1-CZ	-8.04	1.28	1.38
1	E	211	VAL	C-N	7.65	1.51	1.34
2	J	17	GLU	CB-CG	-7.09	1.38	1.52
3	M	14	CYS	CB-SG	-6.31	1.71	1.82
4	Q	21	TRP	CB-CG	-6.09	1.39	1.50
2	L	88	CYS	CB-SG	-6.09	1.72	1.82
4	W	137	CYS	CB-SG	-6.07	1.72	1.82
2	D	194	CYS	CB-SG	-5.88	1.72	1.81
3	O	14	CYS	CB-SG	-5.87	1.72	1.81
4	R	119	TYR	CD1-CE1	-5.47	1.31	1.39
1	A	100(A)	TYR	CE1-CZ	-5.34	1.31	1.38
1	A	79	TYR	CE2-CZ	-5.24	1.31	1.38
1	K	96	LEU	C-N	-5.17	1.22	1.34
4	P	110	TYR	CE1-CZ	-5.16	1.31	1.38
4	R	137	CYS	CB-SG	-5.13	1.73	1.81
3	T	305	CYS	CB-SG	-5.12	1.73	1.81
1	G	96	LEU	C-N	-5.10	1.22	1.34
3	M	64	CYS	CB-SG	-5.10	1.73	1.81
3	M	52	CYS	CB-SG	-5.09	1.73	1.81
4	X	14	TRP	CB-CG	-5.06	1.41	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	277	CYS	CA-CB-SG	-15.68	85.77	114.00
3	S	277	CYS	CA-CB-SG	-8.97	97.85	114.00
3	T	320	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	I	82(B)	SER	N-CA-C	-8.29	88.63	111.00
3	S	30	LEU	CB-CG-CD2	-7.80	97.73	111.00
2	B	30	SER	N-CA-CB	7.50	121.75	110.50
4	V	106	ARG	NE-CZ-NH1	-7.27	116.67	120.30
3	N	277	CYS	CA-CB-SG	-6.82	101.72	114.00
2	B	32	SER	N-CA-C	-6.72	92.85	111.00
2	B	201	LEU	CA-CB-CG	6.65	130.60	115.30
3	T	315	ARG	NE-CZ-NH1	-6.57	117.01	120.30
3	S	315	ARG	NE-CZ-NH1	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	200	GLY	N-CA-C	-6.41	97.08	113.10
2	L	201	LEU	N-CA-C	-6.28	94.04	111.00
3	O	316	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	96	LEU	CA-CB-CG	-6.21	101.02	115.30
1	E	58	LYS	CD-CE-NZ	6.15	125.84	111.70
3	M	30	LEU	CB-CG-CD2	-6.01	100.78	111.00
3	O	30	LEU	CB-CG-CD2	-5.94	100.90	111.00
2	J	17	GLU	N-CA-CB	-5.84	100.08	110.60
2	B	32(A)	TYR	N-CA-C	-5.83	95.27	111.00
2	D	32	SER	N-CA-C	-5.82	95.27	111.00
4	V	39	LYS	CD-CE-NZ	5.76	124.95	111.70
3	M	277	CYS	CA-CB-SG	-5.67	103.80	114.00
4	Q	118	LEU	CB-CG-CD1	-5.67	101.37	111.00
4	Q	106	ARG	NE-CZ-NH1	-5.63	117.49	120.30
3	T	310	LYS	CD-CE-NZ	5.60	124.57	111.70
3	T	320	LEU	CB-CG-CD1	-5.59	101.50	111.00
4	W	1	GLY	N-CA-C	-5.58	99.14	113.10
4	X	102	LEU	CB-CG-CD2	-5.57	101.54	111.00
4	X	106	ARG	NE-CZ-NH1	-5.48	117.56	120.30
4	V	118	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	K	58	LYS	CD-CE-NZ	5.46	124.25	111.70
1	C	82(C)	LEU	N-CA-C	5.45	125.71	111.00
3	T	304	LYS	CG-CD-CE	5.37	128.00	111.90
4	W	102	LEU	CB-CG-CD2	-5.33	101.94	111.00
4	X	24	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	G	58	LYS	CD-CE-NZ	5.24	123.74	111.70
4	R	38	LEU	CB-CG-CD2	-5.22	102.12	111.00
4	W	38	LEU	CB-CG-CD2	-5.19	102.18	111.00
3	M	12	THR	CA-CB-CG2	-5.18	105.14	112.40
2	D	70	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	G	62	LYS	CD-CE-NZ	5.07	123.36	111.70
3	N	320	LEU	CA-CB-CG	5.07	126.96	115.30
1	E	94	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	N	315	ARG	NE-CZ-NH1	-5.03	117.79	120.30
3	S	316	LEU	CB-CG-CD2	-5.02	102.46	111.00
3	U	277	CYS	N-CA-CB	-5.02	101.56	110.60
1	A	82(A)	SER	C-N-CA	5.01	134.23	121.70

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

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	62	0
1	C	1675	0	1642	67	0
1	E	1675	0	1643	43	0
1	G	1675	0	1643	77	0
1	I	1675	0	1643	69	0
1	K	1675	0	1642	45	0
2	B	1628	0	1592	63	0
2	D	1628	0	1591	65	0
2	F	1628	0	1592	30	0
2	H	1628	0	1592	35	0
2	J	1628	0	1590	63	0
2	L	1628	0	1592	36	0
3	M	2529	0	2479	46	0
3	N	2523	0	2474	37	0
3	O	2544	0	2490	54	0
3	S	2529	0	2479	43	0
3	T	2523	0	2474	30	0
3	U	2544	0	2490	47	0
4	P	1406	0	1326	32	0
4	Q	1375	0	1300	28	0
4	R	1375	0	1300	32	0
4	V	1406	0	1326	33	0
4	W	1375	0	1300	23	0
4	X	1375	0	1300	26	0
All	All	43322	0	42142	966	0

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

All (966) 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
2:J:29:VAL:CG2	2:J:68:GLY:O	2.01	1.08
1:A:67:VAL:HG23	1:A:81:ASP:O	1.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:68:THR:OG1	1:A:81:ASP:CG	2.03	0.97
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: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: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:A:68:THR:C	1:A:81:ASP:HB2	1.90	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:C:27:GLY:C	1:C:28:THR:HG23	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:I:96:LEU:HD12	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
2:F:31:SER:OG	2:F:32:SER:N	2.16	0.79
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
2:J:31:SER:OG	2:J:32:SER:N	2.18	0.75
1:G:74:SER:HB3	3:S:291:SER:CB	2.16	0.75
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:VAL:HG22	1:I:108:THR:HG22	1.70	0.73
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.21	0.73
3:U:116(B):PHE:HE1	3:U:260:MET:HE1	1.53	0.73
1:G:74:SER:HB3	3:S:291:SER:OG	1.89	0.73
3:T:117:ARG:HD3	3:T:256:TYR:CD1	2.23	0.72
1:C:74:SER:HB3	3:U:291:SER:HB2	1.69	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: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
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
2:J:27:GLN:O	2:J:28:SER:O	2.09	0.69
1:G:74:SER:HB3	3:S:291:SER:HB2	1.73	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
2:B:27:GLN:O	2:B:28:SER:C	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:OG	1:I:82(B):SER:O	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
4:Q:69:GLU:O	4:R:76:ARG:NH1	2.28	0.64
2:B:94:THR:HG1	2:B:95:PRO:CD	2.09	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
1:G:18:VAL:CG2	1:G:82(C):LEU:HD21	2.28	0.63
3:U:116(B):PHE:CE1	3:U:260:MET:HE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:115:VAL:HG11	3:M:116(B):PHE:HB2	1.80	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
1:C:27:GLY:C	1:C:28:THR:CG2	2.61	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
3:O:38:HIS:CD2	3:O:39:SER:N	2.68	0.61
1:A:74:SER:HB2	4:Q:56:ILE:HG21	1.81	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
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.36	0.60
3:M:229:ARG:NH2	3:O:207:SER:HA	2.10	0.60
1:I:74:SER:HB3	3:O:291:SER:CB	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:TYR:OH	3:M:246:GLU:OE2	2.15	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:OE1	1:A:61:GLN:N	2.35	0.60
1:E:66:ARG:HH11	1:E:82(B):SER:HG	1.42	0.60
2:D:27:GLN:O	2:D:28:SER:C	2.35	0.60
1:E:36:TRP:CE2	1:E:80:MET:HB2	2.36	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
2:D:29:VAL:HG22	2:D:29:VAL:O	2.03	0.59
2:L:29:VAL:HG12	2:L:29:VAL:O	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
2:H:27:GLN:O	2:H:28:SER:C	2.41	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
2:J:32:SER:O	2:J:50:GLY:C	2.40	0.58
1:I:5:VAL:HA	1:I:105:LYS:NZ	2.19	0.58
2:J:61:ARG:NH1	2:J:82:ASP:CG	2.57	0.58
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.38	0.58
2:F:158:ASN:N	2:F:158:ASN:OD1	2.35	0.58
2:F:27:GLN:O	2:F:28:SER:C	2.41	0.58
1:G:53:ILE:HD13	4:V:49:THR:HA	1.85	0.58
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:68:THR:OG1	1:A:81:ASP:HB2	2.02	0.58
2:D:158:ASN:OD1	2:D:158:ASN:N	2.37	0.58
2:D:32(A):TYR:HD1	2:D:91:TYR:CE2	2.22	0.58
1:A:28:THR:CG2	4:Q:53:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OG	1:K:83:SER:O	2.17	0.57
1:A:68:THR:C	1:A:81:ASP:CB	2.59	0.57
3:U:114:SER:HB2	3:U:266:SER:HB2	1.86	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
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:H:166:GLN:HG3	2:H:173:TYR:CZ	2.40	0.56
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:H	1:A:105:LYS:HE2	1.69	0.56
1:E:87:THR:OG1	1:E:110:THR:HA	2.05	0.56
3:M:221:PRO:HG2	3:O:242:LYS:O	2.06	0.56
3:M:207:SER:HA	3:N:229:ARG:HH21	1.71	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:H	1:C:73:ILE:HD12	1.71	0.55
1:G:5:VAL:HA	1:G:105:LYS:HZ3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:94:THR:HG1	2:B:95:PRO:HD3	1.68	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:OG1	2:D:206:THR:O	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
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:N	2:F:136:LEU:HD23	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
3:M:52:CYS:HB3	3:M:277:CYS:O	2.07	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
4:P:148:CYS:O	4:P:151:SER:OG	2.23	0.54
3:T:277:CYS:SG	3:T:277:CYS:O	2.55	0.54
1:I:38:ARG:HG3	1:I:90:TYR:CE1	2.43	0.54
3:N:115:VAL:HG11	3:N:116(B):PHE:HB2	1.90	0.54
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
4:X:27:GLN:HG3	4:X:27:GLN:O	2.08	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
1:C:74:SER:CB	3:U:291:SER:HB2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:96:LEU:C	1:I:96:LEU:HD12	2.22	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: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:N	2:J:158:ASN:OD1	2.40	0.52
3:U:180:TRP:CE2	3:U:233:TYR:HB2	2.44	0.52
4:V:62:GLN:CD	4:V:62:GLN:H	2.13	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
1:I:5:VAL:HA	1:I:105:LYS:HZ1	1.75	0.52
1:A:210:ARG:HH12	1:A:212:GLU:HB3	1.75	0.52
1:A:68:THR:H	1:A:81:ASP:CB	2.08	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
2:J:27:GLN:O	2:J:28:SER:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:74:SER:HB3	3:U:291:SER:CB	2.38	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
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
4:W:62:GLN:H	4:W:62:GLN:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:9:PHE:O	4:P:135:ASN:HA	2.12	0.49
1:K:74:SER:HB3	3:T:291:SER:CB	2.40	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:G:145:TYR:CD1	1:G:145:TYR:C	2.85	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
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
1:E:95:LYS:HE3	1:E:100(E):TYR:CZ	2.48	0.48
1:G:145:TYR:O	1:G:145:TYR:HD1	1.97	0.48
1:G:42:GLY:O	1:G:43:GLN:NE2	2.43	0.48
3:O:284:PRO:HD3	3:O:300:ILE:O	2.14	0.48
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:OG	1:G:25:SER:O	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
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: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:HD12	1:G:73:ILE:H	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
2:D:30:SER:OG	2:D:31:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ILE:HD13	4:P:49:THR:HA	1.96	0.48
1:E:36:TRP:CG	1:E:80:MET:HG3	2.48	0.48
3:O:307:LYS:NZ	4:P:90:ASP:OD2	2.41	0.48
1:C:40:ALA:HB3	1:C:43:GLN:HB2	1.95	0.48
2:D:163:VAL:HG22	2:D:175:LEU:HD13	1.96	0.48
1:I:47:TRP:CG	2:J:96:LEU:HB2	2.49	0.48
1:I:82(C):LEU:HA	1:I:82(C):LEU:HD12	1.53	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
2:D:32:SER:C	2:D:50:GLY:O	2.52	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: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:100(B):PHE:CE1	4:X:19:ASP:HA	2.49	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
3:M:307:LYS:HE2	4:P:61:THR:HG22	1.97	0.47
1:I:100(B):PHE:CE1	4:R:19:ASP:HA	2.49	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:HD23	2:L:136:LEU:N	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
3:S:123:LYS:HZ1	3:S:133:ASN:ND2	2.12	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
1:A:32:TYR:HB3	1:A:100:TYR:CD1	2.50	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:HH11	3:U:262:ARG:HG3	1.78	0.47
3:U:307:LYS:HE2	4:X:61:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:HE2	1:G:105:LYS:H	1.80	0.46
1:K:94:ARG:NE	1:K:95:LYS:O	2.41	0.46
4:X:30:GLN:OE1	4:X:146:ASN:N	2.42	0.46
2:B:21:LEU:HD12	2:B:21:LEU:N	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
4:V:142:HIS:HB2	4:V:165:GLU:CD	2.36	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
4:P:102:LEU:HA	4:P:102:LEU:HD23	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
3:N:163:LYS:CB	3:U:159:ASN:ND2	2.78	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:192:TYR:HB2	2:J:209:PHE:CE1	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:53:ILE:CD1	4:X:49:THR:HA	2.46	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
3:S:284:PRO:HD3	3:S:300:ILE:O	2.15	0.46
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
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
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:145:TYR:O	1:G:145:TYR:CD1	2.70	0.45
1:G:4:LEU:HD11	1:G:94:ARG:HG2	1.99	0.45
1:G:87:THR:HG1	1:G:110:THR:HA	1.81	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:HD23	2:J:136:LEU:N	2.31	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:203:SER:O	2:J:203:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:O:45:ASP:C	3:O:297:ILE:HD11	2.36	0.45
4:W:158:ASP:OD1	4:W:160:PRO:HD2	2.17	0.45
4:X:6:ILE:HG21	4:X:6:ILE:HD13	1.73	0.45
2:D:33:LEU:HD12	2:D:89:GLN:C	2.33	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:38:LEU:HA	4:V:38:LEU:HD23	1.77	0.45
4:V:4:GLY:O	4:V:8:GLY:HA3	2.17	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
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:HA	1:C:209:LYS:HD2	1.86	0.44
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.98	0.44
1:G:197:ASN:ND2	1:G:208:ASP:OD2	2.45	0.44
3:M:314:LEU:HA	3:M:314:LEU:HD23	1.85	0.44
3:T:295:GLN:O	3:T:308:TYR:HA	2.17	0.44
3:T:69:TRP:HE1	3:T:81:THR:CG2	2.31	0.44
4:V:1:GLY:O	4:V:2:LEU:C	2.56	0.44
1:G:53:ILE:CD1	4:V:49:THR:HA	2.47	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:161:GLU:HA	2:D:177:SER:HA	1.99	0.44
2:D:47:LEU:HD23	2:D:58:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:LEU:HD22	2:J:71:PHE:CD2	2.52	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:175:LEU:HD12	2:J:176:SER:H	1.82	0.44
2:J:163:VAL:HG22	2:J:175:LEU:HD13	1.99	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
3:O:180:TRP:CE2	3:O:233:TYR:HB2	2.52	0.44
3:S:30:LEU:HA	3:S:30:LEU:HD23	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:C:32:TYR:HB3	1:C:100:TYR:CD1	2.53	0.44
1:C:154:TRP:CZ3	1:C:196:CYS:HB3	2.52	0.44
1:C:63:PHE:CD2	1:C:66:ARG:HD2	2.51	0.44
2:F:175:LEU:HD12	2:F:176:SER:H	1.83	0.44
2:F:78:LEU:HD23	2:F:78:LEU:HA	1.73	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
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:HD12	2:F:21:LEU:N	2.33	0.44
1:G:178:LEU:C	1:G:178:LEU:HD12	2.38	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:S:314:LEU:HA	3:S:314:LEU:HD23	1.71	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:H	1:A:73:ILE:HD12	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
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:H:175:LEU:HD12	2:H:176:SER:N	2.32	0.44
2:L:202:SER:O	2:L:202:SER:OG	2.30	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:100(A):TYR:HD2	4:R:42:GLN:OE1	2.01	0.44
1:I:53:ILE:HD13	4:R:49:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:ILE:HD12	1:I:73:ILE:H	1.83	0.43
1:I:16:SER:O	1:I:82(C):LEU:HB2	2.17	0.43
2:J:14:SER:O	2:J:17:GLU:OE2	2.36	0.43
3:O:151:LEU:HB3	3:O:252:VAL:HG12	1.99	0.43
3:O:15:ILE:HD11	4:R:122:VAL:HG21	2.00	0.43
1:A:51:ILE:CD1	1:A:71:ALA:HB2	2.48	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:N:45:ASP:C	3:N:297:ILE:HD11	2.39	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
4:P:126:LEU:HD23	4:P:126:LEU:HA	1.70	0.43
4:X:74:GLU:HB3	4:X:77:ILE:HD11	2.00	0.43
1:G:130:SER:HA	2:H:116:PHE:HD1	1.83	0.43
1:G:51:ILE:HD11	1:G:71:ALA:HB2	1.99	0.43
4:W:2:LEU:HA	4:W:2:LEU:HD12	1.54	0.43
2:D:32:SER:O	2:D:50:GLY:O	2.36	0.43
2:D:61:ARG:NH1	2:D:82:ASP:CG	2.72	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
3:M:176:VAL:HA	3:M:258:PHE:O	2.18	0.43
3:T:208:ARG:HH11	4:X:72:HIS:CE1	2.37	0.43
3:O:189:ALA:HA	3:U:189:ALA:HB1	2.00	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
4:P:105:GLU:CG	4:R:106:ARG:HH12	2.31	0.43
4:P:62:GLN:CD	4:P:62:GLN:H	2.22	0.43
4:P:102:LEU:HD21	4:R:103:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:315:ARG:HH11	3:S:315:ARG:HD2	1.62	0.43
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
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
1:K:53:ILE:HD13	4:W:49:THR:HA	2.01	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
4:W:99:LEU:HA	4:W:99:LEU:HD12	1.78	0.43
3:U:308:TYR:HD2	4:X:89:LEU:HD13	1.81	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:R:27:GLN:O	4:R:27:GLN:HG3	2.18	0.43
4:Q:68:LYS:HE3	4:R:79:ASN:HB2	2.00	0.43
3:U:167:SER:OG	3:U:244:THR:HG22	2.18	0.43
1:C:82(C):LEU:HA	1:C:82(C):LEU:HD12	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
2:B:58:ILE:HA	2:B:58:ILE:HD13	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:178:LEU:C	1:E:178:LEU:HD12	2.39	0.42
2:F:61:ARG:NH1	2:F:82:ASP:OD1	2.52	0.42
2:H:204:PRO:O	2:H:205:VAL:C	2.55	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:HA	4:W:102:LEU:HD23	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:T:116(B):PHE:HE1	3:T:260:MET:HE1	1.84	0.42
3:U:103:ILE:N	3:U:103:ILE:HD12	2.34	0.42
1:A:25:SER:OG	1:A:25:SER:O	2.24	0.42
1:A:40:ALA:HB3	1:A:43:GLN:HB2	2.01	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:O	2:J:191:VAL:HG13	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:HD12	4:W:118:LEU:HA	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:198:HIS:CD2	2:L:199:GLN:O	2.72	0.42
2:L:32:SER:HB2	2:L:51:ALA:CB	2.46	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:HA	4:P:168:LEU:HD23	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: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
3:M:106:GLU:CD	4:P:71:ASN:HB3	2.39	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: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:HD23	4:V:168:LEU:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:PRO:HD3	2:H:132:VAL:HG22	2.02	0.42
1:G:181:VAL:HG11	2:H:135:LEU:HD22	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
3:U:119:GLU:CD	3:U:122:PRO:HA	2.39	0.42
2:B:24:ARG:NH1	2:B:70:ASP:OD1	2.53	0.41
1:C:51:ILE:HD13	1:C:51:ILE:HG21	1.71	0.41
1:C:17:SER:HA	1:C:82(A):SER:HA	1.96	0.41
2:H:29:VAL:O	2:H:29:VAL:CG1	2.68	0.41
1:K:61:GLN:OE1	1:K:61:GLN:N	2.52	0.41
1:K:95:LYS:HE2	1:K:97:GLU:O	2.19	0.41
3:O:116(B):PHE:CE1	3:O:260:MET:HE2	2.54	0.41
3:S:45:ASP:C	3:S:297:ILE:HD11	2.40	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:123:GLU:HA	2:H:126:LYS:HE2	2.03	0.41
2:H:32:SER:HB2	2:H:51:ALA:CB	2.49	0.41
2:J:205:VAL:HG12	2:J:205:VAL:H	1.59	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:152:ILE:HD11	3:S:255:ARG:HD2	2.02	0.41
3:S:58:PRO:HB3	3:S:86:TYR:CZ	2.55	0.41
1:E:209:LYS:HA	1:E:209:LYS:HD2	1.77	0.41
1:E:51:ILE:HD13	1:E:51:ILE:HG21	1.72	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:35:TRP:CZ3	2:H:88:CYS:HB3	2.55	0.41
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.55	0.41
2:H:78:LEU:HD23	2:H:78:LEU:HA	1.83	0.41
1:I:129:LYS:HA	1:I:129:LYS:HE2	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:HD2	4:R:170:ARG:HH11	1.72	0.41
3:U:174:LYS:CA	3:U:239:PRO:HG3	2.50	0.41
3:U:8:ASP:N	3:U:9:PRO:CD	2.84	0.41
3:S:11:ASP:OD1	4:V:28:ASN:HA	2.20	0.41
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LYS:HE2	1:E:105:LYS:H	1.84	0.41
3:M:207:SER:OG	3:M:241:ASP:OD1	2.27	0.41
3:S:90(A):PRO:HD2	3:S:271:ASP:OD1	2.19	0.41
3:U:186:SER:HA	3:U:218:ALA:O	2.20	0.41
4:X:102:LEU:HA	4:X:102:LEU:HD23	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
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: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
1:G:74:SER:CB	3:S:291:SER:HB2	2.45	0.41
4:V:1:GLY:O	4:V:4:GLY:N	2.51	0.41
3:S:308:TYR:CD2	4:V:89:LEU:HD13	2.56	0.41
3:M:15:ILE:HD12	3:M:15:ILE:N	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:G:100(A):TYR:OH	4:V:19:ASP:O	2.32	0.41
1:K:100(A):TYR:HB3	4:W:42:GLN:OE1	2.20	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:129:LYS:HZ3	2:L:207:LYS:HD3	1.85	0.41
1:K:146:PHE:CE1	1:K:147:PRO:HB3	2.56	0.41
1:A:53:ILE:CD1	4:Q:49:THR:HA	2.50	0.41
3:S:184:HIS:HB3	3:S:216:GLU:O	2.21	0.41
3:S:41:ASN:ND2	3:S:43:LEU:O	2.54	0.41
3:U:262:ARG:NH1	3:U:262:ARG:HG3	2.36	0.41
2:H:11:LEU:O	2:H:104:VAL:HA	2.20	0.41
1:K:96:LEU:HA	1:K:96:LEU:HD12	1.82	0.41
3:O:176:VAL:HA	3:O:258:PHE:O	2.20	0.41
4:P:1:GLY:O	4:P:2:LEU:C	2.57	0.41
4:P:74:GLU:HB3	4:P:77:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:36:TRP:CZ2	1:C:80:MET:HB2	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
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
1:E:89:VAL:HG22	1:E:108:THR:HG22	2.03	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
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
4:P:2:LEU:HD12	4:P:2:LEU:HA	1.62	0.41
4:V:170:ARG:HH11	4:V:170:ARG:HD2	1.74	0.41
4:X:170:ARG:HD2	4:X:170:ARG:HH11	1.72	0.41
3:N:310:LYS:HA	3:N:310:LYS:HD3	1.90	0.41
3:O:262:ARG:HG3	3:O:262:ARG:HH11	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
4:V:101:LEU:HD23	4:V:101:LEU:HA	1.75	0.41
3:T:303:GLY:HA2	4:W:63:PHE:CE2	2.56	0.41
4:X:99:LEU:HA	4:X:99:LEU:HD12	1.87	0.41
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:146:PHE:HA	1:I:147:PRO:HA	1.90	0.40
1:I:61:GLN:OE1	1:I:61:GLN:N	2.54	0.40
3:M:321:ARG:HD2	3:M:321:ARG:HH11	1.75	0.40
3:M:42:LEU:HD11	3:M:316:LEU:HD22	2.03	0.40
4:P:23:GLY:HA3	4:P:36:ALA:HA	2.02	0.40
4:Q:62:GLN:CD	4:Q:62:GLN:H	2.24	0.40
3:U:52:CYS:HB3	3:U:277:CYS:O	2.20	0.40
4:V:148:CYS:O	4:V:151:SER:OG	2.29	0.40
1:C:100(A):TYR:HD2	4:X:42:GLN:OE1	2.04	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
1:I:145:TYR:CE1	1:I:150:VAL:HG23	2.57	0.40
1:I:38:ARG:NH2	1:I:86:ASP:OD1	2.55	0.40
2:L:13:LEU:HA	2:L:13:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LEU:HD12	2:D:21:LEU:N	2.36	0.40
1:I:12:LYS:HA	1:I:12:LYS:HD2	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:HA	4:Q:73:LEU:HD23	1.84	0.40
4:R:157:TYR:CE2	4:R:159:TYR:HA	2.56	0.40
4:R:141:TYR:O	4:R:166:ALA:HA	2.21	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
3:S:20:ASN:OD1	3:S:20:ASN:C	2.60	0.40
3:T:94:ASN:HA	3:T:94:ASN:HD22	1.75	0.40
1:A:42:GLY:O	1:A:43:GLN:NE2	2.44	0.40
1:C:105:LYS:CE	1:C:105:LYS:H	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:S:42:LEU:HD23	3:S:42:LEU:HA	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%)	14 55
1	C	223/225 (99%)	200 (90%)	20 (9%)	3 (1%)	14 55
1	E	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	38 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	20	63
1	I	223/225 (99%)	205 (92%)	17 (8%)	1 (0%)	38	77
1	K	223/225 (99%)	203 (91%)	17 (8%)	3 (1%)	14	55
2	B	211/213 (99%)	189 (90%)	16 (8%)	6 (3%)	6	39
2	D	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	13	53
2	F	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	13	53
2	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	20	63
2	J	211/213 (99%)	190 (90%)	15 (7%)	6 (3%)	6	39
2	L	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	13	53
3	M	322/331 (97%)	312 (97%)	10 (3%)	0	100	100
3	N	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	44	80
3	O	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	28	70
3	S	322/331 (97%)	312 (97%)	9 (3%)	1 (0%)	44	80
3	T	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	44	80
3	U	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	28	70
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%)	22	65

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
1	K	82(A)	SER
1	A	27	GLY
2	D	31	SER

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Mol	Chain	Res	Type
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%)	175 (93%)	14 (7%)	16	52
1	C	189/189 (100%)	177 (94%)	12 (6%)	21	59
1	E	189/189 (100%)	180 (95%)	9 (5%)	30	67
1	G	189/189 (100%)	176 (93%)	13 (7%)	18	55
1	I	189/189 (100%)	179 (95%)	10 (5%)	26	63
1	K	189/189 (100%)	178 (94%)	11 (6%)	23	61
2	B	184/184 (100%)	176 (96%)	8 (4%)	33	70
2	D	184/184 (100%)	175 (95%)	9 (5%)	29	66
2	F	184/184 (100%)	174 (95%)	10 (5%)	26	63
2	H	184/184 (100%)	173 (94%)	11 (6%)	22	60
2	J	184/184 (100%)	175 (95%)	9 (5%)	29	66
2	L	184/184 (100%)	171 (93%)	13 (7%)	17	54
3	M	284/290 (98%)	278 (98%)	6 (2%)	59	84
3	N	283/290 (98%)	279 (99%)	4 (1%)	71	89
3	O	286/290 (99%)	283 (99%)	3 (1%)	80	91
3	S	284/290 (98%)	279 (98%)	5 (2%)	64	86
3	T	283/290 (98%)	280 (99%)	3 (1%)	78	91
3	U	286/290 (99%)	283 (99%)	3 (1%)	80	91
4	P	150/151 (99%)	150 (100%)	0	100	100
4	Q	146/151 (97%)	145 (99%)	1 (1%)	87	95
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%)	87	95
4	X	146/151 (97%)	146 (100%)	0	100	100
All	All	4828/4884 (99%)	4673 (97%)	155 (3%)	44	76

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	25	SER
1	A	28	THR
1	A	38	ARG
1	A	66	ARG
1	A	81	ASP

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	82(A)	SER
1	A	82(C)	LEU
1	A	83	SER
1	A	100	TYR
1	A	100(F)	MET
1	A	105	LYS
1	A	208	ASP
2	B	22	SER
2	B	28	SER
2	B	122	ASP
2	B	143	GLU
2	B	150	VAL
2	B	199	GLN
2	B	203	SER
2	B	204	PRO
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	100	TYR
1	C	100(F)	MET
1	C	105	LYS
1	C	208	ASP
2	D	22	SER
2	D	32	SER
2	D	61	ARG
2	D	122	ASP
2	D	125	LEU
2	D	143	GLU
2	D	150	VAL
2	D	202	SER
2	D	205	VAL
1	E	11	VAL
1	E	38	ARG
1	E	66	ARG
1	E	81	ASP
1	E	82(B)	SER

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Mol	Chain	Res	Type
1	E	100	TYR
1	E	100(F)	MET
1	E	105	LYS
1	E	208	ASP
2	F	22	SER
2	F	28	SER
2	F	29	VAL
2	F	122	ASP
2	F	125	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	66	ARG
1	G	82(A)	SER
1	G	82(C)	LEU
1	G	83	SER
1	G	84	SER
1	G	100	TYR
1	G	100(F)	MET
1	G	105	LYS
1	G	145	TYR
1	G	148	GLU
1	G	208	ASP
2	H	22	SER
2	H	28	SER
2	H	29	VAL
2	H	30	SER
2	H	122	ASP
2	H	125	LEU
2	H	143	GLU
2	H	150	VAL
2	H	199	GLN
2	H	205	VAL
2	H	206	THR
1	I	38	ARG
1	I	66	ARG
1	I	81	ASP
1	I	82(A)	SER

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Mol	Chain	Res	Type
1	I	82(B)	SER
1	I	83	SER
1	I	100	TYR
1	I	100(F)	MET
1	I	105	LYS
1	I	208	ASP
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	143	GLU
2	J	150	VAL
2	J	199	GLN
1	K	11	VAL
1	K	28	THR
1	K	38	ARG
1	K	66	ARG
1	K	82	LEU
1	K	82(B)	SER
1	K	84	SER
1	K	100	TYR
1	K	100(F)	MET
1	K	105	LYS
1	K	208	ASP
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	61	ARG
2	L	122	ASP
2	L	143	GLU
2	L	150	VAL
2	L	199	GLN
2	L	205	VAL
2	L	206	THR
3	M	63	LYS
3	M	208	ARG
3	M	266	SER

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Mol	Chain	Res	Type
3	M	277	CYS
3	M	283	THR
3	M	320	LEU
3	N	266	SER
3	N	283	THR
3	N	291	SER
3	N	310	LYS
3	O	63	LYS
3	O	266	SER
3	O	283	THR
4	Q	168	LEU
3	S	63	LYS
3	S	208	ARG
3	S	266	SER
3	S	283	THR
3	S	320	LEU
3	T	266	SER
3	T	283	THR
3	T	291	SER
3	U	63	LYS
3	U	266	SER
3	U	283	THR
4	W	168	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	B	38	GLN
2	B	198	HIS
2	B	199	GLN
2	D	38	GLN
2	D	198	HIS
2	D	199	GLN
1	E	39	GLN
1	E	199	ASN
2	F	38	GLN
2	F	198	HIS
2	H	198	HIS
1	I	39	GLN
2	J	38	GLN
2	J	199	GLN

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Mol	Chain	Res	Type
1	K	6	GLN
2	L	198	HIS
2	L	199	GLN
3	M	94	ASN
3	M	133	ASN
3	M	226	GLN
3	N	94	ASN
3	N	111	GLN
3	O	38	HIS
3	O	94	ASN
3	O	159	ASN
3	O	226	GLN
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	79	ASN
3	S	94	ASN
3	S	133	ASN
3	T	111	GLN
3	T	226	GLN
3	U	94	ASN
3	U	159	ASN
3	U	226	GLN
3	U	275	HIS
4	V	43	ASN
4	V	53	ASN
4	V	95	ASN
4	W	25	HIS
4	W	95	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	225/225 (100%)	0.56	15 (6%) 19 16	51, 74, 96, 116	0
1	C	225/225 (100%)	0.53	11 (4%) 30 24	59, 78, 95, 114	0
1	E	225/225 (100%)	0.54	10 (4%) 35 28	55, 79, 99, 111	0
1	G	225/225 (100%)	0.63	12 (5%) 27 22	54, 81, 105, 124	0
1	I	225/225 (100%)	0.91	34 (15%) 3 3	59, 91, 116, 128	0
1	K	225/225 (100%)	0.54	12 (5%) 27 22	51, 72, 98, 114	0
2	B	213/213 (100%)	0.23	1 (0%) 90 86	53, 61, 76, 85	0
2	D	213/213 (100%)	0.38	1 (0%) 90 86	62, 71, 83, 94	0
2	F	213/213 (100%)	0.30	0 100 100	58, 68, 83, 92	0
2	H	213/213 (100%)	0.29	3 (1%) 75 67	54, 68, 86, 98	0
2	J	213/213 (100%)	0.33	4 (1%) 67 59	55, 71, 89, 106	0
2	L	213/213 (100%)	0.17	1 (0%) 90 86	51, 61, 76, 89	0
3	M	324/331 (97%)	2.28	147 (45%) 0 0	55, 175, 212, 218	0
3	N	323/331 (97%)	2.00	137 (42%) 0 0	50, 168, 205, 211	0
3	O	326/331 (98%)	2.48	165 (50%) 0 0	54, 196, 228, 232	0
3	S	324/331 (97%)	1.69	113 (34%) 0 0	55, 153, 182, 186	0
3	T	323/331 (97%)	1.72	114 (35%) 0 0	52, 157, 192, 196	0
3	U	326/331 (98%)	1.73	115 (35%) 0 0	55, 159, 190, 197	0
4	P	175/177 (98%)	0.62	11 (6%) 21 17	51, 73, 141, 170	0
4	Q	171/177 (96%)	0.53	10 (5%) 24 20	50, 72, 133, 157	0
4	R	171/177 (96%)	0.51	8 (4%) 32 26	51, 74, 134, 156	0
4	V	175/177 (98%)	0.57	12 (6%) 18 15	52, 77, 128, 147	0
4	W	171/177 (96%)	0.57	13 (7%) 15 13	51, 72, 113, 141	0
4	X	171/177 (96%)	0.52	10 (5%) 24 20	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%)	1.00	959 (17%) 2 2	50, 80, 199, 232	0

All (959) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	165	SER	13.2
3	O	164	LEU	11.9
3	N	198	ALA	11.7
3	O	250	ASN	10.9
3	M	127	TRP	9.4
3	O	138	ALA	9.3
3	O	154	LEU	9.2
3	M	187	THR	9.1
3	M	250	ASN	9.0
3	M	76	CYS	8.6
1	A	215	SER	8.6
3	M	224	ARG	8.5
3	N	186	SER	8.4
3	N	138	ALA	8.4
3	N	127	TRP	8.4
3	M	195	TYR	8.1
3	M	225	ASP	8.1
3	S	183	HIS	8.1
3	M	74	PRO	8.0
3	M	154	LEU	7.8
3	O	123	LYS	7.8
3	O	246	GLU	7.8
3	S	154	LEU	7.7
3	O	8	ASP	7.7
3	M	260	MET	7.7
3	O	247	ALA	7.6
3	M	142	ALA	7.6
1	G	215	SER	7.4
3	N	167	SER	7.4
3	O	243	ILE	7.3
3	N	199	ASP	7.2
3	O	205	GLY	7.2
3	T	173	GLY	7.1
3	M	55	ARG	7.1
3	O	155	VAL	7.0
3	T	154	LEU	6.9
3	M	172	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
3	U	81	THR	6.8
3	O	163	LYS	6.7
3	M	155	VAL	6.7
3	M	123	LYS	6.7
3	M	217	ILE	6.7
1	I	215	SER	6.7
3	O	133(A)	LYS	6.7
3	O	127	TRP	6.7
3	N	77	GLU	6.6
1	I	131	THR	6.6
3	T	132	SER	6.6
3	T	224	ARG	6.6
3	S	134	GLY	6.6
3	O	141	HIS	6.5
3	O	101	ASP	6.4
3	O	199	ASP	6.4
3	N	224	ARG	6.4
3	T	250	ASN	6.4
3	O	76	CYS	6.3
3	O	159	ASN	6.3
3	M	143	GLY	6.3
3	O	132	SER	6.2
3	O	74	PRO	6.2
3	S	138	ALA	6.2
3	O	213	PHE	6.2
3	U	138	ALA	6.2
3	U	154	LEU	6.2
3	M	229	ARG	6.1
3	U	163	LYS	6.1
3	U	76	CYS	6.1
3	N	216	GLU	6.1
3	O	79	LEU	6.1
3	O	148	TYR	6.0
3	S	155	VAL	6.0
3	U	134	GLY	6.0
3	N	116(C)	GLU	6.0
3	N	154	LEU	6.0
3	S	153	TRP	6.0
3	N	76	CYS	5.9
3	U	153	TRP	5.9
4	P	175	SER	5.9
3	N	155	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
3	T	198	ALA	5.9
3	M	134	GLY	5.8
3	O	216	GLU	5.8
3	O	173	GLY	5.8
3	T	155	VAL	5.8
3	O	187	THR	5.8
4	P	174	ASP	5.8
3	T	123	LYS	5.8
3	O	77	GLU	5.8
3	M	213	PHE	5.7
3	N	187	THR	5.7
3	M	197	ASN	5.7
3	M	230	MET	5.7
3	T	160	SER	5.7
3	T	142	ALA	5.7
3	O	116(C)	GLU	5.7
3	M	186	SER	5.7
3	N	250	ASN	5.6
3	O	153	TRP	5.6
3	N	223	VAL	5.6
3	U	139	CYS	5.6
3	M	147	PHE	5.6
3	O	195	TYR	5.5
3	U	142	ALA	5.5
3	M	80	SER	5.5
3	O	139	CYS	5.5
3	M	93	ASP	5.5
3	U	250	ASN	5.5
3	M	138	ALA	5.5
3	S	172	LYS	5.5
3	T	153	TRP	5.5
3	M	135	VAL	5.5
1	K	215	SER	5.5
3	O	245	PHE	5.4
3	T	195	TYR	5.4
3	M	161	TYR	5.4
3	M	150	ASN	5.3
3	S	64	CYS	5.3
3	N	96	THR	5.3
3	S	116(C)	GLU	5.3
3	O	241	ASP	5.2
3	M	144	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
3	O	93	ASP	5.1
3	N	159	ASN	5.1
3	M	75	GLU	5.0
3	M	97	CYS	5.0
3	M	215	PRO	5.0
3	U	61	LEU	5.0
3	M	200	THR	5.0
3	N	132	SER	5.0
3	M	163	LYS	5.0
3	U	63	LYS	5.0
3	O	88	VAL	4.9
3	M	153	TRP	4.9
3	U	116(C)	GLU	4.9
3	M	82	ALA	4.9
3	M	139	CYS	4.9
3	O	203	PHE	4.9
3	N	141	HIS	4.9
3	T	161	TYR	4.9
3	O	251	LEU	4.8
3	U	8	ASP	4.8
3	N	251	LEU	4.8
3	N	126	SER	4.8
3	O	181	GLY	4.8
3	M	133(A)	LYS	4.8
3	M	183	HIS	4.8
1	K	130	SER	4.8
3	T	196	GLN	4.8
3	S	152	ILE	4.8
3	U	160	SER	4.8
3	O	194	LEU	4.8
3	M	51	LEU	4.8
3	T	127	TRP	4.8
3	T	97	CYS	4.7
3	S	127	TRP	4.7
3	M	116(B)	PHE	4.7
3	N	246	GLU	4.7
3	N	158	GLY	4.7
3	M	121	PHE	4.7
3	M	132	SER	4.7
3	O	9	PRO	4.7
3	U	216	GLU	4.7
3	T	78	SER	4.7

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Mol	Chain	Res	Type	RSRZ
3	U	223	VAL	4.7
3	O	62	GLY	4.7
3	N	173	GLY	4.6
3	T	228	GLY	4.6
3	O	73	ASN	4.6
3	S	230	MET	4.6
3	M	220	ARG	4.6
3	T	141	HIS	4.6
3	U	217	ILE	4.6
3	M	228	GLY	4.6
4	P	173	ILE	4.6
3	O	214	LYS	4.6
3	O	229	ARG	4.6
3	T	122	PRO	4.6
3	O	116(B)	PHE	4.6
3	O	201	TYR	4.5
3	T	129	ASN	4.5
3	N	153	TRP	4.5
3	O	172	LYS	4.5
3	S	197	ASN	4.5
3	U	260	MET	4.5
3	N	194	LEU	4.5
3	O	61	LEU	4.5
3	U	127	TRP	4.5
3	N	260	MET	4.5
3	T	229	ARG	4.5
3	M	141	HIS	4.4
3	O	80	SER	4.4
3	O	166	LYS	4.4
3	O	152	ILE	4.4
1	G	130	SER	4.4
3	N	197	ASN	4.4
3	O	204	VAL	4.4
3	O	90(A)	PRO	4.4
3	M	287	ALA	4.4
1	G	131	THR	4.4
3	O	249	GLY	4.4
3	M	140	PRO	4.3
3	S	79	LEU	4.3
3	T	121	PHE	4.3
3	T	172	LYS	4.3
3	T	126	SER	4.3

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Mol	Chain	Res	Type	RSRZ
3	O	131	ASP	4.3
3	O	134	GLY	4.3
3	U	55(A)	GLY	4.3
3	U	161	TYR	4.3
3	N	163	LYS	4.3
3	T	138	ALA	4.3
3	T	185	PRO	4.3
3	T	77	GLU	4.2
3	O	51	LEU	4.2
3	O	81	THR	4.2
3	S	156	LYS	4.2
3	N	160	SER	4.2
3	U	230	MET	4.2
3	N	245	PHE	4.2
3	O	252	VAL	4.2
3	O	215	PRO	4.2
3	M	73	ASN	4.2
3	T	80	SER	4.2
4	V	174	ASP	4.2
3	M	219	ILE	4.2
3	S	198	ALA	4.2
3	M	162	PRO	4.2
3	T	216	GLU	4.2
3	N	79	LEU	4.1
3	N	161	TYR	4.1
1	A	131	THR	4.1
3	N	229	ARG	4.1
3	S	248	THR	4.1
3	N	241	ASP	4.1
3	M	173	GLY	4.1
3	N	201	TYR	4.1
3	O	207	SER	4.1
3	N	97	CYS	4.1
3	N	157	LYS	4.1
3	T	100	GLY	4.1
3	N	185	PRO	4.1
3	M	196	GLN	4.1
3	M	288	ILE	4.1
4	X	144	CYS	4.1
3	M	126	SER	4.0
3	O	162	PRO	4.0
3	N	152	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	T	79	LEU	4.0
3	M	77	GLU	4.0
3	M	96	THR	4.0
3	N	191	GLN	4.0
3	M	245	PHE	4.0
3	S	166	LYS	4.0
3	S	247	ALA	4.0
3	M	122	PRO	4.0
3	O	104	ASP	4.0
3	T	120	ILE	4.0
3	M	94	ASN	4.0
3	N	129	ASN	4.0
3	O	191	GLN	4.0
3	M	72	GLY	4.0
3	U	215	PRO	4.0
3	M	223	VAL	3.9
3	T	260	MET	3.9
1	I	132	SER	3.9
3	M	81	THR	3.9
3	T	223	VAL	3.9
4	V	143	LYS	3.9
3	O	171	ASP	3.9
3	S	168	TYR	3.9
3	N	83(A)	SER	3.9
3	M	118	PHE	3.9
1	I	214	LYS	3.9
3	O	185	PRO	3.9
3	S	63	LYS	3.9
3	U	116(B)	PHE	3.9
1	K	214	LYS	3.9
3	O	224	ARG	3.9
3	T	134	GLY	3.9
3	N	156	LYS	3.9
1	I	130	SER	3.9
3	O	223	VAL	3.9
3	U	123	LYS	3.9
3	M	92	SER	3.9
3	S	157	LYS	3.9
3	T	11	ASP	3.9
3	N	221	PRO	3.8
3	N	270	SER	3.8
3	S	123	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
3	T	220	ARG	3.8
3	T	157	LYS	3.8
3	O	122	PRO	3.8
1	I	196	CYS	3.8
3	M	64	CYS	3.8
3	M	190	ASP	3.8
3	S	76	CYS	3.8
3	U	214	LYS	3.8
3	T	156	LYS	3.8
3	O	266	SER	3.8
1	I	198	VAL	3.8
1	C	215	SER	3.8
3	N	166	LYS	3.8
3	T	159	ASN	3.8
3	S	160	SER	3.8
3	M	152	ILE	3.8
3	S	161	TYR	3.8
3	U	77	GLU	3.8
3	U	157	LYS	3.8
3	S	139	CYS	3.8
3	T	63	LYS	3.7
3	M	198	ALA	3.7
3	O	156	LYS	3.7
3	M	124	THR	3.7
3	U	164	LEU	3.7
3	U	148	TYR	3.7
1	E	215	SER	3.7
3	U	224	ARG	3.7
3	M	120	ILE	3.7
3	S	118	PHE	3.7
3	O	279	THR	3.7
3	N	184	HIS	3.7
3	M	191	GLN	3.7
4	Q	142	HIS	3.7
3	N	134	GLY	3.6
3	N	183	HIS	3.6
3	M	116(A)	SER	3.6
3	O	228	GLY	3.6
3	M	87	ILE	3.6
3	O	98	TYR	3.6
3	O	124	THR	3.6
3	O	83(A)	SER	3.6

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Mol	Chain	Res	Type	RSRZ
3	T	200	THR	3.6
3	U	80	SER	3.6
3	S	174	LYS	3.6
3	O	116(A)	SER	3.6
3	U	11	ASP	3.6
3	S	77	GLU	3.6
3	O	58	PRO	3.6
3	T	147	PHE	3.6
3	O	150	ASN	3.6
4	V	173	ILE	3.6
3	N	55	ARG	3.5
3	N	195	TYR	3.5
3	N	78	SER	3.5
3	N	140	PRO	3.5
3	M	62	GLY	3.5
3	N	172	LYS	3.5
3	O	59	LEU	3.5
3	T	62	GLY	3.5
3	M	60	HIS	3.5
3	M	83	SER	3.5
3	N	165	SER	3.5
3	T	116	SER	3.5
3	N	259	ALA	3.5
3	U	196	GLN	3.5
3	M	276	ASP	3.5
3	S	261	GLU	3.5
3	U	79	LEU	3.5
3	N	121	PHE	3.5
3	U	62	GLY	3.5
3	U	229	ARG	3.5
3	O	97	CYS	3.5
3	M	137	ALA	3.5
3	N	170	ASN	3.5
3	T	197	ASN	3.5
3	N	74	PRO	3.5
3	S	62	GLY	3.5
3	M	218	ALA	3.5
1	I	112	SER	3.4
3	O	146	SER	3.4
3	O	244	THR	3.4
3	M	100	GLY	3.4
3	U	173	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	N	175	GLU	3.4
3	N	202	VAL	3.4
3	S	74	PRO	3.4
4	V	140	PHE	3.4
1	A	214	LYS	3.4
3	M	151	LEU	3.4
3	S	117	ARG	3.4
3	U	133(A)	LYS	3.4
3	O	157	LYS	3.4
1	E	189	LEU	3.4
3	O	125	SER	3.4
3	O	183	HIS	3.4
4	X	129	ASN	3.4
1	K	131	THR	3.4
1	I	82(B)	SER	3.4
3	M	54	LEU	3.4
3	O	220	ARG	3.4
3	U	247	ALA	3.4
3	S	187	THR	3.4
3	M	251	LEU	3.4
3	S	171	ASP	3.4
3	S	195	TYR	3.4
3	S	245	PHE	3.4
3	M	216	GLU	3.4
3	T	230	MET	3.4
4	P	144	CYS	3.4
3	O	259	ALA	3.3
3	U	147	PHE	3.3
3	S	224	ARG	3.3
3	S	10	GLY	3.3
3	N	88	VAL	3.3
3	M	257	ALA	3.3
3	N	11	ASP	3.3
3	U	97	CYS	3.3
1	E	198	VAL	3.3
3	N	122	PRO	3.3
3	N	139	CYS	3.3
3	S	55	ARG	3.3
3	S	147	PHE	3.3
3	T	139	CYS	3.3
3	O	260	MET	3.3
3	U	199	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
3	O	161	TYR	3.3
1	K	129	LYS	3.3
1	K	189	LEU	3.3
3	S	173	GLY	3.3
3	U	197	ASN	3.3
3	O	126	SER	3.3
3	T	245	PHE	3.3
3	S	251	LEU	3.3
3	M	270	SER	3.3
3	T	76	CYS	3.3
4	W	144	CYS	3.3
3	T	219	ILE	3.2
3	M	79	LEU	3.2
3	N	123	LYS	3.2
3	O	174	LYS	3.2
3	O	202	VAL	3.2
3	U	171	ASP	3.2
3	O	116	SER	3.2
3	O	218	ALA	3.2
3	U	90(A)	PRO	3.2
4	P	143	LYS	3.2
3	S	199	ASP	3.2
1	E	131	THR	3.2
3	T	96	THR	3.2
3	O	282	GLN	3.2
3	O	182	ILE	3.2
3	M	70	ILE	3.2
3	N	118	PHE	3.2
4	X	141	TYR	3.2
1	I	159	LEU	3.2
3	O	167	SER	3.2
3	S	260	MET	3.2
3	T	124	THR	3.2
4	R	144	CYS	3.2
3	T	247	ALA	3.2
3	M	98	TYR	3.2
3	O	273	PRO	3.2
3	M	50	LYS	3.2
3	O	158	GLY	3.2
3	S	246	GLU	3.2
1	I	207	VAL	3.1
3	S	96	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	S	194	LEU	3.1
4	V	144	CYS	3.1
3	S	95	GLY	3.1
3	N	289	ASN	3.1
3	O	94	ASN	3.1
3	O	206	SER	3.1
3	O	192	GLN	3.1
3	T	187	THR	3.1
3	N	61	LEU	3.1
3	O	254	PRO	3.1
3	N	263	ASN	3.1
3	M	104	ASP	3.1
3	S	94	ASN	3.1
1	I	212	GLU	3.1
3	M	240	GLY	3.1
3	O	240	GLY	3.1
3	M	221	PRO	3.1
3	U	73	ASN	3.1
4	Q	162	TYR	3.1
3	O	90	THR	3.1
3	O	147	PHE	3.1
3	U	279	THR	3.1
3	U	155	VAL	3.1
3	M	160	SER	3.0
3	N	219	ILE	3.0
3	O	186	SER	3.0
3	S	93	ASP	3.0
3	S	121	PHE	3.0
3	T	130	HIS	3.0
3	T	201	TYR	3.0
3	S	51	LEU	3.0
3	O	102	PHE	3.0
1	C	210	ARG	3.0
1	I	144	ASP	3.0
3	O	188	SER	3.0
3	M	116(C)	GLU	3.0
3	T	131	ASP	3.0
1	G	191	THR	3.0
3	O	257	ALA	3.0
3	M	259	ALA	3.0
3	U	219	ILE	3.0
3	O	60	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
3	S	61	LEU	3.0
3	N	94	ASN	3.0
3	T	165	SER	3.0
3	U	231	ASN	3.0
4	R	143	LYS	3.0
3	S	290	THR	3.0
3	T	221	PRO	3.0
3	O	149	LYS	3.0
3	T	143	GLY	3.0
3	N	64	CYS	3.0
3	S	250	ASN	3.0
3	O	226	GLN	3.0
1	I	154	TRP	3.0
3	N	142	ALA	3.0
3	O	48	ASN	3.0
3	S	277	CYS	3.0
3	U	288	ILE	2.9
3	S	167	SER	2.9
3	M	68	GLY	2.9
3	M	136	THR	2.9
3	S	215	PRO	2.9
3	S	133(A)	LYS	2.9
3	U	150	ASN	2.9
1	A	189	LEU	2.9
3	O	290	THR	2.9
4	W	27	GLN	2.9
3	U	246	GLU	2.9
3	U	182	ILE	2.9
3	S	263	ASN	2.9
3	O	96	THR	2.9
3	S	88	VAL	2.9
3	T	144	ALA	2.9
3	T	74	PRO	2.9
3	U	207	SER	2.9
3	N	100	GLY	2.9
3	O	118	PHE	2.9
1	A	130	SER	2.9
3	S	55(A)	GLY	2.9
3	O	92	SER	2.9
3	M	236	LEU	2.9
3	S	124	THR	2.9
3	N	208	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
3	M	95	GLY	2.9
3	O	100	GLY	2.9
3	S	122	PRO	2.9
3	S	184	HIS	2.9
3	N	119	GLU	2.9
3	O	190	ASP	2.9
3	S	229	ARG	2.9
3	T	61	LEU	2.9
3	T	158	GLY	2.8
3	U	195	TYR	2.8
3	S	73	ASN	2.8
3	T	82	ALA	2.8
4	R	63	PHE	2.8
3	M	159	ASN	2.8
3	M	71	LEU	2.8
3	M	194	LEU	2.8
3	M	212	LYS	2.8
3	T	81	THR	2.8
1	E	16	SER	2.8
3	S	83(A)	SER	2.8
3	M	263	ASN	2.8
3	N	249	GLY	2.8
3	S	231	ASN	2.8
3	U	141	HIS	2.8
4	W	142	HIS	2.8
3	N	257	ALA	2.8
4	Q	141	TYR	2.8
3	U	186	SER	2.8
3	U	159	ASN	2.8
3	N	144	ALA	2.8
3	O	69	TRP	2.8
3	O	168	TYR	2.8
3	U	245	PHE	2.8
3	O	277	CYS	2.8
3	S	186	SER	2.8
3	T	170	ASN	2.8
3	N	190	ASP	2.8
3	T	64	CYS	2.8
1	K	194	TYR	2.8
3	O	140	PRO	2.8
3	U	248	THR	2.8
3	T	171	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	T	241	ASP	2.8
3	U	60	HIS	2.8
3	M	91	SER	2.8
3	T	118	PHE	2.8
3	U	201	TYR	2.8
3	N	254	PRO	2.7
3	S	282	GLN	2.7
3	T	191	GLN	2.7
3	O	121	PHE	2.7
3	T	202	VAL	2.7
3	M	90(A)	PRO	2.7
3	T	215	PRO	2.7
3	N	124	THR	2.7
1	I	66	ARG	2.7
3	U	168	TYR	2.7
3	S	83	SER	2.7
3	S	287	ALA	2.7
3	N	268	ILE	2.7
3	M	214	LYS	2.7
3	S	78	SER	2.7
3	T	92	SER	2.7
1	I	145	TYR	2.7
3	N	218	ALA	2.7
4	Q	144	CYS	2.7
3	N	90(A)	PRO	2.7
3	S	146	SER	2.7
3	U	51	LEU	2.7
3	U	200	THR	2.7
3	S	202	VAL	2.7
3	U	166	LYS	2.7
3	N	217	ILE	2.7
3	N	51	LEU	2.7
3	S	272	THR	2.7
3	M	63	LYS	2.7
3	M	78	SER	2.7
3	T	184	HIS	2.7
3	U	10	GLY	2.7
4	P	142	HIS	2.7
3	N	147	PHE	2.7
3	N	174	LYS	2.7
3	O	10	GLY	2.7
1	I	206	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	M	222	LYS	2.7
4	W	143	LYS	2.7
4	V	149	MET	2.7
3	N	162	PRO	2.7
1	E	130	SER	2.7
3	S	129	ASN	2.7
4	W	148	CYS	2.7
3	N	200	THR	2.7
3	S	200	THR	2.7
3	N	282	GLN	2.7
3	O	75	GLU	2.7
1	K	128	SER	2.6
3	N	164	LEU	2.6
1	I	1	GLN	2.6
3	M	53	LYS	2.6
3	O	212	LYS	2.6
3	U	99	PRO	2.6
2	L	30	SER	2.6
3	M	157	LYS	2.6
3	M	261	GLU	2.6
3	S	223	VAL	2.6
3	T	50	LYS	2.6
3	U	74	PRO	2.6
3	U	146	SER	2.6
3	N	212	LYS	2.6
3	M	59	LEU	2.6
3	N	102	PHE	2.6
3	O	63	LYS	2.6
2	J	77	ARG	2.6
3	N	278	ASN	2.6
3	N	148	TYR	2.6
3	O	242	LYS	2.6
3	O	120	ILE	2.6
3	M	184	HIS	2.6
3	M	275	HIS	2.6
3	S	270	SER	2.6
3	N	145	LYS	2.6
3	T	270	SER	2.6
1	E	144	ASP	2.6
3	S	289	ASN	2.6
3	S	185	PRO	2.6
3	N	196	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	194	TYR	2.6
3	T	52	CYS	2.6
3	S	11	ASP	2.6
1	I	199	ASN	2.6
3	O	219	ILE	2.6
3	S	75	GLU	2.6
3	S	214	LYS	2.6
1	I	119	PRO	2.6
3	N	99	PRO	2.6
3	S	48	ASN	2.6
1	I	64	GLN	2.6
3	U	218	ALA	2.6
3	N	73	ASN	2.6
3	M	256	TYR	2.5
3	O	119	GLU	2.5
1	I	23	ARG	2.5
3	S	149	LYS	2.5
3	U	118	PHE	2.5
3	U	184	HIS	2.5
3	M	131	ASP	2.5
2	B	62	PHE	2.5
3	U	9	PRO	2.5
3	S	192	GLN	2.5
3	U	262	ARG	2.5
3	U	172	LYS	2.5
3	S	82	ALA	2.5
3	N	236	LEU	2.5
2	J	129	THR	2.5
3	T	133(A)	LYS	2.5
3	N	116(B)	PHE	2.5
3	U	89	GLU	2.5
4	P	165	GLU	2.5
3	U	190	ASP	2.5
1	C	189	LEU	2.5
3	N	54	LEU	2.5
3	N	264	ALA	2.5
1	I	191	THR	2.5
3	M	290	THR	2.5
3	O	49	GLY	2.5
3	M	192	GLN	2.5
3	S	140	PRO	2.5
3	U	198	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	M	208	ARG	2.5
3	U	12	THR	2.5
3	U	187	THR	2.5
3	M	274	VAL	2.5
1	G	112	SER	2.5
3	M	182	ILE	2.5
3	U	270	SER	2.5
3	M	170	ASN	2.5
3	S	158	GLY	2.5
3	N	80	SER	2.5
3	U	116	SER	2.5
4	W	164	GLU	2.5
3	T	12	THR	2.4
4	W	162	TYR	2.4
1	I	126	PRO	2.4
3	S	191	GLN	2.4
3	N	131	ASP	2.4
1	I	129	LYS	2.4
3	N	230	MET	2.4
3	U	54	LEU	2.4
3	T	259	ALA	2.4
3	O	55	ARG	2.4
3	S	221	PRO	2.4
3	U	167	SER	2.4
3	U	220	ARG	2.4
3	O	175	GLU	2.4
3	N	143	GLY	2.4
3	O	71	LEU	2.4
3	S	225	ASP	2.4
3	U	88	VAL	2.4
3	M	148	TYR	2.4
1	I	204	ASN	2.4
3	T	246	GLU	2.4
3	U	129	ASN	2.4
3	U	290	THR	2.4
3	N	98	TYR	2.4
1	G	132	SER	2.4
3	N	215	PRO	2.4
3	T	194	LEU	2.4
3	N	12	THR	2.4
1	G	194	TYR	2.4
3	N	130	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
4	P	141	TYR	2.4
4	Q	157	TYR	2.4
3	O	52	CYS	2.4
3	T	163	LYS	2.4
2	D	62	PHE	2.4
3	S	143	GLY	2.4
3	T	257	ALA	2.4
3	M	11	ASP	2.4
1	E	112	SER	2.4
1	G	1	GLN	2.4
3	N	135	VAL	2.4
3	M	185	PRO	2.4
1	I	205	THR	2.4
3	T	217	ILE	2.4
3	U	66	ILE	2.4
1	G	192	GLN	2.4
3	T	186	SER	2.4
3	N	120	ILE	2.4
1	I	211	VAL	2.3
3	M	88	VAL	2.3
3	M	168	TYR	2.3
1	G	209	LYS	2.3
1	A	207	VAL	2.3
3	O	258	PHE	2.3
3	O	84	TRP	2.3
3	U	183	HIS	2.3
1	K	1	GLN	2.3
3	T	225	ASP	2.3
3	O	217	ILE	2.3
3	O	268	ILE	2.3
4	W	166	ALA	2.3
1	C	214	LYS	2.3
3	U	100	GLY	2.3
3	T	133	ASN	2.3
3	T	183	HIS	2.3
3	U	64	CYS	2.3
3	U	131	ASP	2.3
3	N	128	PRO	2.3
1	A	1	GLN	2.3
4	X	62	GLN	2.3
3	T	93	ASP	2.3
3	T	287	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	Q	60	ASN	2.3
3	N	222	LYS	2.3
3	N	252	VAL	2.3
3	S	204	VAL	2.3
4	V	165	GLU	2.3
3	U	191	GLN	2.3
4	X	30	GLN	2.3
3	T	86	TYR	2.3
3	O	304	LYS	2.3
3	N	243	ILE	2.3
3	S	288	ILE	2.3
3	O	135	VAL	2.3
3	U	130	HIS	2.3
1	C	23	ARG	2.3
1	K	4	LEU	2.3
3	O	302	ILE	2.3
3	M	175	GLU	2.2
4	R	29	GLU	2.2
1	K	211	VAL	2.2
4	X	63	PHE	2.2
3	N	95	GLY	2.2
3	M	234	TRP	2.2
3	T	83(A)	SER	2.2
4	R	142	HIS	2.2
1	C	199	ASN	2.2
4	Q	140	PHE	2.2
1	I	17	SER	2.2
3	T	145	LYS	2.2
3	O	301	THR	2.2
3	T	264	ALA	2.2
3	U	282	GLN	2.2
4	X	162	TYR	2.2
3	O	230	MET	2.2
1	A	81	ASP	2.2
3	O	255	ARG	2.2
3	S	276	ASP	2.2
1	I	140	CYS	2.2
3	T	51	LEU	2.2
1	A	186	SER	2.2
3	N	91	SER	2.2
3	T	116(B)	PHE	2.2
3	M	249	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	T	10	GLY	2.2
3	T	190	ASP	2.2
3	O	262	ARG	2.2
3	T	208	ARG	2.2
3	U	174	LYS	2.2
3	O	55(A)	GLY	2.2
1	C	119	PRO	2.2
3	M	267	ILE	2.2
2	H	70	ASP	2.2
1	I	197	ASN	2.2
3	M	262	ARG	2.2
4	W	72	HIS	2.2
1	I	189	LEU	2.2
3	T	282	GLN	2.2
3	O	170	ASN	2.2
3	S	235	THR	2.2
3	U	121	PHE	2.2
1	A	198	VAL	2.2
3	S	227	GLU	2.2
3	U	202	VAL	2.2
4	Q	165	GLU	2.2
3	S	126	SER	2.2
3	M	211	LYS	2.2
3	N	290	THR	2.2
3	U	212	LYS	2.2
1	C	1	GLN	2.1
4	P	140	PHE	2.1
3	S	104	ASP	2.1
3	U	117	ARG	2.1
3	N	10	GLY	2.1
1	E	159	LEU	2.1
3	U	132	SER	2.1
1	I	213	PRO	2.1
4	W	28	ASN	2.1
3	S	217	ILE	2.1
3	M	199	ASP	2.1
3	O	276	ASP	2.1
4	V	169	ASN	2.1
4	V	170	ARG	2.1
1	G	128	SER	2.1
4	X	142	HIS	2.1
1	C	205	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	T	48	ASN	2.1
3	T	236	LEU	2.1
4	R	170	ARG	2.1
3	N	225	ASP	2.1
3	T	199	ASP	2.1
1	A	199	ASN	2.1
3	S	159	ASN	2.1
1	E	145	TYR	2.1
3	N	146	SER	2.1
3	N	168	TYR	2.1
3	T	256	TYR	2.1
3	O	89	GLU	2.1
3	U	69	TRP	2.1
3	M	279	THR	2.1
3	N	240	GLY	2.1
3	U	143	GLY	2.1
3	U	227	GLU	2.1
3	U	257	ALA	2.1
3	O	253	VAL	2.1
3	O	184	HIS	2.1
3	O	234	TRP	2.1
3	O	297	ILE	2.1
4	Q	72	HIS	2.1
2	H	62	PHE	2.1
3	U	96	THR	2.1
3	U	203	PHE	2.1
1	A	194	TYR	2.1
3	M	201	TYR	2.1
3	T	166	LYS	2.1
1	C	207	VAL	2.1
2	J	32	SER	2.1
3	M	125	SER	2.1
3	N	59	LEU	2.1
4	P	149	MET	2.1
2	H	77	ARG	2.1
3	S	279	THR	2.1
3	T	94	ASN	2.1
4	Q	28	ASN	2.1
4	R	69	GLU	2.1
3	S	142	ALA	2.1
3	S	116(B)	PHE	2.0
3	U	277	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	2.0
3	M	273	PRO	2.0
3	O	133	ASN	2.0
3	S	144	ALA	2.0
4	V	166	ALA	2.0
3	N	112	LEU	2.0
3	M	268	ILE	2.0
3	N	248	THR	2.0
3	O	278	ASN	2.0
3	N	53	LYS	2.0
3	U	265	GLY	2.0
3	T	83	SER	2.0
4	P	171	GLU	2.0
4	W	30	GLN	2.0
4	X	27	GLN	2.0
1	G	189	LEU	2.0
3	T	137	ALA	2.0
4	W	157	TYR	2.0
3	T	164	LEU	2.0
3	U	119	GLU	2.0
4	W	29	GLU	2.0
1	A	144	ASP	2.0
1	I	156	SER	2.0
3	N	116(A)	SER	2.0
4	V	142	HIS	2.0
3	O	256	TYR	2.0
3	S	259	ALA	2.0
1	K	23	ARG	2.0
2	J	125	LEU	2.0
3	M	61	LEU	2.0
3	N	214	LYS	2.0
3	O	66	ILE	2.0
4	R	169	ASN	2.0
4	X	169	ASN	2.0
1	A	112	SER	2.0
3	O	54	LEU	2.0
4	V	162	TYR	2.0
3	S	182	ILE	2.0
3	M	277	CYS	2.0
3	N	232	TYR	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 carbohydrates 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.