



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 5IRO / pdb_00005iro
Title : Crystal structure of a complex between the Human adenovirus type 4 E3-19K protein and MHC class molecule HLA-A2/TAX
Authors : Li, L.; Bouvier, M.
Deposited on : 2016-03-14
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

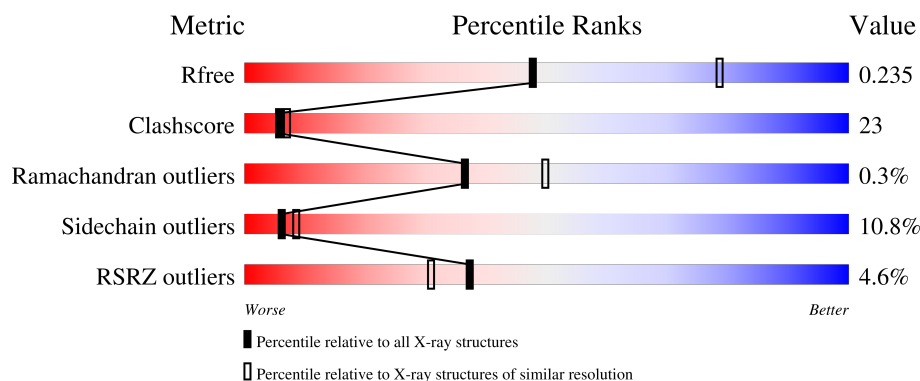
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

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



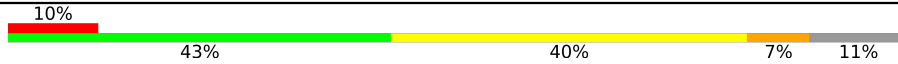
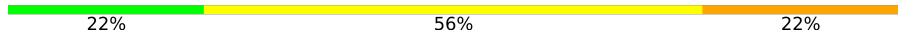
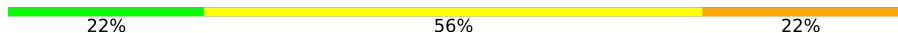
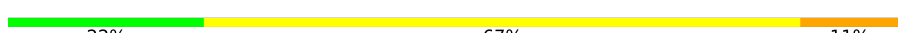
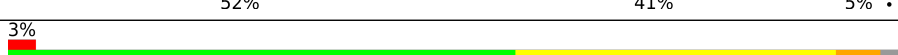
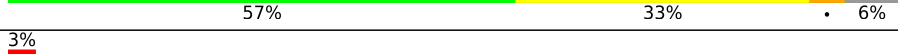
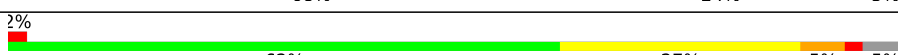
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	275	3% 45% 42% 9% .
1	E	275	5% 51% 40% 6% .
1	I	275	3% 49% 36% 7% 8%
1	M	275	3% 44% 45% 7% .
1	Q	275	4% 42% 44% 9% 6%

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Mol	Chain	Length	Quality of chain
1	U	275	
2	B	9	
2	F	9	
2	J	9	
2	N	9	
2	R	9	
2	V	9	
3	C	100	
3	G	100	
3	K	100	
3	O	100	
3	S	100	
3	W	100	
4	D	108	
4	H	108	
4	L	108	
4	P	108	
4	T	108	
4	X	108	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23039 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2144	1338	389	408	9			
1	E	268	Total	C	N	O	S	0	0	0
			2183	1363	398	413	9			
1	I	252	Total	C	N	O	S	0	0	0
			2053	1282	376	386	9			
1	M	265	Total	C	N	O	S	0	0	0
			2160	1351	392	408	9			
1	Q	259	Total	C	N	O	S	0	0	0
			2111	1315	385	402	9			
1	U	246	Total	C	N	O	S	0	0	0
			2007	1259	363	376	9			

- Molecule 2 is a protein called TAX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	F	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	J	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	N	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	R	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	V	9	Total	C	N	O	0	0	0
			76	56	9	11			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			802	513	136	150	3			
3	G	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	K	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	O	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	S	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	W	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
W	0	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called E3 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			823	520	144	149	10			
4	H	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	L	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	P	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	T	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	X	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			

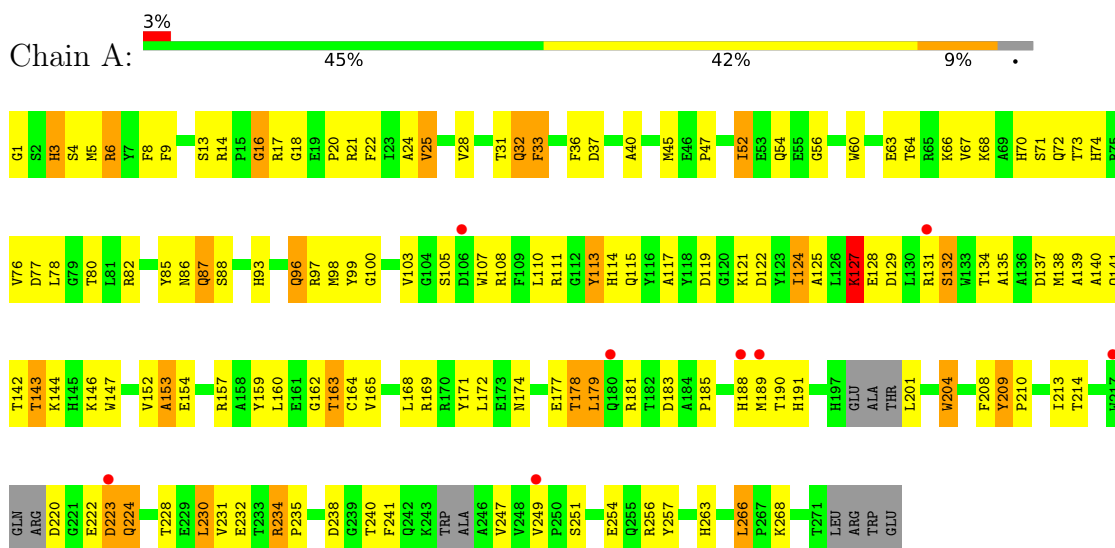
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	D	2	Total 2	O 2	0	0
5	E	3	Total 3	O 3	0	0
5	G	1	Total 1	O 1	0	0
5	I	5	Total 5	O 5	0	0
5	J	1	Total 1	O 1	0	0
5	K	2	Total 2	O 2	0	0
5	L	1	Total 1	O 1	0	0
5	M	4	Total 4	O 4	0	0
5	O	2	Total 2	O 2	0	0
5	P	3	Total 3	O 3	0	0
5	Q	3	Total 3	O 3	0	0
5	S	3	Total 3	O 3	0	0
5	T	3	Total 3	O 3	0	0
5	U	3	Total 3	O 3	0	0
5	W	1	Total 1	O 1	0	0

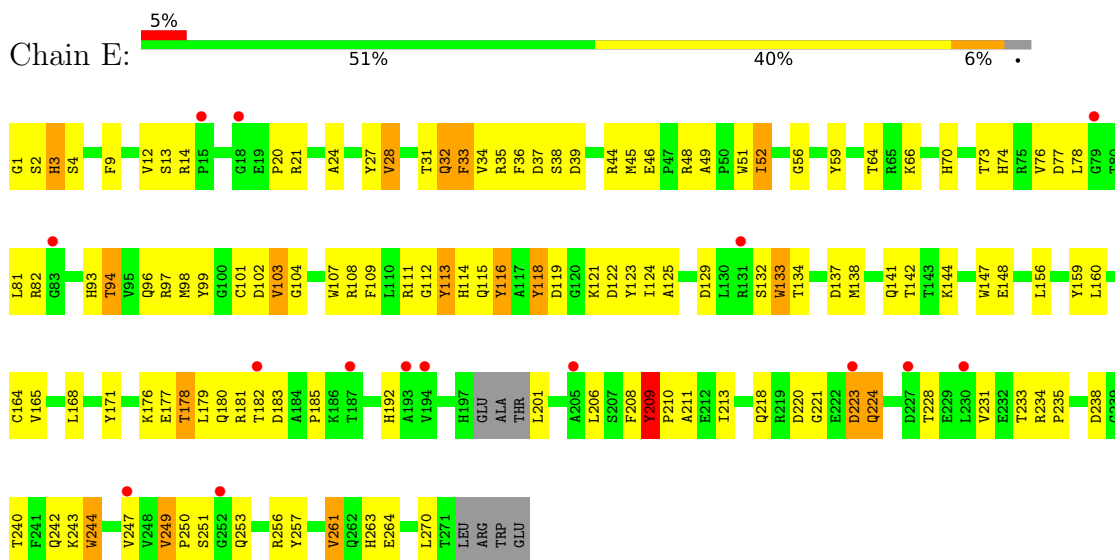
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

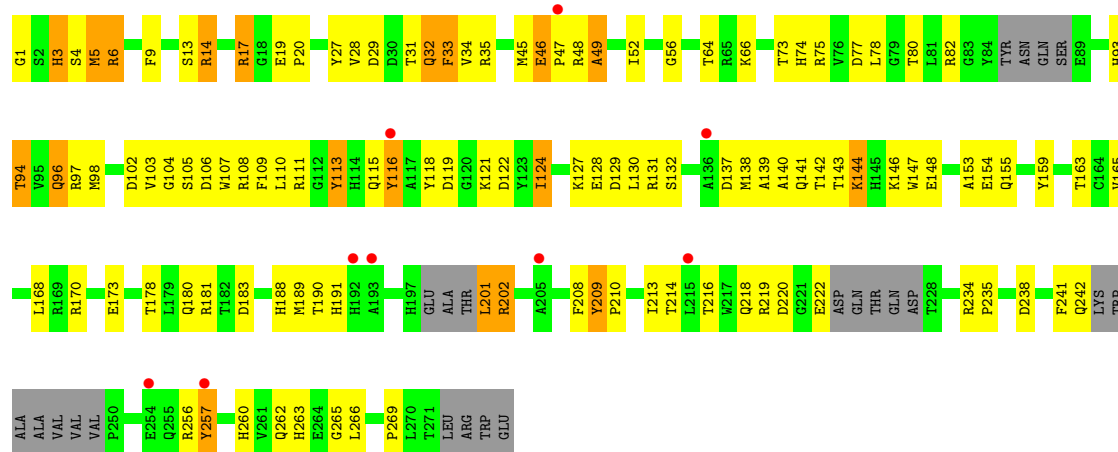


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

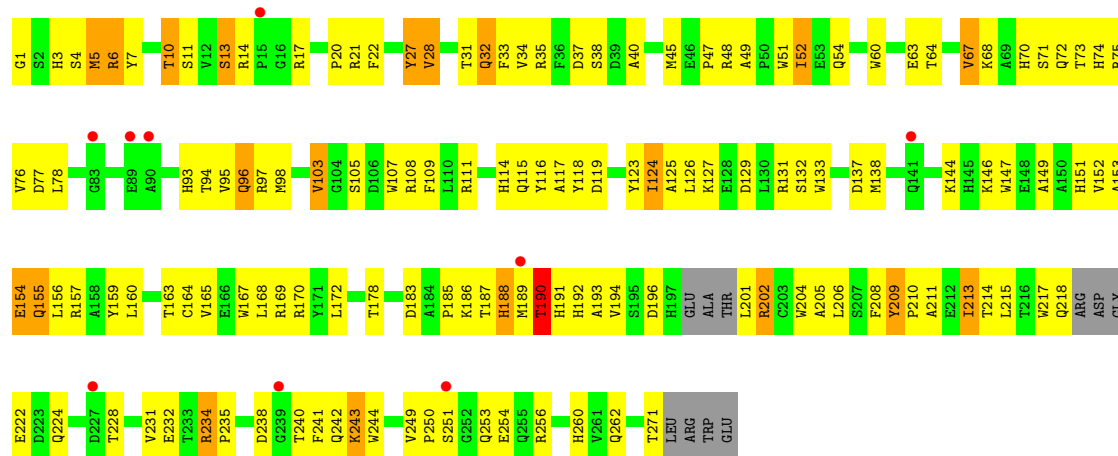
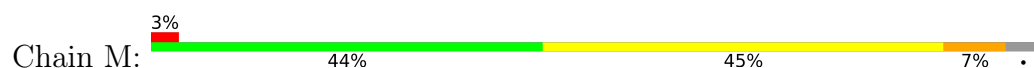


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

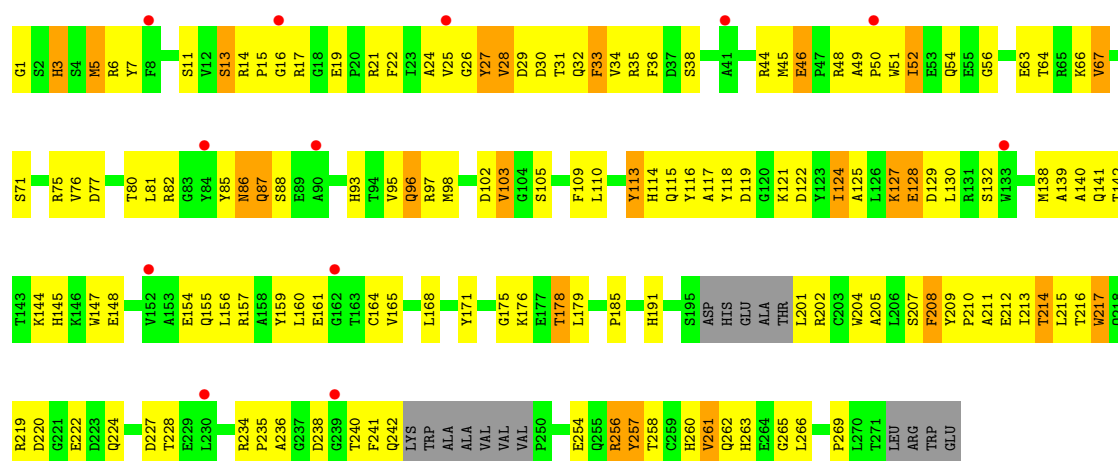
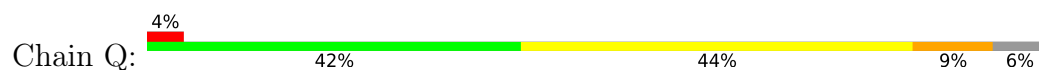




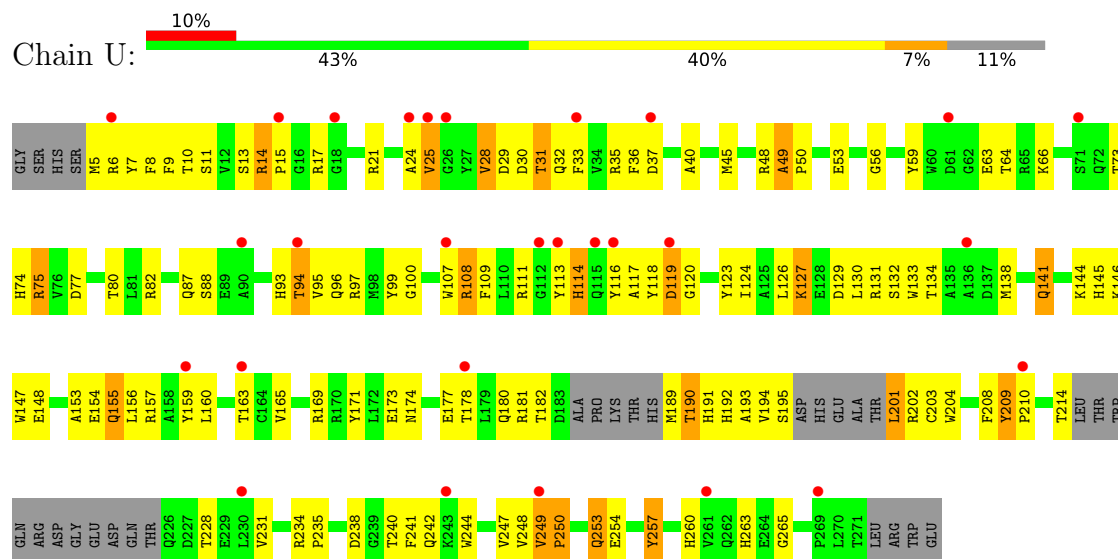
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



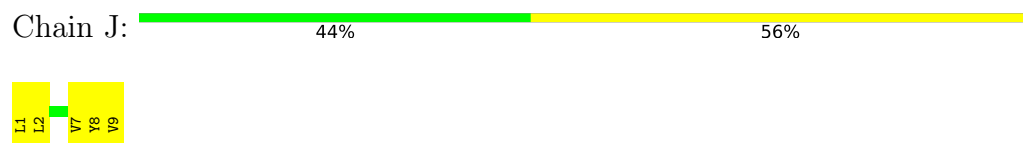
- Molecule 2: TAX protein



- Molecule 2: TAX protein



- Molecule 2: TAX protein



- Molecule 2: TAX protein



- Molecule 2: TAX protein

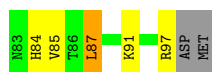




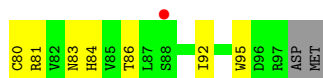
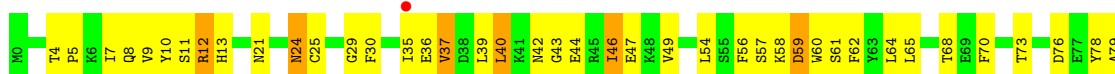
- Molecule 2: TAX protein



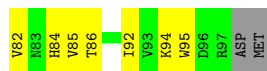
- Molecule 3: Beta-2-microglobulin



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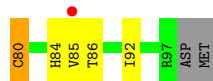
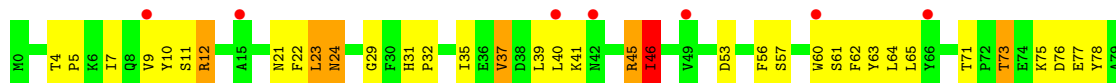


- Molecule 3: Beta-2-microglobulin

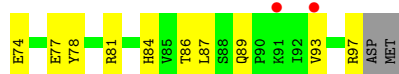




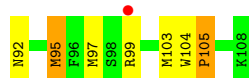
• Molecule 3: Beta-2-microglobulin



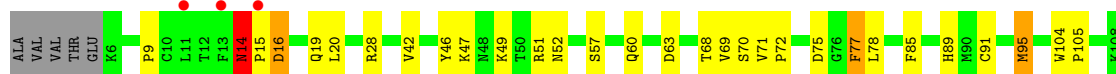
• Molecule 3: Beta-2-microglobulin



• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein

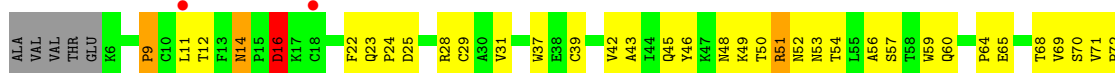


• Molecule 4: E3 19 kDa protein

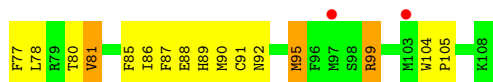




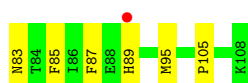
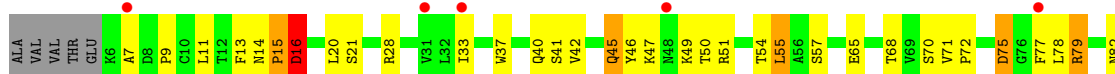
- Molecule 4: E3 19 kDa protein



- Molecule 4: E3 19 kDa protein



- Molecule 4: E3 19 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	165.73Å 165.73Å 122.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.64 49.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.64) 99.3 (49.62-2.64)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.257 , 0.288 0.217 , 0.235	Depositor DCC
R_{free} test set	1983 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.359 for -h,-k,l 0.390 for h,-h-k,-l 0.337 for -k,-h,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 110879 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	1/2202 (0.0%)	0.95	10/2983 (0.3%)
1	E	0.41	0/2245	0.98	9/3045 (0.3%)
1	I	0.34	0/2109	0.92	12/2852 (0.4%)
1	M	0.51	1/2221 (0.0%)	1.02	13/3012 (0.4%)
1	Q	0.43	0/2169	1.03	10/2937 (0.3%)
1	U	0.40	0/2061	1.01	16/2791 (0.6%)
2	B	0.33	0/79	0.79	0/108
2	F	0.41	0/79	0.79	0/108
2	J	0.29	0/79	0.56	0/108
2	N	0.30	0/79	0.55	0/108
2	R	0.28	0/79	0.54	0/108
2	V	0.45	0/79	0.84	0/108
3	C	0.37	0/824	0.95	4/1115 (0.4%)
3	G	0.34	0/843	0.91	3/1141 (0.3%)
3	K	0.34	0/843	0.85	1/1141 (0.1%)
3	O	0.37	0/843	0.85	1/1141 (0.1%)
3	S	0.36	0/843	0.90	5/1141 (0.4%)
3	W	0.37	0/843	0.93	3/1141 (0.3%)
4	D	0.34	0/849	0.95	3/1154 (0.3%)
4	H	0.42	0/858	1.00	4/1165 (0.3%)
4	L	0.34	0/858	0.96	7/1165 (0.6%)
4	P	0.39	0/858	0.98	6/1165 (0.5%)
4	T	0.36	0/858	0.93	5/1165 (0.4%)
4	X	0.37	0/858	1.02	3/1165 (0.3%)
All	All	0.40	2/23659 (0.0%)	0.96	115/32067 (0.4%)

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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	190	THR	CA-C	8.89	1.63	1.52
1	A	153	ALA	CA-CB	-5.29	1.45	1.53

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	TYR	CA-C-N	-12.23	107.18	120.14
1	E	209	TYR	C-N-CA	-12.23	107.18	120.14
4	P	16	ASP	N-CA-C	-9.61	101.44	113.55
4	D	16	ASP	N-CA-C	-9.29	101.84	113.55
3	K	46	ILE	N-CA-C	9.12	115.97	106.21
1	Q	16	GLY	N-CA-C	-8.95	102.86	115.30
1	M	202	ARG	NE-CZ-NH2	-8.75	111.33	119.20
4	X	16	ASP	N-CA-C	-8.72	102.56	113.55
1	M	52	ILE	N-CA-C	-8.48	104.19	113.43
3	C	46	ILE	N-CA-C	8.38	115.17	106.21
3	S	46	ILE	N-CA-C	8.22	115.01	106.21
1	A	209	TYR	CA-C-N	-7.82	111.55	119.99
1	A	209	TYR	C-N-CA	-7.82	111.55	119.99
3	C	8	GLN	N-CA-C	7.81	121.21	107.61
4	H	14	ASN	CA-C-N	-7.63	110.30	119.84
4	H	14	ASN	C-N-CA	-7.63	110.30	119.84
1	M	234	ARG	CA-C-N	7.63	127.92	119.90
1	M	234	ARG	C-N-CA	7.63	127.92	119.90
4	H	16	ASP	N-CA-C	-7.54	104.05	113.55
4	L	52	ASN	CB-CA-C	-7.28	108.18	116.63
1	Q	208	PHE	N-CA-C	7.28	121.39	109.24
1	I	6	ARG	N-CA-C	7.07	119.22	109.18
1	U	209	TYR	CA-C-N	-7.00	112.43	119.99
1	U	209	TYR	C-N-CA	-7.00	112.43	119.99
4	L	16	ASP	N-CA-C	-7.00	104.73	113.55
4	T	16	ASP	N-CA-C	-6.98	104.75	113.55
1	A	52	ILE	N-CA-C	-6.96	105.84	113.43
3	G	42	ASN	N-CA-C	-6.95	104.43	113.12
1	I	110	LEU	N-CA-C	-6.89	100.32	110.52
1	Q	257	TYR	N-CA-C	6.89	119.85	110.55
1	I	180	GLN	N-CA-C	-6.84	104.91	113.18
1	Q	52	ILE	N-CA-C	-6.83	106.58	113.47
3	W	42	ASN	N-CA-C	-6.79	105.00	113.55
3	S	71	THR	CA-C-N	6.77	127.14	119.83
3	S	71	THR	C-N-CA	6.77	127.14	119.83
3	G	46	ILE	N-CA-C	6.75	113.43	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	SER	N-CA-C	6.75	120.37	110.59
1	I	209	TYR	CA-C-N	-6.71	112.55	120.13
1	I	209	TYR	C-N-CA	-6.71	112.55	120.13
1	Q	227	ASP	N-CA-C	6.68	119.55	111.40
1	M	6	ARG	N-CA-C	6.67	118.65	109.18
3	C	57	SER	CB-CA-C	-6.51	109.05	116.54
1	U	194	VAL	N-CA-C	-6.41	106.71	111.90
4	L	52	ASN	N-CA-C	6.36	118.83	108.08
1	M	190	THR	OG1-CB-CG2	-6.19	96.91	109.30
1	U	249	VAL	CA-C-N	6.16	127.54	119.84
1	U	249	VAL	C-N-CA	6.16	127.54	119.84
4	T	91	CYS	N-CA-C	-6.16	105.60	113.23
1	A	16	GLY	N-CA-C	-6.15	106.76	115.30
1	I	56	GLY	CA-C-N	6.10	125.78	119.56
1	I	56	GLY	C-N-CA	6.10	125.78	119.56
1	U	119	ASP	N-CA-C	6.05	117.54	111.07
4	P	11	LEU	N-CA-C	-6.03	105.93	113.28
1	E	165	VAL	N-CA-C	6.00	116.64	110.82
1	M	251	SER	N-CA-C	6.00	120.33	113.19
1	U	260	HIS	N-CA-C	-5.94	100.32	109.76
1	E	52	ILE	N-CA-C	-5.92	106.98	113.43
1	M	196	ASP	N-CA-C	-5.87	105.02	111.82
4	L	101	TYR	N-CA-C	-5.80	105.39	112.88
1	Q	27	TYR	CA-CB-CG	5.79	124.31	113.90
3	O	57	SER	CB-CA-C	-5.76	109.92	116.54
1	U	87	GLN	N-CA-C	5.76	117.36	109.18
1	M	209	TYR	CA-C-N	-5.75	113.77	119.99
1	M	209	TYR	C-N-CA	-5.75	113.77	119.99
3	W	57	SER	CB-CA-C	-5.72	109.96	116.54
1	Q	56	GLY	CA-C-N	5.71	125.39	119.56
1	Q	56	GLY	C-N-CA	5.71	125.39	119.56
1	U	180	GLN	N-CA-C	-5.68	106.31	113.18
1	U	148	GLU	N-CA-C	-5.64	105.89	112.89
4	L	105	PRO	CA-C-N	5.61	126.85	119.84
4	L	105	PRO	C-N-CA	5.61	126.85	119.84
1	U	49	ALA	CA-C-N	5.52	125.04	119.19
1	U	49	ALA	C-N-CA	5.52	125.04	119.19
1	M	254	GLU	N-CA-C	-5.51	103.70	110.65
1	E	133	TRP	N-CA-C	5.48	117.52	109.24
1	M	256	ARG	N-CA-C	-5.45	107.28	114.04
1	I	49	ALA	CA-C-N	5.43	124.95	119.19
1	I	49	ALA	C-N-CA	5.43	124.95	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	127	LYS	N-CA-C	-5.41	103.55	110.53
4	D	105	PRO	CA-C-N	5.41	126.60	119.84
4	D	105	PRO	C-N-CA	5.41	126.60	119.84
1	Q	256	ARG	N-CA-C	-5.40	107.05	113.97
4	T	38	GLU	N-CA-C	-5.40	106.36	113.17
3	G	47	GLU	N-CA-C	-5.38	106.56	113.02
4	P	14	ASN	N-CA-C	5.34	121.60	109.81
4	L	11	LEU	N-CA-C	-5.33	106.78	113.28
3	S	37	VAL	N-CA-C	5.30	117.01	108.85
1	E	56	GLY	CA-C-N	5.28	124.95	119.56
1	E	56	GLY	C-N-CA	5.28	124.95	119.56
4	H	52	ASN	CB-CA-C	-5.28	110.05	117.23
1	A	56	GLY	CA-C-N	5.27	124.94	119.56
1	A	56	GLY	C-N-CA	5.27	124.94	119.56
4	P	105	PRO	CA-C-N	5.27	126.42	119.84
4	P	105	PRO	C-N-CA	5.27	126.42	119.84
1	Q	87	GLN	N-CA-C	5.24	116.62	109.18
1	A	127	LYS	CG-CD-CE	5.24	123.34	111.30
1	U	100	GLY	N-CA-C	5.21	118.60	110.88
1	A	6	ARG	N-CA-C	5.21	116.57	109.18
3	W	70	PHE	N-CA-C	5.21	115.41	108.38
1	I	256	ARG	N-CA-C	-5.19	107.61	114.31
1	I	46	GLU	CA-C-N	5.16	126.29	119.84
1	I	46	GLU	C-N-CA	5.16	126.29	119.84
1	U	56	GLY	CA-C-N	5.13	124.80	119.56
1	U	56	GLY	C-N-CA	5.13	124.80	119.56
1	E	218	GLN	N-CA-C	5.13	116.54	109.15
4	T	105	PRO	CA-C-N	5.13	126.25	119.84
4	T	105	PRO	C-N-CA	5.13	126.25	119.84
3	S	10	TYR	N-CA-C	5.08	114.95	108.24
3	C	57	SER	N-CA-C	5.07	116.02	108.31
1	E	251	SER	N-CA-C	5.05	119.20	113.19
4	X	105	PRO	CA-C-N	5.05	126.15	119.84
4	X	105	PRO	C-N-CA	5.05	126.15	119.84
1	A	110	LEU	N-CA-C	-5.04	103.05	110.52
4	P	52	ASN	CB-CA-C	-5.03	110.39	117.23
1	M	190	THR	CA-CB-OG1	-5.01	102.08	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	189	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	0	1999	136	1
1	E	2183	0	2037	108	0
1	I	2053	0	1916	105	0
1	M	2160	0	2016	151	0
1	Q	2111	0	1966	120	0
1	U	2007	0	1881	116	0
2	B	76	0	79	13	0
2	F	76	0	79	9	0
2	J	76	0	79	6	0
2	N	76	0	79	11	0
2	R	76	0	79	9	0
2	V	76	0	79	9	0
3	C	802	0	770	27	0
3	G	820	0	790	38	0
3	K	820	0	790	31	0
3	O	820	0	790	32	0
3	S	820	0	790	36	0
3	W	820	0	790	42	0
4	D	823	0	773	29	0
4	H	832	0	786	16	0
4	L	832	0	786	23	0
4	P	832	0	786	27	0
4	T	832	0	786	40	0
4	X	832	0	786	28	0
5	A	3	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	2	0	0	1	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	3	0	0	0	0
5	W	1	0	0	0	0
All	All	23039	0	21712	1042	1

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 23.

All (1042) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLN:HB2	1:I:48:ARG:HH12	1.24	1.01
1:M:205:ALA:HB3	1:M:243:LYS:HE2	1.45	0.99
1:Q:5:MET:HG3	1:Q:6:ARG:HG3	1.47	0.96
1:U:250:PRO:O	1:U:253:GLN:NE2	2.01	0.93
1:E:59:TYR:HH	1:E:171:TYR:HH	1.12	0.91
3:W:15:ALA:HB3	3:W:97:ARG:HH12	1.33	0.89
1:E:77:ASP:OD2	1:E:97:ARG:NH2	2.07	0.87
1:A:5:MET:HG2	1:A:6:ARG:HG2	1.58	0.86
1:A:14:ARG:HB3	1:A:17:ARG:HB3	1.58	0.85
1:U:82:ARG:NH2	1:U:88:SER:O	2.10	0.85
3:C:12:ARG:NH2	4:D:97:MET:SD	2.49	0.84
1:A:224:GLN:HE22	1:A:228:THR:H	1.23	0.84
1:Q:77:ASP:OD2	1:Q:97:ARG:NH2	2.10	0.83
1:Q:217:TRP:H	1:Q:217:TRP:CD1	1.95	0.82
1:M:77:ASP:OD2	1:M:97:ARG:NH2	2.13	0.82
1:Q:217:TRP:H	1:Q:217:TRP:HD1	1.25	0.82
4:T:44:ILE:HD13	4:T:55:LEU:HB2	1.60	0.82
1:U:93:HIS:ND1	1:U:119:ASP:OD2	2.12	0.81
1:M:21:ARG:NH1	1:M:22:PHE:H	1.77	0.81
3:C:47:GLU:O	3:W:89:GLN:NE2	2.14	0.80
1:Q:141:GLN:OE1	1:Q:144:LYS:NZ	2.14	0.80
1:E:223:ASP:OD1	1:E:223:ASP:N	2.13	0.80
1:U:173:GLU:O	4:X:51:ARG:NH2	2.14	0.80
1:M:190:THR:O	1:M:202:ARG:HG2	1.82	0.80
1:A:17:ARG:HD3	3:W:44:GLU:HB2	1.63	0.80
1:A:127:LYS:NZ	1:A:132:SER:OG	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:35:ILE:HD11	3:G:84:HIS:CD2	2.17	0.80
3:C:37:VAL:HB	3:C:82:VAL:HG22	1.61	0.79
1:A:177:GLU:O	4:D:28:ARG:NH1	2.15	0.79
1:I:32:GLN:HB2	1:I:48:ARG:NH1	1.96	0.79
1:A:99:TYR:HB3	1:A:114:HIS:HD2	1.48	0.79
1:M:205:ALA:CB	1:M:243:LYS:HE2	2.13	0.79
1:M:188:HIS:HB2	1:M:204:TRP:HZ2	1.49	0.78
4:T:70:SER:HB3	4:T:78:LEU:HD21	1.66	0.78
1:E:201:LEU:N	1:E:247:VAL:O	2.17	0.78
3:G:39:LEU:HB2	3:G:49:VAL:HG11	1.66	0.77
4:T:92:ASN:HA	4:T:99:ARG:NH2	1.99	0.77
1:M:6:ARG:HH22	1:M:115:GLN:HG3	1.50	0.77
1:Q:262:GLN:HE22	1:Q:269:PRO:HB3	1.50	0.76
3:G:54:LEU:HG	3:G:64:LEU:HD11	1.66	0.76
4:X:77:PHE:O	4:X:79:ARG:NH1	2.18	0.76
1:I:6:ARG:NH1	1:I:98:MET:SD	2.58	0.76
1:Q:21:ARG:NH1	1:Q:38:SER:OG	2.18	0.76
1:A:9:PHE:HB2	1:A:97:ARG:HB2	1.67	0.76
3:K:56:PHE:HA	3:K:62:PHE:HA	1.68	0.76
1:I:77:ASP:OD2	1:I:97:ARG:NH2	2.18	0.76
1:U:77:ASP:OD2	1:U:97:ARG:NH2	2.20	0.75
1:M:147:TRP:NE1	2:N:8:TYR:O	2.19	0.75
1:U:14:ARG:HG2	1:U:17:ARG:HB2	1.69	0.75
3:C:56:PHE:HA	3:C:62:PHE:HA	1.69	0.74
4:T:69:VAL:HG23	4:T:81:VAL:HG13	1.70	0.74
1:M:21:ARG:NH2	1:M:37:ASP:HA	2.01	0.74
1:Q:219:ARG:HB2	1:Q:257:TYR:CZ	2.23	0.74
3:S:31:HIS:HD2	3:S:32:PRO:HA	1.51	0.74
4:T:72:PRO:HA	4:T:78:LEU:HA	1.70	0.74
1:Q:5:MET:HG2	1:Q:27:TYR:HE2	1.52	0.74
3:S:56:PHE:HA	3:S:62:PHE:HA	1.69	0.74
4:L:16:ASP:O	4:L:83:ASN:ND2	2.22	0.73
1:Q:238:ASP:OD2	3:S:12:ARG:NH1	2.20	0.73
3:S:73:THR:OG1	3:S:75:LYS:HG2	1.89	0.73
3:G:81:ARG:HG2	3:G:92:ILE:HG12	1.69	0.73
1:I:218:GLN:HB3	1:I:260:HIS:HD2	1.54	0.73
4:T:92:ASN:HA	4:T:99:ARG:HH22	1.54	0.72
3:W:56:PHE:HA	3:W:62:PHE:HA	1.69	0.72
1:E:209:TYR:H	1:E:209:TYR:HD2	1.36	0.72
3:K:54:LEU:HG	3:K:64:LEU:HD11	1.72	0.72
1:Q:14:ARG:HB3	1:Q:17:ARG:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:231:VAL:HG21	1:M:244:TRP:HE3	1.55	0.72
3:G:84:HIS:ND1	3:G:86:THR:HG23	2.05	0.71
3:G:43:GLY:HA2	1:Q:17:ARG:HH11	1.55	0.71
1:M:97:ARG:HG2	1:M:116:TYR:HD1	1.55	0.71
1:M:250:PRO:O	1:M:253:GLN:NE2	2.23	0.71
1:U:109:PHE:O	1:U:111:ARG:NH2	2.22	0.71
1:A:4:SER:HB3	1:A:103:VAL:HG22	1.71	0.71
1:A:8:PHE:HB2	1:A:25:VAL:HG13	1.72	0.71
1:M:1:GLY:H1	1:M:107:TRP:CD1	2.08	0.71
1:A:73:THR:HG23	1:A:97:ARG:HH22	1.55	0.71
1:E:250:PRO:O	1:E:253:GLN:NE2	2.23	0.71
1:E:21:ARG:NH1	1:E:38:SER:OG	2.20	0.70
1:U:9:PHE:HB3	1:U:74:HIS:HE1	1.55	0.70
1:U:120:GLY:N	1:U:123:TYR:OH	2.24	0.70
1:A:223:ASP:OD1	1:A:223:ASP:N	2.24	0.70
3:C:11:SER:OG	3:C:21:ASN:ND2	2.23	0.70
1:A:13:SER:HB3	1:A:93:HIS:H	1.56	0.70
1:I:235:PRO:O	3:K:10:TYR:OH	2.07	0.70
1:Q:35:ARG:HG3	1:Q:46:GLU:HG3	1.74	0.70
3:W:44:GLU:OE2	3:W:81:ARG:NH2	2.22	0.70
1:M:109:PHE:O	1:M:111:ARG:NH2	2.24	0.70
3:K:24:ASN:OD1	3:K:24:ASN:N	2.24	0.70
1:M:98:MET:HE2	3:O:56:PHE:HE1	1.55	0.69
1:I:98:MET:HE2	3:K:56:PHE:HE1	1.56	0.69
3:K:19:LYS:HE2	3:K:20:SER:H	1.57	0.69
1:E:45:MET:H	1:E:64:THR:HG22	1.56	0.69
4:T:13:PHE:HE1	4:T:73:GLY:HA2	1.57	0.69
1:U:13:SER:HB3	1:U:93:HIS:H	1.56	0.69
1:I:27:TYR:HA	1:I:32:GLN:HA	1.75	0.69
1:I:73:THR:OG1	2:J:7:VAL:O	2.11	0.69
1:I:147:TRP:NE1	2:J:8:TYR:O	2.23	0.69
3:S:84:HIS:ND1	3:S:86:THR:HG23	2.07	0.69
1:A:45:MET:H	1:A:64:THR:HG22	1.57	0.69
1:I:124:ILE:HD11	1:I:140:ALA:HA	1.75	0.69
4:H:72:PRO:HA	4:H:78:LEU:HA	1.74	0.68
1:A:124:ILE:HG21	1:A:147:TRP:HZ3	1.58	0.68
1:I:219:ARG:N	1:I:222:GLU:OE2	2.25	0.68
1:M:45:MET:H	1:M:64:THR:HG22	1.57	0.68
1:Q:28:VAL:O	1:Q:31:THR:OG1	2.09	0.68
4:X:70:SER:HB3	4:X:78:LEU:HD21	1.73	0.68
1:M:232:GLU:OE1	3:O:28:SER:OG	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:N	1:A:247:VAL:O	2.27	0.68
3:G:24:ASN:N	3:G:24:ASN:OD1	2.26	0.68
1:M:37:ASP:HB3	1:M:40:ALA:HB2	1.76	0.68
3:C:5:PRO:HB3	3:C:30:PHE:HB3	1.76	0.68
1:E:109:PHE:O	1:E:111:ARG:NH2	2.26	0.68
1:I:4:SER:HB3	1:I:168:LEU:HD21	1.74	0.68
1:I:218:GLN:NE2	1:I:220:ASP:O	2.25	0.68
1:M:13:SER:HA	1:M:20:PRO:HB3	1.76	0.68
1:A:162:GLY:H	1:A:165:VAL:HG22	1.58	0.67
1:U:24:ALA:HB3	1:U:36:PHE:HB3	1.75	0.67
1:E:24:ALA:HB3	1:E:36:PHE:HB3	1.76	0.67
1:E:235:PRO:HB2	3:G:65:LEU:HD22	1.77	0.67
3:G:56:PHE:HA	3:G:62:PHE:HA	1.75	0.67
1:Q:5:MET:HG2	1:Q:27:TYR:CE2	2.29	0.67
3:O:24:ASN:N	3:O:24:ASN:OD1	2.27	0.67
3:O:56:PHE:HA	3:O:62:PHE:HA	1.75	0.67
1:I:4:SER:OG	1:I:102:ASP:OD1	2.12	0.67
4:H:89:HIS:NE2	4:L:19:GLN:OE1	2.27	0.67
1:M:108:ARG:HA	1:M:169:ARG:HH21	1.60	0.67
1:Q:3:HIS:O	1:Q:3:HIS:ND1	2.27	0.67
1:M:6:ARG:NH1	1:M:98:MET:SD	2.68	0.67
4:X:50:THR:O	4:X:51:ARG:HD3	1.95	0.67
1:U:124:ILE:HD11	1:U:133:TRP:HB3	1.75	0.66
4:T:36:GLY:O	4:T:53:ASN:ND2	2.26	0.66
3:G:13:HIS:H	3:G:21:ASN:HD21	1.44	0.66
1:U:189:MET:HG3	1:U:201:LEU:HD23	1.78	0.66
1:M:21:ARG:NH1	1:M:38:SER:OG	2.29	0.66
1:U:13:SER:OG	1:U:82:ARG:NH1	2.27	0.66
1:U:131:ARG:HD3	1:U:153:ALA:HB3	1.76	0.66
1:A:24:ALA:HB3	1:A:36:PHE:HB3	1.77	0.66
1:U:181:ARG:HH21	4:X:28:ARG:HH11	1.44	0.66
3:W:26:TYR:HB2	3:W:65:LEU:HD13	1.78	0.65
1:Q:217:TRP:CD1	1:Q:217:TRP:N	2.64	0.65
3:G:40:LEU:HD11	3:G:79:ALA:HB3	1.78	0.65
1:A:54:GLN:O	4:D:51:ARG:NH2	2.30	0.65
4:L:43:ALA:HB3	4:L:70:SER:HB2	1.77	0.65
1:I:238:ASP:OD2	3:K:12:ARG:NH1	2.29	0.65
1:M:20:PRO:HG2	1:M:75:ARG:HD3	1.78	0.65
1:A:66:LYS:HE3	2:B:2:LEU:HB3	1.77	0.65
3:W:24:ASN:OD1	3:W:24:ASN:N	2.30	0.65
4:P:49:LYS:NZ	4:P:56:ALA:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:147:TRP:NE1	2:R:8:TYR:O	2.30	0.64
3:O:54:LEU:HG	3:O:64:LEU:HD11	1.78	0.64
1:A:213:ILE:HG12	1:A:263:HIS:HD2	1.62	0.64
1:U:45:MET:H	1:U:64:THR:HG22	1.62	0.64
1:E:211:ALA:HB1	1:E:233:THR:HG21	1.79	0.64
1:A:13:SER:OG	1:A:82:ARG:NH1	2.30	0.64
4:P:88:GLU:O	4:P:92:ASN:ND2	2.31	0.64
1:Q:263:HIS:CD2	1:Q:265:GLY:H	2.16	0.64
1:A:93:HIS:ND1	1:A:119:ASP:OD2	2.31	0.64
3:K:30:PHE:CE1	3:K:62:PHE:HB2	2.33	0.64
1:M:231:VAL:HG21	1:M:244:TRP:CE3	2.33	0.64
1:A:157:ARG:HA	1:A:160:LEU:HD12	1.80	0.63
4:P:16:ASP:O	4:P:83:ASN:ND2	2.31	0.63
1:Q:82:ARG:NH2	1:Q:88:SER:O	2.31	0.63
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.11	0.63
1:E:129:ASP:HB2	1:E:132:SER:OG	1.98	0.63
1:Q:157:ARG:HA	1:Q:160:LEU:HD12	1.79	0.63
3:W:13:HIS:H	3:W:21:ASN:HD21	1.43	0.63
1:M:191:HIS:HE1	1:M:193:ALA:HB2	1.62	0.63
1:E:124:ILE:HG23	1:E:133:TRP:CH2	2.34	0.63
3:G:5:PRO:HB3	3:G:30:PHE:HB3	1.81	0.63
2:R:1:LEU:HD23	2:R:2:LEU:HD12	1.81	0.62
3:S:24:ASN:OD1	3:S:24:ASN:N	2.32	0.62
1:M:54:GLN:O	4:P:51:ARG:NH2	2.32	0.62
1:U:191:HIS:CD2	1:U:201:LEU:HD12	2.34	0.62
4:D:28:ARG:NH2	4:D:58:THR:OG1	2.32	0.62
1:M:95:VAL:HG13	1:M:116:TYR:CE1	2.35	0.62
1:U:250:PRO:C	1:U:253:GLN:HE22	2.06	0.62
1:U:73:THR:OG1	2:V:7:VAL:O	2.15	0.62
1:U:234:ARG:HE	1:U:242:GLN:HB2	1.63	0.62
4:T:99:ARG:HH21	4:T:104:TRP:NE1	1.97	0.62
4:X:16:ASP:O	4:X:83:ASN:ND2	2.32	0.62
4:P:43:ALA:HB3	4:P:70:SER:HB2	1.81	0.62
1:U:37:ASP:HB3	1:U:40:ALA:HB2	1.82	0.62
1:A:82:ARG:HD2	1:A:93:HIS:HB2	1.82	0.62
4:P:42:VAL:HG22	4:P:71:VAL:HG12	1.81	0.62
1:I:13:SER:HA	1:I:20:PRO:HB3	1.81	0.61
1:M:35:ARG:HD2	3:O:53:ASP:HB2	1.80	0.61
3:K:79:ALA:HB2	3:K:94:LYS:HG2	1.82	0.61
1:E:234:ARG:HD3	3:G:8:GLN:NE2	2.16	0.61
4:T:92:ASN:O	4:T:99:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:HB3	1:A:204:TRP:HZ2	1.64	0.61
1:I:9:PHE:HB3	1:I:74:HIS:HE1	1.65	0.61
1:Q:51:TRP:H	1:Q:51:TRP:CD1	2.18	0.61
1:U:14:ARG:NH1	1:U:21:ARG:HB2	2.16	0.61
1:A:188:HIS:CD2	1:A:189:MET:H	2.19	0.61
1:A:235:PRO:O	3:C:10:TYR:OH	2.17	0.61
1:E:98:MET:HE3	1:E:115:GLN:HG3	1.83	0.61
1:A:99:TYR:HB3	1:A:114:HIS:CD2	2.32	0.61
3:S:11:SER:OG	3:S:21:ASN:ND2	2.34	0.61
1:I:131:ARG:NH2	1:I:154:GLU:OE1	2.34	0.61
1:E:102:ASP:OD2	1:E:113:TYR:OH	2.16	0.60
3:G:36:GLU:HB3	3:G:83:ASN:ND2	2.16	0.60
1:I:45:MET:H	1:I:64:THR:HG22	1.65	0.60
3:S:29:GLY:HA2	3:S:61:SER:HB2	1.83	0.60
1:U:174:ASN:OD1	4:X:51:ARG:NH1	2.34	0.60
1:I:131:ARG:HD3	1:I:153:ALA:HB3	1.83	0.60
1:U:202:ARG:HG3	1:U:204:TRP:CZ3	2.37	0.60
3:O:73:THR:OG1	3:O:75:LYS:HG2	2.01	0.60
4:P:72:PRO:HA	4:P:78:LEU:HA	1.83	0.60
1:A:141:GLN:N	1:A:141:GLN:OE1	2.33	0.60
1:A:98:MET:HB3	1:A:115:GLN:HG3	1.82	0.60
1:E:112:GLY:HA3	1:E:160:LEU:HD11	1.83	0.60
1:M:71:SER:O	1:M:75:ARG:HG2	2.01	0.60
1:Q:144:LYS:HA	1:Q:147:TRP:CE3	2.37	0.60
4:T:34:LYS:HA	4:T:54:THR:HG22	1.82	0.60
1:Q:124:ILE:HD11	1:Q:140:ALA:HA	1.83	0.60
1:E:116:TYR:N	1:E:124:ILE:O	2.18	0.59
1:M:28:VAL:O	1:M:31:THR:OG1	2.18	0.59
4:D:72:PRO:HA	4:D:78:LEU:HA	1.82	0.59
3:O:7:ILE:HD11	3:O:80:CYS:HB3	1.84	0.59
1:U:249:VAL:HG12	1:U:253:GLN:NE2	2.17	0.59
4:H:15:PRO:HG2	4:H:71:VAL:HG11	1.83	0.59
1:M:191:HIS:HB2	1:M:201:LEU:HG	1.84	0.59
1:E:21:ARG:CZ	1:E:39:ASP:HB2	2.33	0.59
3:G:36:GLU:HB3	3:G:83:ASN:HD21	1.67	0.59
4:X:72:PRO:HA	4:X:78:LEU:HA	1.84	0.59
1:I:262:GLN:HG2	1:I:269:PRO:HB3	1.83	0.59
1:M:21:ARG:NH2	1:M:22:PHE:O	2.36	0.59
1:A:82:ARG:HH21	1:A:87:GLN:HG3	1.66	0.59
1:M:137:ASP:OD1	1:M:138:MET:N	2.28	0.59
1:Q:212:GLU:N	1:Q:212:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:TYR:HH	3:K:63:TYR:HH	1.43	0.59
1:Q:35:ARG:HE	1:Q:48:ARG:HD3	1.68	0.59
3:C:24:ASN:HB3	3:C:65:LEU:HD11	1.83	0.59
1:E:182:THR:HA	1:E:209:TYR:CZ	2.38	0.59
4:L:72:PRO:HA	4:L:78:LEU:HA	1.85	0.59
3:K:19:LYS:HE2	3:K:20:SER:N	2.18	0.59
1:Q:1:GLY:H2	1:Q:105:SER:HA	1.67	0.59
1:Q:44:ARG:HA	1:Q:64:THR:HG23	1.85	0.59
1:I:181:ARG:HH21	4:L:28:ARG:HH11	1.50	0.58
1:A:201:LEU:HD22	1:A:257:TYR:OH	2.04	0.58
3:K:84:HIS:ND1	3:K:86:THR:OG1	2.33	0.58
1:M:157:ARG:HA	1:M:160:LEU:HD12	1.84	0.58
1:M:235:PRO:HA	1:M:241:PHE:HD1	1.69	0.58
1:Q:154:GLU:HA	1:Q:157:ARG:HB3	1.85	0.58
4:T:75:ASP:OD1	4:T:75:ASP:N	2.35	0.58
1:U:5:MET:HG2	1:U:6:ARG:HG2	1.86	0.58
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.38	0.58
3:O:72:PRO:HB3	3:O:95:TRP:HH2	1.67	0.58
1:Q:154:GLU:HG3	1:Q:157:ARG:HD3	1.84	0.58
1:A:63:GLU:OE1	2:B:2:LEU:HB2	2.04	0.58
1:E:159:TYR:OH	2:F:1:LEU:O	2.14	0.58
3:G:29:GLY:HA2	3:G:61:SER:HB2	1.84	0.58
3:G:59:ASP:OD1	3:G:59:ASP:N	2.37	0.58
1:M:146:LYS:HZ1	2:N:8:TYR:HB3	1.68	0.58
1:U:7:TYR:C	1:U:8:PHE:HD2	2.12	0.58
1:A:17:ARG:C	3:W:44:GLU:HB3	2.29	0.57
1:M:22:PHE:HB2	1:M:75:ARG:HH12	1.68	0.57
1:M:73:THR:HG23	1:M:97:ARG:HH12	1.69	0.57
1:A:191:HIS:CE1	1:A:201:LEU:HD21	2.38	0.57
4:D:70:SER:HB3	4:D:78:LEU:HD21	1.86	0.57
1:E:209:TYR:CD1	1:E:210:PRO:HD3	2.39	0.57
1:M:4:SER:OG	1:M:103:VAL:N	2.35	0.57
1:M:204:TRP:HZ3	1:M:206:LEU:HB2	1.69	0.57
4:X:37:TRP:NE1	4:X:54:THR:OG1	2.37	0.57
1:A:3:HIS:O	1:A:3:HIS:ND1	2.32	0.57
1:E:13:SER:HA	1:E:20:PRO:HB3	1.87	0.57
1:Q:213:ILE:HD12	1:Q:263:HIS:HB2	1.87	0.57
1:Q:235:PRO:HB2	3:S:65:LEU:HD22	1.86	0.57
1:U:77:ASP:O	1:U:80:THR:OG1	2.18	0.57
1:U:253:GLN:NE2	1:U:253:GLN:H	2.02	0.57
3:G:35:ILE:HG22	3:G:37:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:ILE:HB	1:I:263:HIS:HD2	1.70	0.57
1:Q:116:TYR:HE1	1:Q:147:TRP:CH2	2.23	0.57
4:D:92:ASN:HA	4:D:99:ARG:NH2	2.20	0.57
1:E:133:TRP:CD1	1:E:144:LYS:HD3	2.40	0.57
1:M:1:GLY:O	1:M:3:HIS:ND1	2.38	0.57
1:M:107:TRP:O	1:M:169:ARG:NE	2.32	0.57
1:M:250:PRO:HB2	1:M:253:GLN:HE22	1.70	0.57
1:Q:102:ASP:OD2	1:Q:113:TYR:OH	2.22	0.57
1:A:99:TYR:HA	1:A:114:HIS:HA	1.87	0.56
1:M:213:ILE:HB	1:M:243:LYS:HZ2	1.69	0.56
1:E:76:VAL:HG23	2:F:8:TYR:HE1	1.69	0.56
1:Q:185:PRO:HB3	1:Q:208:PHE:CZ	2.40	0.56
1:U:177:GLU:OE1	4:X:49:LYS:NZ	2.39	0.56
1:M:124:ILE:HG21	1:M:147:TRP:HZ3	1.70	0.56
1:Q:205:ALA:HB1	1:Q:208:PHE:CE2	2.40	0.56
1:U:174:ASN:HA	4:X:51:ARG:HH12	1.69	0.56
1:M:21:ARG:HH22	1:M:37:ASP:HA	1.70	0.56
1:M:95:VAL:HG13	1:M:116:TYR:HE1	1.69	0.56
1:M:190:THR:HB	1:M:202:ARG:HE	1.71	0.56
1:U:238:ASP:OD2	3:W:12:ARG:NH1	2.38	0.56
1:A:20:PRO:HG3	1:A:78:LEU:HD21	1.86	0.56
1:E:147:TRP:NE1	2:F:8:TYR:O	2.38	0.56
4:P:28:ARG:NH1	4:P:59:TRP:O	2.37	0.56
1:Q:219:ARG:HG3	1:Q:222:GLU:HB2	1.88	0.56
1:U:129:ASP:CG	1:U:130:LEU:H	2.14	0.56
1:U:201:LEU:N	1:U:247:VAL:O	2.39	0.56
1:A:54:GLN:NE2	1:A:174:ASN:O	2.39	0.56
4:D:27:ASN:ND2	4:D:103:MET:HG2	2.21	0.56
1:E:3:HIS:O	1:E:3:HIS:ND1	2.39	0.56
1:E:156:LEU:HA	2:F:3:PHE:CE1	2.40	0.56
1:I:111:ARG:NH1	1:I:111:ARG:HB2	2.20	0.56
4:D:61:PRO:HD3	4:D:104:TRP:CH2	2.41	0.56
1:M:131:ARG:HH22	1:M:151:HIS:CD2	2.24	0.56
3:W:11:SER:OG	3:W:21:ASN:ND2	2.39	0.56
3:W:54:LEU:HD11	3:W:62:PHE:CD1	2.41	0.56
3:G:40:LEU:HB2	3:G:43:GLY:O	2.06	0.55
3:S:45:ARG:NH1	3:S:46:ILE:HG22	2.21	0.55
3:W:31:HIS:HD2	3:W:32:PRO:HA	1.71	0.55
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.39	0.55
1:I:3:HIS:O	1:I:3:HIS:ND1	2.39	0.55
4:L:11:LEU:HD12	4:L:11:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:86:ASN:OD1	1:Q:86:ASN:N	2.37	0.55
1:E:70:HIS:O	1:E:74:HIS:ND1	2.38	0.55
1:A:177:GLU:HG3	4:D:57:SER:HA	1.89	0.55
1:E:20:PRO:HG3	1:E:78:LEU:HD21	1.88	0.55
1:Q:30:ASP:OD2	1:Q:211:ALA:N	2.31	0.55
4:X:75:ASP:OD1	4:X:75:ASP:N	2.40	0.55
1:E:94:THR:OG1	1:E:96:GLN:OE1	2.24	0.55
3:K:13:HIS:H	3:K:21:ASN:HD21	1.55	0.55
1:A:107:TRP:O	1:A:169:ARG:NE	2.35	0.55
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.39	0.55
3:C:11:SER:OG	3:C:13:HIS:O	2.23	0.55
4:H:70:SER:HB3	4:H:78:LEU:HD21	1.88	0.55
3:O:69:GLU:OE2	3:W:19:LYS:NZ	2.29	0.55
1:U:154:GLU:HG2	1:U:157:ARG:HD3	1.89	0.55
1:A:188:HIS:CG	1:A:189:MET:H	2.25	0.55
3:K:35:ILE:HG22	3:K:37:VAL:HG12	1.89	0.55
1:E:144:LYS:O	1:E:148:GLU:HG3	2.05	0.55
1:I:147:TRP:HZ2	2:J:9:VAL:HG12	1.72	0.55
1:U:181:ARG:HH21	4:X:28:ARG:NH1	2.04	0.55
1:A:224:GLN:HE22	1:A:228:THR:N	1.97	0.55
1:I:218:GLN:HB3	1:I:260:HIS:CD2	2.38	0.55
1:M:250:PRO:C	1:M:253:GLN:HE22	2.13	0.55
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.24	0.54
1:A:263:HIS:HB3	1:A:266:LEU:HB2	1.90	0.54
1:I:13:SER:HB3	1:I:93:HIS:H	1.73	0.54
1:Q:77:ASP:O	1:Q:80:THR:OG1	2.22	0.54
4:T:45:GLN:NE2	4:T:47:LYS:O	2.40	0.54
1:U:6:ARG:HD2	1:U:8:PHE:CE2	2.41	0.54
1:A:147:TRP:HZ2	2:B:9:VAL:HG12	1.71	0.54
1:E:33:PHE:CE2	1:E:52:ILE:HB	2.42	0.54
3:K:34:ASP:C	3:K:35:ILE:HD12	2.32	0.54
1:M:14:ARG:HB3	1:M:17:ARG:HG2	1.88	0.54
3:K:37:VAL:HB	3:K:82:VAL:HG22	1.90	0.54
1:M:115:GLN:HA	1:M:125:ALA:HA	1.90	0.54
1:U:114:HIS:CD2	1:U:156:LEU:HD21	2.43	0.54
1:U:201:LEU:HD13	1:U:257:TYR:OH	2.07	0.54
1:I:257:TYR:HD2	1:I:257:TYR:H	1.55	0.54
1:U:202:ARG:HG3	1:U:204:TRP:CE3	2.42	0.54
1:E:118:TYR:H	1:E:118:TYR:HD2	1.56	0.54
1:M:78:LEU:HB3	1:M:95:VAL:HG21	1.88	0.54
1:Q:13:SER:HB2	1:Q:93:HIS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:208:PHE:O	1:Q:240:THR:HA	2.07	0.54
1:E:115:GLN:HA	1:E:125:ALA:HA	1.89	0.54
1:E:185:PRO:HG3	1:E:208:PHE:HB3	1.88	0.54
1:I:77:ASP:O	1:I:80:THR:OG1	2.19	0.54
1:Q:216:THR:O	1:Q:260:HIS:N	2.40	0.54
1:U:238:ASP:OD1	1:U:240:THR:OG1	2.26	0.54
1:M:28:VAL:HG11	1:M:51:TRP:HH2	1.73	0.54
1:U:159:TYR:OH	2:V:1:LEU:O	2.24	0.54
1:E:28:VAL:O	1:E:31:THR:OG1	2.23	0.53
1:E:238:ASP:OD2	3:G:12:ARG:NH1	2.41	0.53
1:M:108:ARG:NH1	1:M:169:ARG:HH22	2.06	0.53
1:Q:127:LYS:NZ	1:Q:129:ASP:OD1	2.38	0.53
1:E:250:PRO:C	1:E:253:GLN:HE22	2.14	0.53
1:I:127:LYS:C	1:I:129:ASP:H	2.16	0.53
1:M:217:TRP:CZ2	1:M:224:GLN:HB2	2.43	0.53
1:E:261:VAL:HG13	1:E:270:LEU:HB2	1.89	0.53
3:W:23:LEU:HG	3:W:70:PHE:CG	2.44	0.53
4:P:75:ASP:OD1	4:P:75:ASP:N	2.41	0.53
3:W:30:PHE:HB2	3:W:84:HIS:NE2	2.24	0.53
1:M:94:THR:OG1	1:M:96:GLN:OE1	2.25	0.53
1:M:103:VAL:HG13	1:M:107:TRP:HA	1.91	0.53
1:Q:127:LYS:HG3	1:Q:128:GLU:N	2.23	0.53
3:G:56:PHE:HB3	3:G:62:PHE:CD1	2.43	0.53
1:M:33:PHE:HD1	1:M:34:VAL:HG23	1.74	0.53
1:M:238:ASP:OD1	1:M:240:THR:OG1	2.23	0.53
1:Q:139:ALA:HA	1:Q:142:THR:HG22	1.90	0.53
4:D:45:GLN:HB3	4:D:68:THR:OG1	2.08	0.53
1:Q:121:LYS:HG3	1:Q:122:ASP:H	1.72	0.53
1:U:11:SER:HA	1:U:21:ARG:O	2.09	0.53
1:A:73:THR:OG1	2:B:7:VAL:O	2.21	0.53
3:C:21:ASN:HB3	3:C:70:PHE:CE2	2.43	0.53
1:I:48:ARG:HG2	1:I:48:ARG:HH21	1.74	0.53
3:O:12:ARG:HH21	4:P:97:MET:HB3	1.74	0.53
4:P:28:ARG:NH2	4:P:60:GLN:HB3	2.24	0.53
1:U:127:LYS:C	1:U:129:ASP:H	2.16	0.53
1:I:19:GLU:OE1	1:I:20:PRO:HD2	2.09	0.53
1:M:1:GLY:HA2	1:M:105:SER:HA	1.90	0.53
4:X:45:GLN:HB3	4:X:68:THR:OG1	2.09	0.53
1:I:147:TRP:CZ2	2:J:9:VAL:HG12	2.44	0.52
1:M:74:HIS:NE2	1:M:97:ARG:HG3	2.24	0.52
1:M:208:PHE:CE1	1:M:241:PHE:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:TYR:CE2	4:H:47:LYS:HE3	2.44	0.52
1:M:14:ARG:HD2	1:M:21:ARG:HB2	1.90	0.52
1:Q:219:ARG:HB2	1:Q:257:TYR:CE1	2.45	0.52
1:U:204:TRP:HZ2	1:U:244:TRP:CD2	2.27	0.52
1:A:66:LYS:HD2	2:B:4:GLY:HA2	1.91	0.52
1:E:124:ILE:HG23	1:E:133:TRP:CZ2	2.44	0.52
1:Q:216:THR:N	1:Q:260:HIS:O	2.42	0.52
3:S:56:PHE:HB3	3:S:62:PHE:CD1	2.44	0.52
3:W:31:HIS:CD2	3:W:32:PRO:HA	2.43	0.52
1:E:73:THR:OG1	2:F:7:VAL:O	2.24	0.52
3:O:30:PHE:CE1	3:O:62:PHE:HB2	2.45	0.52
4:P:28:ARG:HH22	4:P:59:TRP:C	2.16	0.52
1:Q:14:ARG:NE	1:Q:19:GLU:O	2.42	0.52
4:X:20:LEU:HD11	4:X:85:PHE:CD1	2.44	0.52
3:S:35:ILE:CD1	3:S:84:HIS:HD2	2.23	0.52
4:T:65:GLU:HA	4:T:87:PHE:CD2	2.45	0.52
1:U:235:PRO:O	3:W:10:TYR:OH	2.22	0.52
1:A:77:ASP:O	1:A:80:THR:OG1	2.21	0.52
1:E:141:GLN:HA	1:E:144:LYS:HG2	1.91	0.52
3:S:31:HIS:CD2	3:S:32:PRO:HA	2.38	0.52
1:U:191:HIS:HE1	1:U:193:ALA:HB2	1.74	0.52
1:U:263:HIS:CD2	1:U:265:GLY:H	2.28	0.52
3:C:30:PHE:HB2	3:C:84:HIS:HE2	1.74	0.52
3:K:39:LEU:HB2	3:K:49:VAL:HG11	1.90	0.52
1:Q:22:PHE:CE2	1:Q:24:ALA:HB2	2.45	0.52
1:Q:209:TYR:HB3	1:Q:210:PRO:HD3	1.90	0.52
3:S:41:LYS:HB2	3:S:45:ARG:CZ	2.39	0.52
3:W:40:LEU:HG	3:W:43:GLY:O	2.10	0.52
1:Q:63:GLU:OE1	2:R:2:LEU:HD13	2.10	0.52
3:C:11:SER:HG	3:C:21:ASN:HD21	1.57	0.52
1:M:14:ARG:CZ	1:M:17:ARG:HH21	2.22	0.52
3:W:7:ILE:HD11	3:W:93:VAL:HB	1.91	0.52
4:X:49:LYS:HE3	4:X:51:ARG:CZ	2.39	0.52
1:U:29:ASP:CG	1:U:30:ASP:H	2.18	0.51
3:G:57:SER:OG	3:G:58:LYS:N	2.43	0.51
1:M:93:HIS:ND1	1:M:119:ASP:OD2	2.35	0.51
3:O:29:GLY:HA2	3:O:61:SER:HB2	1.91	0.51
4:P:39:CYS:O	4:P:53:ASN:ND2	2.29	0.51
1:A:115:GLN:HA	1:A:125:ALA:HA	1.92	0.51
4:H:49:LYS:HE3	4:H:51:ARG:HH21	1.75	0.51
1:E:235:PRO:O	3:G:10:TYR:OH	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ARG:HG2	1:I:17:ARG:HB3	1.93	0.51
1:M:215:LEU:HD21	1:M:243:LYS:HE3	1.92	0.51
1:A:127:LYS:C	1:A:129:ASP:H	2.19	0.51
1:A:230:LEU:HD23	1:A:230:LEU:H	1.74	0.51
1:E:234:ARG:HE	1:E:242:GLN:HB2	1.75	0.51
1:I:121:LYS:HG3	1:I:122:ASP:H	1.75	0.51
1:A:6:ARG:HG3	1:A:8:PHE:CE2	2.46	0.51
1:I:109:PHE:CZ	1:I:111:ARG:HA	2.46	0.51
1:Q:171:TYR:HE1	2:R:1:LEU:HD13	1.75	0.51
1:A:121:LYS:HG3	1:A:122:ASP:H	1.76	0.51
1:A:137:ASP:O	1:A:141:GLN:NE2	2.43	0.51
1:I:218:GLN:NE2	1:I:222:GLU:H	2.07	0.51
4:T:22:PHE:CD2	4:T:90:MET:HB3	2.46	0.51
4:H:95:MET:HE1	4:H:104:TRP:CG	2.46	0.51
1:M:73:THR:OG1	2:N:7:VAL:O	2.28	0.51
1:Q:159:TYR:OH	2:R:1:LEU:O	2.25	0.51
4:X:33:ILE:HB	4:X:55:LEU:HG	1.93	0.51
1:A:82:ARG:NH2	1:A:88:SER:O	2.43	0.51
3:G:35:ILE:HD11	3:G:84:HIS:HD2	1.71	0.51
1:A:1:GLY:HA2	1:A:105:SER:HA	1.92	0.51
1:A:177:GLU:HG2	4:D:28:ARG:HH22	1.76	0.51
1:E:27:TYR:OH	1:E:32:GLN:NE2	2.44	0.51
1:I:93:HIS:ND1	1:I:119:ASP:OD2	2.33	0.51
3:S:84:HIS:CE1	3:S:86:THR:HG23	2.46	0.51
4:H:14:ASN:O	4:H:16:ASP:N	2.42	0.50
1:I:109:PHE:CE2	1:I:111:ARG:HA	2.46	0.50
1:I:127:LYS:HD3	1:I:128:GLU:N	2.27	0.50
1:Q:11:SER:OG	1:Q:95:VAL:O	2.26	0.50
1:Q:164:CYS:O	1:Q:168:LEU:HB2	2.11	0.50
1:A:108:ARG:HA	1:A:169:ARG:HH21	1.74	0.50
3:G:21:ASN:HB3	3:G:70:PHE:CE2	2.47	0.50
1:I:97:ARG:HD3	1:I:116:TYR:CD2	2.46	0.50
1:Q:33:PHE:CE2	1:Q:52:ILE:HB	2.46	0.50
1:Q:145:HIS:ND1	1:Q:148:GLU:OE1	2.30	0.50
4:L:73:GLY:N	4:L:77:PHE:O	2.41	0.50
1:M:97:ARG:HG2	1:M:116:TYR:CD1	2.42	0.50
1:M:124:ILE:HG21	1:M:147:TRP:CZ3	2.45	0.50
1:Q:109:PHE:CD1	1:Q:161:GLU:HG2	2.46	0.50
1:U:108:ARG:HA	1:U:169:ARG:HH21	1.76	0.50
1:A:32:GLN:H	1:A:32:GLN:CD	2.20	0.50
1:A:171:TYR:CE1	2:B:1:LEU:HD22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ILE:HG23	4:D:89:HIS:HB2	1.93	0.50
1:E:209:TYR:CG	1:E:210:PRO:CD	2.95	0.50
1:U:35:ARG:HD2	1:U:48:ARG:HG3	1.92	0.50
1:U:94:THR:OG1	1:U:96:GLN:OE1	2.27	0.50
1:I:170:ARG:O	1:I:173:GLU:HG2	2.12	0.50
1:I:234:ARG:HD3	3:K:8:GLN:NE2	2.27	0.50
3:K:5:PRO:HB3	3:K:30:PHE:HB3	1.92	0.50
1:M:116:TYR:CE2	1:M:123:TYR:HD2	2.29	0.50
1:Q:262:GLN:HA	1:Q:266:LEU:HD11	1.93	0.50
1:Q:262:GLN:NE2	1:Q:269:PRO:HB3	2.22	0.50
1:U:97:ARG:HD3	1:U:116:TYR:HD1	1.75	0.50
1:I:1:GLY:H1	1:I:107:TRP:CD1	2.29	0.50
1:M:72:GLN:O	1:M:76:VAL:HG22	2.10	0.50
1:M:191:HIS:ND1	1:M:192:HIS:N	2.59	0.50
1:M:209:TYR:HB3	1:M:210:PRO:HD3	1.93	0.50
4:D:68:THR:HG22	4:D:82:ASN:OD1	2.11	0.50
1:E:231:VAL:HG11	1:E:244:TRP:CB	2.41	0.50
1:U:177:GLU:HG3	4:X:57:SER:HA	1.94	0.50
3:C:30:PHE:HB2	3:C:84:HIS:NE2	2.27	0.50
1:M:260:HIS:HE1	1:M:271:THR:HG22	1.76	0.50
4:T:73:GLY:N	4:T:77:PHE:O	2.40	0.50
1:U:254:GLU:HB3	1:U:257:TYR:OH	2.12	0.50
1:Q:93:HIS:ND1	1:Q:119:ASP:OD2	2.45	0.50
1:U:126:LEU:HG	1:U:127:LYS:O	2.11	0.50
3:W:56:PHE:HB3	3:W:62:PHE:CD1	2.47	0.50
1:A:224:GLN:NE2	1:A:228:THR:H	2.01	0.49
1:E:164:CYS:O	1:E:168:LEU:HB2	2.11	0.49
1:E:28:VAL:HG11	1:E:51:TRP:HH2	1.77	0.49
2:V:3:PHE:CE2	2:V:5:TYR:HB2	2.47	0.49
3:S:12:ARG:HB3	3:S:22:PHE:HB2	1.94	0.49
1:M:47:PRO:HB3	1:M:60:TRP:CH2	2.47	0.49
1:U:208:PHE:HB2	1:U:263:HIS:CE1	2.47	0.49
3:C:30:PHE:CE1	3:C:62:PHE:HB2	2.47	0.49
1:M:218:GLN:NE2	1:M:222:GLU:O	2.34	0.49
4:D:57:SER:OG	4:D:58:THR:N	2.44	0.49
1:E:177:GLU:HG3	4:H:57:SER:HA	1.93	0.49
1:I:139:ALA:HA	1:I:142:THR:HG22	1.93	0.49
1:Q:7:TYR:CZ	1:Q:26:GLY:HA3	2.47	0.49
1:A:33:PHE:HE1	1:A:171:TYR:CD1	2.31	0.49
4:T:14:ASN:O	4:T:16:ASP:N	2.42	0.49
1:U:8:PHE:HB2	1:U:25:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:73:THR:HG23	1:U:97:ARG:HH12	1.77	0.49
1:A:152:VAL:HG13	2:B:5:TYR:OH	2.13	0.49
4:D:44:ILE:HD11	4:D:67:TYR:HD1	1.77	0.49
1:I:111:ARG:NH2	1:I:128:GLU:OE2	2.45	0.49
1:M:35:ARG:NH1	3:O:53:ASP:OD2	2.40	0.49
1:M:114:HIS:O	1:M:126:LEU:N	2.41	0.49
4:T:95:MET:O	4:T:99:ARG:NH1	2.45	0.49
1:U:21:ARG:NH1	1:U:37:ASP:OD1	2.46	0.49
1:A:146:LYS:HE2	2:B:8:TYR:HE2	1.78	0.49
4:D:88:GLU:O	4:D:92:ASN:ND2	2.46	0.49
1:I:159:TYR:OH	2:J:1:LEU:O	2.25	0.49
4:L:78:LEU:N	4:P:48:ASN:OD1	2.34	0.49
1:M:5:MET:HB2	1:M:6:ARG:H	1.46	0.49
1:M:146:LYS:NZ	2:N:8:TYR:HB3	2.27	0.49
1:Q:127:LYS:C	1:Q:129:ASP:H	2.20	0.49
3:W:34:ASP:C	3:W:35:ILE:HD12	2.38	0.49
4:L:45:GLN:HB3	4:L:68:THR:OG1	2.13	0.49
1:M:49:ALA:O	1:M:52:ILE:HG22	2.13	0.49
1:M:147:TRP:HZ2	2:N:9:VAL:HG12	1.77	0.49
1:Q:76:VAL:HG13	4:X:7:ALA:O	2.12	0.49
1:I:4:SER:CB	1:I:168:LEU:HD21	2.41	0.48
4:T:22:PHE:CE2	4:T:90:MET:HB3	2.48	0.48
4:L:15:PRO:HG2	4:L:71:VAL:HG11	1.93	0.48
1:E:28:VAL:HG11	1:E:51:TRP:CH2	2.48	0.48
1:I:201:LEU:HD13	1:I:257:TYR:OH	2.13	0.48
1:U:114:HIS:O	1:U:114:HIS:ND1	2.46	0.48
3:G:9:VAL:HG22	3:G:25:CYS:SG	2.54	0.48
1:I:234:ARG:HE	1:I:242:GLN:HB2	1.77	0.48
1:M:183:ASP:HB2	1:M:209:TYR:N	2.27	0.48
1:M:190:THR:HB	1:M:202:ARG:NE	2.26	0.48
3:O:37:VAL:HG12	3:O:82:VAL:HG22	1.94	0.48
3:O:41:LYS:HG3	3:O:78:TYR:CE1	2.49	0.48
1:Q:234:ARG:HE	1:Q:242:GLN:HB2	1.78	0.48
4:X:65:GLU:HA	4:X:87:PHE:CD2	2.49	0.48
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.96	0.48
1:A:232:GLU:O	1:A:234:ARG:HD2	2.14	0.48
1:A:254:GLU:C	1:A:257:TYR:HE2	2.22	0.48
1:Q:103:VAL:HA	1:Q:110:LEU:H	1.77	0.48
3:S:35:ILE:HD11	3:S:84:HIS:HD2	1.78	0.48
4:H:91:CYS:O	4:H:95:MET:HG3	2.14	0.48
1:I:32:GLN:OE1	1:I:32:GLN:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:ASP:HB2	1:I:132:SER:OG	2.14	0.48
1:A:82:ARG:NH2	1:A:87:GLN:HG3	2.29	0.48
1:A:171:TYR:HE1	2:B:1:LEU:HD22	1.79	0.48
1:M:32:GLN:CD	1:M:32:GLN:H	2.21	0.48
1:Q:85:TYR:HB2	1:Q:87:GLN:HE22	1.79	0.48
1:U:28:VAL:O	1:U:31:THR:HG23	2.14	0.48
1:U:114:HIS:NE2	1:U:126:LEU:HB2	2.29	0.48
3:C:34:ASP:C	3:C:35:ILE:HD12	2.39	0.48
3:K:30:PHE:HB2	3:K:84:HIS:NE2	2.29	0.48
1:M:250:PRO:HB2	1:M:253:GLN:NE2	2.28	0.48
1:U:171:TYR:CE1	2:V:1:LEU:HD22	2.48	0.48
1:U:191:HIS:HD2	1:U:201:LEU:HD12	1.79	0.48
3:G:43:GLY:HA3	1:Q:17:ARG:HG2	1.94	0.48
1:M:159:TYR:OH	2:N:1:LEU:O	2.32	0.48
1:U:231:VAL:HG11	1:U:244:TRP:HB3	1.95	0.48
1:E:27:TYR:CZ	1:E:32:GLN:HG3	2.48	0.48
3:K:43:GLY:O	3:K:44:GLU:HG3	2.14	0.48
1:M:116:TYR:CG	1:M:117:ALA:N	2.81	0.48
1:U:96:GLN:HG2	1:U:117:ALA:HB3	1.95	0.48
1:A:154:GLU:HA	1:A:157:ARG:HB3	1.94	0.47
3:G:73:THR:OG1	3:G:76:ASP:HB2	2.14	0.47
1:M:191:HIS:CD2	1:M:201:LEU:HD12	2.49	0.47
1:Q:235:PRO:HA	1:Q:241:PHE:CD1	2.49	0.47
1:A:124:ILE:HG21	1:A:147:TRP:CZ3	2.43	0.47
1:E:14:ARG:HG3	1:E:20:PRO:HA	1.96	0.47
1:M:108:ARG:HD2	1:M:169:ARG:NH2	2.30	0.47
1:A:87:GLN:CD	1:A:88:SER:H	2.21	0.47
1:A:111:ARG:HD2	1:A:128:GLU:O	2.14	0.47
1:A:185:PRO:HD2	1:A:266:LEU:HD23	1.96	0.47
1:E:66:LYS:HD2	2:F:4:GLY:HA2	1.96	0.47
4:H:72:PRO:HA	4:H:77:PHE:O	2.14	0.47
1:I:94:THR:OG1	1:I:96:GLN:OE1	2.32	0.47
1:I:209:TYR:HB3	1:I:210:PRO:HD3	1.96	0.47
1:M:156:LEU:HA	2:N:3:PHE:CE1	2.50	0.47
1:U:234:ARG:HH22	1:U:244:TRP:HZ3	1.60	0.47
1:A:17:ARG:HA	3:W:44:GLU:N	2.29	0.47
1:E:35:ARG:HE	1:E:48:ARG:HD3	1.79	0.47
1:E:35:ARG:HG3	1:E:46:GLU:HB2	1.96	0.47
3:K:19:LYS:O	3:K:72:PRO:HD2	2.13	0.47
1:M:127:LYS:C	1:M:129:ASP:H	2.23	0.47
1:M:234:ARG:HD3	3:O:8:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:201:LEU:HB2	1:Q:254:GLU:CD	2.40	0.47
4:T:44:ILE:HD11	4:T:51:ARG:O	2.15	0.47
4:T:57:SER:OG	4:T:58:THR:N	2.47	0.47
1:U:249:VAL:HG12	1:U:253:GLN:HE21	1.79	0.47
4:D:36:GLY:O	4:D:53:ASN:ND2	2.41	0.47
1:E:231:VAL:HG11	1:E:244:TRP:HB2	1.96	0.47
1:I:208:PHE:CE1	1:I:241:PHE:HB2	2.49	0.47
3:K:15:ALA:HB2	3:K:95:TRP:HZ2	1.79	0.47
1:A:17:ARG:CZ	3:W:40:LEU:HD11	2.44	0.47
4:D:95:MET:O	4:D:99:ARG:NE	2.47	0.47
1:E:21:ARG:HD2	1:E:37:ASP:OD1	2.15	0.47
1:Q:213:ILE:HD11	1:Q:261:VAL:HG23	1.97	0.47
4:T:22:PHE:HE1	4:T:31:VAL:HG13	1.78	0.47
3:W:57:SER:H	3:W:63:TYR:HE2	1.62	0.47
1:A:14:ARG:O	1:A:16:GLY:N	2.45	0.47
1:A:143:THR:OG1	2:B:9:VAL:O	2.29	0.47
1:A:188:HIS:HD2	1:A:190:THR:HG23	1.79	0.47
1:E:209:TYR:CD2	1:E:210:PRO:HD2	2.49	0.47
1:I:190:THR:O	1:I:201:LEU:HG	2.15	0.47
1:M:27:TYR:H	1:M:33:PHE:HE2	1.62	0.47
1:M:214:THR:CG2	1:M:262:GLN:HB2	2.45	0.47
3:O:34:ASP:C	3:O:35:ILE:HD12	2.40	0.47
1:A:1:GLY:H2	1:A:105:SER:HA	1.79	0.47
3:O:80:CYS:O	3:O:92:ILE:HA	2.15	0.47
1:Q:34:VAL:HG21	1:Q:45:MET:SD	2.54	0.47
1:U:118:TYR:CG	1:U:119:ASP:N	2.75	0.47
1:M:138:MET:HE2	1:M:138:MET:HA	1.96	0.47
1:M:164:CYS:O	1:M:168:LEU:HB2	2.15	0.47
1:M:188:HIS:HB2	1:M:204:TRP:CZ2	2.38	0.47
1:Q:24:ALA:HB3	1:Q:36:PHE:HB3	1.95	0.47
1:U:204:TRP:HZ2	1:U:244:TRP:CE2	2.33	0.47
1:A:147:TRP:CZ2	2:B:9:VAL:HG12	2.50	0.47
1:E:51:TRP:CD1	1:E:178:THR:HG21	2.50	0.47
3:O:5:PRO:HB3	3:O:30:PHE:HB3	1.96	0.47
4:P:46:TYR:OH	4:P:59:TRP:HD1	1.98	0.47
1:E:256:ARG:HG3	1:E:257:TYR:HD1	1.80	0.46
1:I:1:GLY:HA2	1:I:105:SER:HA	1.96	0.46
1:I:188:HIS:CD2	1:I:189:MET:H	2.34	0.46
1:M:116:TYR:N	1:M:124:ILE:O	2.40	0.46
4:X:40:GLN:O	4:X:41:SER:OG	2.30	0.46
1:A:4:SER:HB3	1:A:168:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:GLU:HA	1:M:157:ARG:HB3	1.97	0.46
4:D:20:LEU:HD11	4:D:85:PHE:CD1	2.50	0.46
3:G:78:TYR:O	3:G:95:TRP:N	2.44	0.46
1:I:33:PHE:CE2	1:I:52:ILE:HB	2.50	0.46
1:I:109:PHE:HD1	1:I:165:VAL:HG21	1.80	0.46
1:M:5:MET:HG3	1:M:27:TYR:HB3	1.97	0.46
1:M:6:ARG:HH22	1:M:115:GLN:CG	2.25	0.46
1:Q:3:HIS:HB2	1:Q:29:ASP:CG	2.41	0.46
3:W:24:ASN:CB	3:W:65:LEU:HD11	2.45	0.46
1:E:137:ASP:CG	1:E:138:MET:H	2.23	0.46
1:E:177:GLU:H	1:E:177:GLU:CD	2.22	0.46
1:I:257:TYR:N	1:I:257:TYR:CD2	2.84	0.46
3:O:73:THR:HG23	3:O:76:ASP:H	1.79	0.46
1:Q:205:ALA:HB1	1:Q:208:PHE:HE2	1.80	0.46
1:M:54:GLN:HB3	4:P:51:ARG:NH2	2.31	0.46
1:M:108:ARG:HA	1:M:108:ARG:HD2	1.64	0.46
1:M:224:GLN:OE1	1:M:228:THR:OG1	2.24	0.46
1:M:235:PRO:HA	1:M:241:PHE:CD1	2.48	0.46
4:X:49:LYS:HE3	4:X:51:ARG:NH2	2.31	0.46
1:A:100:GLY:O	1:A:113:TYR:N	2.36	0.46
1:Q:109:PHE:HD1	1:Q:165:VAL:HG21	1.80	0.46
1:Q:129:ASP:HB2	1:Q:132:SER:OG	2.15	0.46
1:Q:235:PRO:HA	1:Q:241:PHE:HD1	1.79	0.46
1:M:20:PRO:HG2	1:M:75:ARG:CD	2.44	0.46
1:M:206:LEU:HD11	3:O:14:PRO:HD3	1.96	0.46
1:Q:256:ARG:HG3	1:Q:257:TYR:CD1	2.51	0.46
3:S:80:CYS:O	3:S:92:ILE:HA	2.15	0.46
1:A:127:LYS:HG2	1:A:132:SER:OG	2.15	0.46
1:A:154:GLU:HG2	1:A:157:ARG:HD3	1.98	0.46
1:A:164:CYS:O	1:A:168:LEU:HB2	2.16	0.46
3:C:9:VAL:HG22	3:C:25:CYS:SG	2.55	0.46
3:C:87:LEU:HD11	3:C:91:LYS:HE3	1.98	0.46
3:K:73:THR:OG1	3:K:76:ASP:HB2	2.15	0.46
1:Q:44:ARG:HG3	1:Q:64:THR:OG1	2.15	0.46
4:X:14:ASN:OD1	4:X:15:PRO:HD3	2.15	0.46
1:E:14:ARG:HH11	1:E:21:ARG:HB2	1.81	0.46
4:L:99:ARG:HD2	4:L:104:TRP:O	2.16	0.46
1:M:21:ARG:NH2	1:M:37:ASP:OD1	2.48	0.46
3:S:56:PHE:HD1	3:S:60:TRP:HA	1.81	0.46
1:M:76:VAL:HG23	2:N:8:TYR:HE1	1.81	0.45
1:Q:115:GLN:C	1:Q:116:TYR:HD2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:178:THR:O	1:Q:209:TYR:OH	2.24	0.45
3:S:31:HIS:HD2	3:S:32:PRO:CA	2.26	0.45
3:K:13:HIS:O	3:K:21:ASN:ND2	2.49	0.45
1:M:127:LYS:HB3	1:M:132:SER:OG	2.16	0.45
1:E:249:VAL:HG21	1:E:257:TYR:HE2	1.81	0.45
1:I:5:MET:HB3	1:I:6:ARG:H	1.56	0.45
1:I:257:TYR:HD2	1:I:257:TYR:N	2.15	0.45
1:Q:214:THR:HG23	1:Q:262:GLN:HB2	1.97	0.45
1:U:123:TYR:CD2	1:U:123:TYR:N	2.83	0.45
1:A:108:ARG:HH11	1:A:169:ARG:HH22	1.65	0.45
1:I:141:GLN:OE1	1:I:144:LYS:NZ	2.41	0.45
4:L:70:SER:HB3	4:L:78:LEU:HD11	1.98	0.45
3:S:23:LEU:HD23	3:S:39:LEU:HD22	1.99	0.45
1:U:114:HIS:CD2	1:U:126:LEU:HB2	2.51	0.45
1:U:155:GLN:O	1:U:155:GLN:HG2	2.15	0.45
3:G:46:ILE:O	3:G:49:VAL:HG13	2.16	0.45
1:I:219:ARG:HG2	1:I:257:TYR:HB2	1.98	0.45
4:T:6:LYS:HE2	1:U:75:ARG:NH2	2.32	0.45
1:I:6:ARG:HH22	1:I:115:GLN:HG2	1.81	0.45
1:M:108:ARG:HH11	1:M:169:ARG:HH22	1.63	0.45
1:U:190:THR:HG23	1:U:202:ARG:HD3	1.99	0.45
4:X:45:GLN:OE1	4:X:50:THR:HG22	2.16	0.45
4:D:8:ASP:CG	4:D:11:LEU:HG	2.42	0.45
1:E:49:ALA:O	1:E:52:ILE:HG22	2.16	0.45
1:E:224:GLN:NE2	1:E:228:THR:H	2.14	0.45
1:M:208:PHE:CD1	1:M:213:ILE:HD11	2.51	0.45
1:E:96:GLN:HG3	3:G:60:TRP:HE3	1.82	0.45
1:I:118:TYR:CG	1:I:119:ASP:N	2.81	0.45
4:L:88:GLU:O	4:L:92:ASN:ND2	2.49	0.45
1:M:14:ARG:NE	1:M:17:ARG:HE	2.15	0.45
1:M:215:LEU:HD11	1:M:243:LYS:CD	2.46	0.45
4:T:9:PRO:HD2	2:V:8:TYR:OH	2.15	0.45
4:T:86:ILE:HD11	4:T:88:GLU:HB3	1.98	0.45
4:X:14:ASN:O	4:X:16:ASP:N	2.49	0.45
4:X:50:THR:O	4:X:50:THR:OG1	2.31	0.45
1:A:178:THR:O	1:A:178:THR:OG1	2.33	0.45
3:C:37:VAL:HG13	3:C:66:TYR:CE1	2.51	0.45
1:E:213:ILE:HB	1:E:263:HIS:HD2	1.82	0.45
4:L:77:PHE:CZ	4:P:64:PRO:HD3	2.52	0.45
1:Q:201:LEU:HD13	1:Q:254:GLU:OE1	2.17	0.45
1:U:99:TYR:HA	1:U:114:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ARG:HB3	1:E:64:THR:HG21	1.99	0.45
1:I:6:ARG:NE	1:I:113:TYR:HD1	2.15	0.45
1:I:66:LYS:HE3	2:J:2:LEU:HB2	1.98	0.45
1:M:21:ARG:CZ	1:M:38:SER:H	2.29	0.45
1:M:118:TYR:HD2	1:M:123:TYR:HB2	1.82	0.45
1:M:147:TRP:CZ2	2:N:9:VAL:HG12	2.51	0.45
1:Q:220:ASP:O	1:Q:222:GLU:N	2.49	0.45
1:U:7:TYR:C	1:U:8:PHE:CD2	2.95	0.45
1:U:203:CYS:C	1:U:204:TRP:HE3	2.25	0.45
3:W:37:VAL:HG21	3:W:66:TYR:CD1	2.52	0.45
1:E:208:PHE:HZ	1:E:243:LYS:HG3	1.82	0.44
1:E:209:TYR:CG	1:E:210:PRO:HD3	2.52	0.44
4:L:6:LYS:HA	4:L:6:LYS:NZ	2.32	0.44
1:Q:236:ALA:O	3:S:12:ARG:HD2	2.17	0.44
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.53	0.44
3:C:9:VAL:CG2	3:C:80:CYS:HB2	2.47	0.44
1:I:183:ASP:HB2	1:I:209:TYR:N	2.33	0.44
1:M:186:LYS:HD2	1:M:186:LYS:HA	1.79	0.44
1:M:211:ALA:HB2	1:M:241:PHE:CE2	2.52	0.44
3:S:73:THR:HG1	3:S:75:LYS:H	1.64	0.44
1:U:49:ALA:HA	1:U:50:PRO:HD3	1.74	0.44
3:W:23:LEU:HG	3:W:70:PHE:CD2	2.52	0.44
3:C:23:LEU:HB2	3:C:68:THR:HG22	1.99	0.44
4:D:8:ASP:OD1	4:D:11:LEU:HG	2.16	0.44
1:E:70:HIS:NE2	1:E:99:TYR:OH	2.50	0.44
1:E:178:THR:HG23	1:E:179:LEU:HD12	1.98	0.44
1:M:116:TYR:CD2	1:M:123:TYR:HD2	2.36	0.44
1:U:107:TRP:O	1:U:169:ARG:NH2	2.49	0.44
1:A:66:LYS:HG2	2:B:2:LEU:HD23	1.99	0.44
1:I:6:ARG:HG3	1:I:113:TYR:HE1	1.82	0.44
1:I:144:LYS:O	1:I:148:GLU:HG3	2.17	0.44
1:M:6:ARG:HD3	1:M:98:MET:HG2	2.00	0.44
1:Q:21:ARG:HH11	1:Q:38:SER:HG	1.62	0.44
3:W:86:THR:OG1	3:W:87:LEU:N	2.50	0.44
3:K:11:SER:OG	3:K:21:ASN:ND2	2.50	0.44
4:L:19:GLN:O	4:L:34:LYS:N	2.49	0.44
1:M:107:TRP:CH2	1:M:172:LEU:HB3	2.53	0.44
3:S:46:ILE:HG23	3:S:46:ILE:O	2.17	0.44
1:U:154:GLU:HA	1:U:157:ARG:HB3	1.99	0.44
3:W:30:PHE:CE1	3:W:62:PHE:HB2	2.53	0.44
1:E:124:ILE:HG23	1:E:133:TRP:HH2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:THR:O	1:I:202:ARG:HB2	2.17	0.44
1:M:108:ARG:HH11	1:M:169:ARG:NH2	2.15	0.44
1:M:204:TRP:CZ3	1:M:206:LEU:HB2	2.51	0.44
1:A:45:MET:SD	1:A:67:VAL:HG21	2.58	0.44
1:A:235:PRO:HB2	3:C:65:LEU:HD22	1.99	0.44
4:H:28:ARG:NH2	4:H:60:GLN:HB3	2.33	0.44
1:M:160:LEU:O	1:M:165:VAL:HG23	2.17	0.44
1:Q:176:LYS:HA	1:Q:179:LEU:HG	2.00	0.44
1:E:224:GLN:CD	1:E:228:THR:H	2.25	0.44
3:K:11:SER:OG	3:K:13:HIS:O	2.31	0.44
1:Q:49:ALA:HA	1:Q:50:PRO:HD3	1.84	0.44
1:Q:115:GLN:HA	1:Q:125:ALA:HA	1.99	0.44
1:U:204:TRP:CZ2	1:U:244:TRP:CD2	3.06	0.44
2:B:2:LEU:HD12	2:B:2:LEU:HA	1.89	0.44
1:E:108:ARG:HA	1:E:108:ARG:HD2	1.76	0.44
1:E:138:MET:O	1:E:141:GLN:HG2	2.18	0.44
3:G:30:PHE:CE1	3:G:62:PHE:HB2	2.53	0.44
3:O:3:ARG:NH1	5:O:101:HOH:O	2.50	0.44
1:U:6:ARG:HD2	1:U:8:PHE:CZ	2.53	0.44
1:U:50:PRO:O	1:U:53:GLU:HG2	2.17	0.44
1:U:156:LEU:HA	2:V:3:PHE:HE1	1.83	0.44
1:U:234:ARG:HD3	3:W:8:GLN:NE2	2.33	0.44
3:W:39:LEU:HD23	3:W:39:LEU:HA	1.91	0.44
4:D:65:GLU:HA	4:D:87:PHE:CD2	2.53	0.43
1:E:2:SER:HB2	1:E:264:GLU:OE2	2.18	0.43
1:I:127:LYS:HB3	1:I:132:SER:OG	2.18	0.43
3:O:35:ILE:HG13	3:O:84:HIS:HD2	1.83	0.43
4:P:9:PRO:O	4:P:12:THR:OG1	2.36	0.43
1:U:177:GLU:H	1:U:177:GLU:CD	2.26	0.43
1:A:18:GLY:N	3:W:44:GLU:HB3	2.33	0.43
1:A:68:LYS:O	1:A:72:GLN:HG2	2.19	0.43
1:E:103:VAL:HG13	1:E:107:TRP:HA	1.99	0.43
3:G:44:GLU:CD	1:Q:17:ARG:HB3	2.43	0.43
1:Q:49:ALA:O	1:Q:52:ILE:HG22	2.17	0.43
1:Q:63:GLU:O	1:Q:67:VAL:HG22	2.18	0.43
3:W:35:ILE:HD11	3:W:84:HIS:CD2	2.53	0.43
3:W:77:GLU:HG2	3:W:78:TYR:N	2.33	0.43
1:A:17:ARG:HA	3:W:43:GLY:C	2.43	0.43
1:M:215:LEU:HD11	1:M:243:LYS:CE	2.49	0.43
4:T:40:GLN:O	4:T:41:SER:OG	2.29	0.43
3:W:31:HIS:HD2	3:W:32:PRO:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:CB	1:A:168:LEU:HD21	2.48	0.43
1:E:121:LYS:HG3	1:E:122:ASP:H	1.82	0.43
1:I:181:ARG:HH21	4:L:28:ARG:NH1	2.15	0.43
1:I:191:HIS:HB2	1:I:201:LEU:CD1	2.48	0.43
4:L:75:ASP:HB2	4:L:77:PHE:CD2	2.53	0.43
4:P:28:ARG:HH11	4:P:29:CYS:H	1.66	0.43
4:T:65:GLU:OE2	4:T:88:GLU:HB2	2.19	0.43
1:U:114:HIS:CE1	1:U:126:LEU:HB2	2.53	0.43
1:U:208:PHE:CE1	1:U:241:PHE:HB2	2.53	0.43
1:E:66:LYS:HE3	2:F:2:LEU:HB2	2.01	0.43
1:I:1:GLY:N	1:I:104:GLY:O	2.46	0.43
1:Q:54:GLN:HA	4:T:54:THR:OG1	2.19	0.43
1:Q:114:HIS:CG	1:Q:156:LEU:HD21	2.54	0.43
2:R:3:PHE:CE2	2:R:5:TYR:HB2	2.53	0.43
3:S:9:VAL:HG22	3:S:80:CYS:HB2	1.99	0.43
1:U:97:ARG:HD3	1:U:116:TYR:CD1	2.52	0.43
1:A:137:ASP:CG	1:A:138:MET:H	2.26	0.43
1:A:172:LEU:HD22	1:A:179:LEU:HD22	2.00	0.43
3:K:80:CYS:O	3:K:92:ILE:HA	2.18	0.43
3:O:7:ILE:HD12	3:O:82:VAL:HG21	2.00	0.43
1:M:60:TRP:O	1:M:64:THR:HG23	2.18	0.43
1:M:234:ARG:HG3	1:M:242:GLN:HB2	1.99	0.43
3:S:45:ARG:HG3	3:S:45:ARG:HH11	1.84	0.43
4:T:59:TRP:CD1	4:T:87:PHE:HB2	2.53	0.43
1:U:204:TRP:CZ2	1:U:244:TRP:CG	3.07	0.43
1:A:208:PHE:CG	1:A:213:ILE:HD11	2.54	0.43
3:C:23:LEU:HG	3:C:70:PHE:CD2	2.54	0.43
3:C:57:SER:H	3:C:63:TYR:HE2	1.67	0.43
4:D:65:GLU:HA	4:D:87:PHE:CE2	2.54	0.43
4:D:104:TRP:HA	4:D:105:PRO:C	2.44	0.43
1:Q:7:TYR:CE1	2:R:2:LEU:HD11	2.54	0.43
1:U:191:HIS:ND1	1:U:192:HIS:N	2.66	0.43
1:A:33:PHE:CE2	1:A:52:ILE:HB	2.54	0.43
1:A:234:ARG:HA	1:A:235:PRO:HD3	1.84	0.43
1:E:118:TYR:CD2	1:E:123:TYR:HB2	2.53	0.43
1:I:188:HIS:CG	1:I:189:MET:H	2.37	0.43
1:U:141:GLN:HG3	1:U:145:HIS:CE1	2.54	0.43
1:U:209:TYR:HB3	1:U:210:PRO:HD3	2.01	0.43
1:E:82:ARG:HD2	1:E:93:HIS:HB2	2.00	0.43
1:E:133:TRP:CG	1:E:134:THR:N	2.86	0.43
1:E:256:ARG:HG3	1:E:257:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:GLU:HG2	1:Q:17:ARG:C	2.44	0.43
3:K:19:LYS:HZ3	3:K:19:LYS:HG3	1.73	0.43
1:M:238:ASP:OD2	3:O:12:ARG:NH1	2.52	0.43
3:O:71:THR:HA	3:O:72:PRO:HD2	1.87	0.43
1:Q:219:ARG:HB2	1:Q:257:TYR:CE2	2.53	0.43
4:T:44:ILE:HG22	4:T:69:VAL:HG12	2.01	0.43
1:U:96:GLN:HB2	3:W:56:PHE:CE2	2.53	0.43
1:U:114:HIS:CD2	1:U:126:LEU:HD22	2.54	0.43
1:M:11:SER:HA	1:M:21:ARG:O	2.19	0.42
1:M:95:VAL:HG13	1:M:116:TYR:OH	2.19	0.42
4:T:20:LEU:HD11	4:T:85:PHE:CD1	2.54	0.42
3:C:35:ILE:HG22	3:C:37:VAL:HG12	2.01	0.42
1:I:35:ARG:CZ	1:I:48:ARG:HD3	2.49	0.42
1:I:74:HIS:NE2	1:I:97:ARG:HG3	2.34	0.42
3:O:57:SER:H	3:O:63:TYR:HE2	1.66	0.42
1:Q:66:LYS:HD2	2:R:3:PHE:O	2.19	0.42
1:A:1:GLY:H1	1:A:107:TRP:CD1	2.37	0.42
1:A:127:LYS:HZ2	1:A:132:SER:HG	1.52	0.42
3:C:26:TYR:HB2	3:C:65:LEU:HD13	2.00	0.42
2:F:1:LEU:HD12	2:F:2:LEU:N	2.33	0.42
3:G:11:SER:OG	3:G:21:ASN:ND2	2.52	0.42
1:I:137:ASP:CG	1:I:138:MET:H	2.26	0.42
1:M:260:HIS:CE1	1:M:271:THR:HA	2.54	0.42
4:P:37:TRP:NE1	4:P:54:THR:OG1	2.52	0.42
1:Q:51:TRP:CE3	1:Q:175:GLY:HA3	2.54	0.42
4:T:22:PHE:CZ	4:T:87:PHE:HD1	2.37	0.42
1:A:251:SER:HA	1:A:254:GLU:OE2	2.20	0.42
1:M:253:GLN:NE2	1:M:253:GLN:H	2.16	0.42
4:P:65:GLU:HA	4:P:87:PHE:CD2	2.55	0.42
1:U:6:ARG:HB2	1:U:8:PHE:HE2	1.85	0.42
1:A:63:GLU:O	1:A:67:VAL:HG23	2.20	0.42
1:E:1:GLY:N	1:E:104:GLY:O	2.50	0.42
1:I:49:ALA:O	1:I:52:ILE:HG22	2.20	0.42
1:M:129:ASP:HB2	1:M:132:SER:OG	2.19	0.42
4:P:45:GLN:HB3	4:P:68:THR:OG1	2.19	0.42
1:Q:22:PHE:CD2	1:Q:71:SER:HB2	2.55	0.42
4:T:44:ILE:HG13	4:T:52:ASN:O	2.20	0.42
1:A:204:TRP:CE3	1:A:204:TRP:N	2.87	0.42
1:A:204:TRP:N	1:A:204:TRP:HE3	2.18	0.42
1:M:191:HIS:O	1:M:202:ARG:NH1	2.53	0.42
1:Q:66:LYS:HE3	2:R:2:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:35:ILE:HG22	3:S:37:VAL:HG13	2.01	0.42
3:W:29:GLY:HA2	3:W:61:SER:HB2	2.01	0.42
1:A:177:GLU:HG2	4:D:28:ARG:NH2	2.35	0.42
1:E:181:ARG:HB3	1:E:183:ASP:OD2	2.19	0.42
3:K:41:LYS:HG3	3:K:78:TYR:CE1	2.54	0.42
1:M:149:ALA:O	1:M:151:HIS:ND1	2.52	0.42
3:S:63:TYR:C	3:S:64:LEU:HD12	2.44	0.42
1:A:108:ARG:NH1	1:A:169:ARG:HH22	2.17	0.42
1:I:46:GLU:HA	1:I:47:PRO:HD3	1.71	0.42
1:I:108:ARG:HA	1:I:108:ARG:HD2	1.82	0.42
1:Q:30:ASP:OD2	1:Q:210:PRO:HA	2.20	0.42
1:Q:85:TYR:HB2	1:Q:87:GLN:OE1	2.18	0.42
1:Q:144:LYS:HE2	1:Q:148:GLU:OE2	2.19	0.42
4:T:45:GLN:O	4:T:67:TYR:HB2	2.20	0.42
1:U:124:ILE:HA	1:U:134:THR:O	2.19	0.42
3:W:23:LEU:HB2	3:W:68:THR:HG22	2.02	0.42
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.54	0.42
1:A:85:TYR:HB3	1:A:86:ASN:H	1.64	0.42
1:Q:191:HIS:HB2	1:Q:201:LEU:HD12	2.02	0.42
4:D:66:TRP:HZ3	4:D:68:THR:HG23	1.84	0.42
1:E:234:ARG:HA	1:E:235:PRO:HD3	1.82	0.42
1:I:3:HIS:HB2	1:I:29:ASP:OD2	2.19	0.42
4:L:27:ASN:HA	4:L:95:MET:HE1	2.02	0.42
1:M:191:HIS:HD2	1:M:201:LEU:HD12	1.84	0.42
1:U:141:GLN:HG3	1:U:145:HIS:HE1	1.84	0.42
1:U:171:TYR:OH	2:V:1:LEU:HD22	2.20	0.42
1:A:188:HIS:O	1:A:189:MET:HG2	2.20	0.41
1:E:98:MET:HE2	3:G:60:TRP:CH2	2.55	0.41
1:M:167:TRP:CE3	1:M:170:ARG:HD3	2.55	0.41
1:M:185:PRO:CB	1:M:205:ALA:HB1	2.49	0.41
1:Q:118:TYR:CG	1:Q:119:ASP:N	2.79	0.41
3:S:57:SER:H	3:S:63:TYR:HE2	1.68	0.41
4:T:76:GLY:HA2	1:U:146:LYS:HG3	2.01	0.41
1:A:96:GLN:HG2	1:A:117:ALA:HB3	2.02	0.41
1:I:31:THR:HG21	1:I:209:TYR:OH	2.19	0.41
1:I:111:ARG:NH1	1:I:128:GLU:HG2	2.34	0.41
4:L:28:ARG:CD	4:L:106:PRO:HG3	2.50	0.41
1:M:70:HIS:CE1	2:N:2:LEU:HD22	2.55	0.41
3:S:4:THR:HA	3:S:5:PRO:HD3	1.84	0.41
3:S:40:LEU:HA	3:S:45:ARG:HH12	1.85	0.41
1:A:18:GLY:HA3	3:W:44:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HD3	1:A:153:ALA:HB3	2.01	0.41
1:A:135:ALA:HB1	1:A:140:ALA:HB1	2.02	0.41
1:I:33:PHE:HD2	1:I:33:PHE:HA	1.73	0.41
1:I:48:ARG:HG2	1:I:48:ARG:NH2	2.34	0.41
1:M:63:GLU:O	1:M:67:VAL:HG22	2.19	0.41
1:M:155:GLN:O	1:M:155:GLN:HG2	2.21	0.41
4:P:104:TRP:HA	4:P:105:PRO:C	2.45	0.41
3:W:21:ASN:HB3	3:W:70:PHE:CE2	2.56	0.41
1:E:66:LYS:HE2	1:E:66:LYS:HB2	1.85	0.41
4:H:104:TRP:HA	4:H:105:PRO:C	2.45	0.41
1:I:13:SER:OG	1:I:82:ARG:NH1	2.53	0.41
1:A:76:VAL:O	1:A:80:THR:HG23	2.21	0.41
1:A:168:LEU:O	1:A:172:LEU:HG	2.21	0.41
3:G:13:HIS:N	3:G:21:ASN:HD21	2.15	0.41
4:H:60:GLN:HG2	4:H:63:ASP:OD2	2.20	0.41
1:Q:25:VAL:HG13	1:Q:48:ARG:NH1	2.35	0.41
1:Q:96:GLN:HG2	1:Q:117:ALA:HB3	2.02	0.41
1:U:156:LEU:HA	2:V:3:PHE:CE1	2.55	0.41
1:A:70:HIS:HA	1:A:73:THR:HG22	2.03	0.41
1:I:4:SER:HB3	1:I:103:VAL:HG22	2.01	0.41
1:Q:15:PRO:HD2	1:Q:17:ARG:HG3	2.03	0.41
1:Q:219:ARG:NH1	1:Q:257:TYR:OH	2.48	0.41
1:A:33:PHE:HD2	1:A:33:PHE:HA	1.69	0.41
1:A:220:ASP:O	1:A:222:GLU:N	2.54	0.41
1:E:101:CYS:HB3	1:E:160:LEU:HD12	2.03	0.41
1:I:14:ARG:HE	1:I:17:ARG:HD2	1.86	0.41
1:I:127:LYS:HD3	1:I:128:GLU:H	1.85	0.41
1:I:181:ARG:NH2	4:L:106:PRO:HB3	2.35	0.41
3:O:41:LYS:HE3	3:O:78:TYR:OH	2.21	0.41
4:P:29:CYS:HB2	4:P:95:MET:HG3	2.02	0.41
3:S:12:ARG:CB	3:S:22:PHE:HB2	2.50	0.41
3:S:77:GLU:HG2	3:S:78:TYR:N	2.36	0.41
1:U:141:GLN:O	1:U:145:HIS:ND1	2.54	0.41
1:E:176:LYS:O	1:E:180:GLN:N	2.54	0.41
4:H:20:LEU:HD11	4:H:85:PHE:CD1	2.56	0.41
1:I:143:THR:O	1:I:146:LYS:HB2	2.21	0.41
3:K:12:ARG:HB3	3:K:22:PHE:HB2	2.02	0.41
1:Q:3:HIS:HB2	1:Q:29:ASP:OD2	2.20	0.41
1:Q:80:THR:OG1	1:Q:81:LEU:N	2.54	0.41
4:T:65:GLU:HA	4:T:87:PHE:HD2	1.85	0.41
1:U:14:ARG:HA	1:U:15:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:59:TYR:O	1:U:63:GLU:HB2	2.21	0.41
1:A:6:ARG:CZ	1:A:8:PHE:HZ	2.33	0.41
1:A:45:MET:H	1:A:64:THR:CG2	2.30	0.41
1:A:159:TYR:CD1	1:A:163:THR:HB	2.55	0.41
1:E:206:LEU:HD23	1:E:206:LEU:HA	1.78	0.41
1:E:250:PRO:HB2	1:E:253:GLN:OE1	2.21	0.41
3:G:21:ASN:HB3	3:G:70:PHE:HE2	1.83	0.41
1:I:20:PRO:HG3	1:I:78:LEU:HD21	2.01	0.41
1:I:33:PHE:CE1	1:I:52:ILE:HD13	2.55	0.41
1:I:189:MET:HG3	1:I:201:LEU:CD2	2.51	0.41
1:I:214:THR:CG2	1:I:262:GLN:HB2	2.51	0.41
1:M:147:TRP:HB3	1:M:152:VAL:CG1	2.51	0.41
1:M:201:LEU:HB3	1:M:202:ARG:H	1.52	0.41
4:P:45:GLN:HG3	4:P:46:TYR:N	2.34	0.41
4:T:68:THR:HB	4:T:80:THR:CG2	2.50	0.41
1:U:95:VAL:HA	1:U:117:ALA:O	2.21	0.41
1:U:129:ASP:HB3	1:U:132:SER:OG	2.21	0.41
1:U:147:TRP:CH2	2:V:9:VAL:HG12	2.56	0.41
1:U:160:LEU:O	1:U:165:VAL:HG23	2.21	0.41
1:A:231:VAL:HG22	1:A:234:ARG:CZ	2.50	0.41
4:D:13:PHE:HE1	4:D:73:GLY:HA2	1.85	0.41
1:E:35:ARG:HG3	1:E:35:ARG:O	2.21	0.41
1:I:201:LEU:HD23	1:I:202:ARG:H	1.86	0.41
1:M:64:THR:O	1:M:68:LYS:HG3	2.21	0.41
4:P:22:PHE:CE1	4:P:31:VAL:HG13	2.56	0.41
3:S:73:THR:HG21	3:S:76:ASP:HB2	2.02	0.41
1:A:266:LEU:HD12	1:A:268:LYS:O	2.22	0.40
1:E:99:TYR:HB3	1:E:114:HIS:HD2	1.86	0.40
1:E:123:TYR:CD2	1:E:124:ILE:HG12	2.56	0.40
1:E:181:ARG:HA	1:E:181:ARG:HD3	1.84	0.40
1:M:10:THR:HG21	3:O:62:PHE:HE1	1.87	0.40
1:Q:29:ASP:C	1:Q:31:THR:H	2.28	0.40
1:Q:266:LEU:HD12	1:Q:266:LEU:O	2.20	0.40
4:D:27:ASN:HD22	4:D:103:MET:HG2	1.87	0.40
4:H:72:PRO:HD3	4:H:78:LEU:HD12	2.02	0.40
3:O:23:LEU:O	3:O:67:TYR:HA	2.21	0.40
4:P:23:GLN:HA	4:P:24:PRO:HD3	1.92	0.40
4:T:99:ARG:HH21	4:T:104:TRP:HE1	1.69	0.40
4:T:104:TRP:CD1	4:T:104:TRP:C	2.99	0.40
1:U:9:PHE:HB3	1:U:74:HIS:CE1	2.45	0.40
1:A:139:ALA:O	1:A:142:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:HB3	1:A:204:TRP:CZ2	2.52	0.40
3:C:41:LYS:HE3	3:C:78:TYR:OH	2.21	0.40
1:E:250:PRO:HB2	1:E:253:GLN:HE22	1.86	0.40
4:L:57:SER:OG	4:L:58:THR:N	2.51	0.40
1:Q:127:LYS:HG2	1:Q:132:SER:OG	2.21	0.40
1:Q:213:ILE:HD11	1:Q:261:VAL:CG2	2.51	0.40
4:T:22:PHE:HZ	4:T:87:PHE:CD1	2.40	0.40
1:U:66:LYS:HE2	1:U:66:LYS:HB2	1.91	0.40
4:X:68:THR:HG22	4:X:82:ASN:OD1	2.21	0.40
1:A:209:TYR:HB3	1:A:210:PRO:HD3	2.02	0.40
1:E:4:SER:HB2	1:E:102:ASP:HA	2.04	0.40
1:E:220:ASP:HB3	1:E:221:GLY:H	1.76	0.40
1:E:249:VAL:HG12	1:E:253:GLN:HE21	1.87	0.40
4:L:46:TYR:CE2	4:L:47:LYS:HE3	2.56	0.40
1:M:6:ARG:NH2	1:M:115:GLN:HG3	2.28	0.40
1:M:156:LEU:HA	2:N:3:PHE:HE1	1.86	0.40
3:S:84:HIS:CG	3:S:85:VAL:H	2.40	0.40
1:U:118:TYR:N	1:U:123:TYR:CE2	2.87	0.40
1:U:191:HIS:CE1	1:U:193:ALA:HB2	2.55	0.40
4:X:46:TYR:CE2	4:X:47:LYS:HE3	2.57	0.40
1:A:181:ARG:HB3	1:A:183:ASP:OD1	2.20	0.40
3:C:15:ALA:HB3	3:C:97:ARG:NH1	2.37	0.40
1:E:9:PHE:HZ	2:F:2:LEU:HD21	1.85	0.40
1:E:115:GLN:C	1:E:116:TYR:HD2	2.29	0.40
1:E:238:ASP:OD1	1:E:240:THR:OG1	2.37	0.40
1:I:234:ARG:HA	1:I:235:PRO:HD3	1.81	0.40
1:I:263:HIS:CE1	1:I:265:GLY:H	2.39	0.40
1:M:133:TRP:CZ2	1:M:153:ALA:HB2	2.57	0.40
3:O:36:GLU:N	3:O:36:GLU:OE1	2.55	0.40
1:Q:33:PHE:HD2	1:Q:33:PHE:HA	1.72	0.40
3:S:9:VAL:CG2	3:S:80:CYS:HB2	2.51	0.40
1:U:118:TYR:HB3	1:U:123:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:OG	1:A:129:ASP:OD1[3_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/275 (93%)	229 (90%)	27 (10%)	0	100	100
1	E	264/275 (96%)	233 (88%)	31 (12%)	0	100	100
1	I	242/275 (88%)	216 (89%)	26 (11%)	0	100	100
1	M	259/275 (94%)	230 (89%)	29 (11%)	0	100	100
1	Q	253/275 (92%)	225 (89%)	27 (11%)	1 (0%)	30	42
1	U	238/275 (86%)	214 (90%)	23 (10%)	1 (0%)	30	42
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	V	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	C	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
3	G	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
3	K	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
3	O	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	S	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	W	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
4	D	100/108 (93%)	88 (88%)	11 (11%)	1 (1%)	12	18
4	H	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	L	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	P	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	T	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	12	18
4	X	101/108 (94%)	89 (88%)	10 (10%)	2 (2%)	6	8
All	All	2731/2952 (92%)	2424 (89%)	298 (11%)	9 (0%)	36	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	9	PRO
4	P	9	PRO
4	X	9	PRO
4	H	9	PRO
4	T	9	PRO
4	D	9	PRO
1	Q	128	GLU
1	U	250	PRO
4	X	15	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	222/231 (96%)	196 (88%)	26 (12%)	5	7
1	E	225/231 (97%)	203 (90%)	22 (10%)	7	11
1	I	211/231 (91%)	186 (88%)	25 (12%)	5	6
1	M	223/231 (96%)	199 (89%)	24 (11%)	6	8
1	Q	218/231 (94%)	188 (86%)	30 (14%)	3	4
1	U	206/231 (89%)	179 (87%)	27 (13%)	4	5
2	B	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
2	J	8/8 (100%)	8 (100%)	0	100	100
2	N	8/8 (100%)	7 (88%)	1 (12%)	4	6
2	R	8/8 (100%)	7 (88%)	1 (12%)	4	6
2	V	8/8 (100%)	6 (75%)	2 (25%)	0	0
3	C	91/95 (96%)	85 (93%)	6 (7%)	15	25
3	G	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	K	93/95 (98%)	81 (87%)	12 (13%)	4	5
3	O	93/95 (98%)	85 (91%)	8 (9%)	10	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	93/95 (98%)	84 (90%)	9 (10%)	8	11
3	W	93/95 (98%)	88 (95%)	5 (5%)	20	33
4	D	91/96 (95%)	85 (93%)	6 (7%)	15	25
4	H	92/96 (96%)	84 (91%)	8 (9%)	9	15
4	L	92/96 (96%)	82 (89%)	10 (11%)	6	8
4	P	92/96 (96%)	82 (89%)	10 (11%)	6	8
4	T	92/96 (96%)	84 (91%)	8 (9%)	9	15
4	X	92/96 (96%)	80 (87%)	12 (13%)	4	5
All	All	2460/2580 (95%)	2194 (89%)	266 (11%)	6	8

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	25	VAL
1	A	28	VAL
1	A	31	THR
1	A	32	GLN
1	A	33	PHE
1	A	74	HIS
1	A	87	GLN
1	A	96	GLN
1	A	113	TYR
1	A	124	ILE
1	A	127	LYS
1	A	134	THR
1	A	143	THR
1	A	144	LYS
1	A	163	THR
1	A	178	THR
1	A	179	LEU
1	A	204	TRP
1	A	214	THR
1	A	223	ASP
1	A	224	GLN
1	A	230	LEU
1	A	234	ARG
1	A	249	VAL
1	A	266	LEU

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Mol	Chain	Res	Type
2	B	5	TYR
2	B	8	TYR
3	C	7	ILE
3	C	37	VAL
3	C	40	LEU
3	C	80	CYS
3	C	85	VAL
3	C	87	LEU
4	D	16	ASP
4	D	39	CYS
4	D	42	VAL
4	D	50	THR
4	D	58	THR
4	D	95	MET
1	E	3	HIS
1	E	12	VAL
1	E	28	VAL
1	E	32	GLN
1	E	33	PHE
1	E	34	VAL
1	E	81	LEU
1	E	94	THR
1	E	103	VAL
1	E	113	TYR
1	E	116	TYR
1	E	118	TYR
1	E	119	ASP
1	E	142	THR
1	E	178	THR
1	E	192	HIS
1	E	209	TYR
1	E	223	ASP
1	E	224	GLN
1	E	244	TRP
1	E	249	VAL
1	E	261	VAL
2	F	1	LEU
2	F	7	VAL
2	F	9	VAL
3	G	4	THR
3	G	7	ILE
3	G	12	ARG

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Mol	Chain	Res	Type
3	G	24	ASN
3	G	37	VAL
3	G	40	LEU
3	G	59	ASP
3	G	68	THR
3	G	80	CYS
4	H	14	ASN
4	H	19	GLN
4	H	42	VAL
4	H	68	THR
4	H	69	VAL
4	H	75	ASP
4	H	77	PHE
4	H	95	MET
1	I	3	HIS
1	I	5	MET
1	I	14	ARG
1	I	17	ARG
1	I	28	VAL
1	I	32	GLN
1	I	33	PHE
1	I	34	VAL
1	I	75	ARG
1	I	94	THR
1	I	96	GLN
1	I	106	ASP
1	I	113	TYR
1	I	116	TYR
1	I	124	ILE
1	I	130	LEU
1	I	144	LYS
1	I	155	GLN
1	I	163	THR
1	I	178	THR
1	I	201	LEU
1	I	202	ARG
1	I	216	THR
1	I	257	TYR
1	I	266	LEU
3	K	7	ILE
3	K	12	ARG
3	K	19	LYS

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Mol	Chain	Res	Type
3	K	24	ASN
3	K	37	VAL
3	K	40	LEU
3	K	47	GLU
3	K	53	ASP
3	K	55	SER
3	K	70	PHE
3	K	80	CYS
3	K	85	VAL
4	L	6	LYS
4	L	11	LEU
4	L	16	ASP
4	L	42	VAL
4	L	50	THR
4	L	68	THR
4	L	69	VAL
4	L	71	VAL
4	L	75	ASP
4	L	78	LEU
1	M	5	MET
1	M	7	TYR
1	M	10	THR
1	M	13	SER
1	M	27	TYR
1	M	28	VAL
1	M	32	GLN
1	M	48	ARG
1	M	67	VAL
1	M	96	GLN
1	M	103	VAL
1	M	124	ILE
1	M	144	LYS
1	M	154	GLU
1	M	155	GLN
1	M	163	THR
1	M	178	THR
1	M	187	THR
1	M	188	HIS
1	M	190	THR
1	M	194	VAL
1	M	213	ILE
1	M	243	LYS

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Mol	Chain	Res	Type
1	M	249	VAL
2	N	7	VAL
3	O	7	ILE
3	O	12	ARG
3	O	24	ASN
3	O	40	LEU
3	O	47	GLU
3	O	67	TYR
3	O	68	THR
3	O	70	PHE
4	P	14	ASN
4	P	16	ASP
4	P	25	ASP
4	P	50	THR
4	P	51	ARG
4	P	57	SER
4	P	69	VAL
4	P	75	ASP
4	P	89	HIS
4	P	95	MET
1	Q	3	HIS
1	Q	5	MET
1	Q	13	SER
1	Q	28	VAL
1	Q	32	GLN
1	Q	33	PHE
1	Q	46	GLU
1	Q	67	VAL
1	Q	75	ARG
1	Q	86	ASN
1	Q	96	GLN
1	Q	98	MET
1	Q	103	VAL
1	Q	113	TYR
1	Q	124	ILE
1	Q	127	LYS
1	Q	130	LEU
1	Q	138	MET
1	Q	155	GLN
1	Q	178	THR
1	Q	202	ARG
1	Q	204	TRP

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Mol	Chain	Res	Type
1	Q	207	SER
1	Q	214	THR
1	Q	215	LEU
1	Q	217	TRP
1	Q	224	GLN
1	Q	228	THR
1	Q	258	THR
1	Q	261	VAL
2	R	1	LEU
3	S	7	ILE
3	S	12	ARG
3	S	23	LEU
3	S	24	ASN
3	S	45	ARG
3	S	46	ILE
3	S	53	ASP
3	S	73	THR
3	S	80	CYS
4	T	11	LEU
4	T	42	VAL
4	T	44	ILE
4	T	75	ASP
4	T	81	VAL
4	T	89	HIS
4	T	95	MET
4	T	99	ARG
1	U	10	THR
1	U	14	ARG
1	U	25	VAL
1	U	28	VAL
1	U	31	THR
1	U	32	GLN
1	U	33	PHE
1	U	75	ARG
1	U	94	THR
1	U	108	ARG
1	U	113	TYR
1	U	114	HIS
1	U	138	MET
1	U	141	GLN
1	U	144	LYS
1	U	155	GLN

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Mol	Chain	Res	Type
1	U	163	THR
1	U	178	THR
1	U	182	THR
1	U	190	THR
1	U	195	SER
1	U	201	LEU
1	U	214	THR
1	U	228	THR
1	U	248	VAL
1	U	253	GLN
1	U	257	TYR
2	V	2	LEU
2	V	7	VAL
3	W	7	ILE
3	W	24	ASN
3	W	49	VAL
3	W	73	THR
3	W	74	GLU
4	X	11	LEU
4	X	13	PHE
4	X	16	ASP
4	X	21	SER
4	X	42	VAL
4	X	45	GLN
4	X	55	LEU
4	X	71	VAL
4	X	75	ASP
4	X	79	ARG
4	X	89	HIS
4	X	95	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	114	HIS
1	A	145	HIS
1	A	188	HIS
1	A	192	HIS
1	A	197	HIS
1	A	224	GLN
3	C	42	ASN

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Mol	Chain	Res	Type
4	D	27	ASN
4	D	52	ASN
4	D	100	GLN
1	E	151	HIS
1	E	253	GLN
3	G	13	HIS
3	G	21	ASN
3	G	31	HIS
4	H	48	ASN
4	H	100	GLN
1	I	115	GLN
1	I	188	HIS
1	I	197	HIS
1	I	260	HIS
3	K	21	ASN
4	L	92	ASN
1	M	188	HIS
1	M	253	GLN
1	M	262	GLN
3	O	8	GLN
3	O	42	ASN
4	P	52	ASN
4	P	92	ASN
4	P	102	HIS
1	Q	87	GLN
1	Q	188	HIS
1	Q	192	HIS
1	Q	224	GLN
1	Q	260	HIS
1	Q	262	GLN
3	S	31	HIS
3	S	42	ASN
4	T	83	ASN
4	T	92	ASN
1	U	114	HIS
3	W	31	HIS
4	X	19	GLN
4	X	100	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	264/275 (96%)	0.22	8 (3%)	52	47	20, 49, 98, 218	0
1	E	268/275 (97%)	0.33	15 (5%)	30	25	18, 49, 126, 173	0
1	I	252/275 (91%)	0.20	9 (3%)	46	40	14, 41, 85, 176	0
1	M	265/275 (96%)	0.36	9 (3%)	48	42	18, 51, 117, 161	0
1	Q	259/275 (94%)	0.64	12 (4%)	37	31	22, 61, 134, 238	0
1	U	246/275 (89%)	0.70	28 (11%)	10	8	27, 59, 131, 224	0
2	B	9/9 (100%)	0.07	0	100	100	29, 33, 52, 58	0
2	F	9/9 (100%)	0.26	0	100	100	34, 53, 82, 85	0
2	J	9/9 (100%)	0.15	0	100	100	22, 33, 49, 83	0
2	N	9/9 (100%)	0.13	0	100	100	20, 39, 61, 77	0
2	R	9/9 (100%)	0.66	0	100	100	33, 41, 70, 75	0
2	V	9/9 (100%)	0.51	0	100	100	41, 51, 77, 80	0
3	C	96/100 (96%)	0.26	3 (3%)	51	45	30, 54, 130, 166	0
3	G	98/100 (98%)	0.07	2 (2%)	65	61	16, 42, 73, 218	0
3	K	98/100 (98%)	0.07	2 (2%)	65	61	15, 40, 74, 180	0
3	O	98/100 (98%)	0.18	3 (3%)	51	45	26, 48, 121, 147	0
3	S	98/100 (98%)	0.66	8 (8%)	17	14	23, 57, 142, 203	0
3	W	98/100 (98%)	0.69	8 (8%)	17	14	20, 57, 115, 186	0
4	D	102/108 (94%)	0.06	2 (1%)	65	61	15, 42, 79, 193	0
4	H	103/108 (95%)	0.09	3 (2%)	53	48	22, 38, 76, 132	0
4	L	103/108 (95%)	0.05	2 (1%)	66	62	17, 36, 81, 129	0
4	P	103/108 (95%)	0.08	2 (1%)	66	62	16, 44, 115, 147	0
4	T	103/108 (95%)	0.37	7 (6%)	23	19	19, 54, 114, 160	0
4	X	103/108 (95%)	0.47	6 (5%)	29	24	18, 49, 92, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2811/2952 (95%)	0.34	129 (4%) 37 31	14, 49, 118, 238	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	93	VAL	6.7
3	W	20	SER	6.0
1	E	223	ASP	5.7
1	I	254	GLU	5.0
1	M	90	ALA	4.8
1	E	227	ASP	4.8
1	U	112	GLY	4.5
1	U	26	GLY	4.5
3	S	42	ASN	4.2
1	U	119	ASP	4.1
1	M	83	GLY	4.1
1	A	189	MET	3.9
1	Q	133	TRP	3.9
3	S	85	VAL	3.9
4	H	13	PHE	3.8
1	E	131	ARG	3.8
1	A	188	HIS	3.7
3	S	15	ALA	3.6
1	U	210	PRO	3.6
4	X	31	VAL	3.6
1	U	33	PHE	3.6
3	G	88	SER	3.5
1	M	89	GLU	3.4
1	E	194	VAL	3.2
4	H	15	PRO	3.2
1	Q	16	GLY	3.2
3	S	66	TYR	3.2
1	U	115	GLN	3.1
1	A	217	TRP	3.1
1	I	136	ALA	3.1
1	U	159	TYR	3.1
3	S	40	LEU	3.1
4	D	11	LEU	3.1
3	K	54	LEU	3.0
1	I	47	PRO	3.0
1	E	193	ALA	3.0
4	H	11	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	T	15	PRO	3.0
4	L	8	ASP	3.0
1	M	239	GLY	3.0
3	C	54	LEU	3.0
1	U	37	ASP	3.0
1	E	83	GLY	3.0
1	I	193	ALA	3.0
1	E	15	PRO	2.9
3	G	35	ILE	2.9
4	T	7	ALA	2.9
4	L	11	LEU	2.9
4	P	11	LEU	2.9
3	O	44	GLU	2.9
4	X	7	ALA	2.9
1	Q	25	VAL	2.9
1	A	223	ASP	2.8
1	E	182	THR	2.8
1	A	106	ASP	2.8
1	E	247	VAL	2.8
1	M	15	PRO	2.8
4	T	35	CYS	2.7
1	I	205	ALA	2.7
3	W	27	VAL	2.7
1	E	230	LEU	2.7
1	E	252	GLY	2.6
1	U	116	TYR	2.6
1	E	79	GLY	2.6
3	S	9	VAL	2.6
1	U	94	THR	2.5
1	Q	152	VAL	2.5
1	E	187	THR	2.5
1	U	178	THR	2.5
4	X	33	ILE	2.5
1	U	15	PRO	2.5
1	U	269	PRO	2.5
1	U	230	LEU	2.4
1	U	61	ASP	2.4
3	W	16	GLU	2.4
4	T	103	MET	2.4
1	U	6	ARG	2.4
3	W	91	LYS	2.4
1	U	243	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	239	GLY	2.4
1	A	180	GLN	2.4
1	Q	8	PHE	2.4
1	I	215	LEU	2.3
1	M	189	MET	2.3
1	Q	50	PRO	2.3
3	O	74	GLU	2.3
1	Q	162	GLY	2.3
1	U	25	VAL	2.3
3	W	65	LEU	2.3
1	U	163	THR	2.3
1	U	261	VAL	2.3
3	O	88	SER	2.3
1	M	141	GLN	2.3
1	E	205	ALA	2.2
1	Q	41	ALA	2.2
1	Q	90	ALA	2.2
4	P	18	CYS	2.2
1	A	131	ARG	2.2
4	T	21	SER	2.2
1	I	192	HIS	2.2
4	X	89	HIS	2.2
4	D	99	ARG	2.2
1	U	113	TYR	2.2
3	W	9	VAL	2.2
1	U	136	ALA	2.2
1	Q	230	LEU	2.2
1	M	251	SER	2.2
1	I	257	TYR	2.1
4	T	97	MET	2.1
1	U	90	ALA	2.1
1	U	107	TRP	2.1
1	Q	84	TYR	2.1
1	U	18	GLY	2.1
3	S	49	VAL	2.1
3	C	33	SER	2.1
3	C	15	ALA	2.1
3	S	60	TRP	2.1
1	E	18	GLY	2.1
3	W	18	GLY	2.1
1	M	227	ASP	2.1
3	K	45	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	X	48	ASN	2.1
1	U	249	VAL	2.1
1	U	71	SER	2.0
4	T	56	ALA	2.0
1	A	249	VAL	2.0
4	X	77	PHE	2.0
1	U	24	ALA	2.0
1	I	116	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.