



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:53 PM UTC

PDB ID : 7U8M / pdb_00007u8m
Title : Crystal structure of chimeric hemagglutinin cH15/3 in complex with broad protective antibodies 31.a.83 and FluA-20
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2022-03-08
Resolution : 5.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

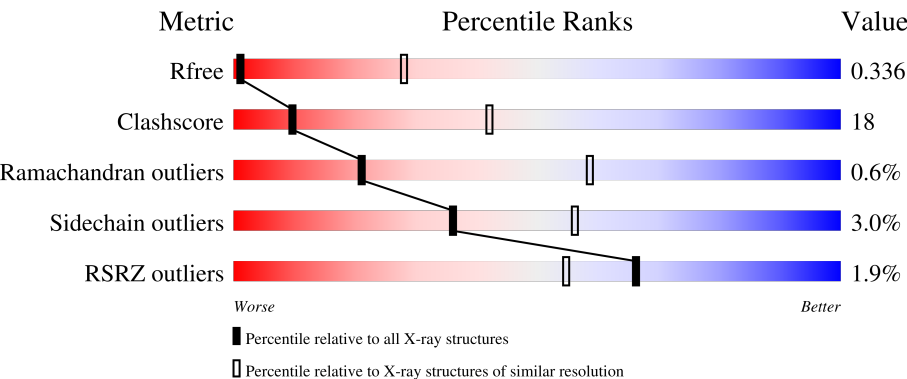
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.39 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	1060 (6.80-4.00)
Clashscore	190562	1117 (6.80-4.00)
Ramachandran outliers	187476	1020 (6.80-3.96)
Sidechain outliers	187428	1019 (6.86-3.94)
RSRZ outliers	180081	1053 (6.80-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	333	2% 54% 38% 5% .
1	C	333	3% 55% 37% 5% .
1	G	333	2% 53% 39% 5% .
2	B	176	3% 85% 13% . .
2	D	176	6% 90% 7% . .

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Mol	Chain	Length	Quality of chain
2	I	176	
3	E	214	
3	J	214	
3	L	214	
4	F	234	
4	H	234	
4	K	234	
5	N	229	
5	Q	229	
5	T	229	
6	O	214	
6	R	214	
6	U	214	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31560 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 hemagglutinin HA1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2482	1545	444	480	13			
1	C	321	Total	C	N	O	S	0	0	0
			2474	1539	443	479	13			
1	G	322	Total	C	N	O	S	0	0	0
			2482	1545	444	480	13			

- Molecule 2 is a protein called hemagglutinin HA2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1396	869	247	274	6			
2	D	172	Total	C	N	O	S	0	0	0
			1390	866	246	272	6			
2	I	173	Total	C	N	O	S	0	0	0
			1396	869	247	274	6			

- Molecule 3 is a protein called Antibody 31.a.83 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1643	1025	281	331	6			
3	E	213	Total	C	N	O	S	0	0	0
			1643	1025	281	331	6			
3	J	213	Total	C	N	O	S	0	0	0
			1643	1025	281	331	6			

- Molecule 4 is a protein called antibody 31.a.83 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	226	Total	C	N	O	S	0	0	0
			1699	1074	280	338	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	226	Total	C	N	O	S	0	0	0
			1699	1074	280	338	7			
4	K	226	Total	C	N	O	S	0	0	0
			1699	1074	280	338	7			

- Molecule 5 is a protein called antibody FluA-20 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	222	Total	C	N	O	S	0	0	0
			1662	1050	273	332	7			
5	Q	221	Total	C	N	O	S	0	0	0
			1658	1048	272	331	7			
5	T	221	Total	C	N	O	S	0	0	0
			1656	1047	272	330	7			

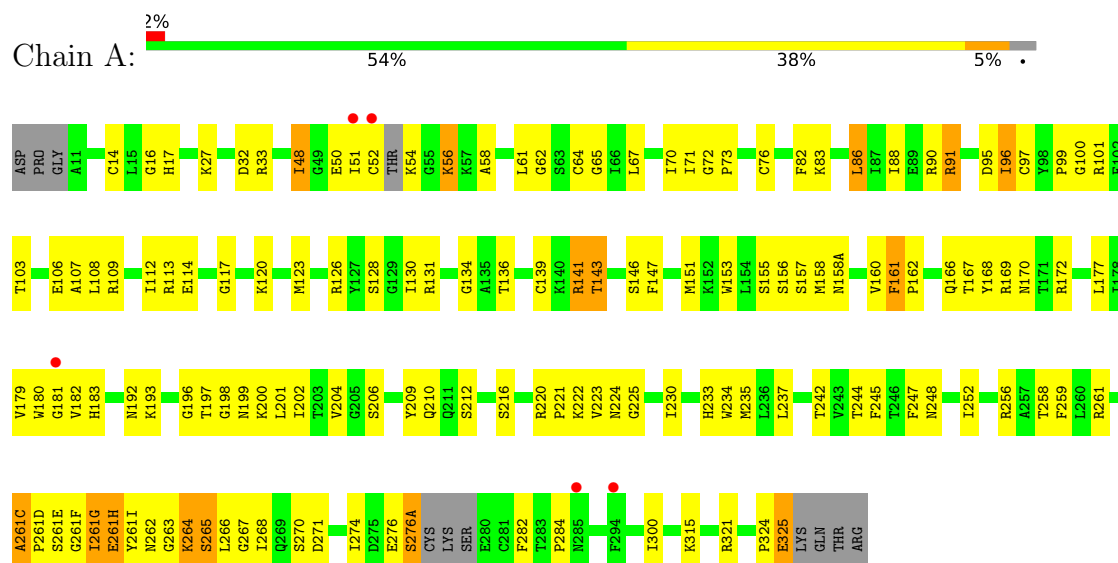
- Molecule 6 is a protein called antibody FluA-20 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			
6	R	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			
6	U	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			

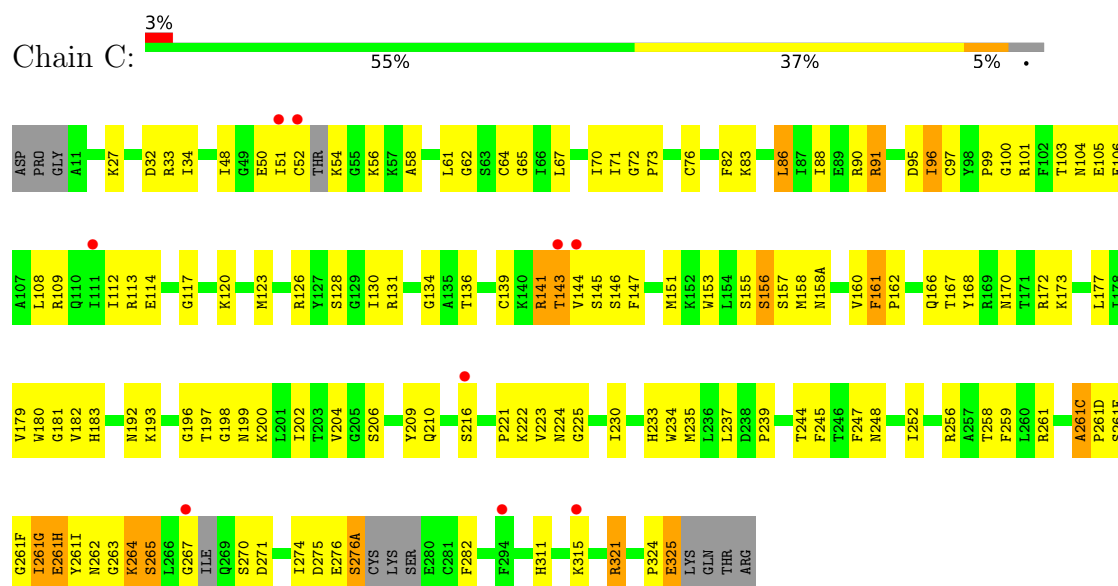
3 Residue-property plots

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.

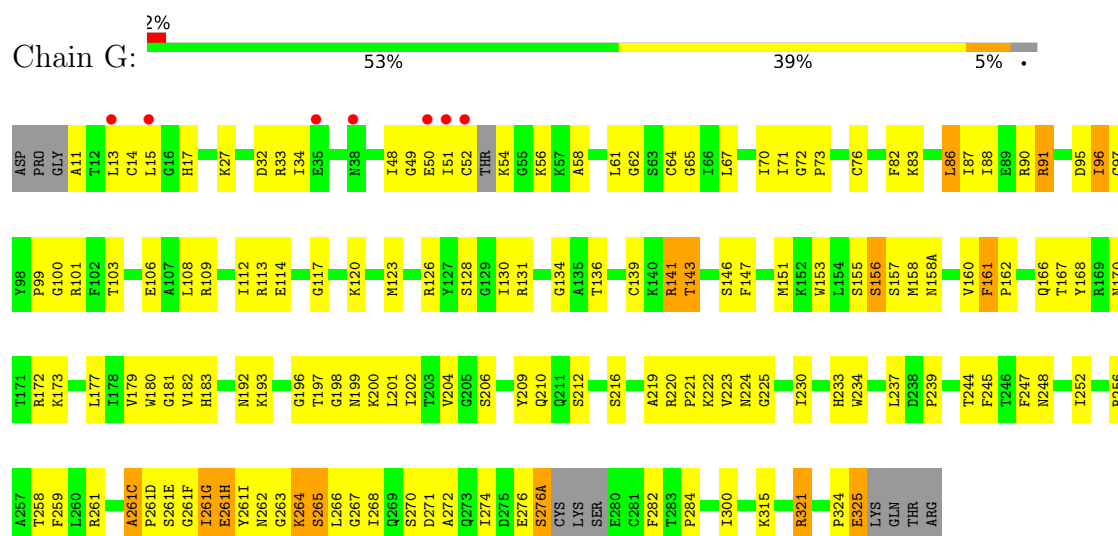
• Molecule 1: hemagglutinin HA1 subunit



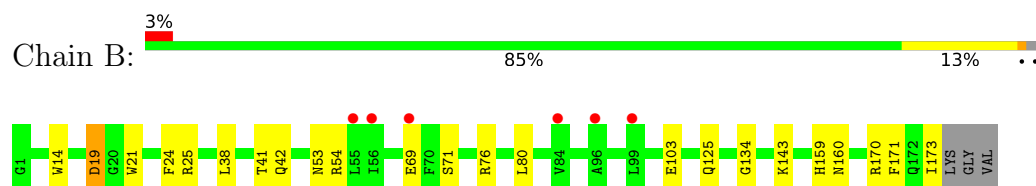
• Molecule 1: hemagglutinin HA1 subunit



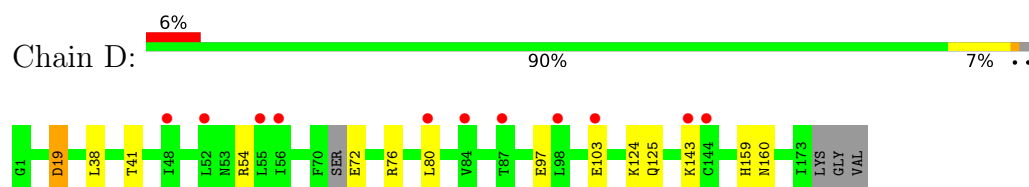
• Molecule 1: hemagglutinin HA1 subunit



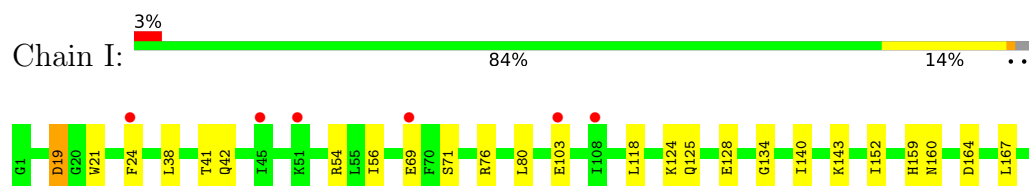
• Molecule 2: hemagglutinin HA2 subunit



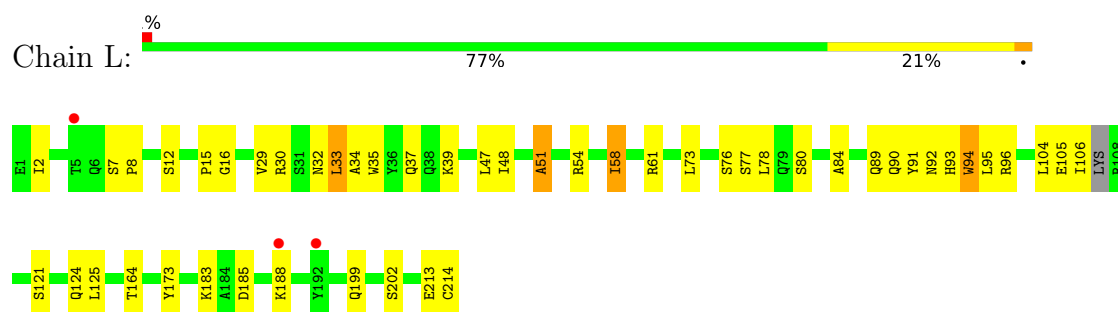
• Molecule 2: hemagglutinin HA2 subunit



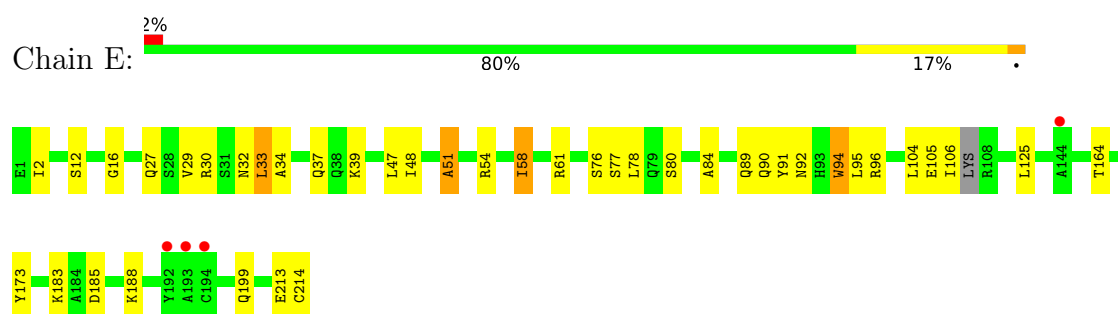
• Molecule 2: hemagglutinin HA2 subunit



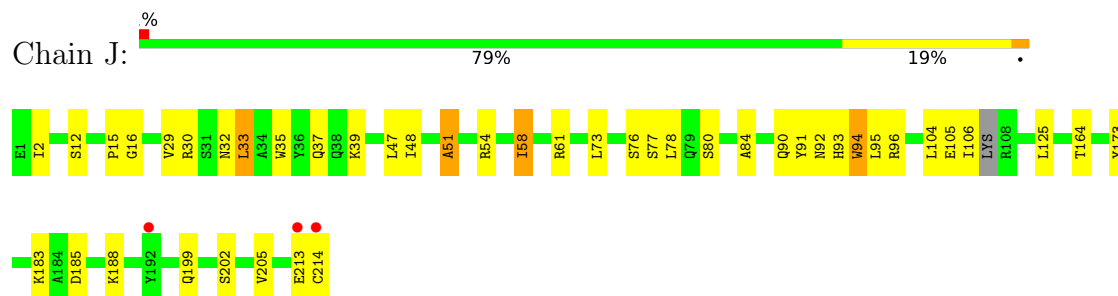
• Molecule 3: Antibody 31.a.83 Fab light chain



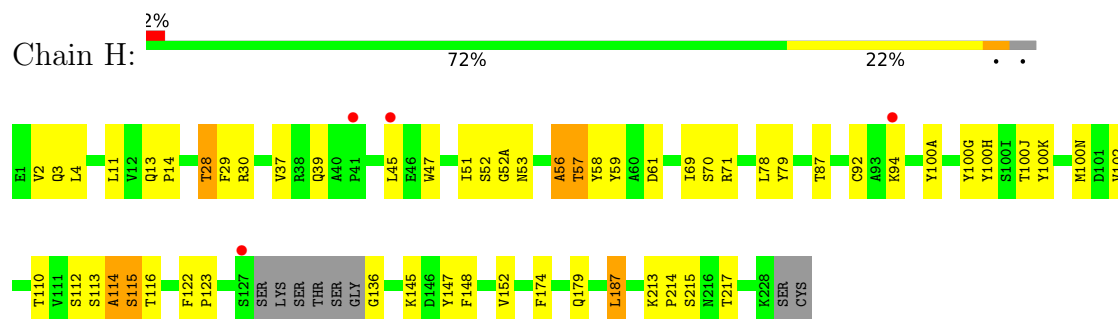
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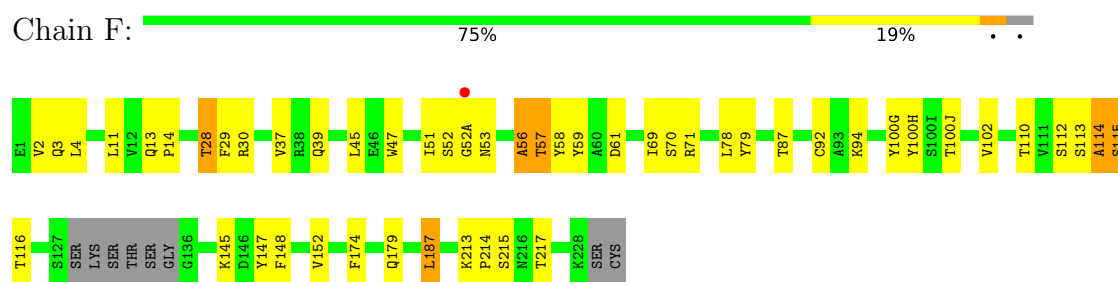
- Molecule 3: Antibody 31.a.83 Fab light chain



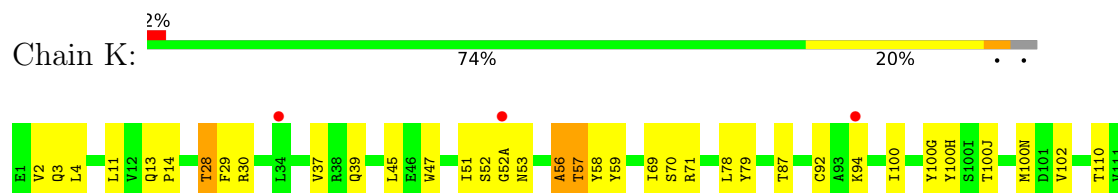
- Molecule 4: antibody 31.a.83 Fab heavy chain



- Molecule 4: antibody 31.a.83 Fab heavy chain

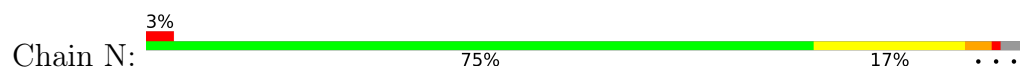


- Molecule 4: antibody 31.a.83 Fab heavy chain

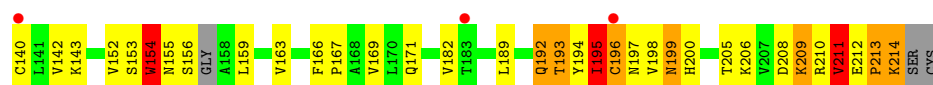
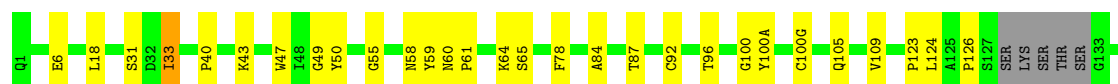




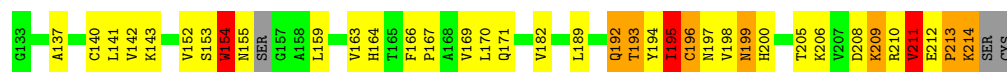
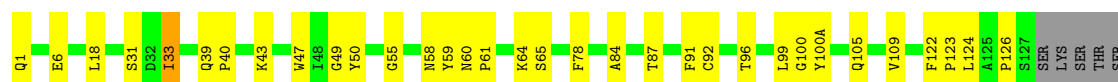
- Molecule 5: antibody FluA-20 Fab heavy chain



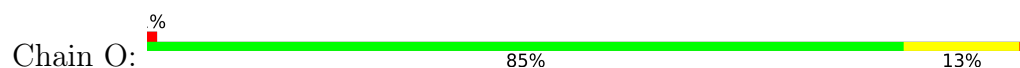
- Molecule 5: antibody FluA-20 Fab heavy chain



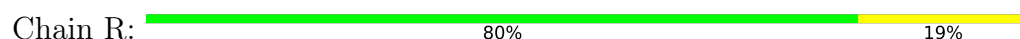
- Molecule 5: antibody FluA-20 Fab heavy chain

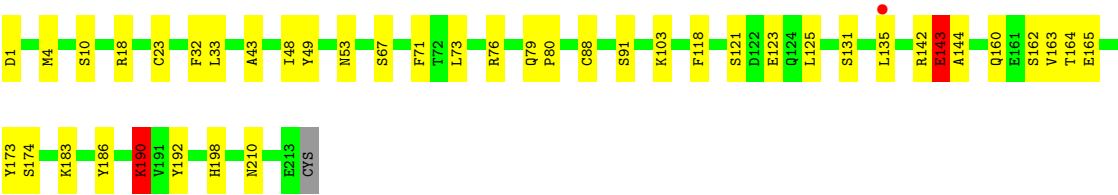


- Molecule 6: antibody FluA-20 Fab light chain

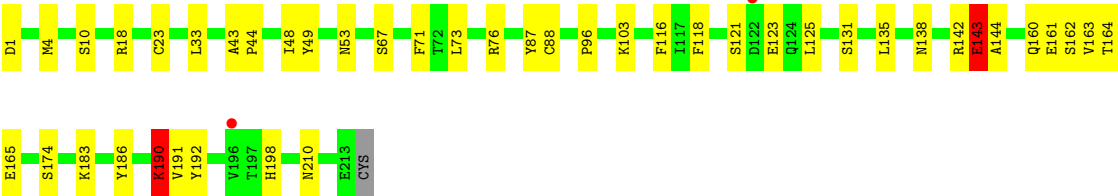
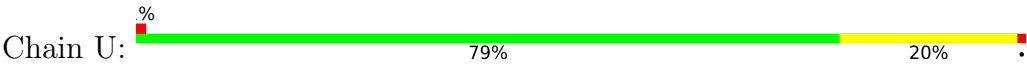


- Molecule 6: antibody FluA-20 Fab light chain





● Molecule 6: antibody FluA-20 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.92Å 155.73Å 156.89Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	49.94 – 5.39 49.94 – 5.39	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.94-5.39) 95.8 (49.94-5.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 5.39Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.304 , 0.342 0.300 , 0.336	Depositor DCC
R_{free} test set	1074 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 338.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	31560	wwPDB-VP
Average B, all atoms (Å ²)	312.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.63	1/2531 (0.0%)	1.16	15/3422 (0.4%)
1	C	0.63	1/2522 (0.0%)	1.16	15/3408 (0.4%)
1	G	0.63	1/2531 (0.0%)	1.16	15/3422 (0.4%)
2	B	0.34	0/1420	0.68	1/1906 (0.1%)
2	D	0.35	0/1413	0.68	1/1895 (0.1%)
2	I	0.35	0/1420	0.68	1/1906 (0.1%)
3	E	0.45	0/1677	0.59	0/2277
3	J	0.45	0/1677	0.59	0/2277
3	L	0.45	0/1677	0.59	0/2277
4	F	0.39	0/1741	0.60	2/2376 (0.1%)
4	H	0.39	0/1741	0.60	2/2376 (0.1%)
4	K	0.39	0/1741	0.61	2/2376 (0.1%)
5	N	0.72	2/1704 (0.1%)	1.09	12/2330 (0.5%)
5	Q	0.72	2/1699 (0.1%)	1.08	11/2322 (0.5%)
5	T	0.72	2/1697 (0.1%)	1.06	11/2319 (0.5%)
6	O	0.62	1/1683 (0.1%)	0.99	3/2285 (0.1%)
6	R	0.63	1/1683 (0.1%)	0.99	3/2285 (0.1%)
6	U	0.63	1/1683 (0.1%)	0.99	3/2285 (0.1%)
All	All	0.56	12/32240 (0.0%)	0.91	97/43744 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	N	0	1
5	Q	0	1
5	T	0	1
6	O	0	1
6	R	0	1
6	U	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	40	PRO	CA-C	-6.42	1.48	1.51
5	Q	40	PRO	CA-C	-6.15	1.48	1.51
5	N	40	PRO	CA-C	-5.97	1.48	1.51
5	N	33	ILE	C-O	-5.63	1.17	1.24
5	Q	33	ILE	C-O	-5.55	1.17	1.24
5	T	33	ILE	C-O	-5.48	1.18	1.24
1	A	143	THR	CA-CB	5.28	1.62	1.53
1	G	143	THR	CA-CB	5.21	1.62	1.53
1	C	143	THR	CA-CB	5.20	1.62	1.53
6	O	143	GLU	C-N	-5.04	1.27	1.33
6	R	143	GLU	C-N	-5.02	1.27	1.33
6	U	143	GLU	C-N	-5.01	1.27	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLY	N-CA-C	15.24	131.80	112.14
1	C	263	GLY	N-CA-C	15.19	131.74	112.14
1	G	263	GLY	N-CA-C	15.19	131.73	112.14
1	A	261(H)	GLU	N-CA-C	-13.90	95.74	113.12
1	C	261(H)	GLU	N-CA-C	-13.87	95.78	113.12
1	G	261(H)	GLU	N-CA-C	-13.87	95.78	113.12
1	G	264	LYS	N-CA-C	12.76	128.84	111.24
1	C	264	LYS	N-CA-C	12.75	128.84	111.24
1	A	264	LYS	N-CA-C	12.72	128.80	111.24
6	O	144	ALA	N-CA-C	-10.89	90.13	108.75
6	U	144	ALA	N-CA-C	-10.88	90.14	108.75
6	R	144	ALA	N-CA-C	-10.85	90.19	108.75
1	G	161	PHE	CA-C-N	9.73	130.34	119.83
1	G	161	PHE	C-N-CA	9.73	130.34	119.83
1	A	161	PHE	CA-C-N	9.70	130.31	119.83
1	A	161	PHE	C-N-CA	9.70	130.31	119.83
1	C	161	PHE	CA-C-N	9.68	130.29	119.83
1	C	161	PHE	C-N-CA	9.68	130.29	119.83
1	C	261(C)	ALA	C-N-CD	-9.17	100.43	120.60
1	G	261(C)	ALA	C-N-CD	-9.15	100.47	120.60
1	A	261(C)	ALA	C-N-CD	-9.15	100.48	120.60
1	G	72	GLY	N-CA-C	8.59	129.85	112.34
1	A	72	GLY	N-CA-C	8.57	129.82	112.34
1	C	72	GLY	N-CA-C	8.56	129.81	112.34
5	T	193	THR	N-CA-C	8.52	123.31	109.76
5	Q	193	THR	N-CA-C	8.51	123.28	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	193	THR	N-CA-C	8.48	123.25	109.76
5	Q	154	TRP	CA-C-N	-7.89	110.76	122.36
5	Q	154	TRP	C-N-CA	-7.89	110.76	122.36
5	N	154	TRP	CA-C-N	-7.87	110.80	122.36
5	N	154	TRP	C-N-CA	-7.87	110.80	122.36
1	C	91	ARG	N-CA-C	7.68	119.43	111.14
1	A	91	ARG	N-CA-C	7.61	119.36	111.14
1	G	91	ARG	N-CA-C	7.40	119.42	111.36
5	N	154	TRP	O-C-N	-7.14	113.70	123.12
5	T	154	TRP	O-C-N	-7.14	113.69	123.12
5	Q	154	TRP	O-C-N	-7.09	113.76	123.12
5	N	156	SER	N-CA-C	6.94	120.74	111.30
1	C	265	SER	N-CA-C	6.89	119.63	110.53
1	A	265	SER	N-CA-C	6.86	119.58	110.53
1	G	265	SER	N-CA-C	6.82	119.54	110.53
5	N	192	GLN	N-CA-C	6.82	120.57	109.59
5	Q	192	GLN	N-CA-C	6.81	120.56	109.59
5	T	192	GLN	N-CA-C	6.78	120.50	109.59
6	U	190	LYS	CG-CD-CE	-6.69	95.90	111.30
6	O	190	LYS	CG-CD-CE	-6.67	95.96	111.30
6	R	190	LYS	CG-CD-CE	-6.67	95.97	111.30
5	T	211	VAL	N-CA-C	6.48	117.82	108.48
1	A	65	GLY	N-CA-C	-6.48	104.25	112.54
5	N	211	VAL	N-CA-C	6.47	117.80	108.48
1	G	65	GLY	N-CA-C	-6.43	104.30	112.54
5	Q	211	VAL	N-CA-C	6.42	117.73	108.48
1	C	65	GLY	N-CA-C	-6.42	104.33	112.54
5	T	154	TRP	CA-C-N	-6.05	110.81	121.70
5	T	154	TRP	C-N-CA	-6.05	110.81	121.70
1	C	128	SER	N-CA-C	5.87	120.24	111.96
5	N	199	ASN	CB-CA-C	5.87	120.44	109.71
1	A	128	SER	N-CA-C	5.85	120.20	111.96
1	G	128	SER	N-CA-C	5.84	120.20	111.96
5	T	199	ASN	CB-CA-C	5.83	120.38	109.71
5	Q	199	ASN	CB-CA-C	5.81	120.35	109.71
1	G	96	ILE	N-CA-C	5.70	116.69	108.48
1	C	96	ILE	N-CA-C	5.70	116.68	108.48
6	U	142	ARG	CG-CD-NE	5.70	124.53	112.00
1	A	96	ILE	N-CA-C	5.66	116.63	108.48
6	O	142	ARG	CG-CD-NE	5.66	124.46	112.00
6	R	142	ARG	CG-CD-NE	5.63	124.38	112.00
4	F	56	ALA	CA-C-N	5.58	131.74	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	56	ALA	C-N-CA	5.58	131.74	121.70
4	K	56	ALA	CA-C-N	5.57	131.72	121.70
4	K	56	ALA	C-N-CA	5.57	131.72	121.70
4	H	56	ALA	CA-C-N	5.55	131.70	121.70
4	H	56	ALA	C-N-CA	5.55	131.70	121.70
5	T	195	ILE	CA-C-N	-5.44	113.64	121.42
5	T	195	ILE	C-N-CA	-5.44	113.64	121.42
5	Q	195	ILE	CA-C-N	-5.43	113.65	121.42
5	Q	195	ILE	C-N-CA	-5.43	113.65	121.42
1	A	156	SER	N-CA-C	5.41	118.98	112.38
5	N	195	ILE	CA-C-N	-5.40	113.70	121.42
5	N	195	ILE	C-N-CA	-5.40	113.70	121.42
1	C	156	SER	N-CA-C	5.40	118.96	112.38
1	G	156	SER	N-CA-C	5.39	118.96	112.38
5	T	140	CYS	CA-CB-SG	5.32	126.63	114.40
5	Q	140	CYS	CA-CB-SG	5.31	126.61	114.40
5	N	140	CYS	CA-CB-SG	5.31	126.61	114.40
2	B	76	ARG	N-CA-C	5.29	117.47	111.02
2	D	76	ARG	N-CA-C	5.24	117.41	111.02
2	I	76	ARG	N-CA-C	5.22	117.39	111.02
1	G	216	SER	CA-C-N	5.18	125.34	119.90
1	G	216	SER	C-N-CA	5.18	125.34	119.90
1	C	216	SER	CA-C-N	5.11	125.27	119.90
1	C	216	SER	C-N-CA	5.11	125.27	119.90
1	A	216	SER	CA-C-N	5.09	125.24	119.90
1	A	216	SER	C-N-CA	5.09	125.24	119.90
5	N	33	ILE	N-CA-C	5.04	118.92	113.43
5	T	196	CYS	N-CA-CB	5.01	117.62	110.06
5	Q	196	CYS	N-CA-CB	5.00	117.61	110.06

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	N	154	TRP	Mainchain
6	O	143	GLU	Mainchain
5	Q	154	TRP	Mainchain
6	R	143	GLU	Mainchain
5	T	154	TRP	Mainchain
6	U	143	GLU	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	2482	0	2431	164	0
1	C	2474	0	2418	148	0
1	G	2482	0	2430	184	0
2	B	1396	0	1331	50	0
2	D	1390	0	1324	26	0
2	I	1396	0	1330	41	0
3	E	1643	0	1592	41	0
3	J	1643	0	1592	46	0
3	L	1643	0	1592	47	0
4	F	1699	0	1650	67	0
4	H	1699	0	1650	86	0
4	K	1699	0	1650	58	0
5	N	1662	0	1618	61	0
5	Q	1658	0	1614	90	0
5	T	1656	0	1612	123	0
6	O	1646	0	1608	41	0
6	R	1646	0	1608	66	0
6	U	1646	0	1608	80	0
All	All	31560	0	30658	1099	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 18.

All (1099) 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:G:51:ILE:HD11	1:G:268:ILE:CG2	1.37	1.51
1:A:106:GLU:CB	2:B:71:SER:HB2	1.47	1.43
1:C:101:ARG:NE	5:N:100:GLY:HA2	1.40	1.32
1:G:106:GLU:CB	2:I:71:SER:HB2	1.60	1.31
1:G:106:GLU:HB3	2:I:71:SER:CB	1.60	1.31
5:T:169:VAL:CG1	6:U:162:SER:HB3	1.61	1.30
1:A:106:GLU:HB3	2:B:71:SER:CB	1.62	1.27
1:C:101:ARG:HE	5:N:100:GLY:CA	1.50	1.23
1:G:106:GLU:CG	2:I:71:SER:HB3	1.67	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:166:PHE:CD1	6:U:164:THR:HG23	1.74	1.21
1:A:33:ARG:HH22	3:J:2:ILE:CD1	1.56	1.17
1:G:86:LEU:HD22	1:G:86:LEU:C	1.70	1.17
2:I:42:GLN:OE1	4:K:100(G):TYR:HB3	1.43	1.16
1:C:51:ILE:HB	1:C:86:LEU:CD2	1.76	1.16
1:G:220:ARG:HG2	5:T:96:THR:HG21	1.17	1.15
5:Q:212:GLU:HG3	5:Q:213:PRO:HD2	1.29	1.14
1:G:51:ILE:HD11	1:G:268:ILE:HG23	1.17	1.14
5:T:169:VAL:HG13	6:U:162:SER:HB3	1.17	1.14
1:A:221:PRO:HB2	6:R:49:TYR:CE2	1.80	1.14
1:A:268:ILE:HB	1:A:284:PRO:O	1.46	1.13
1:G:51:ILE:HB	1:G:86:LEU:HG	1.31	1.13
5:N:212:GLU:HG3	5:N:213:PRO:HD2	1.29	1.13
1:C:51:ILE:HD12	1:C:86:LEU:HD13	1.27	1.12
1:C:51:ILE:CB	1:C:86:LEU:HD22	1.78	1.12
5:T:212:GLU:HG3	5:T:213:PRO:HD2	1.29	1.12
1:G:86:LEU:C	1:G:86:LEU:CD2	2.20	1.12
1:G:51:ILE:HG13	1:G:268:ILE:HD13	1.29	1.12
1:G:52:CYS:O	1:G:56:LYS:HG3	1.48	1.11
1:A:106:GLU:HG3	2:B:71:SER:HB3	1.28	1.10
1:G:106:GLU:CG	2:I:71:SER:CB	2.30	1.10
1:G:51:ILE:HD11	1:G:268:ILE:HG21	1.14	1.09
1:A:33:ARG:HH22	3:J:2:ILE:HD12	1.17	1.09
1:C:101:ARG:CZ	5:N:100:GLY:HA2	1.82	1.09
2:B:41:THR:HG21	4:H:100(G):TYR:CE1	1.88	1.09
5:T:124:LEU:HB3	6:U:118:PHE:CE1	1.87	1.09
1:A:33:ARG:NH2	3:J:2:ILE:HD12	1.67	1.08
1:G:268:ILE:HB	1:G:284:PRO:O	1.54	1.08
1:G:51:ILE:CD1	1:G:268:ILE:CG2	2.33	1.06
1:C:221:PRO:HB2	6:O:49:TYR:CE2	1.89	1.06
1:G:52:CYS:C	1:G:56:LYS:HG3	1.80	1.05
2:D:38:LEU:CD2	4:F:53:ASN:HB3	1.86	1.05
3:L:2:ILE:CD1	1:C:33:ARG:HH22	1.67	1.05
5:Q:169:VAL:CG1	6:R:162:SER:HB2	1.86	1.05
2:D:41:THR:HG21	4:F:100(G):TYR:CE1	1.90	1.05
4:F:114:ALA:HB3	4:F:148:PHE:CE2	1.94	1.03
1:G:106:GLU:HG3	2:I:71:SER:HB3	1.38	1.02
4:H:114:ALA:HB3	4:H:148:PHE:CE2	1.94	1.02
1:G:106:GLU:CB	2:I:71:SER:CB	2.25	1.02
4:K:114:ALA:HB3	4:K:148:PHE:CE2	1.94	1.02
3:L:2:ILE:HD12	1:C:33:ARG:HH22	1.21	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LYS:HE2	5:T:55:GLY:HA3	1.42	1.01
5:Q:166:PHE:CD1	6:R:164:THR:HG23	1.94	1.01
1:G:220:ARG:HG2	5:T:96:THR:CG2	1.90	1.00
1:A:268:ILE:HG22	1:A:284:PRO:HA	1.43	1.00
4:H:114:ALA:CB	4:H:148:PHE:CE2	2.45	1.00
4:F:114:ALA:CB	4:F:148:PHE:CE2	2.45	1.00
4:K:114:ALA:CB	4:K:148:PHE:CE2	2.45	1.00
3:L:93:HIS:HB2	1:C:33:ARG:HH11	1.25	0.99
1:G:51:ILE:CD1	1:G:268:ILE:HG23	1.91	0.99
1:A:51:ILE:HD11	1:A:268:ILE:CG2	1.92	0.99
1:A:106:GLU:CG	2:B:71:SER:CB	2.40	0.99
2:B:38:LEU:HA	4:H:100(G):TYR:OH	1.62	0.99
3:E:2:ILE:HD12	1:G:33:ARG:HH22	1.28	0.98
1:G:49:GLY:HA3	1:G:272:ALA:HB3	1.43	0.98
5:N:214:LYS:HD3	5:N:214:LYS:H	1.28	0.98
2:B:38:LEU:O	4:H:100(G):TYR:HE2	1.46	0.98
3:L:2:ILE:HD12	1:C:33:ARG:NH2	1.78	0.98
5:Q:212:GLU:CG	5:Q:213:PRO:HD2	1.93	0.98
5:N:212:GLU:CG	5:N:213:PRO:HD2	1.93	0.97
5:T:61:PRO:HA	5:T:64:LYS:HE2	1.41	0.97
1:A:51:ILE:HB	1:A:86:LEU:HD22	1.45	0.97
1:C:101:ARG:HE	5:N:100:GLY:HA2	0.91	0.97
5:Q:214:LYS:H	5:Q:214:LYS:HD3	1.28	0.97
1:A:106:GLU:CB	2:B:71:SER:CB	2.29	0.97
5:T:212:GLU:CG	5:T:213:PRO:HD2	1.93	0.97
6:U:190:LYS:HZ1	6:U:210:ASN:HA	1.30	0.97
5:T:214:LYS:H	5:T:214:LYS:HD3	1.28	0.96
1:G:86:LEU:HD22	1:G:86:LEU:O	1.64	0.96
1:G:106:GLU:HB3	2:I:71:SER:HB2	0.96	0.95
1:G:261(E):SER:OG	5:Q:64:LYS:HE2	1.67	0.95
1:A:106:GLU:CG	2:B:71:SER:HB3	1.94	0.94
1:G:49:GLY:HA3	1:G:272:ALA:CB	1.97	0.94
1:A:101:ARG:HG3	5:Q:100:GLY:HA2	1.49	0.93
5:T:124:LEU:HD12	6:U:118:PHE:CG	2.03	0.93
2:B:38:LEU:CD2	4:H:53:ASN:HB3	1.98	0.93
1:A:101:ARG:HG3	5:Q:100:GLY:CA	1.99	0.93
3:E:2:ILE:CD1	1:G:33:ARG:HH22	1.82	0.93
1:G:51:ILE:CG1	1:G:268:ILE:HD13	1.99	0.92
5:T:166:PHE:HE1	6:U:174:SER:C	1.76	0.92
5:T:166:PHE:CD1	6:U:164:THR:CG2	2.52	0.92
1:G:51:ILE:CD1	1:G:268:ILE:HG21	1.97	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:169:VAL:HG13	6:U:162:SER:CB	2.01	0.91
5:T:124:LEU:HB3	6:U:118:PHE:CZ	2.04	0.91
5:T:154:TRP:O	5:T:155:ASN:HB2	1.70	0.90
5:Q:124:LEU:HB3	6:R:118:PHE:CE1	2.07	0.90
1:G:51:ILE:HB	1:G:86:LEU:CG	2.02	0.90
1:C:221:PRO:HB2	6:O:49:TYR:CD2	2.07	0.89
1:C:51:ILE:CD1	1:C:86:LEU:HD13	2.01	0.89
5:Q:169:VAL:HG13	6:R:162:SER:HB2	1.51	0.89
1:G:86:LEU:HD23	1:G:87:ILE:N	1.88	0.88
5:Q:154:TRP:O	5:Q:155:ASN:HB2	1.69	0.88
1:G:221:PRO:HB2	6:U:49:TYR:CE2	2.08	0.88
5:N:154:TRP:O	5:N:155:ASN:HB2	1.70	0.88
1:A:51:ILE:HD11	1:A:268:ILE:HG21	1.53	0.88
2:B:38:LEU:O	4:H:100(G):TYR:CE2	2.27	0.88
1:C:51:ILE:HD12	1:C:86:LEU:CD1	2.03	0.88
5:T:61:PRO:CA	5:T:64:LYS:HE2	2.04	0.88
5:T:159:LEU:HD22	5:T:194:TYR:CE1	2.09	0.88
1:G:52:CYS:C	1:G:56:LYS:CG	2.47	0.87
5:Q:166:PHE:CE1	6:R:164:THR:HG23	2.09	0.87
2:B:41:THR:HB	4:H:100(G):TYR:CZ	2.09	0.87
5:N:159:LEU:HD22	5:N:194:TYR:CE1	2.09	0.87
6:O:190:LYS:HZ1	6:O:210:ASN:HA	1.39	0.87
5:Q:159:LEU:HD22	5:Q:194:TYR:CE1	2.09	0.87
1:C:222:LYS:O	6:O:53:ASN:HB3	1.75	0.86
6:R:190:LYS:HZ1	6:R:210:ASN:HA	1.40	0.86
1:G:106:GLU:HG2	2:I:71:SER:HB3	1.57	0.86
5:T:166:PHE:CE1	6:U:164:THR:HG23	2.10	0.86
1:C:101:ARG:NH2	5:N:100:GLY:HA2	1.91	0.86
1:C:261:ARG:NH1	1:C:261(H):GLU:HG3	1.91	0.85
3:E:2:ILE:HD12	1:G:33:ARG:NH2	1.89	0.85
1:G:51:ILE:CB	1:G:86:LEU:HG	2.07	0.85
5:Q:59:TYR:HB2	5:Q:64:LYS:HG2	1.57	0.85
1:G:261:ARG:NH1	1:G:261(H):GLU:HG3	1.91	0.84
1:G:220:ARG:CG	5:T:96:THR:HG21	2.03	0.84
4:H:100(J):THR:HG23	4:H:100(K):TYR:CE1	2.12	0.84
1:G:58:ALA:CB	1:G:86:LEU:HD13	2.08	0.84
2:B:41:THR:CG2	4:H:100(G):TYR:CE1	2.61	0.83
1:A:261:ARG:NH1	1:A:261(H):GLU:HG3	1.91	0.83
5:N:212:GLU:OE2	5:N:213:PRO:HD3	1.78	0.83
5:T:212:GLU:OE2	5:T:213:PRO:HD3	1.78	0.83
2:D:41:THR:HG21	4:F:100(G):TYR:CZ	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:212:GLU:OE2	5:Q:213:PRO:HD3	1.78	0.83
5:T:166:PHE:HZ	6:U:174:SER:HB3	1.42	0.83
5:T:59:TYR:HB2	5:T:64:LYS:HG2	1.58	0.82
1:G:268:ILE:HG22	1:G:284:PRO:HA	1.61	0.82
2:D:38:LEU:HD21	4:F:53:ASN:HB3	1.60	0.81
5:T:166:PHE:HA	6:U:164:THR:HG22	1.62	0.81
1:A:221:PRO:CB	6:R:49:TYR:CE2	2.63	0.81
1:A:33:ARG:CZ	3:J:2:ILE:HD12	2.11	0.81
1:C:221:PRO:HG2	6:O:49:TYR:CZ	2.16	0.81
5:T:169:VAL:CG1	6:U:162:SER:CB	2.53	0.81
1:A:131:ARG:HG3	1:A:157:SER:HA	1.63	0.81
1:A:48:ILE:HD13	1:A:50:GLU:OE1	1.81	0.80
1:C:101:ARG:NE	5:N:100:GLY:CA	2.22	0.80
1:C:131:ARG:HG3	1:C:157:SER:HA	1.63	0.80
1:A:51:ILE:HD11	1:A:268:ILE:HG23	1.63	0.80
3:L:93:HIS:HB2	1:C:33:ARG:NH1	1.96	0.80
1:A:261(F):GLY:O	1:A:261(G):ILE:HG13	1.82	0.79
2:B:42:GLN:HB2	4:H:100(G):TYR:HD2	1.47	0.79
1:C:51:ILE:HB	1:C:86:LEU:HD22	0.86	0.79
1:G:131:ARG:HG3	1:G:157:SER:HA	1.63	0.79
1:G:261(F):GLY:O	1:G:261(G):ILE:HG13	1.82	0.79
1:A:48:ILE:CD1	1:A:50:GLU:OE1	2.31	0.79
5:T:169:VAL:HG11	6:U:162:SER:HB3	1.60	0.78
1:G:86:LEU:CD2	1:G:87:ILE:N	2.45	0.78
5:Q:166:PHE:CD1	6:R:164:THR:CG2	2.65	0.78
5:T:166:PHE:CZ	6:U:174:SER:HB3	2.19	0.78
2:I:42:GLN:OE1	4:K:100(G):TYR:CB	2.30	0.78
6:R:190:LYS:NZ	6:R:190:LYS:O	2.17	0.78
1:A:71:ILE:HG22	1:A:151:MET:HE3	1.66	0.77
1:C:261(F):GLY:O	1:C:261(G):ILE:HG13	1.82	0.77
1:C:311:HIS:CE1	2:D:97:GLU:OE1	2.37	0.77
6:O:190:LYS:O	6:O:190:LYS:NZ	2.17	0.77
6:U:190:LYS:NZ	6:U:190:LYS:O	2.17	0.77
1:G:58:ALA:HB2	1:G:86:LEU:HD13	1.67	0.77
1:G:106:GLU:HG2	2:I:71:SER:CB	2.09	0.77
1:A:33:ARG:NH2	3:J:2:ILE:CD1	2.33	0.77
5:T:159:LEU:HD22	5:T:194:TYR:HE1	1.50	0.76
1:C:71:ILE:HG22	1:C:151:MET:HE3	1.66	0.76
1:G:71:ILE:HG22	1:G:151:MET:HE3	1.66	0.76
5:T:124:LEU:HD12	6:U:118:PHE:CD2	2.20	0.76
1:A:261(E):SER:O	5:N:59:TYR:CD2	2.37	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:166:PHE:CZ	6:U:174:SER:CB	2.69	0.76
4:K:14:PRO:HD3	4:K:112:SER:O	1.86	0.76
5:N:153:SER:HB2	5:N:197:ASN:ND2	2.01	0.75
1:G:261(E):SER:OG	5:Q:64:LYS:CE	2.35	0.75
1:C:170:ASN:HB2	1:C:237:LEU:HD23	1.68	0.75
1:G:51:ILE:HB	1:G:86:LEU:CD1	2.16	0.75
5:T:153:SER:HB2	5:T:197:ASN:ND2	2.01	0.75
1:G:170:ASN:HB2	1:G:237:LEU:HD23	1.68	0.75
4:H:52:SER:HB3	4:H:100(H):TYR:HD1	1.52	0.75
1:G:51:ILE:HG13	1:G:268:ILE:CD1	2.15	0.75
2:B:38:LEU:HD23	4:H:53:ASN:HB3	1.68	0.75
3:E:32:ASN:HB3	3:E:91:TYR:HB3	1.69	0.75
5:T:167:PRO:HD3	6:U:164:THR:HA	1.67	0.75
4:F:52:SER:HB3	4:F:100(H):TYR:HD1	1.52	0.74
5:Q:153:SER:HB2	5:Q:197:ASN:ND2	2.01	0.74
1:A:222:LYS:HE2	1:A:225:GLY:HA2	1.69	0.74
3:L:32:ASN:HB3	3:L:91:TYR:HB3	1.69	0.74
4:H:14:PRO:HD3	4:H:112:SER:O	1.86	0.74
1:G:51:ILE:O	1:G:86:LEU:HD12	1.87	0.74
5:T:167:PRO:CD	6:U:164:THR:HA	2.17	0.74
1:G:86:LEU:C	1:G:86:LEU:HD23	2.09	0.74
4:F:14:PRO:HD3	4:F:112:SER:O	1.86	0.74
5:T:143:LYS:HE3	6:U:131:SER:OG	1.87	0.74
1:C:221:PRO:CB	6:O:49:TYR:CE2	2.69	0.74
4:K:52:SER:HB3	4:K:100(H):TYR:HD1	1.52	0.74
3:J:32:ASN:HB3	3:J:91:TYR:HB3	1.69	0.74
5:N:214:LYS:H	5:N:214:LYS:CD	2.00	0.74
1:A:170:ASN:HB2	1:A:237:LEU:HD23	1.68	0.73
1:G:222:LYS:HE2	1:G:225:GLY:HA2	1.70	0.73
1:C:222:LYS:HE2	1:C:225:GLY:HA2	1.69	0.73
5:T:171:GLN:HA	6:U:160:GLN:OE1	1.89	0.73
1:A:51:ILE:HD13	1:A:266:LEU:HD23	1.70	0.73
5:Q:124:LEU:HD12	6:R:118:PHE:CG	2.24	0.73
5:Q:159:LEU:HD22	5:Q:194:TYR:HE1	1.50	0.72
4:F:28:THR:HG21	4:F:94:LYS:HZ1	1.54	0.72
5:T:166:PHE:CE1	6:U:174:SER:C	2.65	0.72
5:T:214:LYS:H	5:T:214:LYS:CD	2.00	0.72
1:G:27:LYS:NZ	1:G:32:ASP:OD1	2.23	0.72
1:C:221:PRO:CB	6:O:49:TYR:CD2	2.73	0.72
1:C:27:LYS:NZ	1:C:32:ASP:OD1	2.23	0.72
2:B:42:GLN:HB2	4:H:100(G):TYR:CD2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:190:LYS:NZ	6:R:190:LYS:C	2.48	0.71
6:U:190:LYS:NZ	6:U:190:LYS:C	2.48	0.71
1:A:131:ARG:HB2	1:A:155:SER:HB2	1.71	0.71
1:A:220:ARG:HG2	5:Q:96:THR:HG21	1.71	0.71
4:H:28:THR:HG21	4:H:94:LYS:HZ1	1.55	0.71
5:N:159:LEU:HD22	5:N:194:TYR:HE1	1.50	0.71
5:N:208:ASP:O	5:N:209:LYS:HD2	1.91	0.71
6:O:190:LYS:NZ	6:O:190:LYS:C	2.48	0.71
4:K:11:LEU:HD11	4:K:148:PHE:HE2	1.54	0.71
1:C:90:ARG:NH1	1:C:270:SER:O	2.24	0.71
1:C:131:ARG:HB2	1:C:155:SER:HB2	1.71	0.71
2:D:41:THR:CG2	4:F:100(G):TYR:CZ	2.74	0.71
5:T:208:ASP:O	5:T:209:LYS:HD2	1.91	0.71
1:C:104:ASN:OD1	2:D:72:GLU:HG3	1.90	0.71
5:Q:208:ASP:O	5:Q:209:LYS:HD2	1.91	0.71
1:A:27:LYS:NZ	1:A:32:ASP:OD1	2.23	0.71
1:A:90:ARG:NH1	1:A:270:SER:O	2.24	0.71
1:A:141:ARG:O	1:A:143:THR:HG22	1.91	0.71
1:C:141:ARG:O	1:C:143:THR:HG22	1.91	0.71
1:G:90:ARG:NH1	1:G:270:SER:O	2.24	0.71
1:A:106:GLU:CG	2:B:71:SER:HB2	2.09	0.70
1:C:311:HIS:NE2	2:D:97:GLU:OE1	2.24	0.70
1:G:141:ARG:O	1:G:143:THR:HG22	1.91	0.70
3:J:96:ARG:NH1	4:K:47:TRP:CD1	2.59	0.70
1:A:101:ARG:HG3	5:Q:100:GLY:HA3	1.73	0.70
2:B:41:THR:CB	4:H:100(G):TYR:CZ	2.75	0.70
1:C:261(G):ILE:CG2	5:T:65:SER:O	2.39	0.70
4:F:56:ALA:HA	4:F:57:THR:HG22	1.74	0.70
1:G:131:ARG:HB2	1:G:155:SER:HB2	1.72	0.70
1:G:222:LYS:O	6:U:53:ASN:HB3	1.92	0.70
6:R:190:LYS:HE2	6:R:210:ASN:HB3	1.73	0.70
1:A:221:PRO:HG2	6:R:49:TYR:CZ	2.26	0.70
6:U:190:LYS:HE2	6:U:210:ASN:HB3	1.73	0.70
6:U:190:LYS:C	6:U:190:LYS:HZ3	2.00	0.70
2:B:80:LEU:HG	2:D:80:LEU:HD21	1.74	0.70
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.24	0.69
3:E:164:THR:HG23	4:F:174:PHE:CD2	2.28	0.69
6:O:190:LYS:HE2	6:O:210:ASN:HB3	1.73	0.69
2:B:41:THR:CG2	4:H:100(G):TYR:CZ	2.75	0.69
4:F:11:LEU:HD11	4:F:148:PHE:HE2	1.54	0.69
1:A:136:THR:HG23	1:A:139:CYS:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HB2	6:R:49:TYR:CD2	2.27	0.69
1:C:136:THR:HG23	1:C:139:CYS:H	1.58	0.69
6:O:123:GLU:OE1	6:O:123:GLU:N	2.25	0.69
4:H:56:ALA:HA	4:H:57:THR:HG22	1.74	0.69
4:K:56:ALA:HA	4:K:57:THR:HG22	1.74	0.69
5:Q:212:GLU:OE2	5:Q:213:PRO:CD	2.41	0.68
5:T:212:GLU:OE2	5:T:213:PRO:CD	2.41	0.68
6:R:79:GLN:HG2	6:R:80:PRO:HD2	1.75	0.68
5:Q:214:LYS:H	5:Q:214:LYS:CD	2.00	0.68
5:T:167:PRO:HG2	6:U:163:VAL:O	1.94	0.68
1:A:261(F):GLY:HA2	5:N:59:TYR:HE2	1.59	0.68
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.24	0.68
5:N:212:GLU:OE2	5:N:213:PRO:CD	2.42	0.68
1:G:219:ALA:HB3	5:T:1:GLN:OE1	1.95	0.67
4:K:114:ALA:HB1	4:K:148:PHE:CD2	2.28	0.67
4:F:114:ALA:HB1	4:F:148:PHE:CD2	2.28	0.67
5:N:195:ILE:HG12	5:N:195:ILE:O	1.94	0.67
4:H:114:ALA:HB1	4:H:148:PHE:CD2	2.28	0.67
2:D:41:THR:HB	4:F:100(G):TYR:CE2	2.30	0.67
1:G:58:ALA:HB1	1:G:86:LEU:HD13	1.76	0.67
1:G:136:THR:HG23	1:G:139:CYS:H	1.58	0.67
1:A:51:ILE:HG23	1:A:282:PHE:CD1	2.29	0.67
1:G:219:ALA:CB	5:T:1:GLN:HE22	2.08	0.67
3:J:202:SER:HB3	6:R:173:TYR:OH	1.95	0.67
2:I:54:ARG:NH2	2:I:103:GLU:OE2	2.24	0.67
1:C:51:ILE:HG23	1:C:282:PHE:CD1	2.29	0.67
1:C:101:ARG:HH21	5:N:100:GLY:HA2	1.60	0.66
1:A:200:LYS:HA	1:A:248:ASN:ND2	2.11	0.66
1:G:51:ILE:HG23	1:G:282:PHE:CD1	2.30	0.66
1:G:200:LYS:HA	1:G:248:ASN:ND2	2.11	0.66
4:K:112:SER:OG	4:K:114:ALA:N	2.29	0.66
5:Q:60:ASN:O	5:Q:64:LYS:HG3	1.94	0.66
5:Q:195:ILE:HG12	5:Q:195:ILE:O	1.94	0.66
6:R:123:GLU:OE1	6:R:123:GLU:N	2.25	0.66
1:C:96:ILE:HD13	1:C:99:PRO:HA	1.78	0.66
1:A:33:ARG:NH1	3:J:2:ILE:HD12	2.11	0.66
5:Q:166:PHE:HE1	6:R:174:SER:C	2.04	0.66
1:A:96:ILE:HD13	1:A:99:PRO:HA	1.78	0.66
3:L:78:LEU:HD11	3:L:104:LEU:HD21	1.78	0.66
1:G:221:PRO:HB2	6:U:49:TYR:CD2	2.30	0.66
4:K:28:THR:HG21	4:K:94:LYS:HZ1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:195:ILE:HG12	5:T:195:ILE:O	1.94	0.66
1:C:101:ARG:HH21	5:N:100:GLY:C	2.04	0.66
2:D:41:THR:CG2	4:F:100(G):TYR:CE1	2.75	0.65
1:G:101:ARG:NH2	5:T:99:LEU:HD12	2.11	0.65
4:H:112:SER:OG	4:H:114:ALA:N	2.29	0.65
5:T:105:GLN:HG2	6:U:43:ALA:H	1.62	0.65
1:A:200:LYS:HA	1:A:248:ASN:HD21	1.61	0.65
1:C:200:LYS:HA	1:C:248:ASN:ND2	2.11	0.65
1:G:200:LYS:HA	1:G:248:ASN:HD21	1.61	0.65
1:A:180:TRP:CE2	1:A:233:HIS:HB2	2.32	0.65
4:F:11:LEU:HD11	4:F:148:PHE:CE2	2.32	0.65
1:G:96:ILE:HD13	1:G:99:PRO:HA	1.78	0.65
1:G:180:TRP:CE2	1:G:233:HIS:HB2	2.32	0.65
3:J:78:LEU:HD11	3:J:104:LEU:HD21	1.78	0.65
4:K:11:LEU:HD11	4:K:148:PHE:CE2	2.32	0.65
1:G:50:GLU:OE1	1:G:274:ILE:HG12	1.96	0.65
5:T:59:TYR:O	5:T:64:LYS:HD3	1.97	0.65
3:L:125:LEU:O	3:L:183:LYS:HD2	1.97	0.65
1:A:202:ILE:HG23	1:A:247:PHE:HB3	1.80	0.64
1:C:261:ARG:HH12	1:C:261(H):GLU:HG3	1.60	0.64
1:C:200:LYS:HA	1:C:248:ASN:HD21	1.61	0.64
4:F:112:SER:OG	4:F:114:ALA:N	2.29	0.64
5:Q:124:LEU:HB3	6:R:118:PHE:CZ	2.32	0.64
1:A:268:ILE:CB	1:A:284:PRO:O	2.35	0.64
1:G:101:ARG:HD3	5:T:100:GLY:N	2.12	0.64
3:J:125:LEU:O	3:J:183:LYS:HD2	1.97	0.64
4:K:28:THR:HG21	4:K:94:LYS:NZ	2.13	0.64
1:G:86:LEU:HD21	1:G:88:ILE:HG12	1.79	0.64
2:B:41:THR:HG21	4:H:100(G):TYR:CZ	2.32	0.64
3:E:96:ARG:NH1	4:F:47:TRP:CD1	2.66	0.64
5:N:159:LEU:HD22	5:N:194:TYR:CD1	2.33	0.64
5:Q:205:THR:O	5:Q:206:LYS:HD3	1.98	0.64
5:T:105:GLN:HA	6:U:43:ALA:HA	1.78	0.64
5:T:205:THR:O	5:T:206:LYS:HD3	1.98	0.64
1:C:180:TRP:CE2	1:C:233:HIS:HB2	2.32	0.64
3:E:125:LEU:O	3:E:183:LYS:HD2	1.97	0.64
1:C:202:ILE:HG23	1:C:247:PHE:HB3	1.80	0.63
2:B:41:THR:HB	4:H:100(G):TYR:CE2	2.33	0.63
3:E:78:LEU:HD11	3:E:104:LEU:HD21	1.78	0.63
1:G:261:ARG:HH12	1:G:261(H):GLU:HG3	1.60	0.63
5:Q:84:ALA:O	5:Q:87:THR:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:166:PHE:CE1	6:U:174:SER:HB2	2.33	0.63
6:R:190:LYS:C	6:R:190:LYS:HZ2	2.05	0.63
5:T:61:PRO:HA	5:T:64:LYS:CE	2.23	0.63
5:Q:159:LEU:HD22	5:Q:194:TYR:CD1	2.33	0.63
4:H:28:THR:HG21	4:H:94:LYS:NZ	2.13	0.63
4:F:28:THR:HG21	4:F:94:LYS:NZ	2.13	0.63
1:G:49:GLY:CA	1:G:272:ALA:HB3	2.23	0.63
6:R:18:ARG:HH21	6:R:76:ARG:NH2	1.97	0.63
5:T:84:ALA:O	5:T:87:THR:HG22	1.98	0.63
5:T:166:PHE:CZ	6:U:174:SER:HB2	2.33	0.63
6:U:18:ARG:HH21	6:U:76:ARG:NH2	1.97	0.63
6:U:123:GLU:OE1	6:U:123:GLU:N	2.25	0.63
1:A:261:ARG:HH12	1:A:261(H):GLU:HG3	1.60	0.62
1:C:173:LYS:CE	5:T:55:GLY:HA3	2.24	0.62
6:R:4:MET:HE3	6:R:23:CYS:SG	2.39	0.62
6:U:4:MET:HE3	6:U:23:CYS:SG	2.39	0.62
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.81	0.62
1:G:202:ILE:HG23	1:G:247:PHE:HB3	1.80	0.62
5:N:84:ALA:O	5:N:87:THR:HG22	1.98	0.62
5:T:159:LEU:HD22	5:T:194:TYR:CD1	2.33	0.62
5:Q:169:VAL:HG11	6:R:162:SER:HB2	1.77	0.62
3:J:199:GLN:HB3	6:R:10:SER:OG	1.99	0.62
6:O:4:MET:HE3	6:O:23:CYS:SG	2.39	0.62
2:I:56:ILE:HG13	4:K:100:ILE:HG12	1.82	0.62
6:O:18:ARG:HH21	6:O:76:ARG:NH2	1.97	0.62
1:C:58:ALA:HB2	1:C:86:LEU:HD23	1.82	0.62
6:R:190:LYS:NZ	6:R:210:ASN:HA	2.13	0.62
1:A:220:ARG:HG2	5:Q:96:THR:CG2	2.30	0.62
1:A:101:ARG:CG	5:Q:100:GLY:HA3	2.30	0.62
1:A:170:ASN:ND2	1:A:237:LEU:O	2.32	0.62
2:D:38:LEU:HD21	4:F:53:ASN:CB	2.30	0.62
1:A:120:LYS:HB2	1:A:256:ARG:HH21	1.65	0.61
4:K:13:GLN:HE22	4:K:113:SER:CB	2.13	0.61
3:J:37:GLN:HB2	3:J:47:LEU:HD11	1.81	0.61
5:Q:212:GLU:CG	5:Q:213:PRO:CD	2.76	0.61
5:T:105:GLN:HG2	6:U:43:ALA:N	2.14	0.61
1:A:106:GLU:HB3	2:B:71:SER:HB2	0.66	0.61
1:C:101:ARG:HH21	5:N:100:GLY:CA	2.13	0.61
1:G:101:ARG:HG2	1:G:101:ARG:HH11	1.64	0.61
5:T:60:ASN:O	5:T:64:LYS:HG3	2.00	0.61
3:E:37:GLN:HB2	3:E:47:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:LYS:HB2	1:G:256:ARG:HH21	1.65	0.61
1:G:170:ASN:ND2	1:G:237:LEU:O	2.32	0.61
1:A:71:ILE:CG2	1:A:151:MET:HE3	2.31	0.61
5:T:166:PHE:CE1	6:U:174:SER:CB	2.84	0.61
1:A:33:ARG:HH12	3:J:2:ILE:CD1	2.14	0.61
4:H:13:GLN:HE22	4:H:113:SER:CB	2.14	0.61
4:H:100(A):TYR:CE1	4:H:100(K):TYR:CE2	2.88	0.61
5:Q:60:ASN:C	5:Q:64:LYS:HG3	2.26	0.61
2:B:38:LEU:C	4:H:100(G):TYR:HE2	2.09	0.61
2:I:41:THR:HG21	4:K:100(G):TYR:CZ	2.36	0.61
6:O:190:LYS:C	6:O:190:LYS:HZ2	2.06	0.61
4:F:13:GLN:HE22	4:F:113:SER:CB	2.14	0.60
5:T:60:ASN:C	5:T:64:LYS:HG3	2.26	0.60
1:A:58:ALA:HB2	1:A:86:LEU:CD2	2.31	0.60
1:A:160:VAL:HA	1:A:196:GLY:HA3	1.83	0.60
1:C:71:ILE:CG2	1:C:151:MET:HE3	2.30	0.60
1:C:100:GLY:HA3	1:C:230:ILE:O	2.01	0.60
1:C:160:VAL:HA	1:C:196:GLY:HA3	1.83	0.60
1:G:15:LEU:CD1	2:I:118:LEU:HG	2.31	0.60
1:C:170:ASN:ND2	1:C:237:LEU:O	2.32	0.60
1:G:100:GLY:HA3	1:G:230:ILE:O	2.01	0.60
2:B:19:ASP:OD1	2:B:19:ASP:N	2.35	0.60
3:J:94:TRP:HZ3	4:K:59:TYR:O	1.84	0.60
1:A:261(D):PRO:O	1:A:261(E):SER:HB2	2.02	0.60
1:G:172:ARG:HD3	1:G:259:PHE:CZ	2.37	0.60
1:G:261(D):PRO:O	1:G:261(E):SER:HB2	2.02	0.60
1:A:33:ARG:HH22	3:J:2:ILE:HD11	1.57	0.60
1:C:261(D):PRO:O	1:C:261(E):SER:HB2	2.02	0.60
1:G:71:ILE:CG2	1:G:151:MET:HE3	2.31	0.60
1:A:100:GLY:HA3	1:A:230:ILE:O	2.01	0.60
1:C:172:ARG:HD3	1:C:259:PHE:CZ	2.37	0.60
3:J:96:ARG:HH12	4:K:47:TRP:CD1	2.19	0.60
6:O:190:LYS:NZ	6:O:210:ASN:HA	2.14	0.60
5:T:137:ALA:CB	6:U:116:PHE:CZ	2.85	0.60
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.37	0.60
1:A:221:PRO:HB2	6:R:49:TYR:CZ	2.34	0.60
1:C:120:LYS:HB2	1:C:256:ARG:HH21	1.65	0.60
2:D:38:LEU:HD23	4:F:53:ASN:HB3	1.82	0.60
1:G:130:ILE:HG23	1:G:155:SER:O	2.02	0.60
5:T:137:ALA:HB3	6:U:116:PHE:CZ	2.35	0.60
2:D:124:LYS:HD3	2:I:134:GLY:HA2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:CYS:O	1:G:224:ASN:ND2	2.35	0.60
1:G:261(G):ILE:CG2	5:Q:65:SER:O	2.49	0.60
2:I:19:ASP:OD1	2:I:19:ASP:N	2.34	0.60
3:L:124:GLN:HA	4:H:122:PHE:CE1	2.37	0.60
5:T:6:GLU:HG3	5:T:92:CYS:SG	2.42	0.60
4:H:114:ALA:HB1	4:H:148:PHE:CE2	2.36	0.59
1:A:130:ILE:HG23	1:A:155:SER:O	2.02	0.59
1:G:268:ILE:CG2	1:G:284:PRO:HA	2.31	0.59
5:Q:210:ARG:HG3	5:Q:210:ARG:HH11	1.67	0.59
2:B:38:LEU:CD2	4:H:53:ASN:CB	2.75	0.59
1:G:160:VAL:HA	1:G:196:GLY:HA3	1.83	0.59
5:N:212:GLU:CG	5:N:213:PRO:CD	2.76	0.59
1:A:221:PRO:CB	6:R:49:TYR:CZ	2.86	0.59
1:A:261(F):GLY:HA2	5:N:59:TYR:CE2	2.37	0.59
2:B:38:LEU:HA	4:H:100(G):TYR:CZ	2.36	0.59
2:D:41:THR:HB	4:F:100(G):TYR:CZ	2.37	0.59
1:A:52:CYS:O	1:A:56:LYS:HG2	2.03	0.59
3:L:96:ARG:NH1	4:H:47:TRP:CD1	2.71	0.59
1:G:219:ALA:HB1	5:T:1:GLN:HE22	1.66	0.59
1:C:50:GLU:OE1	1:C:274:ILE:HG12	2.03	0.59
5:N:18:LEU:HD13	5:N:109:VAL:HG11	1.85	0.59
5:Q:6:GLU:HG3	5:Q:92:CYS:SG	2.42	0.59
5:Q:143:LYS:HE3	6:R:131:SER:OG	2.01	0.59
1:A:70:ILE:HG21	1:A:179:VAL:HG21	1.85	0.59
1:A:97:CYS:O	1:A:224:ASN:ND2	2.34	0.59
3:E:105:GLU:CD	3:E:173:TYR:HH	2.11	0.59
5:N:6:GLU:HG3	5:N:92:CYS:SG	2.42	0.59
5:N:210:ARG:HG3	5:N:210:ARG:HH11	1.67	0.59
5:Q:18:LEU:HD13	5:Q:109:VAL:HG11	1.84	0.59
1:C:97:CYS:O	1:C:224:ASN:ND2	2.35	0.58
1:C:130:ILE:HG23	1:C:155:SER:O	2.02	0.58
1:G:15:LEU:HD12	2:I:118:LEU:HG	1.85	0.58
2:I:41:THR:HG21	4:K:100(G):TYR:CE1	2.38	0.58
1:C:261(G):ILE:HG22	5:T:65:SER:O	2.02	0.58
5:N:199:ASN:OD1	5:N:206:LYS:HG3	2.03	0.58
5:Q:153:SER:HB2	5:Q:197:ASN:HD21	1.67	0.58
5:T:210:ARG:HG3	5:T:210:ARG:HH11	1.67	0.58
1:C:101:ARG:HE	5:N:100:GLY:HA3	1.60	0.58
5:T:18:LEU:HD13	5:T:109:VAL:HG11	1.85	0.58
1:C:70:ILE:HG21	1:C:179:VAL:HG21	1.85	0.58
3:E:27:GLN:OE1	1:G:33:ARG:CZ	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ILE:HG21	1:G:179:VAL:HG21	1.85	0.58
6:O:143:GLU:O	6:O:198:HIS:HD2	1.87	0.58
6:R:143:GLU:O	6:R:198:HIS:HD2	1.87	0.58
5:T:214:LYS:HD3	5:T:214:LYS:N	2.10	0.58
6:U:143:GLU:O	6:U:198:HIS:HD2	1.87	0.58
1:G:261(E):SER:CB	5:Q:64:LYS:HE2	2.34	0.58
1:G:86:LEU:HD21	1:G:88:ILE:CG1	2.33	0.58
1:G:101:ARG:CZ	5:T:99:LEU:HB2	2.33	0.58
1:G:261(E):SER:HB3	5:Q:64:LYS:HB3	1.85	0.58
1:C:50:GLU:HG2	1:C:275:ASP:O	2.03	0.57
3:E:2:ILE:HD12	1:G:33:ARG:CZ	2.33	0.57
1:A:261(C):ALA:HB3	1:A:261(I):TYR:HB2	1.87	0.57
3:L:164:THR:HG23	4:H:174:PHE:CD2	2.39	0.57
6:U:190:LYS:NZ	6:U:210:ASN:HA	2.13	0.57
5:T:153:SER:HB2	5:T:197:ASN:HD21	1.67	0.57
4:H:114:ALA:CB	4:H:148:PHE:CD2	2.87	0.57
1:C:261(C):ALA:HB3	1:C:261(I):TYR:HB2	1.87	0.57
4:H:70:SER:HB3	4:H:79:TYR:HB2	1.86	0.57
4:F:70:SER:HB3	4:F:79:TYR:HB2	1.86	0.57
4:F:100(H):TYR:CE2	4:F:100(J):THR:HA	2.40	0.57
3:L:202:SER:OG	6:O:142:ARG:CB	2.53	0.57
3:J:202:SER:CB	6:R:173:TYR:OH	2.51	0.57
4:K:70:SER:HB3	4:K:79:TYR:HB2	1.86	0.57
5:T:124:LEU:CB	6:U:118:PHE:CE1	2.77	0.57
1:A:103:THR:HG22	1:A:233:HIS:HA	1.87	0.57
4:H:100(H):TYR:CE2	4:H:100(J):THR:HA	2.40	0.57
4:F:114:ALA:CB	4:F:148:PHE:CD2	2.86	0.57
5:N:152:VAL:HG22	5:N:198:VAL:HG22	1.87	0.56
1:A:206:SER:HB3	1:A:209:TYR:HB3	1.87	0.56
6:O:103:LYS:NZ	6:O:165:GLU:OE2	2.38	0.56
5:Q:100(A):TYR:C	6:R:32:PHE:CE2	2.83	0.56
5:T:61:PRO:CB	5:T:64:LYS:HE2	2.35	0.56
5:T:212:GLU:CG	5:T:213:PRO:CD	2.76	0.56
1:A:14:CYS:O	2:B:24:PHE:HA	2.05	0.56
5:T:105:GLN:HA	6:U:43:ALA:CA	2.35	0.56
1:A:221:PRO:CB	6:R:49:TYR:CD2	2.88	0.56
1:C:206:SER:HB3	1:C:209:TYR:HB3	1.87	0.56
1:C:261(G):ILE:O	1:C:261(G):ILE:HD12	2.06	0.56
1:G:261(G):ILE:HD12	1:G:261(G):ILE:O	2.06	0.56
3:J:105:GLU:CD	3:J:173:TYR:OH	2.49	0.56
1:C:52:CYS:C	1:C:56:LYS:HB2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2:ILE:HD12	1:G:33:ARG:NH1	2.20	0.56
3:E:94:TRP:HZ3	4:F:59:TYR:O	1.87	0.56
1:G:103:THR:HG22	1:G:233:HIS:HA	1.87	0.56
1:C:103:THR:HG22	1:C:233:HIS:HA	1.87	0.56
1:G:261(C):ALA:HB3	1:G:261(I):TYR:HB2	1.86	0.56
5:Q:142:VAL:HG22	5:Q:198:VAL:HG21	1.88	0.56
5:Q:152:VAL:HG22	5:Q:198:VAL:HG22	1.87	0.56
2:D:41:THR:CB	4:F:100(G):TYR:CZ	2.88	0.56
1:G:51:ILE:CD1	1:G:268:ILE:HD13	2.36	0.56
4:K:100(H):TYR:CE2	4:K:100(J):THR:HA	2.40	0.56
3:E:105:GLU:CD	3:E:173:TYR:OH	2.49	0.56
1:A:51:ILE:CD1	1:A:266:LEU:HD23	2.36	0.55
4:F:114:ALA:HB3	4:F:148:PHE:HE2	1.68	0.55
1:A:261(G):ILE:HG22	5:N:64:LYS:O	2.06	0.55
1:C:58:ALA:HB2	1:C:86:LEU:CD2	2.36	0.55
5:T:152:VAL:HG22	5:T:198:VAL:HG22	1.87	0.55
2:B:53:ASN:HB2	4:H:100(K):TYR:CZ	2.40	0.55
5:N:142:VAL:HG22	5:N:198:VAL:HG21	1.88	0.55
3:E:2:ILE:HD12	1:G:33:ARG:HH12	1.71	0.55
1:G:206:SER:HB3	1:G:209:TYR:HB3	1.87	0.55
4:F:4:LEU:HD23	4:F:94:LYS:HE2	1.89	0.55
1:G:268:ILE:HB	1:G:284:PRO:C	2.30	0.55
4:K:4:LEU:HD23	4:K:94:LYS:HE2	1.89	0.55
4:K:114:ALA:HB1	4:K:148:PHE:CE2	2.37	0.55
5:T:142:VAL:HG22	5:T:198:VAL:HG21	1.87	0.55
3:L:105:GLU:CD	3:L:173:TYR:OH	2.49	0.55
1:A:58:ALA:HB2	1:A:86:LEU:HD23	1.88	0.55
1:A:261(G):ILE:HD12	1:A:261(G):ILE:O	2.06	0.55
1:A:52:CYS:O	1:A:282:PHE:CE1	2.60	0.54
1:C:156:SER:O	1:C:157:SER:OG	2.23	0.54
1:G:52:CYS:O	1:G:282:PHE:CE1	2.60	0.54
6:U:103:LYS:NZ	6:U:165:GLU:OE2	2.38	0.54
4:H:4:LEU:HD23	4:H:94:LYS:HE2	1.89	0.54
4:F:87:THR:HG23	4:F:110:THR:HA	1.90	0.54
1:A:204:VAL:O	1:A:210:GLN:HA	2.08	0.54
2:D:38:LEU:O	4:F:100(G):TYR:HE2	1.89	0.54
1:G:67:LEU:N	1:G:95:ASP:OD1	2.41	0.54
1:G:139:CYS:HB2	1:G:146:SER:O	2.07	0.54
6:R:121:SER:O	6:R:125:LEU:HD13	2.08	0.54
1:C:52:CYS:O	1:C:282:PHE:CE1	2.60	0.54
5:N:153:SER:HB2	5:N:197:ASN:HD21	1.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:121:SER:O	6:O:125:LEU:HD13	2.08	0.54
5:T:166:PHE:HE1	6:U:174:SER:O	1.90	0.54
1:A:139:CYS:HB2	1:A:146:SER:O	2.07	0.54
1:C:204:VAL:O	1:C:210:GLN:HA	2.08	0.54
1:G:204:VAL:O	1:G:210:GLN:HA	2.08	0.54
5:T:164:HIS:NE2	6:U:138:ASN:OD1	2.41	0.54
3:L:202:SER:OG	6:O:142:ARG:HB2	2.07	0.54
2:D:19:ASP:OD1	2:D:19:ASP:N	2.35	0.54
3:E:164:THR:HG23	4:F:174:PHE:CE2	2.42	0.54
4:H:87:THR:HG23	4:H:110:THR:HA	1.89	0.53
1:C:221:PRO:HG2	6:O:49:TYR:CE1	2.42	0.53
1:A:14:CYS:N	2:B:25:ARG:O	2.28	0.53
2:D:38:LEU:HA	4:F:100(G):TYR:CE2	2.43	0.53
5:Q:166:PHE:HZ	6:R:174:SER:HB3	1.73	0.53
1:C:51:ILE:CG1	1:C:86:LEU:HD13	2.38	0.53
1:C:139:CYS:HB2	1:C:146:SER:O	2.07	0.53
5:Q:163:VAL:HG22	5:Q:182:VAL:CG1	2.38	0.53
1:C:61:LEU:HB3	1:C:64:CYS:HB3	1.90	0.53
4:F:187:LEU:C	4:F:187:LEU:HD12	2.34	0.53
1:G:156:SER:O	1:G:157:SER:OG	2.23	0.53
2:I:42:GLN:NE2	4:K:100(H):TYR:O	2.42	0.53
5:N:163:VAL:HG22	5:N:182:VAL:CG1	2.38	0.53
5:T:208:ASP:C	5:T:209:LYS:HD2	2.33	0.53
6:U:121:SER:O	6:U:125:LEU:HD13	2.08	0.53
1:A:61:LEU:HB3	1:A:64:CYS:HB3	1.89	0.53
1:A:120:LYS:HB2	1:A:256:ARG:NH2	2.24	0.53
3:L:48:ILE:HA	3:L:54:ARG:HA	1.91	0.53
3:E:48:ILE:HA	3:E:54:ARG:HA	1.91	0.53
1:G:61:LEU:HB3	1:G:64:CYS:HB3	1.89	0.53
5:Q:208:ASP:C	5:Q:209:LYS:HD2	2.32	0.53
3:E:30:ARG:H	3:E:91:TYR:HE1	1.57	0.53
1:G:222:LYS:CE	1:G:225:GLY:HA2	2.39	0.53
2:I:42:GLN:OE1	4:K:100(G):TYR:CD2	2.62	0.53
4:K:112:SER:OG	4:K:113:SER:N	2.42	0.53
5:N:208:ASP:C	5:N:209:LYS:HD2	2.32	0.53
4:H:112:SER:OG	4:H:113:SER:N	2.42	0.53
4:H:187:LEU:C	4:H:187:LEU:HD12	2.34	0.53
3:J:105:GLU:CD	3:J:173:TYR:HH	2.17	0.53
6:R:103:LYS:NZ	6:R:165:GLU:OE2	2.38	0.53
3:L:164:THR:HG23	4:H:174:PHE:CE2	2.44	0.53
1:C:88:ILE:HD12	1:C:274:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:LEU:HD21	4:K:53:ASN:HB3	1.90	0.53
4:K:87:THR:HG23	4:K:110:THR:HA	1.90	0.53
5:Q:59:TYR:O	5:Q:64:LYS:HD2	2.09	0.53
5:T:199:ASN:CG	5:T:206:LYS:HD2	2.34	0.53
1:A:67:LEU:N	1:A:95:ASP:OD1	2.41	0.53
3:L:124:GLN:CA	4:H:122:PHE:CE1	2.92	0.53
4:F:51:ILE:HG23	4:F:71:ARG:HH21	1.74	0.53
5:Q:210:ARG:HG3	5:Q:210:ARG:NH1	2.24	0.53
1:C:120:LYS:HB2	1:C:256:ARG:NH2	2.24	0.53
1:G:173:LYS:HE2	5:Q:55:GLY:HA3	1.90	0.53
4:K:187:LEU:C	4:K:187:LEU:HD12	2.34	0.53
5:Q:199:ASN:CG	5:Q:206:LYS:HD2	2.34	0.53
5:T:163:VAL:HG22	5:T:182:VAL:CG1	2.38	0.53
4:H:51:ILE:HG23	4:H:71:ARG:HH21	1.74	0.52
1:G:88:ILE:HD12	1:G:274:ILE:HD11	1.90	0.52
3:J:48:ILE:HA	3:J:54:ARG:HA	1.91	0.52
5:T:163:VAL:HG22	5:T:182:VAL:HG12	1.92	0.52
5:T:210:ARG:HG3	5:T:210:ARG:NH1	2.24	0.52
3:L:96:ARG:HH12	4:H:47:TRP:CD1	2.27	0.52
5:N:210:ARG:HG3	5:N:210:ARG:NH1	2.24	0.52
5:T:154:TRP:O	5:T:155:ASN:C	2.52	0.52
5:T:159:LEU:CD2	5:T:194:TYR:CE1	2.90	0.52
1:A:221:PRO:CG	6:R:49:TYR:CZ	2.92	0.52
1:G:120:LYS:HB2	1:G:256:ARG:NH2	2.24	0.52
1:C:192:ASN:HA	1:C:196:GLY:O	2.10	0.52
4:F:112:SER:OG	4:F:113:SER:N	2.42	0.52
3:L:124:GLN:HG3	4:H:122:PHE:CZ	2.45	0.52
1:A:91:ARG:NH2	1:A:271:ASP:OD2	2.43	0.52
1:A:113:ARG:HB3	1:A:267:GLY:HA3	1.92	0.52
1:G:91:ARG:NH2	1:G:271:ASP:OD2	2.43	0.52
4:K:51:ILE:HG23	4:K:71:ARG:HH21	1.74	0.52
6:U:190:LYS:HZ1	6:U:210:ASN:CA	2.13	0.52
1:A:192:ASN:HA	1:A:196:GLY:O	2.10	0.52
1:C:261(G):ILE:HG21	5:T:65:SER:O	2.10	0.52
1:G:219:ALA:CB	5:T:1:GLN:NE2	2.72	0.52
5:N:47:TRP:CH2	5:N:49:GLY:HA2	2.44	0.52
5:T:47:TRP:CH2	5:T:49:GLY:HA2	2.44	0.52
2:B:170:ARG:HH21	2:I:128:GLU:CD	2.18	0.52
4:F:100(H):TYR:HE2	4:F:100(J):THR:HA	1.75	0.52
5:N:163:VAL:HG22	5:N:182:VAL:HG12	1.92	0.52
1:A:88:ILE:HD12	1:A:274:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:30:ARG:H	3:L:91:TYR:HE1	1.57	0.52
1:G:50:GLU:OE1	1:G:50:GLU:HA	2.09	0.52
3:J:39:LYS:HG3	3:J:84:ALA:HB2	1.92	0.52
4:K:115:SER:O	4:K:116:THR:C	2.52	0.52
5:Q:47:TRP:CH2	5:Q:49:GLY:HA2	2.44	0.52
1:C:91:ARG:NH2	1:C:271:ASP:OD2	2.43	0.51
4:K:100(H):TYR:HE2	4:K:100(J):THR:HA	1.75	0.51
1:A:268:ILE:CG2	1:A:284:PRO:HA	2.28	0.51
5:T:47:TRP:CD2	6:U:96:PRO:HD2	2.45	0.51
5:T:47:TRP:CE3	6:U:96:PRO:HD2	2.45	0.51
4:H:136:GLY:HA2	6:O:156:SER:HB3	1.92	0.51
1:C:222:LYS:CE	1:C:225:GLY:HA2	2.39	0.51
1:A:261(G):ILE:CG2	5:N:64:LYS:O	2.59	0.51
3:J:30:ARG:H	3:J:91:TYR:HE1	1.57	0.51
5:Q:163:VAL:HG22	5:Q:182:VAL:HG12	1.92	0.51
1:C:221:PRO:CG	6:O:49:TYR:CZ	2.92	0.51
1:G:113:ARG:HB3	1:G:267:GLY:HA3	1.92	0.51
1:G:192:ASN:HA	1:G:196:GLY:O	2.10	0.51
5:N:154:TRP:CH2	5:N:196:CYS:HB3	2.46	0.51
6:R:18:ARG:HE	6:R:76:ARG:NH1	2.09	0.51
1:A:181:GLY:HA3	1:A:252:ILE:HB	1.93	0.51
4:H:115:SER:O	4:H:116:THR:C	2.53	0.51
4:F:13:GLN:OE1	4:F:113:SER:HA	2.11	0.51
5:Q:154:TRP:O	5:Q:155:ASN:CB	2.35	0.51
5:T:154:TRP:CH2	5:T:196:CYS:HB3	2.46	0.51
1:A:48:ILE:HD12	1:A:50:GLU:OE1	2.11	0.51
3:E:39:LYS:HG3	3:E:84:ALA:HB2	1.93	0.51
3:J:54:ARG:HB2	3:J:58:ILE:HD11	1.93	0.51
1:C:113:ARG:HB3	1:C:267:GLY:HA3	1.92	0.51
3:E:2:ILE:CD1	1:G:33:ARG:HH12	2.24	0.51
3:E:199:GLN:CD	6:U:10:SER:OG	2.54	0.51
4:F:115:SER:O	4:F:116:THR:C	2.52	0.51
3:L:94:TRP:HZ3	4:H:59:TYR:O	1.93	0.50
2:I:38:LEU:CD2	4:K:53:ASN:HB3	2.41	0.50
4:K:13:GLN:OE1	4:K:113:SER:HA	2.11	0.50
6:O:18:ARG:HE	6:O:76:ARG:NH1	2.09	0.50
5:Q:154:TRP:O	5:Q:155:ASN:C	2.52	0.50
5:Q:154:TRP:CH2	5:Q:196:CYS:HB3	2.46	0.50
4:H:13:GLN:OE1	4:H:113:SER:HA	2.11	0.50
1:G:139:CYS:O	1:G:146:SER:HB3	2.11	0.50
6:U:18:ARG:HE	6:U:76:ARG:NH1	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:CYS:O	1:C:56:LYS:HG2	2.10	0.50
1:G:106:GLU:HB3	2:I:71:SER:OG	2.09	0.50
3:L:213:GLU:O	3:L:214:CYS:SG	2.70	0.50
4:H:100(A):TYR:CD1	4:H:100(K):TYR:CE2	2.98	0.50
2:D:38:LEU:HA	4:F:100(G):TYR:OH	2.12	0.50
3:E:213:GLU:O	3:E:214:CYS:SG	2.70	0.50
6:R:143:GLU:O	6:R:198:HIS:CD2	2.65	0.50
6:U:186:TYR:O	6:U:192:TYR:OH	2.30	0.50
3:L:39:LYS:HG3	3:L:84:ALA:HB2	1.92	0.50
1:C:139:CYS:O	1:C:146:SER:HB3	2.11	0.50
6:O:186:TYR:O	6:O:192:TYR:OH	2.30	0.50
1:A:139:CYS:O	1:A:146:SER:HB3	2.11	0.50
1:G:101:ARG:NE	5:T:99:LEU:HB2	2.27	0.50
4:H:100(H):TYR:HE2	4:H:100(J):THR:HA	1.75	0.50
4:H:136:GLY:HA3	6:O:156:SER:HB2	1.94	0.50
4:F:114:ALA:CB	4:F:148:PHE:CZ	2.95	0.50
4:F:59:TYR:CE1	4:F:69:ILE:HD13	2.47	0.50
4:K:59:TYR:CE1	4:K:69:ILE:HD13	2.47	0.50
3:L:199:GLN:HG3	6:O:10:SER:OG	2.11	0.49
1:G:14:CYS:O	2:I:24:PHE:HA	2.11	0.49
1:G:181:GLY:HA3	1:G:252:ILE:HB	1.93	0.49
6:O:143:GLU:O	6:O:198:HIS:CD2	2.65	0.49
3:L:54:ARG:HB2	3:L:58:ILE:HD11	1.93	0.49
4:H:213:LYS:N	4:H:214:PRO:CD	2.76	0.49
1:C:67:LEU:N	1:C:95:ASP:OD1	2.41	0.49
4:K:13:GLN:HE22	4:K:113:SER:HB2	1.77	0.49
6:R:186:TYR:O	6:R:192:TYR:OH	2.30	0.49
3:E:95:LEU:HG	4:F:47:TRP:HZ3	1.77	0.49
4:K:213:LYS:N	4:K:214:PRO:CD	2.75	0.49
5:N:154:TRP:O	5:N:155:ASN:C	2.52	0.49
5:Q:171:GLN:HA	6:R:160:GLN:OE1	2.12	0.49
6:U:143:GLU:O	6:U:198:HIS:CD2	2.65	0.49
3:E:96:ARG:NH1	4:F:47:TRP:NE1	2.60	0.49
3:J:213:GLU:O	3:J:214:CYS:SG	2.69	0.49
1:A:153:TRP:HZ2	1:A:183:HIS:CE1	2.31	0.49
1:C:181:GLY:HA3	1:C:252:ILE:HB	1.93	0.49
3:E:54:ARG:HB2	3:E:58:ILE:HD11	1.93	0.49
4:H:13:GLN:HE22	4:H:113:SER:HB2	1.77	0.49
1:C:167:THR:HG22	1:C:244:THR:OG1	2.13	0.49
6:U:103:LYS:CE	6:U:165:GLU:OE2	2.61	0.49
2:B:41:THR:HB	4:H:100(G):TYR:OH	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:LEU:HD12	3:L:51:ALA:HA	1.95	0.49
3:L:124:GLN:HG3	4:H:122:PHE:CE2	2.48	0.49
4:F:213:LYS:N	4:F:214:PRO:CD	2.76	0.49
6:R:103:LYS:CE	6:R:165:GLU:OE2	2.61	0.49
1:A:167:THR:HG22	1:A:244:THR:OG1	2.13	0.49
4:H:59:TYR:CE1	4:H:69:ILE:HD13	2.47	0.49
1:C:153:TRP:HZ2	1:C:183:HIS:CE1	2.31	0.49
4:K:114:ALA:CB	4:K:148:PHE:CZ	2.95	0.49
1:A:222:LYS:CE	1:A:225:GLY:HA2	2.39	0.49
1:A:51:ILE:HB	1:A:86:LEU:CD2	2.32	0.48
1:G:51:ILE:HD13	1:G:266:LEU:HD23	1.94	0.48
1:G:167:THR:HG22	1:G:244:THR:OG1	2.13	0.48
1:G:324:PRO:O	1:G:325:GLU:HB2	2.13	0.48
4:H:147:TYR:CE2	4:H:152:VAL:HG13	2.48	0.48
5:Q:200:HIS:HB3	5:Q:205:THR:OG1	2.13	0.48
1:A:261(E):SER:O	5:N:59:TYR:HD2	1.92	0.48
4:F:147:TYR:CE2	4:F:152:VAL:HG13	2.48	0.48
3:J:96:ARG:NH1	4:K:100(N):MET:HE1	2.27	0.48
5:N:200:HIS:HB3	5:N:205:THR:OG1	2.13	0.48
5:N:212:GLU:CD	5:N:213:PRO:CD	2.86	0.48
6:O:103:LYS:CE	6:O:165:GLU:OE2	2.61	0.48
5:N:50:TYR:CE2	5:N:58:ASN:HB3	2.49	0.48
1:A:117:GLY:C	1:A:261:ARG:HG3	2.39	0.48
3:E:33:LEU:HD12	3:E:51:ALA:HA	1.94	0.48
4:F:13:GLN:HE22	4:F:113:SER:HB2	1.77	0.48
5:Q:43:LYS:HE2	5:Q:43:LYS:HB3	1.57	0.48
5:T:212:GLU:CD	5:T:213:PRO:CD	2.86	0.48
1:A:33:ARG:NH1	3:J:2:ILE:CD1	2.75	0.48
1:G:51:ILE:HG23	1:G:282:PHE:HD1	1.79	0.48
1:G:67:LEU:HB2	1:G:95:ASP:OD1	2.14	0.48
1:G:153:TRP:HZ2	1:G:183:HIS:CE1	2.31	0.48
5:Q:212:GLU:CD	5:Q:213:PRO:CD	2.86	0.48
5:T:166:PHE:HD1	6:U:164:THR:HG23	1.62	0.48
1:A:70:ILE:HD11	1:A:112:ILE:HG13	1.96	0.48
1:C:101:ARG:NH2	5:N:100:GLY:CA	2.68	0.48
5:N:126:PRO:HG3	5:N:189:LEU:HD22	1.96	0.48
2:B:38:LEU:HA	4:H:100(G):TYR:CE2	2.49	0.48
1:C:67:LEU:HB2	1:C:95:ASP:OD1	2.14	0.48
1:C:70:ILE:HD11	1:C:112:ILE:HG13	1.95	0.48
4:K:37:VAL:HG22	4:K:47:TRP:HA	1.96	0.48
5:T:126:PRO:HG3	5:T:189:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:200:HIS:HB3	5:T:205:THR:OG1	2.13	0.48
1:A:51:ILE:HD12	1:A:86:LEU:HD13	1.95	0.48
1:G:101:ARG:HH21	5:T:99:LEU:HD12	1.78	0.48
2:I:42:GLN:OE1	4:K:100(G):TYR:HD2	1.96	0.48
1:C:50:GLU:CD	1:C:274:ILE:HG23	2.39	0.47
1:A:324:PRO:O	1:A:325:GLU:HB2	2.13	0.47
1:C:117:GLY:C	1:C:261:ARG:HG3	2.39	0.47
1:G:300:ILE:HD11	2:I:69:GLU:HG3	1.96	0.47
5:Q:166:PHE:CE1	6:R:164:THR:CG2	2.91	0.47
5:Q:169:VAL:HG13	6:R:162:SER:CB	2.35	0.47
1:A:33:ARG:HH12	3:J:2:ILE:HD12	1.74	0.47
1:A:52:CYS:C	1:A:56:LYS:HG2	2.40	0.47
3:L:95:LEU:HD11	4:H:61:ASP:H	1.79	0.47
2:D:38:LEU:O	4:F:100(G):TYR:CE2	2.68	0.47
3:E:96:ARG:HH12	4:F:47:TRP:CD1	2.30	0.47
5:Q:166:PHE:HA	6:R:164:THR:HG22	1.96	0.47
5:T:50:TYR:CE2	5:T:58:ASN:HB3	2.49	0.47
5:T:91:PHE:CE1	6:U:44:PRO:HD3	2.49	0.47
1:C:161:PHE:HB3	1:C:248:ASN:O	2.15	0.47
2:D:38:LEU:HA	4:F:100(G):TYR:HE2	1.79	0.47
2:D:159:HIS:CE1	2:D:160:ASN:OD1	2.67	0.47
5:N:212:GLU:CD	5:N:213:PRO:HD2	2.40	0.47
1:A:67:LEU:HG	1:A:109:ARG:HG2	1.97	0.47
1:A:101:ARG:CG	5:Q:100:GLY:CA	2.82	0.47
4:H:100(A):TYR:CD1	4:H:100(K):TYR:HE2	2.31	0.47
1:G:51:ILE:HB	1:G:86:LEU:HD12	1.94	0.47
3:J:199:GLN:CB	6:R:10:SER:OG	2.62	0.47
5:Q:61:PRO:HA	5:Q:64:LYS:HD3	1.95	0.47
1:A:222:LYS:O	6:R:53:ASN:HB3	2.13	0.47
1:C:51:ILE:HD12	1:C:86:LEU:HB2	1.96	0.47
1:C:161:PHE:HA	1:C:162:PRO:HD3	1.74	0.47
1:G:161:PHE:HB3	1:G:248:ASN:O	2.15	0.47
5:T:124:LEU:C	6:U:118:PHE:CE1	2.93	0.47
1:A:51:ILE:CB	1:A:86:LEU:HD22	2.32	0.47
1:A:67:LEU:HB2	1:A:95:ASP:OD1	2.14	0.47
1:A:182:VAL:HG22	1:A:202:ILE:HD12	1.97	0.47
2:B:53:ASN:OD1	2:B:53:ASN:O	2.33	0.47
4:H:100(J):THR:HG23	4:H:100(K):TYR:CZ	2.49	0.47
4:H:114:ALA:HB3	4:H:148:PHE:HE2	1.68	0.47
1:C:324:PRO:O	1:C:325:GLU:HB2	2.13	0.47
1:G:70:ILE:HD11	1:G:112:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:GLY:C	1:G:261:ARG:HG3	2.39	0.47
2:I:159:HIS:CE1	2:I:160:ASN:OD1	2.67	0.47
4:K:147:TYR:CE2	4:K:152:VAL:HG13	2.48	0.47
5:T:137:ALA:HB3	6:U:116:PHE:CE1	2.50	0.47
5:T:212:GLU:CD	5:T:213:PRO:HD2	2.40	0.47
4:H:14:PRO:HD3	4:H:112:SER:C	2.40	0.47
4:H:37:VAL:HG22	4:H:47:TRP:HA	1.96	0.47
3:J:33:LEU:HD12	3:J:51:ALA:HA	1.95	0.47
5:Q:50:TYR:CE2	5:Q:58:ASN:HB3	2.49	0.47
5:Q:124:LEU:HD12	6:R:118:PHE:CD2	2.50	0.47
3:J:199:GLN:CG	6:R:10:SER:OG	2.63	0.47
5:Q:159:LEU:CD2	5:Q:194:TYR:CE1	2.90	0.47
2:B:159:HIS:CE1	2:B:160:ASN:OD1	2.68	0.46
4:H:114:ALA:CB	4:H:148:PHE:CZ	2.95	0.46
5:Q:212:GLU:CD	5:Q:213:PRO:HD2	2.39	0.46
1:C:223:VAL:HG22	6:O:53:ASN:ND2	2.29	0.46
1:G:67:LEU:HG	1:G:109:ARG:HG2	1.97	0.46
4:K:14:PRO:HD3	4:K:112:SER:C	2.40	0.46
5:T:170:LEU:O	6:U:160:GLN:NE2	2.46	0.46
1:A:180:TRP:NE1	1:A:233:HIS:HB2	2.31	0.46
4:F:14:PRO:HD3	4:F:112:SER:C	2.40	0.46
5:N:154:TRP:O	5:N:155:ASN:CB	2.35	0.46
1:G:177:LEU:HB3	1:G:258:THR:HB	1.98	0.46
5:N:159:LEU:CD2	5:N:194:TYR:CE1	2.90	0.46
5:T:137:ALA:HB2	6:U:116:PHE:CZ	2.49	0.46
1:C:62:GLY:HA2	1:C:90:ARG:HG3	1.98	0.46
1:C:177:LEU:HB3	1:C:258:THR:HB	1.98	0.46
6:O:67:SER:HA	6:O:71:PHE:CE2	2.51	0.46
5:Q:126:PRO:HG3	5:Q:189:LEU:HD22	1.96	0.46
6:U:190:LYS:C	6:U:190:LYS:HZ2	2.21	0.46
1:A:161:PHE:HB3	1:A:248:ASN:O	2.15	0.46
3:L:121:SER:HB3	4:H:123:PRO:HD2	1.96	0.46
4:H:39:GLN:HB2	4:H:45:LEU:HD13	1.98	0.46
1:C:67:LEU:HG	1:C:109:ARG:HG2	1.97	0.46
1:G:158(A):ASN:OD1	1:G:193:LYS:HE2	2.16	0.46
5:T:59:TYR:CB	5:T:64:LYS:HG2	2.37	0.46
3:L:105:GLU:CD	3:L:173:TYR:HH	2.22	0.46
4:F:37:VAL:HG22	4:F:47:TRP:HA	1.96	0.46
1:G:17:HIS:HA	2:I:21:TRP:O	2.16	0.46
4:F:145:LYS:HE3	4:F:179:GLN:OE1	2.16	0.46
1:G:51:ILE:HD12	1:G:86:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:GLY:HA2	1:G:90:ARG:HG3	1.98	0.46
2:B:53:ASN:HB2	4:H:100(K):TYR:OH	2.15	0.46
3:L:91:TYR:HB2	3:L:92:ASN:HB3	1.98	0.46
1:G:182:VAL:HG22	1:G:202:ILE:HD12	1.97	0.46
4:H:145:LYS:HE3	4:H:179:GLN:OE1	2.16	0.46
3:E:95:LEU:HD11	4:F:61:ASP:H	1.81	0.46
2:B:38:LEU:HD22	4:H:53:ASN:HB3	1.93	0.45
1:C:182:VAL:HG22	1:C:202:ILE:HD12	1.97	0.45
1:G:13:LEU:CD2	2:I:152:ILE:HG21	2.45	0.45
5:Q:166:PHE:CZ	6:R:174:SER:HB3	2.51	0.45
5:T:166:PHE:HZ	6:U:174:SER:CB	2.13	0.45
1:A:158(A):ASN:OD1	1:A:193:LYS:HE2	2.16	0.45
1:A:177:LEU:HB3	1:A:258:THR:HB	1.98	0.45
1:A:300:ILE:HD11	2:B:69:GLU:HG3	1.98	0.45
1:G:108:LEU:HD13	1:G:234:TRP:CE3	2.52	0.45
1:A:56:LYS:HD3	1:A:56:LYS:HA	1.76	0.45
1:C:180:TRP:NE1	1:C:233:HIS:HB2	2.31	0.45
1:C:200:LYS:HD3	1:C:248:ASN:ND2	2.31	0.45
1:G:13:LEU:HD22	2:I:152:ILE:HG21	1.98	0.45
1:G:123:MET:HE3	1:G:168:TYR:CD2	2.52	0.45
1:G:166:GLN:HB2	1:G:245:PHE:HB2	1.98	0.45
1:G:219:ALA:CB	5:T:1:GLN:OE1	2.64	0.45
3:J:91:TYR:HB2	3:J:92:ASN:HB3	1.98	0.45
1:A:200:LYS:HA	1:A:200:LYS:HD3	1.78	0.45
1:C:123:MET:HE3	1:C:168:TYR:CD2	2.52	0.45
1:C:157:SER:O	1:C:158:MET:HG3	2.17	0.45
1:C:173:LYS:HD2	1:C:173:LYS:N	2.32	0.45
3:E:91:TYR:HB2	3:E:92:ASN:HB3	1.98	0.45
1:G:52:CYS:O	1:G:282:PHE:HE1	2.00	0.45
1:G:157:SER:O	1:G:158:MET:HG3	2.17	0.45
1:G:200:LYS:HD3	1:G:248:ASN:ND2	2.31	0.45
1:C:108:LEU:HD13	1:C:234:TRP:CE3	2.52	0.45
1:C:166:GLN:HB2	1:C:245:PHE:HB2	1.99	0.45
5:N:214:LYS:CD	5:N:214:LYS:N	2.75	0.45
5:T:91:PHE:CE1	6:U:44:PRO:CD	2.99	0.45
6:U:67:SER:HA	6:U:71:PHE:CE2	2.51	0.45
1:A:33:ARG:HH11	3:J:93:HIS:HB2	1.81	0.45
1:A:51:ILE:O	1:A:86:LEU:HD22	2.17	0.45
1:A:200:LYS:HD3	1:A:248:ASN:ND2	2.31	0.45
3:E:12:SER:HA	3:E:105:GLU:HB2	1.99	0.45
3:E:95:LEU:HA	4:F:47:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:TRP:NE1	1:G:233:HIS:HB2	2.31	0.45
1:A:131:ARG:CG	1:A:157:SER:HA	2.41	0.45
1:A:157:SER:O	1:A:158:MET:HG3	2.17	0.45
1:A:261(D):PRO:O	5:N:57:THR:O	2.35	0.45
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.98	0.45
6:R:67:SER:HA	6:R:71:PHE:CE2	2.51	0.45
1:A:108:LEU:HD13	1:A:234:TRP:CE3	2.52	0.45
1:C:158(A):ASN:OD1	1:C:193:LYS:HE2	2.16	0.45
4:K:39:GLN:HB2	4:K:45:LEU:HD13	1.98	0.45
5:Q:166:PHE:CZ	6:R:174:SER:CB	3.00	0.45
1:A:48:ILE:H	1:A:48:ILE:HG13	1.55	0.45
2:B:173:ILE:HA	2:I:164:ASP:OD1	2.17	0.45
3:L:124:GLN:HB2	4:H:122:PHE:CD1	2.52	0.45
4:F:30:ARG:NH2	4:F:71:ARG:HG3	2.32	0.45
3:J:164:THR:HG23	4:K:174:PHE:CE2	2.52	0.45
5:Q:100(A):TYR:C	6:R:32:PHE:HE2	2.24	0.45
5:Q:105:GLN:HG2	6:R:43:ALA:N	2.32	0.45
1:C:108:LEU:HD13	1:C:234:TRP:CD2	2.52	0.44
1:A:58:ALA:CB	1:A:86:LEU:HG	2.47	0.44
1:A:108:LEU:HD13	1:A:234:TRP:CD2	2.52	0.44
1:A:123:MET:HE3	1:A:168:TYR:CD2	2.52	0.44
1:A:172:ARG:HD3	1:A:259:PHE:CE2	2.52	0.44
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.98	0.44
4:K:145:LYS:HE3	4:K:179:GLN:OE1	2.16	0.44
5:Q:214:LYS:CD	5:Q:214:LYS:N	2.75	0.44
1:C:52:CYS:O	1:C:282:PHE:HE1	2.00	0.44
1:C:223:VAL:O	1:C:224:ASN:HB2	2.17	0.44
2:D:38:LEU:CA	4:F:100(G):TYR:HE2	2.30	0.44
1:G:223:VAL:O	1:G:224:ASN:HB2	2.18	0.44
3:L:12:SER:HA	3:L:105:GLU:HB2	1.99	0.44
4:F:39:GLN:HB2	4:F:45:LEU:HD13	1.98	0.44
1:A:62:GLY:HA2	1:A:90:ARG:HG3	1.98	0.44
1:A:130:ILE:HG22	1:A:131:ARG:O	2.18	0.44
3:L:199:GLN:CG	6:O:10:SER:OG	2.66	0.44
4:H:30:ARG:NH2	4:H:71:ARG:HG3	2.32	0.44
1:G:130:ILE:HG22	1:G:131:ARG:O	2.18	0.44
1:G:172:ARG:HD3	1:G:259:PHE:CE2	2.52	0.44
1:G:54:LYS:HD2	1:G:276(A):SER:O	2.18	0.44
6:R:123:GLU:H	6:R:123:GLU:CD	2.21	0.44
1:A:221:PRO:HG2	6:R:49:TYR:CE1	2.52	0.44
1:A:223:VAL:O	1:A:224:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:100(N):MET:H	4:H:100(N):MET:HG2	1.60	0.44
1:C:54:LYS:HD2	1:C:276(A):SER:O	2.18	0.44
1:C:172:ARG:HD3	1:C:259:PHE:CE2	2.52	0.44
1:G:173:LYS:HD2	1:G:173:LYS:N	2.32	0.44
1:G:221:PRO:CB	6:U:49:TYR:CD2	3.01	0.44
5:T:123:PRO:HB3	5:T:211:VAL:HG13	2.00	0.44
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.98	0.44
1:A:166:GLN:HB2	1:A:245:PHE:HB2	1.99	0.44
2:B:53:ASN:ND2	4:H:100(K):TYR:CE1	2.79	0.44
4:H:100(J):THR:HG23	4:H:100(K):TYR:CD1	2.52	0.44
1:G:221:PRO:HG2	6:U:49:TYR:CZ	2.52	0.44
5:Q:167:PRO:HG2	6:R:163:VAL:O	2.18	0.44
6:U:33:LEU:HD21	6:U:88:CYS:HB2	2.00	0.44
6:U:48:ILE:HD12	6:U:73:LEU:HD13	1.99	0.44
6:U:123:GLU:H	6:U:123:GLU:CD	2.21	0.44
3:L:121:SER:CB	4:H:123:PRO:HD2	2.48	0.44
4:H:4:LEU:HD11	4:H:92:CYS:O	2.18	0.44
1:C:82:PHE:CE2	1:C:117:GLY:HA2	2.53	0.44
1:A:54:LYS:HD2	1:A:276(A):SER:O	2.18	0.43
1:C:51:ILE:HG23	1:C:282:PHE:HD1	1.79	0.43
1:G:108:LEU:HD13	1:G:234:TRP:CD2	2.52	0.43
6:O:48:ILE:HD12	6:O:73:LEU:HD13	1.99	0.43
1:G:82:PHE:CE2	1:G:117:GLY:HA2	2.53	0.43
5:N:123:PRO:HB3	5:N:211:VAL:HG13	2.00	0.43
1:A:51:ILE:HG23	1:A:282:PHE:HD1	1.78	0.43
1:A:82:PHE:CE2	1:A:117:GLY:HA2	2.53	0.43
1:A:114:GLU:HA	1:A:265:SER:O	2.18	0.43
4:H:11:LEU:HG	4:H:110:THR:OG1	2.18	0.43
1:G:96:ILE:HD11	5:T:100(A):TYR:OH	2.17	0.43
4:K:4:LEU:HD11	4:K:92:CYS:O	2.18	0.43
6:O:33:LEU:HD21	6:O:88:CYS:HB2	2.00	0.43
6:O:190:LYS:HZ1	6:O:210:ASN:CA	2.21	0.43
6:R:33:LEU:HD21	6:R:88:CYS:HB2	2.00	0.43
5:T:169:VAL:HG11	6:U:161:GLU:O	2.18	0.43
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.64	0.43
1:C:86:LEU:HG	1:C:86:LEU:O	2.19	0.43
1:C:114:GLU:HA	1:C:265:SER:O	2.18	0.43
1:C:130:ILE:HG22	1:C:131:ARG:O	2.18	0.43
1:C:221:PRO:HB3	6:O:49:TYR:CG	2.53	0.43
4:F:4:LEU:HD11	4:F:92:CYS:O	2.18	0.43
3:J:16:GLY:H	3:J:78:LEU:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:167:PRO:HD3	6:R:164:THR:HA	2.00	0.43
5:T:205:THR:C	5:T:206:LYS:HD3	2.42	0.43
2:B:80:LEU:HD21	2:I:80:LEU:HG	2.01	0.43
3:J:12:SER:HA	3:J:105:GLU:HB2	1.99	0.43
3:J:47:LEU:HB3	3:J:48:ILE:HD12	2.00	0.43
6:R:48:ILE:HD12	6:R:73:LEU:HD13	1.99	0.43
1:C:52:CYS:HA	1:C:54:LYS:N	2.34	0.43
3:E:47:LEU:HB3	3:E:48:ILE:HD12	2.01	0.43
2:I:42:GLN:CD	4:K:100(G):TYR:HB3	2.33	0.43
3:E:92:ASN:OD1	3:E:92:ASN:N	2.52	0.43
1:G:11:ALA:O	2:I:140:ILE:HB	2.18	0.43
3:J:80:SER:HA	3:J:106:ILE:HG12	2.01	0.43
4:K:30:ARG:NH2	4:K:71:ARG:HG3	2.32	0.43
5:Q:100(A):TYR:O	6:R:32:PHE:CD2	2.71	0.43
2:B:80:LEU:CG	2:D:80:LEU:HD21	2.46	0.43
2:B:134:GLY:HA2	2:I:124:LYS:HD3	2.00	0.43
3:L:7:SER:HA	3:L:8:PRO:HA	1.87	0.43
4:F:94:LYS:HG3	4:F:102:VAL:HB	2.01	0.43
1:G:101:ARG:HG2	1:G:101:ARG:NH1	2.32	0.43
1:G:131:ARG:CG	1:G:157:SER:HA	2.41	0.43
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.54	0.43
5:Q:205:THR:C	5:Q:206:LYS:HD3	2.42	0.43
1:A:106:GLU:C	2:B:71:SER:CB	2.92	0.42
3:L:47:LEU:HB3	3:L:48:ILE:HD12	2.00	0.42
3:L:185:ASP:HA	3:L:188:LYS:HD3	2.01	0.42
4:H:94:LYS:HG3	4:H:102:VAL:HB	2.01	0.42
1:G:114:GLU:HA	1:G:265:SER:O	2.18	0.42
1:A:86:LEU:HG	1:A:86:LEU:O	2.20	0.42
1:C:101:ARG:NH1	1:C:105:GLU:OE2	2.52	0.42
1:C:235:MET:HE3	1:C:235:MET:HB2	1.78	0.42
3:E:16:GLY:H	3:E:78:LEU:HB3	1.84	0.42
1:G:108:LEU:HD22	1:G:234:TRP:CD1	2.55	0.42
6:R:125:LEU:HB3	6:R:183:LYS:HD2	2.01	0.42
6:U:125:LEU:HB3	6:U:183:LYS:HD2	2.00	0.42
1:A:161:PHE:HA	1:A:162:PRO:HD3	1.74	0.42
4:H:51:ILE:HG21	4:H:78:LEU:HD13	2.02	0.42
1:C:131:ARG:CG	1:C:157:SER:HA	2.41	0.42
4:F:51:ILE:HG21	4:F:78:LEU:HD13	2.02	0.42
3:J:205:VAL:CG2	6:R:143:GLU:OE1	2.67	0.42
5:T:78:PHE:CZ	5:T:92:CYS:HB2	2.54	0.42
1:A:197:THR:HG22	1:A:198:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:O	1:A:248:ASN:ND2	2.52	0.42
3:L:92:ASN:OD1	3:L:92:ASN:N	2.52	0.42
3:J:92:ASN:OD1	3:J:92:ASN:N	2.52	0.42
4:K:13:GLN:HA	4:K:112:SER:O	2.19	0.42
1:A:108:LEU:HD22	1:A:234:TRP:CD1	2.54	0.42
1:C:105:GLU:HG3	1:C:106:GLU:OE1	2.20	0.42
1:G:146:SER:OG	1:G:147:PHE:N	2.53	0.42
3:J:91:TYR:HA	3:J:92:ASN:HA	1.80	0.42
5:N:78:PHE:CZ	5:N:92:CYS:HB2	2.54	0.42
5:T:59:TYR:O	5:T:64:LYS:CG	2.68	0.42
3:E:185:ASP:HA	3:E:188:LYS:HD3	2.02	0.42
1:G:199:ASN:O	1:G:248:ASN:ND2	2.52	0.42
4:K:114:ALA:HB3	4:K:148:PHE:HE2	1.68	0.42
5:T:124:LEU:HB3	6:U:118:PHE:CD1	2.46	0.42
1:A:52:CYS:O	1:A:282:PHE:HE1	2.00	0.42
3:L:80:SER:HA	3:L:106:ILE:HG12	2.01	0.42
4:H:58:TYR:HE2	4:H:100(H):TYR:CG	2.38	0.42
1:C:146:SER:OG	1:C:147:PHE:N	2.53	0.42
1:C:197:THR:HG22	1:C:198:GLY:N	2.35	0.42
1:G:11:ALA:O	2:I:140:ILE:N	2.38	0.42
1:A:17:HIS:HA	2:B:21:TRP:O	2.20	0.42
1:C:199:ASN:O	1:C:248:ASN:ND2	2.52	0.42
4:K:215:SER:O	4:K:217:THR:HG23	2.20	0.42
1:A:51:ILE:HG13	1:A:268:ILE:HD13	2.01	0.42
1:A:73:PRO:HD2	1:A:76:CYS:HB2	2.02	0.42
3:L:61:ARG:HD2	3:L:77:SER:O	2.20	0.42
1:C:200:LYS:HA	1:C:200:LYS:HD3	1.77	0.42
3:E:80:SER:HA	3:E:106:ILE:HG12	2.01	0.42
2:I:56:ILE:HG21	4:K:100:ILE:HG21	2.00	0.42
1:A:83:LYS:HD3	1:A:262:ASN:HB2	2.02	0.42
3:E:30:ARG:N	3:E:91:TYR:HE1	2.18	0.42
4:F:215:SER:O	4:F:217:THR:HG23	2.20	0.42
5:N:212:GLU:CD	5:N:213:PRO:HD3	2.44	0.42
6:O:125:LEU:HB3	6:O:183:LYS:HD2	2.00	0.42
5:Q:78:PHE:CZ	5:Q:92:CYS:HB2	2.54	0.42
5:Q:123:PRO:HB3	5:Q:211:VAL:HG13	2.00	0.42
3:L:16:GLY:H	3:L:78:LEU:HB3	1.84	0.41
1:C:108:LEU:HD22	1:C:234:TRP:CD1	2.55	0.41
4:F:13:GLN:HA	4:F:112:SER:O	2.19	0.41
3:E:34:ALA:HB3	3:E:89:GLN:HG2	2.02	0.41
1:G:73:PRO:HD2	1:G:76:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:61:ARG:HD2	3:J:77:SER:O	2.20	0.41
3:J:185:ASP:HA	3:J:188:LYS:HD3	2.02	0.41
4:K:94:LYS:HG3	4:K:102:VAL:HB	2.01	0.41
1:A:109:ARG:O	1:A:113:ARG:HG3	2.21	0.41
1:A:235:MET:HE3	1:A:235:MET:HB2	1.78	0.41
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.41
1:C:52:CYS:O	1:C:56:LYS:CG	2.68	0.41
1:C:73:PRO:HD2	1:C:76:CYS:HB2	2.02	0.41
3:E:61:ARG:HD2	3:E:77:SER:O	2.20	0.41
4:F:58:TYR:HE2	4:F:100(H):TYR:CG	2.38	0.41
1:G:197:THR:HG22	1:G:198:GLY:N	2.35	0.41
1:G:201:LEU:HD11	1:G:212:SER:HB2	2.03	0.41
5:N:142:VAL:CG2	5:N:198:VAL:HG21	2.51	0.41
6:O:123:GLU:H	6:O:123:GLU:CD	2.21	0.41
5:Q:100(G):CYS:SG	6:R:91:SER:CB	3.09	0.41
5:T:142:VAL:CG2	5:T:198:VAL:HG21	2.51	0.41
4:H:13:GLN:HA	4:H:112:SER:O	2.19	0.41
5:Q:100(G):CYS:SG	6:R:91:SER:HB2	2.61	0.41
1:A:48:ILE:HB	1:A:50:GLU:OE1	2.20	0.41
2:B:171:PHE:HD1	2:I:167:LEU:HD13	1.86	0.41
1:C:83:LYS:HD3	1:C:262:ASN:HB2	2.02	0.41
1:G:83:LYS:HD3	1:G:262:ASN:HB2	2.02	0.41
5:Q:59:TYR:O	5:Q:64:LYS:CG	2.68	0.41
1:C:86:LEU:HD11	1:C:88:ILE:HG12	2.03	0.41
1:C:261(G):ILE:HG22	5:T:65:SER:HA	2.02	0.41
1:G:161:PHE:HA	1:G:162:PRO:HD3	1.74	0.41
1:A:169:ARG:HB2	1:A:242:THR:HG22	2.02	0.41
3:L:30:ARG:N	3:L:91:TYR:HE1	2.18	0.41
1:C:221:PRO:HB3	6:O:49:TYR:CD2	2.55	0.41
3:J:35:TRP:CE3	3:J:73:LEU:HD22	2.56	0.41
3:J:95:LEU:HA	4:K:47:TRP:CZ3	2.56	0.41
4:K:51:ILE:HG21	4:K:78:LEU:HD13	2.02	0.41
4:K:58:TYR:HE2	4:K:100(H):TYR:CG	2.38	0.41
5:N:124:LEU:HB3	6:O:118:PHE:CD1	2.56	0.41
5:Q:142:VAL:CG2	5:Q:198:VAL:HG21	2.51	0.41
5:Q:214:LYS:HD3	5:Q:214:LYS:N	2.10	0.41
5:T:122:PHE:O	5:T:141:LEU:N	2.46	0.41
3:E:95:LEU:HG	4:F:47:TRP:CZ3	2.56	0.41
1:G:52:CYS:C	1:G:56:LYS:HG2	2.42	0.41
5:T:59:TYR:O	5:T:64:LYS:CD	2.67	0.41
3:L:34:ALA:HB3	3:L:89:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:15:PRO:HA	3:J:78:LEU:HD22	2.03	0.40
5:T:39:GLN:NE2	6:U:87:TYR:OH	2.32	0.40
1:A:107:ALA:N	2:B:71:SER:OG	2.54	0.40
1:A:166:GLN:O	1:A:245:PHE:N	2.38	0.40
1:A:201:LEU:HD11	1:A:212:SER:HB2	2.03	0.40
3:L:35:TRP:CE3	3:L:73:LEU:HD22	2.56	0.40
1:C:34:ILE:HD11	1:C:321:ARG:NE	2.37	0.40
1:C:144:VAL:HG22	1:C:145:SER:N	2.37	0.40
1:C:173:LYS:O	1:C:239:PRO:HG3	2.22	0.40
1:G:15:LEU:HD11	2:I:118:LEU:HG	2.00	0.40
1:G:261(C):ALA:HA	1:G:261(D):PRO:HD2	1.90	0.40
6:O:18:ARG:HH21	6:O:76:ARG:CZ	2.34	0.40
6:U:18:ARG:HH21	6:U:76:ARG:CZ	2.34	0.40
3:L:15:PRO:HA	3:L:78:LEU:HD22	2.03	0.40
1:C:109:ARG:O	1:C:113:ARG:HG3	2.20	0.40
1:G:34:ILE:HD11	1:G:321:ARG:NE	2.37	0.40
4:H:215:SER:O	4:H:217:THR:HG23	2.20	0.40
1:C:221:PRO:HD2	5:N:98:ASP:OD2	2.21	0.40
6:R:18:ARG:HH21	6:R:76:ARG:CZ	2.34	0.40
5:T:171:GLN:HA	6:U:160:GLN:CD	2.46	0.40
2:B:38:LEU:CA	4:H:100(G):TYR:CE2	3.04	0.40
1:G:173:LYS:O	1:G:239:PRO:HG3	2.22	0.40
5:T:43:LYS:HE2	5:T:43:LYS:HB3	1.57	0.40
6:U:190:LYS:HZ2	6:U:191:VAL:HA	1.86	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	316/333 (95%)	307 (97%)	7 (2%)	2 (1%)	21 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	313/333 (94%)	306 (98%)	5 (2%)	2 (1%)	21	59
1	G	316/333 (95%)	308 (98%)	6 (2%)	2 (1%)	21	59
2	B	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	D	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
2	I	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
3	E	209/214 (98%)	193 (92%)	13 (6%)	3 (1%)	9	38
3	J	209/214 (98%)	193 (92%)	13 (6%)	3 (1%)	9	38
3	L	209/214 (98%)	193 (92%)	13 (6%)	3 (1%)	9	38
4	F	222/234 (95%)	209 (94%)	11 (5%)	2 (1%)	14	50
4	H	222/234 (95%)	209 (94%)	11 (5%)	2 (1%)	14	50
4	K	222/234 (95%)	209 (94%)	11 (5%)	2 (1%)	14	50
5	N	218/229 (95%)	209 (96%)	8 (4%)	1 (0%)	24	63
5	Q	215/229 (94%)	208 (97%)	6 (3%)	1 (0%)	24	63
5	T	215/229 (94%)	208 (97%)	6 (3%)	1 (0%)	24	63
6	O	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	R	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	U	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	4029/4200 (96%)	3862 (96%)	143 (4%)	24 (1%)	21	59

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	94	TRP
3	E	94	TRP
3	J	94	TRP
1	A	141	ARG
3	L	76	SER
1	C	141	ARG
3	E	76	SER
1	G	141	ARG
3	J	76	SER
3	L	51	ALA
3	E	51	ALA
3	J	51	ALA
4	H	114	ALA
4	F	114	ALA

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Mol	Chain	Res	Type
4	K	114	ALA
1	A	261(G)	ILE
1	C	261(G)	ILE
1	G	261(G)	ILE
4	H	52(A)	GLY
4	F	52(A)	GLY
4	K	52(A)	GLY
5	N	213	PRO
5	Q	213	PRO
5	T	213	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	275/285 (96%)	265 (96%)	10 (4%)	31	52
1	C	274/285 (96%)	265 (97%)	9 (3%)	33	54
1	G	275/285 (96%)	266 (97%)	9 (3%)	33	54
2	B	146/148 (99%)	143 (98%)	3 (2%)	47	64
2	D	145/148 (98%)	142 (98%)	3 (2%)	47	64
2	I	146/148 (99%)	143 (98%)	3 (2%)	47	64
3	E	186/187 (100%)	182 (98%)	4 (2%)	45	63
3	J	186/187 (100%)	182 (98%)	4 (2%)	45	63
3	L	186/187 (100%)	182 (98%)	4 (2%)	45	63
4	F	189/196 (96%)	182 (96%)	7 (4%)	30	51
4	H	189/196 (96%)	182 (96%)	7 (4%)	30	51
4	K	189/196 (96%)	181 (96%)	8 (4%)	26	47
5	N	192/199 (96%)	183 (95%)	9 (5%)	23	44
5	Q	192/199 (96%)	183 (95%)	9 (5%)	23	44
5	T	191/199 (96%)	183 (96%)	8 (4%)	26	47
6	O	189/190 (100%)	186 (98%)	3 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	189/190 (100%)	186 (98%)	3 (2%)	55	69
6	U	189/190 (100%)	186 (98%)	3 (2%)	55	69
All	All	3528/3615 (98%)	3422 (97%)	106 (3%)	36	56

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	56	LYS
1	A	86	LEU
1	A	126	ARG
1	A	264	LYS
1	A	276	GLU
1	A	276(A)	SER
1	A	315	LYS
1	A	321	ARG
1	A	325	GLU
2	B	19	ASP
2	B	125	GLN
2	B	143	LYS
3	L	29	VAL
3	L	33	LEU
3	L	58	ILE
3	L	90	GLN
4	H	2	VAL
4	H	3	GLN
4	H	28	THR
4	H	29	PHE
4	H	57	THR
4	H	115	SER
4	H	187	LEU
1	C	48	ILE
1	C	86	LEU
1	C	126	ARG
1	C	264	LYS
1	C	276	GLU
1	C	276(A)	SER
1	C	315	LYS
1	C	321	ARG
1	C	325	GLU
2	D	19	ASP

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Mol	Chain	Res	Type
2	D	125	GLN
2	D	143	LYS
3	E	29	VAL
3	E	33	LEU
3	E	58	ILE
3	E	90	GLN
4	F	2	VAL
4	F	3	GLN
4	F	28	THR
4	F	29	PHE
4	F	57	THR
4	F	115	SER
4	F	187	LEU
1	G	48	ILE
1	G	86	LEU
1	G	126	ARG
1	G	264	LYS
1	G	276	GLU
1	G	276(A)	SER
1	G	315	LYS
1	G	321	ARG
1	G	325	GLU
2	I	19	ASP
2	I	125	GLN
2	I	143	LYS
3	J	29	VAL
3	J	33	LEU
3	J	58	ILE
3	J	90	GLN
4	K	2	VAL
4	K	3	GLN
4	K	28	THR
4	K	29	PHE
4	K	57	THR
4	K	115	SER
4	K	187	LEU
4	K	216	ASN
5	N	31	SER
5	N	33	ILE
5	N	156	SER
5	N	192	GLN
5	N	193	THR

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Mol	Chain	Res	Type
5	N	195	ILE
5	N	209	LYS
5	N	211	VAL
5	N	214	LYS
6	O	1	ASP
6	O	135	LEU
6	O	190	LYS
5	Q	31	SER
5	Q	33	ILE
5	Q	156	SER
5	Q	192	GLN
5	Q	193	THR
5	Q	195	ILE
5	Q	209	LYS
5	Q	211	VAL
5	Q	214	LYS
6	R	1	ASP
6	R	135	LEU
6	R	190	LYS
5	T	31	SER
5	T	33	ILE
5	T	192	GLN
5	T	193	THR
5	T	195	ILE
5	T	209	LYS
5	T	211	VAL
5	T	214	LYS
6	U	1	ASP
6	U	135	LEU
6	U	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	311	HIS
2	B	27	GLN
2	B	159	HIS
3	L	37	GLN
3	L	147	GLN
3	L	210	ASN
4	H	13	GLN

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Mol	Chain	Res	Type
4	H	216	ASN
1	C	166	GLN
2	D	27	GLN
2	D	105	GLN
2	D	159	HIS
3	E	37	GLN
3	E	147	GLN
3	E	210	ASN
4	F	13	GLN
4	F	216	ASN
1	G	165	ASN
1	G	166	GLN
1	G	199	ASN
1	G	311	HIS
2	I	27	GLN
2	I	105	GLN
2	I	159	HIS
3	J	147	GLN
3	J	210	ASN
4	K	13	GLN
4	K	172	HIS
4	K	211	ASN
6	O	38	HIS
6	O	79	GLN
6	O	147	GLN
6	O	152	ASN
6	O	199	GLN
6	R	38	HIS
6	R	138	ASN
6	R	152	ASN
6	R	199	GLN
6	U	38	HIS
6	U	79	GLN
6	U	152	ASN
6	U	199	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	322/333 (96%)	0.07	5 (1%) 70 58	219, 365, 393, 401	0
1	C	321/333 (96%)	0.03	9 (2%) 55 46	219, 348, 383, 391	0
1	G	322/333 (96%)	0.05	7 (2%) 62 52	219, 375, 402, 405	0
2	B	173/176 (98%)	0.13	6 (3%) 47 41	213, 245, 324, 353	0
2	D	172/176 (97%)	0.35	11 (6%) 25 28	214, 248, 328, 355	0
2	I	173/176 (98%)	0.27	6 (3%) 47 41	215, 248, 325, 359	0
3	E	213/214 (99%)	-0.02	4 (1%) 66 55	246, 298, 321, 344	0
3	J	213/214 (99%)	-0.04	3 (1%) 73 60	244, 289, 328, 366	0
3	L	213/214 (99%)	0.03	3 (1%) 73 60	245, 279, 309, 331	0
4	F	226/234 (96%)	0.03	1 (0%) 88 78	230, 276, 345, 359	0
4	H	226/234 (96%)	0.03	4 (1%) 67 56	238, 268, 306, 315	0
4	K	226/234 (96%)	0.07	4 (1%) 67 56	228, 267, 327, 340	0
5	N	222/229 (96%)	0.09	6 (2%) 56 46	303, 333, 349, 359	0
5	Q	221/229 (96%)	-0.06	3 (1%) 73 60	328, 347, 373, 381	0
5	T	221/229 (96%)	-0.05	0 100 100	337, 370, 384, 388	0
6	O	213/214 (99%)	0.01	2 (0%) 81 68	287, 309, 343, 348	0
6	R	213/214 (99%)	-0.14	1 (0%) 87 76	330, 347, 366, 372	0
6	U	213/214 (99%)	-0.03	2 (0%) 81 68	336, 357, 385, 388	0
All	All	4103/4200 (97%)	0.04	77 (1%) 66 55	213, 317, 386, 405	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	51	ILE	5.9
1	C	51	ILE	4.9
1	A	51	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
3	L	5	THR	4.1
1	G	13	LEU	3.8
2	B	84	VAL	3.7
1	C	294	PHE	3.6
1	C	52	CYS	3.4
1	G	52	CYS	3.4
2	B	99	LEU	3.3
3	E	194	CYS	3.3
3	J	213	GLU	3.2
4	K	94	LYS	3.2
2	D	80	LEU	3.1
3	J	214	CYS	3.0
1	A	52	CYS	2.9
1	C	111	ILE	2.8
1	G	50	GLU	2.8
3	L	192	TYR	2.8
4	H	41	PRO	2.8
5	Q	183	THR	2.7
2	D	144	CYS	2.7
5	Q	196	CYS	2.7
6	U	122	ASP	2.7
2	D	84	VAL	2.7
5	N	140	CYS	2.7
1	G	15	LEU	2.6
5	N	142	VAL	2.6
1	G	35	GLU	2.6
2	I	24	PHE	2.6
1	C	315	LYS	2.6
2	D	55	LEU	2.6
5	N	127	SER	2.6
2	D	98	LEU	2.6
4	K	127	SER	2.6
2	D	52	LEU	2.6
1	C	143	THR	2.5
5	N	138	LEU	2.5
2	B	56	ILE	2.4
2	D	103	GLU	2.4
1	C	144	VAL	2.4
2	I	108	ILE	2.4
4	K	34	LEU	2.4
4	F	52(A)	GLY	2.3
2	B	96	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	K	52(A)	GLY	2.3
4	H	94	LYS	2.3
1	A	181	GLY	2.3
2	I	51	LYS	2.3
4	H	45	LEU	2.3
6	O	73	LEU	2.2
2	I	69	GLU	2.2
3	J	192	TYR	2.2
3	L	188	LYS	2.2
3	E	144	ALA	2.2
2	D	87	THR	2.2
5	N	44	GLY	2.2
2	D	56	ILE	2.2
6	U	196	VAL	2.2
1	A	294	PHE	2.2
2	D	48	ILE	2.2
1	C	216	SER	2.2
3	E	192	TYR	2.2
2	I	103	GLU	2.2
2	B	69	GLU	2.1
5	Q	140	CYS	2.1
6	O	62	PHE	2.1
1	A	285	ASN	2.1
2	B	55	LEU	2.1
2	I	45	ILE	2.1
1	G	38	ASN	2.1
1	C	267	GLY	2.0
3	E	193	ALA	2.0
5	N	141	LEU	2.0
2	D	143	LYS	2.0
6	R	135	LEU	2.0
4	H	127	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.