



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 8JAI / pdb_00008jai
Title : Crystal Structure of Human H-Ferritin variant 123F assembling in solution 1
Authors : Chen, X.; Zhao, G.
Deposited on : 2023-05-06
Resolution : 2.56 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

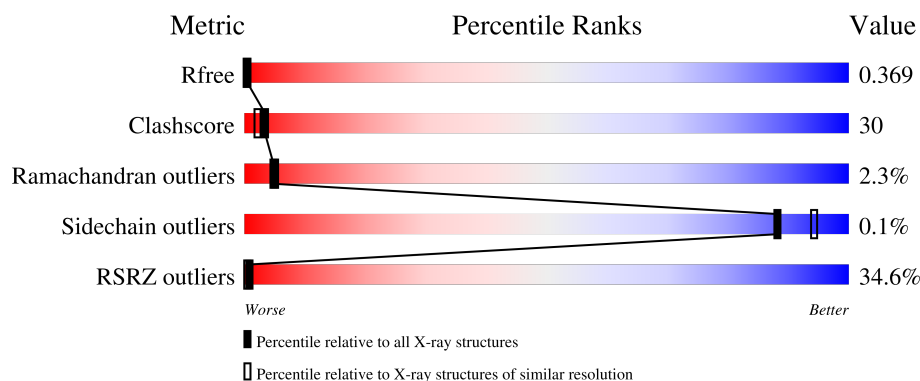
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	183	15% 45% 48% 6%
1	B	183	9% 48% 46% 6%
1	C	183	52% 41% 52% 6%
1	D	183	53% 33% 60% 6%
1	E	183	19% 50% 43% 6%

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Mol	Chain	Length	Quality of chain
1	F	183	
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	
1	M	183	
1	N	183	
1	O	183	
1	P	183	
1	Q	183	
1	R	183	
1	S	183	
1	T	183	
1	U	183	
1	V	183	
1	W	183	
1	X	183	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34001 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	B	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	C	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	D	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	E	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	F	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	G	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	H	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	I	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	J	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	K	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	L	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	M	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	N	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	O	172	Total	C	N	O	S	0	0	0
			1413	889	248	270	6			
1	P	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	R	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	S	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	T	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	U	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	V	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	W	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			
1	X	172	Total	C	N	O	S	0	0	0
			1416	891	248	270	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	ASP	engineered mutation	UNP P02794
B	123	PHE	ASP	engineered mutation	UNP P02794
C	123	PHE	ASP	engineered mutation	UNP P02794
D	123	PHE	ASP	engineered mutation	UNP P02794
E	123	PHE	ASP	engineered mutation	UNP P02794
F	123	PHE	ASP	engineered mutation	UNP P02794
G	123	PHE	ASP	engineered mutation	UNP P02794
H	123	PHE	ASP	engineered mutation	UNP P02794
I	123	PHE	ASP	engineered mutation	UNP P02794
J	123	PHE	ASP	engineered mutation	UNP P02794
K	123	PHE	ASP	engineered mutation	UNP P02794
L	123	PHE	ASP	engineered mutation	UNP P02794
M	123	PHE	ASP	engineered mutation	UNP P02794
N	123	PHE	ASP	engineered mutation	UNP P02794
O	123	PHE	ASP	engineered mutation	UNP P02794
P	123	PHE	ASP	engineered mutation	UNP P02794
Q	123	PHE	ASP	engineered mutation	UNP P02794
R	123	PHE	ASP	engineered mutation	UNP P02794
S	123	PHE	ASP	engineered mutation	UNP P02794
T	123	PHE	ASP	engineered mutation	UNP P02794
U	123	PHE	ASP	engineered mutation	UNP P02794
V	123	PHE	ASP	engineered mutation	UNP P02794
W	123	PHE	ASP	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
X	123	PHE	ASP	engineered mutation	UNP P02794

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	2	Total Fe 2 2	0	0
2	D	1	Total Fe 1 1	0	0
2	E	2	Total Fe 2 2	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0
2	P	2	Total Fe 2 2	0	0
2	Q	1	Total Fe 1 1	0	0
2	S	2	Total Fe 2 2	0	0
2	W	1	Total Fe 1 1	0	0

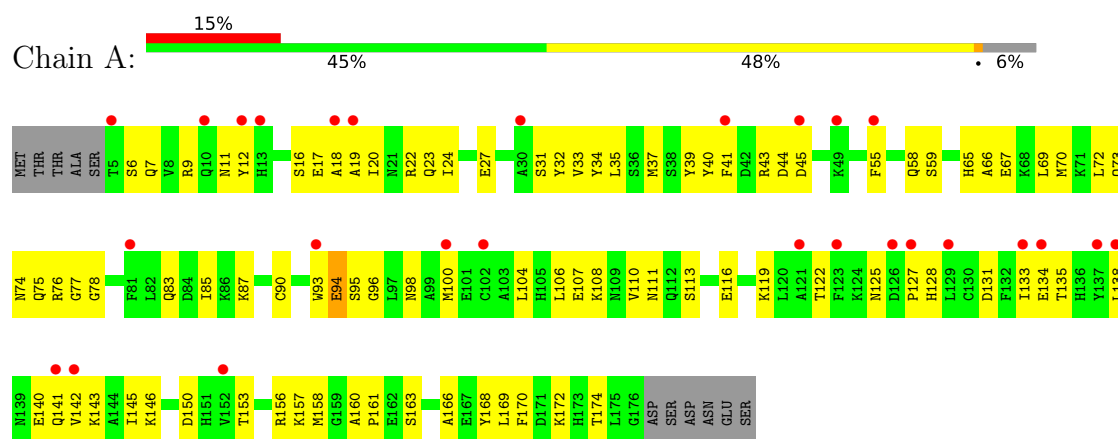
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0

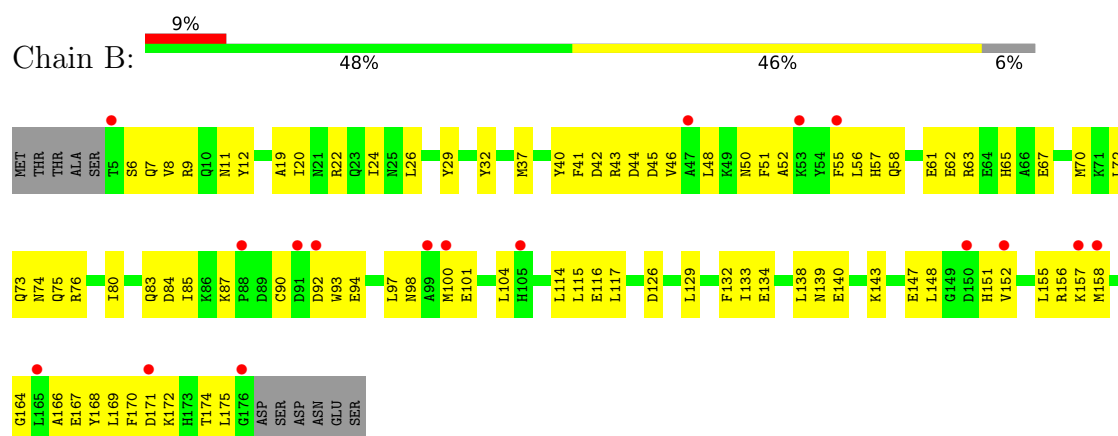
3 Residue-property plots [i](#)

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

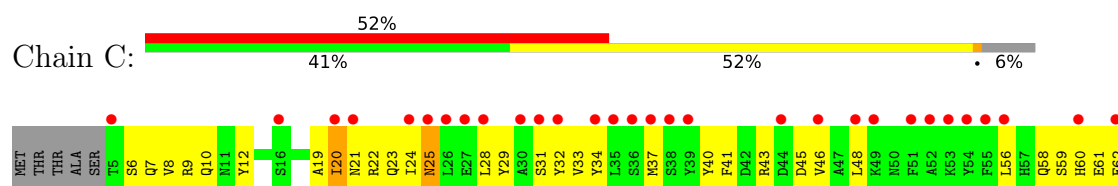
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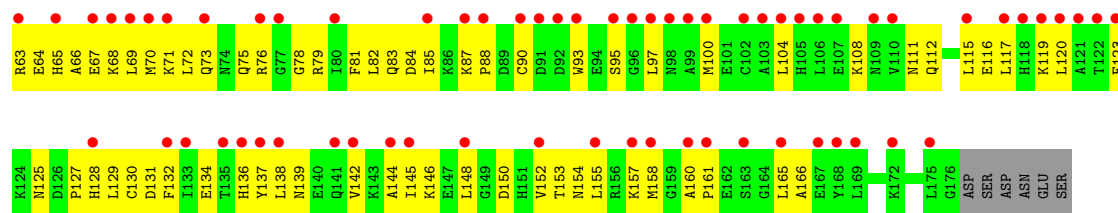


• Molecule 1: Ferritin heavy chain

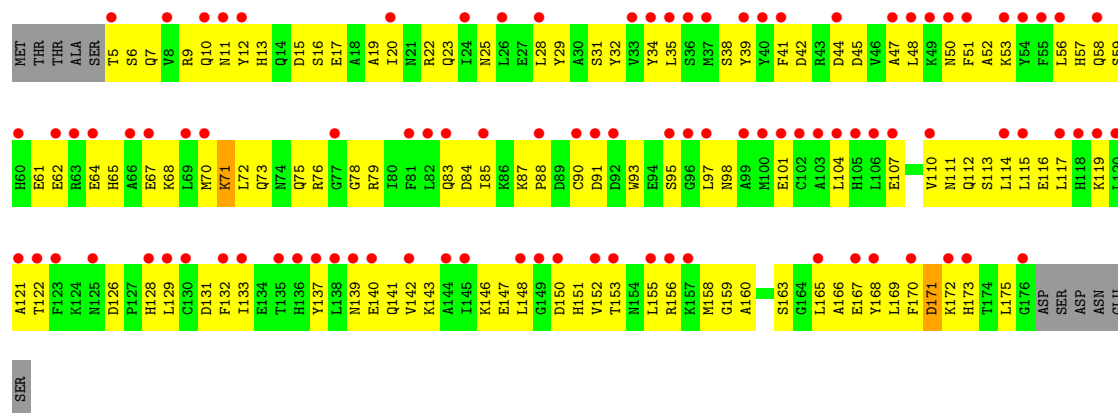


• Molecule 1: Ferritin heavy chain

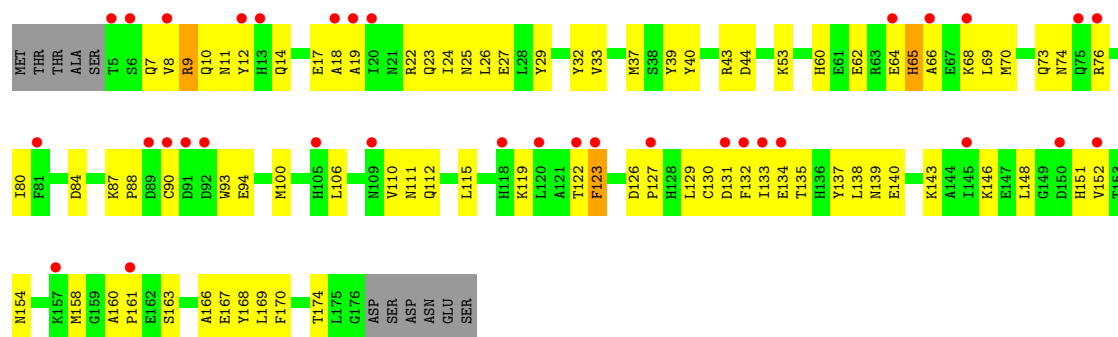




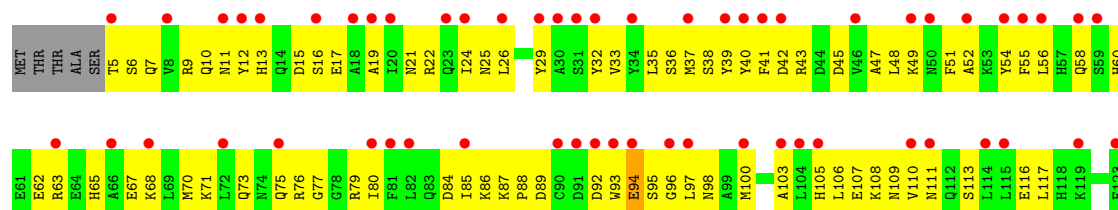
● Molecule 1: Ferritin heavy chain

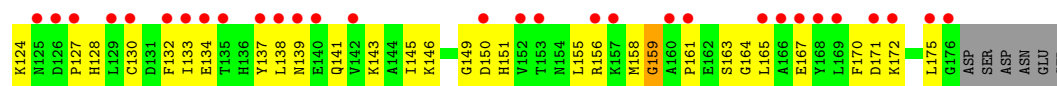


● Molecule 1: Ferritin heavy chain

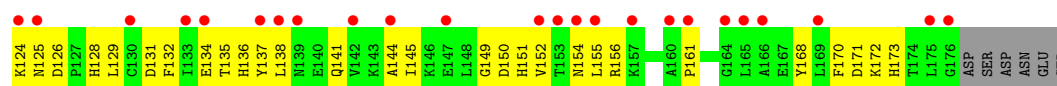
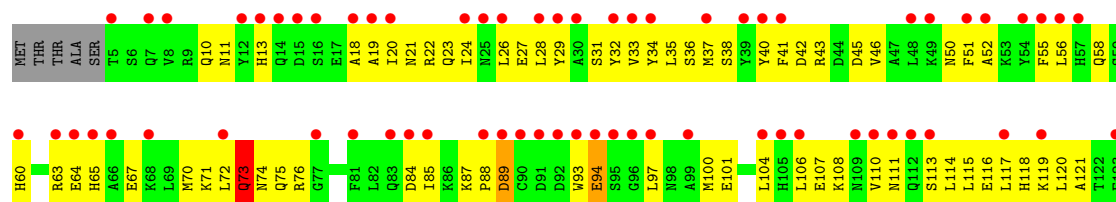
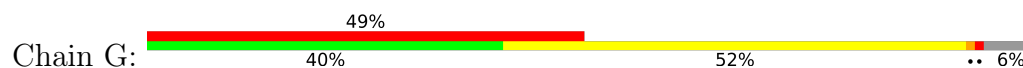


● Molecule 1: Ferritin heavy chain

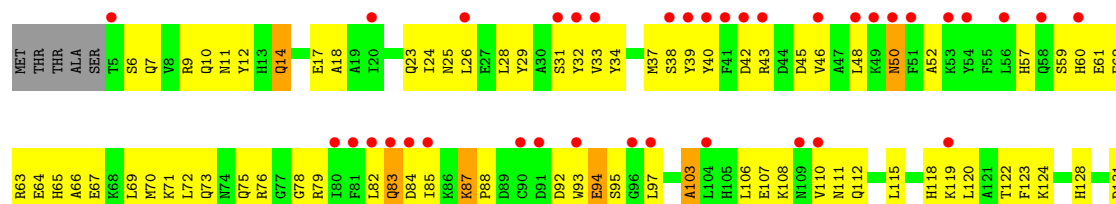




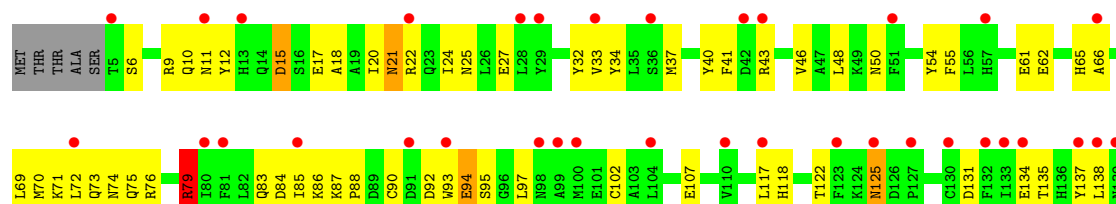
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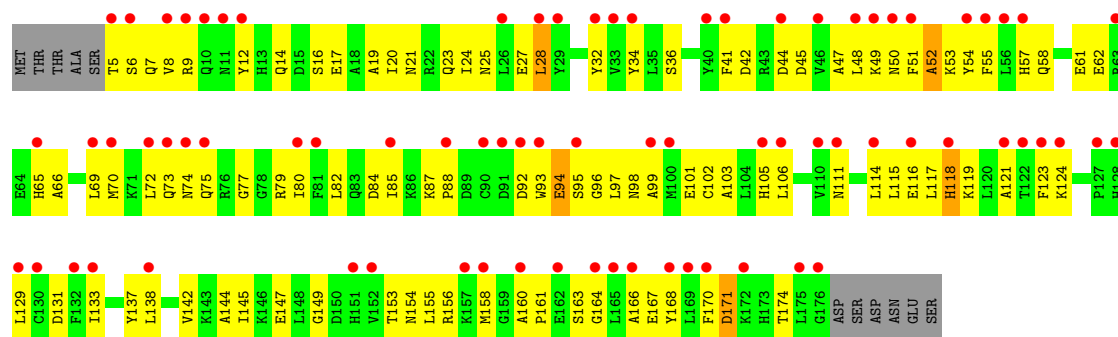


• Molecule 1: Ferritin heavy chain

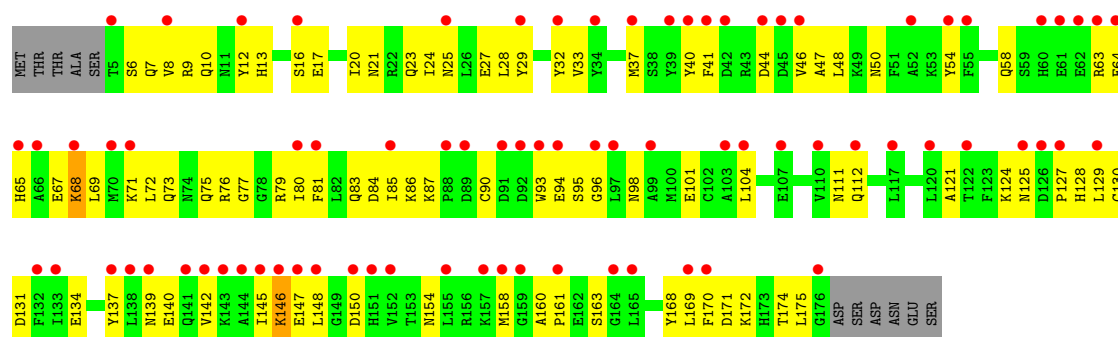
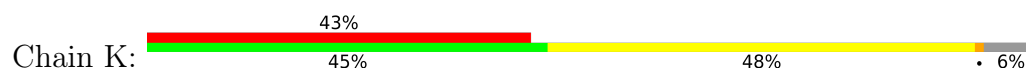


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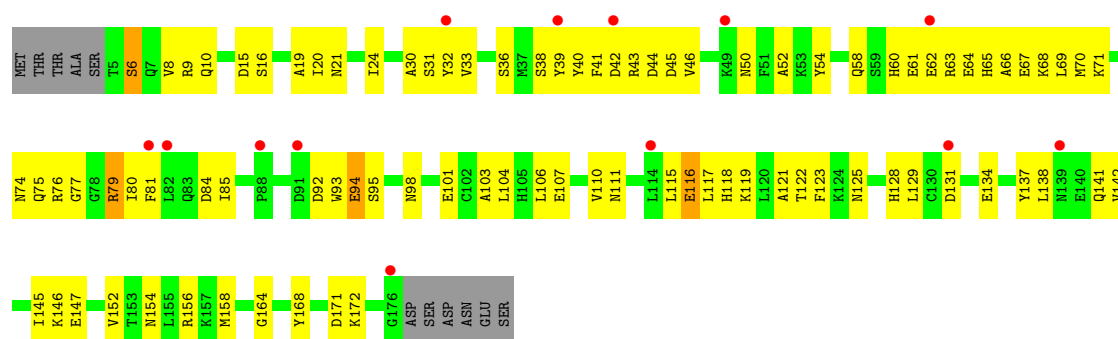




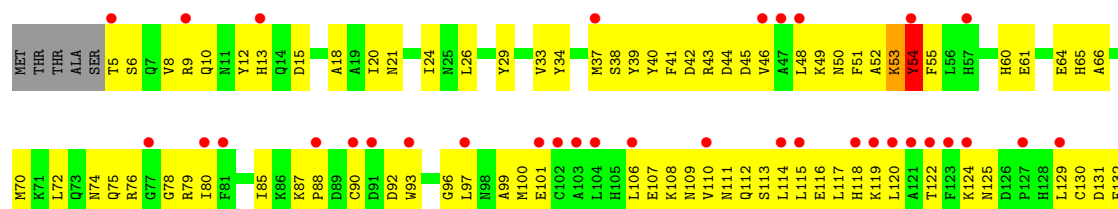
• Molecule 1: Ferritin heavy chain

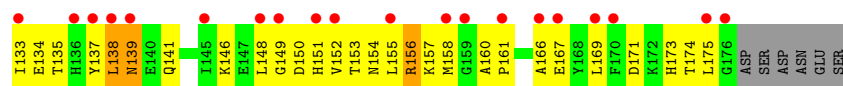


• Molecule 1: Ferritin heavy chain

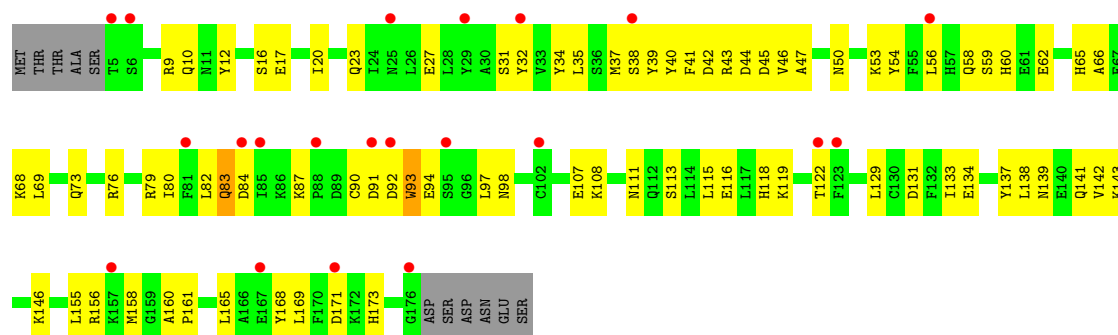


• Molecule 1: Ferritin heavy chain

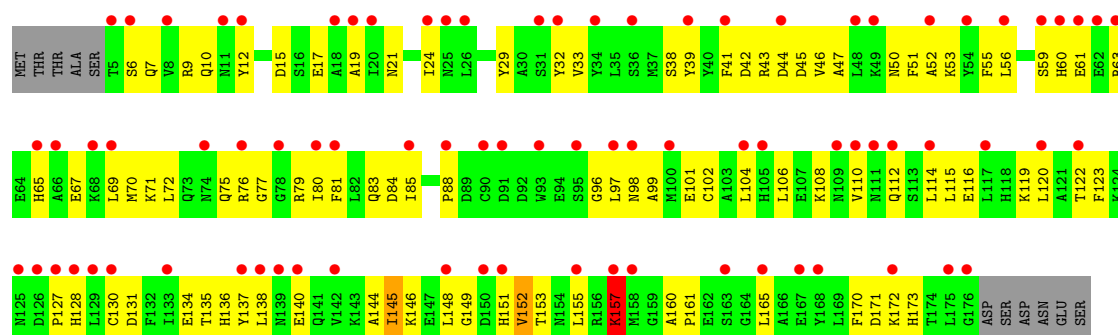
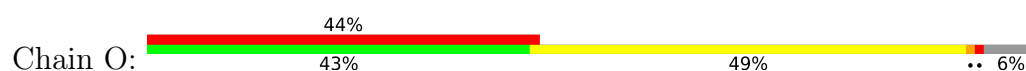




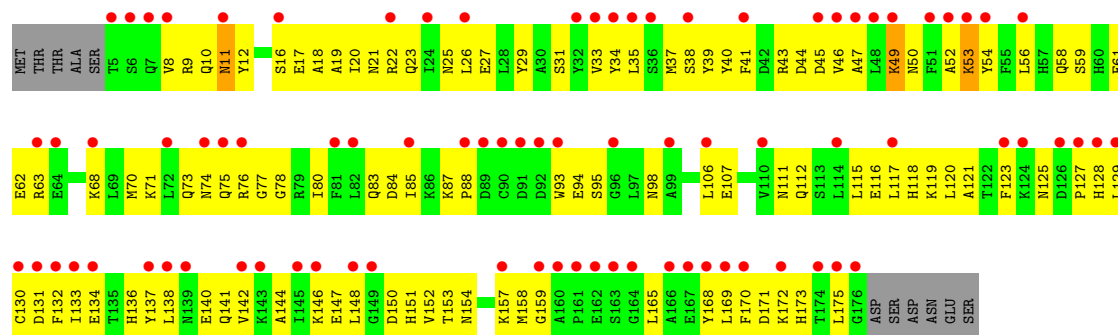
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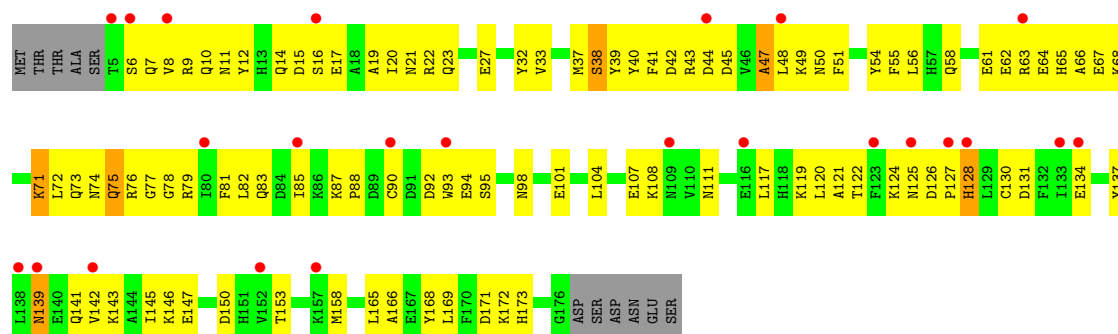


• Molecule 1: Ferritin heavy chain

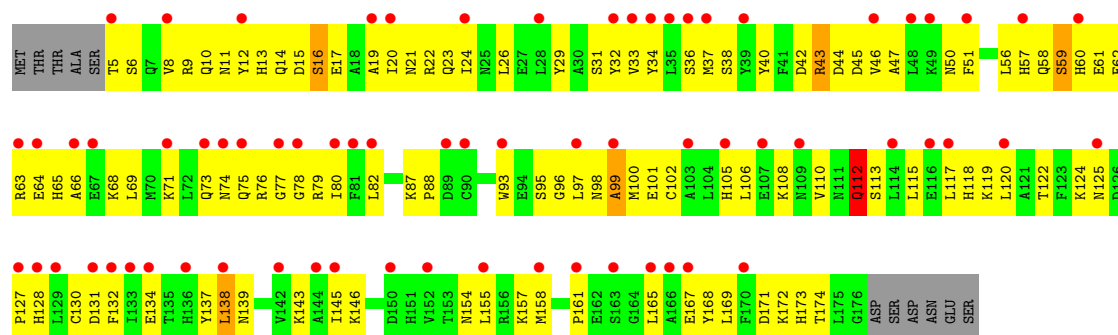


• Molecule 1: Ferritin heavy chain

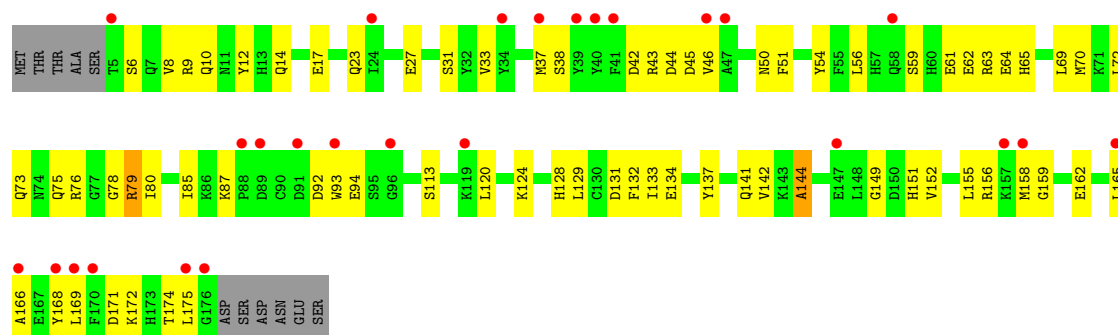




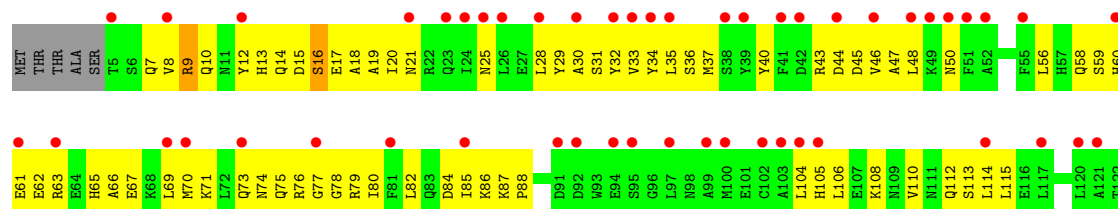
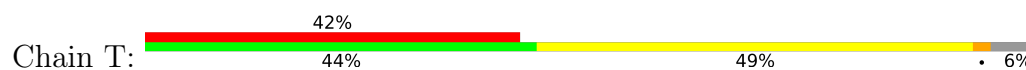
• Molecule 1: Ferritin heavy chain

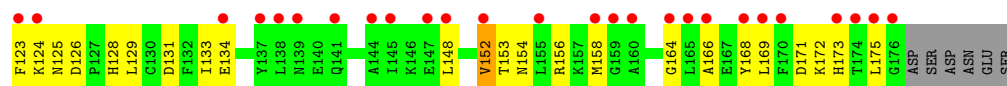


• Molecule 1: Ferritin heavy chain

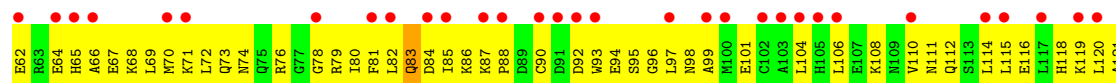
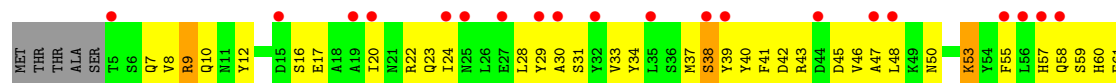


• Molecule 1: Ferritin heavy chain

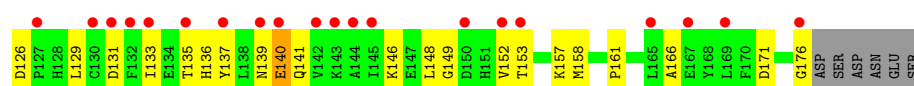
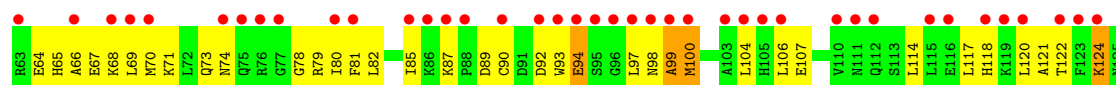




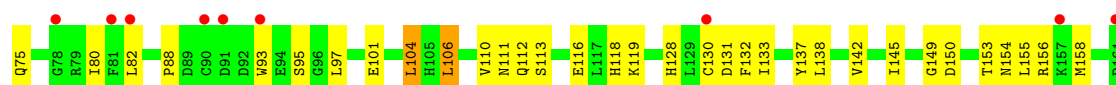
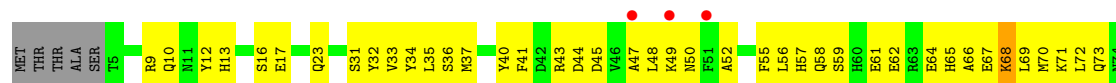
• Molecule 1: Ferritin heavy chain



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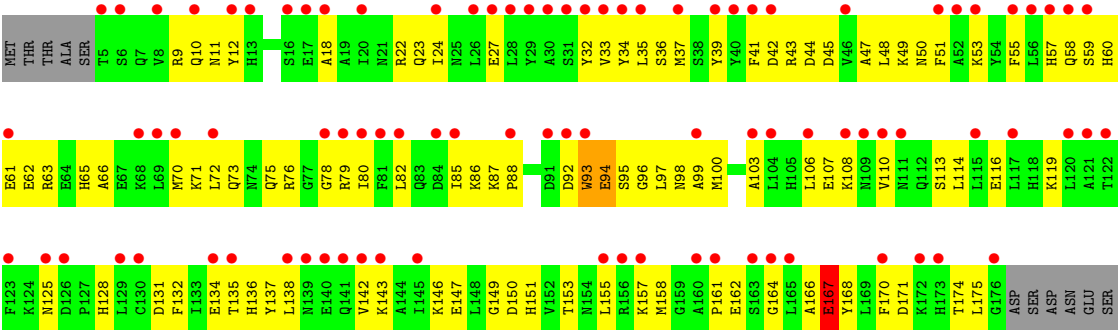


• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	301.66Å 301.66Å 316.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.59 – 2.56 65.59 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.59-2.56) 93.3 (65.59-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.335 , 0.368 0.335 , 0.369	Depositor DCC
R_{free} test set	11628 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.089 for -l,-k,-h 0.095 for -h,l,k	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.52	0/1446	0.71	0/1947
1	B	0.56	0/1446	0.68	0/1947
1	C	0.49	0/1446	0.71	1/1947 (0.1%)
1	D	0.58	1/1446 (0.1%)	0.72	1/1947 (0.1%)
1	E	0.47	0/1446	0.68	0/1947
1	F	0.51	0/1446	0.72	0/1947
1	G	0.46	0/1446	0.76	1/1947 (0.1%)
1	H	0.54	0/1446	0.78	2/1947 (0.1%)
1	I	0.77	2/1446 (0.1%)	0.80	2/1947 (0.1%)
1	J	0.49	0/1446	0.72	2/1947 (0.1%)
1	K	0.50	1/1446 (0.1%)	0.66	0/1947
1	L	0.63	2/1446 (0.1%)	0.81	3/1947 (0.2%)
1	M	0.64	2/1446 (0.1%)	0.89	8/1947 (0.4%)
1	N	0.58	1/1446 (0.1%)	0.70	1/1947 (0.1%)
1	O	0.53	1/1443 (0.1%)	0.70	0/1944
1	P	0.48	1/1446 (0.1%)	0.65	0/1947
1	Q	0.54	1/1446 (0.1%)	0.76	1/1947 (0.1%)
1	R	0.61	2/1446 (0.1%)	0.80	0/1947
1	S	0.52	1/1446 (0.1%)	0.72	1/1947 (0.1%)
1	T	0.51	0/1446	0.68	0/1947
1	U	0.50	0/1446	0.81	6/1947 (0.3%)
1	V	0.61	0/1446	0.80	0/1947
1	W	0.58	1/1446 (0.1%)	0.72	2/1947 (0.1%)
1	X	0.51	1/1446 (0.1%)	0.70	0/1947
All	All	0.55	17/34701 (0.0%)	0.74	31/46725 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	M	0	1
1	V	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	79	ARG	NE-CZ	17.44	1.52	1.33
1	I	79	ARG	CZ-NH1	11.92	1.49	1.32
1	W	68	LYS	CE-NZ	10.34	1.80	1.49
1	R	112	GLN	CG-CD	8.76	1.74	1.52
1	X	167	GLU	CB-CG	6.40	1.71	1.52
1	L	79	ARG	CA-CB	6.39	1.62	1.53
1	O	157	LYS	CE-NZ	6.22	1.68	1.49
1	N	83	GLN	CD-NE2	6.18	1.46	1.33
1	D	17	GLU	CB-CG	5.88	1.70	1.52
1	S	79	ARG	CD-NE	-5.77	1.38	1.46
1	L	79	ARG	CB-CG	-5.65	1.35	1.52
1	R	174	THR	CA-C	5.57	1.56	1.52
1	Q	71	LYS	CG-CD	5.55	1.69	1.52
1	M	54	TYR	CG-CD2	5.35	1.50	1.39
1	M	156	ARG	CG-CD	5.34	1.68	1.52
1	P	53	LYS	CE-NZ	5.20	1.65	1.49
1	K	146	LYS	CG-CD	5.00	1.67	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	79	ARG	CG-CD-NE	12.09	138.60	112.00
1	M	156	ARG	N-CA-C	-10.46	100.70	113.15
1	L	6	SER	CA-C-N	-7.81	109.69	122.65
1	L	6	SER	C-N-CA	-7.81	109.69	122.65
1	M	156	ARG	NE-CZ-NH2	7.54	125.98	119.20
1	U	53	LYS	CD-CE-NZ	7.33	135.36	111.90
1	U	149	GLY	CA-C-N	-7.15	109.56	121.92
1	U	149	GLY	C-N-CA	-7.15	109.56	121.92
1	G	73	GLN	O-C-N	-6.98	113.31	122.59
1	N	83	GLN	CA-CB-CG	6.62	127.34	114.10
1	H	14	GLN	N-CA-C	-6.57	104.12	111.28
1	I	79	ARG	CD-NE-CZ	-6.56	115.21	124.40
1	M	53	LYS	CA-C-N	-6.41	110.38	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	53	LYS	C-N-CA	-6.41	110.38	121.66
1	U	83	GLN	CA-C-N	6.21	130.13	120.75
1	U	83	GLN	C-N-CA	6.21	130.13	120.75
1	D	71	LYS	N-CA-CB	-6.07	101.27	110.07
1	M	156	ARG	CA-CB-CG	5.92	125.95	114.10
1	C	25	ASN	N-CA-C	-5.88	106.73	112.97
1	Q	139	ASN	CB-CA-C	5.86	121.61	109.95
1	M	54	TYR	CA-C-N	-5.78	111.03	121.14
1	M	54	TYR	C-N-CA	-5.78	111.03	121.14
1	S	79	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	W	104	LEU	CA-C-N	5.45	128.99	120.82
1	W	104	LEU	C-N-CA	5.45	128.99	120.82
1	U	150	ASP	N-CA-C	-5.34	106.94	113.50
1	L	79	ARG	CA-CB-CG	-5.32	103.46	114.10
1	M	54	TYR	CD1-CG-CD2	-5.32	110.12	118.10
1	H	87	LYS	CD-CE-NZ	-5.12	95.51	111.90
1	J	28	LEU	CA-C-N	5.09	127.52	120.29
1	J	28	LEU	C-N-CA	5.09	127.52	120.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	50	ASN	Peptide
1	I	79	ARG	Sidechain
1	M	54	TYR	Sidechain
1	V	124	LYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1416	0	1362	81	0
1	B	1416	0	1362	81	0
1	C	1416	0	1362	105	0
1	D	1416	0	1362	124	0
1	E	1416	0	1362	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1416	0	1362	115	0
1	G	1416	0	1362	103	0
1	H	1416	0	1362	97	0
1	I	1416	0	1362	89	0
1	J	1416	0	1362	108	0
1	K	1416	0	1362	93	0
1	L	1416	0	1362	78	0
1	M	1416	0	1362	115	1
1	N	1416	0	1362	87	0
1	O	1413	0	1355	100	1
1	P	1416	0	1361	115	0
1	Q	1416	0	1362	111	0
1	R	1416	0	1362	113	0
1	S	1416	0	1362	62	0
1	T	1416	0	1362	99	0
1	U	1416	0	1362	108	0
1	V	1416	0	1362	96	0
1	W	1416	0	1362	73	0
1	X	1416	0	1362	123	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	S	2	0	0	0	0
2	W	1	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
All	All	34001	0	32680	2016	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 30.

All (2016) 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:O:157:LYS:NZ	1:O:157:LYS:CE	1.68	1.55
1:W:68:LYS:NZ	1:W:68:LYS:CE	1.80	1.43
1:R:37:MET:HE1	1:R:99:ALA:HB1	1.33	1.11
1:M:101:GLU:OE2	1:M:156:ARG:NH1	1.94	1.00
1:D:10:GLN:O	1:D:76:ARG:NH2	1.93	0.99
1:N:83:GLN:OE1	1:N:84:ASP:N	1.95	0.99
1:O:120:LEU:HA	1:O:123:PHE:HD2	1.28	0.97
1:L:10:GLN:O	1:L:76:ARG:NH2	2.00	0.94
1:R:157:LYS:NZ	1:U:46:VAL:O	2.02	0.93
1:J:77:GLY:O	1:J:79:ARG:NH1	2.02	0.93
1:R:11:ASN:ND2	1:R:125:ASN:O	2.03	0.91
1:U:131:ASP:HA	1:U:134:GLU:HB2	1.50	0.90
1:K:10:GLN:O	1:K:76:ARG:NH2	2.04	0.90
1:E:27:GLU:OE1	1:E:65:HIS:ND1	2.05	0.89
1:K:17:GLU:HG3	1:K:73:GLN:HE22	1.37	0.89
1:M:54:TYR:HD2	1:M:175:LEU:HD13	1.37	0.89
1:G:132:PHE:O	1:G:136:HIS:ND1	2.05	0.88
1:U:66:ALA:HA	1:U:69:LEU:HD12	1.56	0.88
1:R:15:ASP:HB2	1:R:124:LYS:HE3	1.55	0.87
1:O:44:ASP:OD1	1:O:45:ASP:N	2.06	0.87
1:B:48:LEU:HD21	1:B:167:GLU:HB3	1.55	0.87
1:M:133:ILE:HG22	1:M:138:LEU:HG	1.57	0.87
1:L:152:VAL:HG12	1:L:156:ARG:HH11	1.42	0.85
1:F:107:GLU:OE1	1:F:141:GLN:NE2	2.10	0.85
1:V:21:ASN:OD1	1:V:73:GLN:NE2	2.09	0.85
1:N:43:ARG:NH2	1:N:45:ASP:OD2	2.09	0.84
1:R:134:GLU:HA	1:R:138:LEU:HD12	1.59	0.84
1:F:111:ASN:HD22	1:F:141:GLN:CG	1.89	0.84
1:H:111:ASN:ND2	1:L:10:GLN:OE1	2.09	0.84
1:X:143:LYS:O	1:X:147:GLU:N	2.09	0.84
1:P:10:GLN:O	1:P:76:ARG:NH2	2.10	0.84
1:C:112:GLN:NE2	1:C:116:GLU:OE1	2.12	0.83
1:P:9:ARG:NH2	1:P:12:TYR:O	2.11	0.83
1:Q:153:THR:HG21	1:X:45:ASP:HA	1.60	0.83
1:J:24:ILE:HG12	1:J:69:LEU:HB3	1.59	0.83
1:M:42:ASP:OD1	1:M:49:LYS:NZ	2.11	0.83
1:G:18:ALA:HA	1:G:21:ASN:HB2	1.61	0.83
1:W:43:ARG:NH2	1:W:45:ASP:OD2	2.10	0.83
1:X:23:GLN:OE1	1:X:113:SER:OG	1.96	0.83
1:P:33:VAL:HG22	1:P:88:PRO:HG3	1.59	0.82
1:O:97:LEU:HD13	1:O:161:PRO:HD3	1.60	0.82
1:X:12:TYR:HB2	1:X:76:ARG:HE	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLN:O	1:C:76:ARG:NH2	2.12	0.82
1:C:43:ARG:NH2	1:C:45:ASP:OD2	2.11	0.82
1:D:153:THR:OG1	1:K:44:ASP:O	1.96	0.82
1:I:9:ARG:NH2	1:I:17:GLU:OE2	2.12	0.82
1:J:163:SER:HB3	1:J:166:ALA:HB2	1.62	0.82
1:R:139:ASN:OD1	1:R:143:LYS:NZ	2.13	0.82
1:C:85:ILE:HB	1:X:85:ILE:HB	1.60	0.82
1:F:111:ASN:HB2	1:F:141:GLN:HG2	1.60	0.82
1:V:9:ARG:NH2	1:V:13:HIS:O	2.12	0.82
1:D:34:TYR:HB3	1:D:59:SER:HB2	1.62	0.82
1:K:83:GLN:HA	1:P:87:LYS:HD2	1.62	0.82
1:L:62:GLU:OE1	1:L:65:HIS:ND1	2.13	0.81
1:H:39:TYR:HE1	1:R:71:LYS:HG3	1.45	0.81
1:N:62:GLU:OE1	1:N:65:HIS:ND1	2.13	0.81
1:J:156:ARG:NH1	1:U:7:GLN:OE1	2.13	0.81
1:Q:63:ARG:NH1	1:Q:64:GLU:OE2	2.14	0.81
1:N:111:ASN:ND2	1:W:10:GLN:OE1	2.12	0.81
1:R:62:GLU:OE1	1:R:62:GLU:N	2.14	0.81
1:S:6:SER:HB3	1:S:9:ARG:HG3	1.60	0.81
1:I:87:LYS:HB3	1:N:83:GLN:O	1.81	0.81
1:D:97:LEU:HD11	1:D:152:VAL:HG13	1.63	0.81
1:O:108:LYS:NZ	1:Q:9:ARG:O	2.14	0.80
1:B:174:THR:OG1	1:I:168:TYR:OH	1.98	0.80
1:E:131:ASP:HA	1:E:134:GLU:HB2	1.61	0.80
1:J:74:ASN:ND2	1:O:42:ASP:OD2	2.15	0.80
1:G:134:GLU:HB3	1:K:131:ASP:OD2	1.82	0.80
1:T:16:SER:O	1:T:20:ILE:HG12	1.82	0.80
1:O:108:LYS:HD3	1:Q:10:GLN:HE21	1.47	0.80
1:C:46:VAL:O	1:P:157:LYS:NZ	2.15	0.80
1:J:149:GLY:O	1:J:153:THR:OG1	1.99	0.79
1:M:150:ASP:O	1:M:154:ASN:ND2	2.16	0.79
1:O:104:LEU:HG	1:O:145:ILE:HG23	1.63	0.79
1:G:74:ASN:ND2	1:U:42:ASP:OD2	2.15	0.79
1:M:148:LEU:HA	1:M:151:HIS:HB2	1.63	0.78
1:X:37:MET:HE1	1:X:103:ALA:HB2	1.64	0.78
1:J:93:TRP:HB3	1:J:99:ALA:HB2	1.65	0.78
1:W:169:LEU:O	1:W:173:HIS:ND1	2.15	0.78
1:R:12:TYR:OH	1:R:73:GLN:OE1	1.98	0.78
1:R:31:SER:OG	1:R:59:SER:O	2.01	0.78
1:J:121:ALA:HB2	1:J:129:LEU:HD23	1.66	0.78
1:I:97:LEU:HD21	1:I:156:ARG:HE	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:HG1	1:I:168:TYR:HH	1.31	0.77
1:C:97:LEU:HA	1:C:155:LEU:HD13	1.67	0.77
1:G:32:TYR:OH	1:U:83:GLN:O	1.99	0.77
1:T:112:GLN:NE2	1:T:112:GLN:O	2.16	0.77
1:F:11:ASN:HD22	1:U:115:LEU:HD13	1.49	0.77
1:N:40:TYR:OH	1:N:94:GLU:O	2.02	0.77
1:M:119:LYS:O	1:M:122:THR:OG1	2.02	0.77
1:P:11:ASN:O	1:P:76:ARG:NH2	2.17	0.77
1:R:50:ASN:ND2	1:R:171:ASP:OD2	2.17	0.76
1:G:42:ASP:OD1	1:U:71:LYS:NZ	2.18	0.76
1:K:9:ARG:HG2	1:K:77:GLY:HA3	1.68	0.76
1:G:42:ASP:OD2	1:U:74:ASN:ND2	2.18	0.76
1:Q:9:ARG:NH2	1:Q:12:TYR:O	2.17	0.76
1:T:34:TYR:HA	1:T:37:MET:SD	2.25	0.76
1:A:31:SER:O	1:A:59:SER:OG	2.02	0.76
1:I:25:ASN:ND2	1:I:83:GLN:O	2.17	0.76
1:H:38:SER:OG	1:H:52:ALA:O	2.03	0.76
1:J:115:LEU:O	1:J:118:HIS:HB3	1.85	0.76
1:J:17:GLU:O	1:J:73:GLN:NE2	2.18	0.76
1:L:121:ALA:HB2	1:L:129:LEU:HD23	1.66	0.76
1:C:73:GLN:HE21	1:C:78:GLY:HA3	1.48	0.76
1:R:95:SER:OG	1:R:98:ASN:OD1	2.03	0.76
1:X:24:ILE:HG21	1:X:70:MET:HE3	1.67	0.76
1:O:65:HIS:HB3	1:O:137:TYR:HE1	1.50	0.76
1:T:168:TYR:HH	1:U:174:THR:HG1	1.31	0.76
1:D:158:MET:HE1	1:D:169:LEU:HB2	1.69	0.75
1:A:107:GLU:OE1	1:A:141:GLN:NE2	2.17	0.75
1:K:12:TYR:HB2	1:K:76:ARG:HH21	1.50	0.75
1:Q:131:ASP:HA	1:Q:134:GLU:HB2	1.66	0.75
1:T:7:GLN:HG3	1:T:8:VAL:HG13	1.66	0.75
1:A:134:GLU:HA	1:A:138:LEU:HD12	1.68	0.75
1:A:12:TYR:OH	1:A:17:GLU:HA	1.85	0.75
1:O:145:ILE:HG22	1:Q:8:VAL:HG12	1.69	0.75
1:G:63:ARG:NH2	1:U:59:SER:OG	2.19	0.74
1:S:79:ARG:HA	1:S:79:ARG:HE	1.50	0.74
1:H:14:GLN:O	1:H:18:ALA:N	2.14	0.74
1:X:73:GLN:HG3	1:X:78:GLY:O	1.87	0.74
1:U:133:ILE:HG22	1:U:138:LEU:HG	1.69	0.74
1:P:40:TYR:O	1:P:43:ARG:HB2	1.87	0.74
1:B:9:ARG:NH2	1:B:12:TYR:O	2.20	0.74
1:I:6:SER:OG	1:N:44:ASP:OD2	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:116:GLU:HA	1:O:119:LYS:HB2	1.69	0.74
1:D:131:ASP:HB2	1:X:134:GLU:HG3	1.70	0.74
1:H:48:LEU:HD21	1:H:168:TYR:HA	1.68	0.74
1:A:9:ARG:NH2	1:A:17:GLU:OE1	2.21	0.74
1:U:53:LYS:O	1:U:53:LYS:CD	2.36	0.74
1:J:85:ILE:HB	1:O:85:ILE:HB	1.70	0.73
1:M:49:LYS:O	1:M:52:ALA:N	2.21	0.73
1:V:98:ASN:O	1:V:100:MET:N	2.20	0.73
1:B:67:GLU:HA	1:B:70:MET:HE3	1.70	0.73
1:B:93:TRP:O	1:B:98:ASN:ND2	2.20	0.73
1:U:53:LYS:O	1:U:53:LYS:HD2	1.89	0.73
1:D:168:TYR:OH	1:M:174:THR:OG1	2.07	0.73
1:I:138:LEU:O	1:T:128:HIS:ND1	2.20	0.73
1:M:92:ASP:OD1	1:M:93:TRP:N	2.22	0.73
1:B:11:ASN:O	1:B:76:ARG:NH2	2.22	0.73
1:X:158:MET:HE1	1:X:170:PHE:HB2	1.70	0.73
1:A:94:GLU:OE1	1:A:98:ASN:ND2	2.21	0.73
1:L:54:TYR:OH	1:L:147:GLU:OE2	2.05	0.73
1:M:54:TYR:CD2	1:M:175:LEU:HD13	2.23	0.73
1:N:65:HIS:O	1:N:137:TYR:OH	2.06	0.73
1:Q:7:GLN:HG3	1:Q:8:VAL:HG13	1.69	0.73
1:S:31:SER:OG	1:S:59:SER:O	2.04	0.73
1:D:25:ASN:HA	1:D:28:LEU:HD12	1.71	0.73
1:F:73:GLN:HG2	1:F:80:ILE:HG12	1.69	0.73
1:R:66:ALA:HA	1:R:69:LEU:HD12	1.69	0.73
1:R:155:LEU:HD23	1:R:158:MET:HE3	1.69	0.72
1:W:36:SER:O	1:W:93:TRP:NE1	2.22	0.72
1:D:128:HIS:HA	1:X:138:LEU:HD13	1.70	0.72
1:N:94:GLU:OE2	1:N:98:ASN:ND2	2.23	0.72
1:O:112:GLN:NE2	1:O:116:GLU:OE1	2.21	0.72
1:G:41:PHE:CD2	1:G:51:PHE:HB3	2.25	0.72
1:Q:19:ALA:HA	1:Q:22:ARG:HD3	1.69	0.72
1:W:31:SER:OG	1:W:59:SER:O	2.07	0.72
1:C:108:LYS:NZ	1:O:7:GLN:O	2.22	0.72
1:V:65:HIS:NE2	1:V:140:GLU:OE1	2.23	0.72
1:J:21:ASN:HA	1:J:24:ILE:HD12	1.71	0.72
1:O:43:ARG:NH2	1:O:45:ASP:OD2	2.22	0.72
1:P:134:GLU:HA	1:P:138:LEU:HB2	1.72	0.72
1:V:43:ARG:NH2	1:V:45:ASP:OD2	2.21	0.72
1:F:127:PRO:HA	1:F:130:CYS:HB2	1.71	0.71
1:O:115:LEU:O	1:O:119:LYS:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:18:ALA:O	1:T:21:ASN:N	2.22	0.71
1:L:41:PHE:HA	1:L:46:VAL:HG11	1.70	0.71
1:M:78:GLY:O	1:M:79:ARG:NH1	2.22	0.71
1:O:50:ASN:HA	1:O:53:LYS:HG3	1.70	0.71
1:O:120:LEU:HA	1:O:123:PHE:CD2	2.19	0.71
1:D:173:HIS:O	1:K:172:LYS:NZ	2.23	0.71
1:H:26:LEU:HD11	1:H:110:VAL:HG22	1.73	0.71
1:V:124:LYS:N	1:V:124:LYS:HD2	2.05	0.71
1:X:164:GLY:HA2	1:X:167:GLU:OE2	1.89	0.71
1:G:107:GLU:OE1	1:G:141:GLN:NE2	2.19	0.71
1:Q:15:ASP:HB3	1:Q:120:LEU:HD21	1.73	0.71
1:Q:77:GLY:O	1:Q:79:ARG:NH2	2.22	0.71
1:W:64:GLU:HG2	1:W:68:LYS:HZ2	1.55	0.71
1:B:44:ASP:O	1:Q:7:GLN:NE2	2.24	0.71
1:F:36:SER:OG	1:F:88:PRO:HG2	1.90	0.71
1:F:37:MET:O	1:F:40:TYR:N	2.22	0.71
1:P:50:ASN:HA	1:P:53:LYS:HE2	1.73	0.71
1:X:87:LYS:NZ	1:X:88:PRO:O	2.24	0.71
1:D:7:GLN:NE2	1:X:149:GLY:O	2.24	0.71
1:M:129:LEU:O	1:M:133:ILE:HG12	1.90	0.71
1:M:50:ASN:HA	1:M:53:LYS:HG2	1.72	0.70
1:A:66:ALA:HA	1:A:69:LEU:HD13	1.71	0.70
1:J:42:ASP:OD2	1:O:71:LYS:NZ	2.22	0.70
1:K:6:SER:OG	1:P:44:ASP:OD2	2.09	0.70
1:L:63:ARG:NH2	1:L:67:GLU:OE1	2.24	0.70
1:N:43:ARG:HB2	1:N:46:VAL:HG22	1.73	0.70
1:T:8:VAL:O	1:T:10:GLN:N	2.23	0.70
1:F:111:ASN:OD1	1:F:111:ASN:O	2.09	0.70
1:R:21:ASN:HA	1:R:24:ILE:HD12	1.71	0.70
1:H:71:LYS:NZ	1:R:42:ASP:OD1	2.25	0.70
1:E:154:ASN:HB3	1:E:170:PHE:HE2	1.55	0.70
1:P:19:ALA:HA	1:P:22:ARG:HG3	1.72	0.70
1:J:9:ARG:HG3	1:J:12:TYR:HB3	1.72	0.69
1:X:11:ASN:O	1:X:11:ASN:ND2	2.25	0.69
1:A:142:VAL:HG21	1:M:76:ARG:HD2	1.74	0.69
1:C:165:LEU:HD13	1:P:158:MET:HB3	1.73	0.69
1:E:44:ASP:OD1	1:E:44:ASP:N	2.23	0.69
1:F:108:LYS:NZ	1:J:7:GLN:O	2.25	0.69
1:U:118:HIS:NE2	1:U:134:GLU:OE2	2.25	0.69
1:P:146:LYS:HD3	1:X:75:GLN:HA	1.74	0.69
1:A:72:LEU:HD11	1:A:128:HIS:CE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:61:GLU:O	1:T:65:HIS:ND1	2.25	0.69
1:D:85:ILE:HB	1:V:85:ILE:HB	1.75	0.69
1:F:7:GLN:O	1:U:108:LYS:NZ	2.26	0.69
1:J:142:VAL:HA	1:J:145:ILE:HD12	1.75	0.69
1:O:38:SER:OG	1:O:52:ALA:O	2.09	0.69
1:R:9:ARG:NH2	1:R:12:TYR:O	2.23	0.69
1:V:27:GLU:HG2	1:V:65:HIS:HB3	1.75	0.69
1:C:139:ASN:HA	1:O:128:HIS:CD2	2.28	0.69
1:G:40:TYR:OH	1:G:94:GLU:O	2.11	0.69
1:U:134:GLU:HA	1:U:138:LEU:HD12	1.73	0.69
1:V:94:GLU:HG3	1:V:98:ASN:HD22	1.58	0.69
1:G:141:GLN:O	1:G:144:ALA:N	2.26	0.68
1:Q:12:TYR:CE2	1:Q:17:GLU:HB3	2.27	0.68
1:H:118:HIS:O	1:H:122:THR:OG1	2.05	0.68
1:B:44:ASP:OD2	1:Q:6:SER:OG	2.10	0.68
1:B:114:LEU:O	1:B:116:GLU:N	2.27	0.68
1:L:118:HIS:O	1:L:122:THR:OG1	2.10	0.68
1:G:34:TYR:CE2	1:G:58:GLN:HB3	2.29	0.68
1:G:118:HIS:HE1	1:G:134:GLU:HG3	1.57	0.68
1:B:114:LEU:O	1:B:117:LEU:N	2.26	0.68
1:B:114:LEU:HA	1:B:117:LEU:HD12	1.75	0.68
1:G:100:MET:HB3	1:G:152:VAL:HG12	1.75	0.68
1:H:168:TYR:OH	1:K:174:THR:OG1	2.12	0.68
1:M:146:LYS:HZ1	1:V:74:ASN:C	2.01	0.68
1:B:57:HIS:NE2	1:B:61:GLU:OE1	2.27	0.68
1:C:97:LEU:HD13	1:C:155:LEU:HB3	1.74	0.68
1:G:119:LYS:HE3	1:K:125:ASN:HB3	1.76	0.68
1:H:107:GLU:OE2	1:H:141:GLN:NE2	2.26	0.68
1:F:150:ASP:OD1	1:O:44:ASP:HA	1.93	0.68
1:O:148:LEU:O	1:O:152:VAL:N	2.26	0.68
1:R:15:ASP:CB	1:R:124:LYS:HE3	2.23	0.68
1:B:63:ARG:NH1	1:Q:63:ARG:HD2	2.09	0.68
1:B:157:LYS:HG3	1:I:164:GLY:HA3	1.76	0.68
1:E:53:LYS:HE2	1:E:53:LYS:HA	1.74	0.68
1:S:165:LEU:O	1:S:169:LEU:HD12	1.92	0.68
1:B:83:GLN:HA	1:Q:87:LYS:HD2	1.76	0.68
1:F:48:LEU:HD22	1:F:171:ASP:HB2	1.74	0.68
1:I:27:GLU:HG2	1:I:65:HIS:HB2	1.75	0.68
1:V:114:LEU:HA	1:V:117:LEU:HB3	1.74	0.68
1:C:71:LYS:O	1:C:75:GLN:N	2.22	0.67
1:C:139:ASN:OD1	1:O:128:HIS:NE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:ASN:HA	1:J:28:LEU:HD12	1.77	0.67
1:Q:120:LEU:O	1:Q:124:LYS:N	2.28	0.67
1:D:65:HIS:CE1	1:D:140:GLU:HG3	2.29	0.67
1:E:74:ASN:ND2	1:S:42:ASP:OD2	2.20	0.67
1:P:70:MET:O	1:P:74:ASN:ND2	2.27	0.67
1:S:92:ASP:OD1	1:S:93:TRP:N	2.26	0.67
1:M:65:HIS:HD2	1:M:137:TYR:HE1	1.41	0.67
1:D:68:LYS:HB3	1:D:132:PHE:HZ	1.59	0.67
1:F:45:ASP:OD2	1:T:79:ARG:NH2	2.28	0.67
1:G:45:ASP:OD1	1:G:45:ASP:N	2.26	0.67
1:J:133:ILE:HG23	1:J:137:TYR:HB2	1.75	0.67
1:T:112:GLN:HA	1:T:115:LEU:HD12	1.77	0.67
1:F:146:LYS:HZ3	1:J:74:ASN:HB3	1.60	0.67
1:A:145:ILE:HG13	1:A:146:LYS:N	2.10	0.67
1:C:29:TYR:O	1:C:33:VAL:HG23	1.94	0.67
1:D:13:HIS:CD2	1:D:15:ASP:HB2	2.29	0.67
1:K:111:ASN:ND2	1:R:10:GLN:OE1	2.27	0.67
1:W:67:GLU:O	1:W:71:LYS:N	2.26	0.67
1:K:131:ASP:HA	1:K:134:GLU:HB2	1.77	0.67
1:W:64:GLU:HG2	1:W:68:LYS:NZ	2.09	0.67
1:D:50:ASN:ND2	1:D:171:ASP:O	2.16	0.66
1:O:41:PHE:HA	1:O:46:VAL:HG11	1.77	0.66
1:C:112:GLN:HA	1:C:115:LEU:HB2	1.75	0.66
1:G:145:ILE:HG22	1:K:8:VAL:HG12	1.76	0.66
1:J:20:ILE:O	1:J:24:ILE:HG13	1.94	0.66
1:O:65:HIS:HB3	1:O:137:TYR:CE1	2.29	0.66
1:F:105:HIS:CE1	1:F:109:ASN:HD21	2.13	0.66
1:F:134:GLU:HG2	1:J:131:ASP:HB2	1.76	0.66
1:K:171:ASP:HA	1:K:175:LEU:HD23	1.75	0.66
1:B:84:ASP:OD1	1:Q:87:LYS:N	2.26	0.66
1:V:12:TYR:OH	1:V:73:GLN:OE1	2.13	0.66
1:D:42:ASP:OD1	1:V:71:LYS:NZ	2.19	0.66
1:F:171:ASP:HA	1:F:175:LEU:HD12	1.78	0.66
1:I:86:LYS:HD3	1:N:84:ASP:OD1	1.96	0.66
1:J:5:THR:HG22	1:J:6:SER:H	1.60	0.66
1:P:12:TYR:OH	1:P:20:ILE:HG13	1.94	0.66
1:S:23:GLN:OE1	1:S:113:SER:OG	2.13	0.66
1:M:155:LEU:C	1:M:157:LYS:H	2.01	0.66
1:R:10:GLN:O	1:R:76:ARG:NH2	2.28	0.66
1:V:62:GLU:OE2	1:V:141:GLN:NE2	2.29	0.66
1:M:156:ARG:HA	1:M:160:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:172:LYS:HE3	1:T:173:HIS:HB3	1.77	0.66
1:V:6:SER:HB3	1:V:9:ARG:HB2	1.78	0.66
1:T:33:VAL:O	1:T:36:SER:OG	2.12	0.66
1:X:9:ARG:NH1	1:X:12:TYR:O	2.28	0.66
1:F:70:MET:HE1	1:T:35:LEU:HD21	1.78	0.66
1:H:97:LEU:HD11	1:H:156:ARG:HG2	1.77	0.66
1:H:153:THR:HG21	1:M:45:ASP:HA	1.77	0.66
1:K:33:VAL:HG12	1:K:37:MET:HE3	1.78	0.66
1:T:17:GLU:OE1	1:T:79:ARG:N	2.25	0.66
1:E:18:ALA:O	1:E:22:ARG:NH2	2.28	0.65
1:G:138:LEU:HD11	1:K:127:PRO:HG2	1.78	0.65
1:V:120:LEU:HG	1:V:124:LYS:HD3	1.77	0.65
1:C:29:TYR:OH	1:C:88:PRO:HA	1.96	0.65
1:E:11:ASN:O	1:E:76:ARG:NH2	2.29	0.65
1:I:118:HIS:ND1	1:I:122:THR:OG1	2.29	0.65
1:R:127:PRO:HA	1:R:130:CYS:HB2	1.78	0.65
1:E:65:HIS:O	1:E:137:TYR:OH	2.14	0.65
1:K:154:ASN:O	1:K:158:MET:N	2.30	0.65
1:C:7:GLN:O	1:Q:108:LYS:NZ	2.30	0.65
1:J:6:SER:HB2	1:J:79:ARG:HH12	1.62	0.65
1:S:79:ARG:HA	1:S:79:ARG:NE	2.10	0.65
1:S:158:MET:HE2	1:S:166:ALA:HB1	1.77	0.65
1:T:15:ASP:OD2	1:T:124:LYS:NZ	2.29	0.65
1:T:29:TYR:O	1:T:33:VAL:HG23	1.97	0.65
1:E:111:ASN:ND2	1:I:10:GLN:OE1	2.30	0.65
1:S:33:VAL:HG12	1:S:37:MET:HE3	1.78	0.65
1:C:33:VAL:O	1:C:37:MET:HG3	1.96	0.65
1:D:28:LEU:HD22	1:D:85:ILE:HD11	1.79	0.65
1:T:44:ASP:O	1:U:153:THR:OG1	2.10	0.65
1:J:87:LYS:N	1:O:84:ASP:OD1	2.24	0.65
1:B:43:ARG:NH2	1:B:45:ASP:OD2	2.30	0.65
1:H:171:ASP:HA	1:H:175:LEU:HD12	1.79	0.65
1:J:62:GLU:O	1:J:65:HIS:HB2	1.96	0.65
1:J:124:LYS:HE2	1:J:124:LYS:HA	1.78	0.65
1:G:87:LYS:NZ	1:G:89:ASP:O	2.31	0.64
1:Q:61:GLU:HA	1:Q:64:GLU:HG2	1.77	0.64
1:X:47:ALA:HA	1:X:49:LYS:NZ	2.12	0.64
1:D:113:SER:O	1:D:117:LEU:N	2.25	0.64
1:F:139:ASN:O	1:F:143:LYS:NZ	2.28	0.64
1:H:146:LYS:HD3	1:L:75:GLN:HA	1.78	0.64
1:X:93:TRP:O	1:X:95:SER:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASP:OD2	1:E:135:THR:OG1	2.15	0.64
1:R:51:PHE:N	1:R:171:ASP:OD1	2.30	0.64
1:A:131:ASP:OD1	1:A:135:THR:OG1	2.16	0.64
1:A:174:THR:OG1	1:L:168:TYR:OH	2.15	0.64
1:J:23:GLN:HG3	1:J:117:LEU:HD12	1.78	0.64
1:R:95:SER:O	1:R:99:ALA:N	2.30	0.64
1:V:19:ALA:HA	1:V:22:ARG:HG2	1.78	0.64
1:G:117:LEU:HA	1:G:120:LEU:HB3	1.80	0.64
1:S:27:GLU:CD	1:S:65:HIS:HB3	2.22	0.64
1:Q:43:ARG:O	1:Q:47:ALA:N	2.29	0.64
1:F:130:CYS:O	1:F:134:GLU:HB2	1.97	0.64
1:G:23:GLN:HE22	1:G:113:SER:HB3	1.63	0.64
1:G:26:LEU:HD11	1:G:110:VAL:HG22	1.79	0.64
1:P:23:GLN:OE1	1:P:26:LEU:HD23	1.97	0.64
1:P:133:ILE:HG22	1:P:138:LEU:HG	1.79	0.64
1:Q:41:PHE:CD2	1:Q:51:PHE:HB3	2.33	0.64
1:T:168:TYR:O	1:T:171:ASP:HB3	1.98	0.64
1:H:158:MET:HB3	1:H:166:ALA:HB1	1.80	0.64
1:M:97:LEU:HD11	1:M:156:ARG:HG2	1.80	0.64
1:U:111:ASN:O	1:U:115:LEU:N	2.22	0.64
1:X:34:TYR:HE2	1:X:62:GLU:HG3	1.63	0.64
1:R:62:GLU:HA	1:R:65:HIS:CG	2.33	0.64
1:R:87:LYS:NZ	1:R:88:PRO:O	2.31	0.64
1:E:119:LYS:O	1:E:122:THR:HB	1.98	0.63
1:G:118:HIS:CE1	1:K:127:PRO:HB2	2.33	0.63
1:K:98:ASN:HA	1:K:101:GLU:CD	2.23	0.63
1:O:41:PHE:HA	1:O:46:VAL:CG1	2.27	0.63
1:D:107:GLU:O	1:D:141:GLN:NE2	2.31	0.63
1:H:34:TYR:OH	1:H:107:GLU:OE1	2.13	0.63
1:U:65:HIS:O	1:U:137:TYR:OH	2.14	0.63
1:B:43:ARG:HB3	1:B:45:ASP:OD1	1.98	0.63
1:C:127:PRO:HA	1:C:130:CYS:SG	2.37	0.63
1:E:148:LEU:O	1:E:152:VAL:HG23	1.99	0.63
1:T:34:TYR:O	1:T:37:MET:HB2	1.97	0.63
1:C:69:LEU:HD21	1:C:137:TYR:HE2	1.63	0.63
1:D:20:ILE:HD13	1:D:117:LEU:HD21	1.80	0.63
1:F:111:ASN:HD22	1:F:141:GLN:HG3	1.64	0.63
1:H:103:ALA:O	1:H:106:LEU:N	2.31	0.63
1:P:9:ARG:NH1	1:P:17:GLU:OE1	2.24	0.63
1:M:131:ASP:HA	1:M:134:GLU:HB2	1.80	0.63
1:S:62:GLU:HA	1:S:65:HIS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:GLN:NE2	1:U:108:LYS:O	2.29	0.63
1:O:9:ARG:NH1	1:O:17:GLU:OE1	2.32	0.63
1:Q:93:TRP:O	1:Q:95:SER:N	2.30	0.63
1:P:154:ASN:O	1:P:158:MET:HG3	1.99	0.63
1:Q:98:ASN:HA	1:Q:101:GLU:OE2	1.99	0.63
1:T:76:ARG:C	1:T:78:GLY:H	2.07	0.63
1:U:28:LEU:O	1:U:31:SER:OG	2.14	0.63
1:B:45:ASP:OD1	1:B:45:ASP:N	2.29	0.63
1:I:32:TYR:HE2	1:I:87:LYS:HA	1.64	0.63
1:L:58:GLN:HA	1:L:61:GLU:HB2	1.81	0.63
1:T:32:TYR:CD2	1:T:88:PRO:HD3	2.34	0.63
1:A:145:ILE:HD12	1:M:8:VAL:HB	1.81	0.62
1:D:35:LEU:HD21	1:V:70:MET:HE1	1.80	0.62
1:J:158:MET:HE1	1:J:170:PHE:HB2	1.80	0.62
1:D:128:HIS:CE1	1:X:142:VAL:HG21	2.35	0.62
1:M:96:GLY:N	1:M:167:GLU:OE1	2.32	0.62
1:B:133:ILE:HG22	1:B:138:LEU:HG	1.80	0.62
1:C:142:VAL:O	1:O:75:GLN:NE2	2.26	0.62
1:D:13:HIS:CD2	1:D:15:ASP:H	2.16	0.62
1:V:40:TYR:OH	1:V:94:GLU:O	2.16	0.62
1:I:79:ARG:NE	1:N:43:ARG:NE	2.47	0.62
1:K:27:GLU:N	1:K:27:GLU:OE1	2.32	0.62
1:R:97:LEU:HD13	1:R:161:PRO:HD3	1.82	0.62
1:X:107:GLU:O	1:X:110:VAL:N	2.31	0.62
1:A:72:LEU:HA	1:A:75:GLN:CD	2.24	0.62
1:B:63:ARG:HH12	1:Q:63:ARG:HD2	1.65	0.62
1:D:158:MET:HE2	1:D:166:ALA:HA	1.81	0.62
1:L:103:ALA:O	1:L:106:LEU:HB3	2.00	0.62
1:M:49:LYS:HE2	1:M:49:LYS:HA	1.80	0.62
1:O:116:GLU:O	1:O:120:LEU:N	2.30	0.62
1:Q:168:TYR:HD2	1:Q:169:LEU:HD23	1.65	0.62
1:I:74:ASN:ND2	1:N:42:ASP:HB3	2.15	0.62
1:H:29:TYR:HA	1:H:85:ILE:HG23	1.82	0.62
1:A:12:TYR:CE1	1:A:16:SER:HB2	2.35	0.61
1:E:133:ILE:HG22	1:E:138:LEU:HG	1.82	0.61
1:F:146:LYS:NZ	1:J:74:ASN:HB3	2.15	0.61
1:G:128:HIS:ND1	1:G:129:LEU:HD12	2.15	0.61
1:L:54:TYR:HH	1:L:147:GLU:CD	2.07	0.61
1:A:111:ASN:HD22	1:M:10:GLN:HE22	1.48	0.61
1:H:34:TYR:HE2	1:H:62:GLU:HG3	1.65	0.61
1:M:112:GLN:O	1:M:116:GLU:N	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:20:ILE:HD13	1:Q:117:LEU:HD11	1.82	0.61
1:U:24:ILE:HG23	1:U:66:ALA:HB1	1.81	0.61
1:U:38:SER:OG	1:U:39:TYR:N	2.28	0.61
1:W:9:ARG:NH2	1:W:13:HIS:O	2.33	0.61
1:D:110:VAL:HB	1:D:141:GLN:NE2	2.16	0.61
1:I:32:TYR:CE2	1:I:87:LYS:HA	2.35	0.61
1:O:29:TYR:O	1:O:33:VAL:N	2.33	0.61
1:X:60:HIS:CG	1:X:63:ARG:HH21	2.17	0.61
1:C:33:VAL:HG12	1:C:37:MET:HE2	1.82	0.61
1:D:101:GLU:OE2	1:D:156:ARG:NH2	2.33	0.61
1:D:170:PHE:C	1:D:172:LYS:H	2.08	0.61
1:N:16:SER:O	1:N:20:ILE:HG12	2.00	0.61
1:R:12:TYR:HB2	1:R:76:ARG:NH2	2.15	0.61
1:H:11:ASN:ND2	1:H:11:ASN:O	2.33	0.61
1:H:93:TRP:O	1:H:95:SER:N	2.33	0.61
1:J:114:LEU:HD22	1:J:133:ILE:CG2	2.30	0.61
1:O:131:ASP:OD1	1:O:135:THR:OG1	2.19	0.61
1:W:13:HIS:O	1:W:16:SER:OG	2.16	0.61
1:H:87:LYS:HD2	1:H:88:PRO:O	2.01	0.61
1:I:79:ARG:HE	1:N:43:ARG:NE	1.98	0.61
1:R:36:SER:O	1:R:93:TRP:NE1	2.33	0.61
1:D:12:TYR:OH	1:D:73:GLN:OE1	2.15	0.61
1:N:23:GLN:NE2	1:N:113:SER:OG	2.23	0.61
1:T:63:ARG:NE	1:T:67:GLU:OE1	2.34	0.61
1:W:93:TRP:O	1:W:95:SER:N	2.30	0.61
1:X:150:ASP:OD1	1:X:150:ASP:N	2.33	0.61
1:R:99:ALA:O	1:R:101:GLU:N	2.34	0.61
1:B:65:HIS:NE2	1:B:140:GLU:OE1	2.22	0.61
1:I:131:ASP:HA	1:I:134:GLU:HB2	1.83	0.61
1:R:40:TYR:O	1:R:43:ARG:HD3	2.01	0.61
1:G:115:LEU:O	1:G:119:LYS:HG2	2.01	0.60
1:K:98:ASN:HA	1:K:101:GLU:OE1	2.01	0.60
1:P:12:TYR:OH	1:P:73:GLN:OE1	2.16	0.60
1:R:19:ALA:HA	1:R:22:ARG:HE	1.65	0.60
1:R:113:SER:O	1:R:117:LEU:N	2.32	0.60
1:R:169:LEU:O	1:R:173:HIS:N	2.33	0.60
1:Q:65:HIS:O	1:Q:137:TYR:OH	2.16	0.60
1:F:43:ARG:HG2	1:T:74:ASN:OD1	2.02	0.60
1:G:13:HIS:CD2	1:G:124:LYS:HD2	2.36	0.60
1:J:111:ASN:O	1:J:114:LEU:HB2	2.00	0.60
1:M:119:LYS:HG3	1:M:120:LEU:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:61:GLU:O	1:O:65:HIS:ND1	2.34	0.60
1:W:65:HIS:O	1:W:68:LYS:HB2	2.01	0.60
1:X:11:ASN:ND2	1:X:125:ASN:O	2.27	0.60
1:B:170:PHE:HA	1:I:168:TYR:OH	2.01	0.60
1:C:72:LEU:HD22	1:C:132:PHE:HE2	1.66	0.60
1:G:10:GLN:NE2	1:R:108:LYS:O	2.20	0.60
1:N:31:SER:O	1:N:59:SER:OG	2.20	0.60
1:W:23:GLN:OE1	1:W:113:SER:OG	2.19	0.60
1:E:111:ASN:HB3	1:I:10:GLN:HE22	1.66	0.60
1:U:72:LEU:O	1:U:76:ARG:HG2	2.00	0.60
1:V:17:GLU:OE1	1:V:79:ARG:N	2.32	0.60
1:K:174:THR:HB	1:K:175:LEU:HD22	1.84	0.60
1:U:43:ARG:NH2	1:U:45:ASP:OD2	2.29	0.60
1:P:54:TYR:O	1:P:58:GLN:HG2	2.02	0.60
1:E:127:PRO:HA	1:E:130:CYS:SG	2.42	0.60
1:L:65:HIS:O	1:L:137:TYR:OH	2.18	0.60
1:N:73:GLN:HG2	1:N:80:ILE:HG13	1.83	0.60
1:R:23:GLN:NE2	1:R:23:GLN:O	2.34	0.60
1:T:34:TYR:CE2	1:T:58:GLN:HG3	2.37	0.60
1:W:138:LEU:O	1:W:142:VAL:HG23	2.01	0.60
1:K:68:LYS:HB3	1:K:137:TYR:OH	2.02	0.60
1:U:95:SER:H	1:U:98:ASN:HB3	1.67	0.60
1:V:19:ALA:HA	1:V:22:ARG:HE	1.66	0.60
1:K:21:ASN:ND2	1:K:81:PHE:H	2.00	0.60
1:D:19:ALA:HA	1:D:22:ARG:HD2	1.83	0.59
1:E:84:ASP:OD1	1:S:87:LYS:N	2.35	0.59
1:H:9:ARG:NE	1:H:12:TYR:HB3	2.16	0.59
1:H:65:HIS:HB3	1:H:137:TYR:HE2	1.67	0.59
1:L:24:ILE:HD13	1:L:70:MET:HG3	1.84	0.59
1:L:145:ILE:HG22	1:S:8:VAL:HG12	1.83	0.59
1:O:98:ASN:O	1:O:101:GLU:HB2	2.02	0.59
1:C:146:LYS:HB2	1:O:75:GLN:HG3	1.83	0.59
1:D:53:LYS:HA	1:D:56:LEU:HB3	1.84	0.59
1:G:87:LYS:NZ	1:G:88:PRO:O	2.27	0.59
1:H:82:LEU:O	1:R:87:LYS:HE2	2.02	0.59
1:I:150:ASP:O	1:I:154:ASN:HB2	2.01	0.59
1:E:25:ASN:O	1:E:29:TYR:N	2.29	0.59
1:H:61:GLU:O	1:H:65:HIS:ND1	2.34	0.59
1:H:131:ASP:HA	1:H:134:GLU:HB2	1.85	0.59
1:M:65:HIS:CD2	1:M:137:TYR:HE1	2.21	0.59
1:T:148:LEU:O	1:T:152:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:OG	1:A:7:GLN:N	2.35	0.59
1:A:133:ILE:HG22	1:A:138:LEU:HG	1.84	0.59
1:M:24:ILE:HD13	1:M:70:MET:HG2	1.85	0.59
1:M:131:ASP:O	1:M:135:THR:N	2.35	0.59
1:S:120:LEU:O	1:S:124:LYS:HG2	2.02	0.59
1:U:9:ARG:HE	1:U:12:TYR:HD2	1.49	0.59
1:E:87:LYS:HD2	1:E:88:PRO:O	2.02	0.59
1:P:115:LEU:HB3	1:P:119:LYS:NZ	2.18	0.59
1:Q:127:PRO:HA	1:Q:130:CYS:HB2	1.84	0.59
1:E:174:THR:OG1	1:N:168:TYR:OH	2.20	0.59
1:J:28:LEU:HB3	1:J:85:ILE:HG12	1.84	0.59
1:J:155:LEU:HB3	1:J:160:ALA:HB3	1.83	0.59
1:S:72:LEU:C	1:S:72:LEU:HD23	2.28	0.59
1:T:29:TYR:OH	1:T:86:LYS:NZ	2.25	0.59
1:F:10:GLN:HE22	1:U:108:LYS:C	2.10	0.59
1:O:76:ARG:HH12	1:O:128:HIS:HB3	1.66	0.59
1:P:111:ASN:HB3	1:X:10:GLN:NE2	2.17	0.59
1:V:9:ARG:NH2	1:V:17:GLU:OE2	2.34	0.59
1:I:18:ALA:HA	1:I:21:ASN:OD1	2.03	0.58
1:J:58:GLN:O	1:J:62:GLU:N	2.30	0.58
1:R:65:HIS:O	1:R:137:TYR:OH	2.12	0.58
1:S:73:GLN:HG2	1:S:80:ILE:HG12	1.85	0.58
1:U:139:ASN:O	1:U:143:LYS:NZ	2.35	0.58
1:W:17:GLU:HB2	1:W:73:GLN:HE22	1.68	0.58
1:B:6:SER:OG	1:Q:44:ASP:OD2	2.21	0.58
1:C:138:LEU:HG	1:O:128:HIS:HB2	1.83	0.58
1:E:134:GLU:HA	1:E:138:LEU:HD12	1.84	0.58
1:G:151:HIS:O	1:G:155:LEU:HD13	2.03	0.58
1:I:15:ASP:O	1:I:18:ALA:N	2.36	0.58
1:Q:71:LYS:HG3	1:Q:75:GLN:HG3	1.85	0.58
1:F:36:SER:HG	1:F:88:PRO:HG2	1.68	0.58
1:G:56:LEU:HG	1:G:60:HIS:CE1	2.38	0.58
1:H:63:ARG:HH12	1:R:60:HIS:CD2	2.21	0.58
1:M:51:PHE:N	1:M:171:ASP:OD2	2.36	0.58
1:B:50:ASN:HB2	1:B:171:ASP:CG	2.28	0.58
1:P:68:LYS:HE2	1:P:136:HIS:CG	2.38	0.58
1:Q:19:ALA:HA	1:Q:22:ARG:HB2	1.85	0.58
1:X:50:ASN:HB3	1:X:175:LEU:HB2	1.83	0.58
1:D:72:LEU:HA	1:D:75:GLN:HB2	1.86	0.58
1:I:9:ARG:HG3	1:I:12:TYR:HB3	1.85	0.58
1:K:41:PHE:HD1	1:K:46:VAL:HG11	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:GLU:HA	1:O:70:MET:SD	2.43	0.58
1:V:44:ASP:OD1	1:V:45:ASP:N	2.36	0.58
1:E:66:ALA:O	1:E:70:MET:HG3	2.03	0.58
1:J:58:GLN:O	1:J:62:GLU:HG2	2.03	0.58
1:L:152:VAL:O	1:L:156:ARG:HB2	2.02	0.58
1:O:9:ARG:NH2	1:O:12:TYR:O	2.37	0.58
1:C:20:ILE:O	1:C:23:GLN:N	2.36	0.58
1:P:127:PRO:HA	1:P:130:CYS:HB2	1.84	0.58
1:V:62:GLU:OE2	1:V:65:HIS:ND1	2.36	0.58
1:W:68:LYS:NZ	1:W:68:LYS:CD	2.67	0.58
1:D:170:PHE:HA	1:K:168:TYR:OH	2.04	0.58
1:F:73:GLN:HG2	1:F:80:ILE:CG1	2.34	0.58
1:C:131:ASP:HA	1:C:134:GLU:OE1	2.04	0.58
1:F:67:GLU:HA	1:F:70:MET:HE3	1.86	0.58
1:R:68:LYS:HE2	1:R:137:TYR:CZ	2.38	0.58
1:C:41:PHE:HB3	1:C:48:LEU:O	2.03	0.58
1:S:72:LEU:HA	1:S:75:GLN:HB2	1.85	0.58
1:X:134:GLU:HA	1:X:138:LEU:HD12	1.85	0.58
1:G:75:GLN:HA	1:R:146:LYS:HD3	1.86	0.57
1:M:106:LEU:O	1:M:109:ASN:N	2.37	0.57
1:R:51:PHE:HE2	1:R:96:GLY:HA3	1.69	0.57
1:F:84:ASP:OD1	1:F:85:ILE:N	2.34	0.57
1:G:120:LEU:HD11	1:G:124:LYS:HE2	1.86	0.57
1:R:97:LEU:O	1:R:101:GLU:HG3	2.04	0.57
1:S:27:GLU:OE2	1:S:65:HIS:ND1	2.37	0.57
1:S:137:TYR:O	1:S:141:GLN:HG2	2.04	0.57
1:V:61:GLU:O	1:V:64:GLU:HG2	2.04	0.57
1:X:11:ASN:O	1:X:76:ARG:NH2	2.38	0.57
1:G:11:ASN:O	1:G:76:ARG:NH2	2.38	0.57
1:I:40:TYR:O	1:I:43:ARG:HG3	2.04	0.57
1:J:57:HIS:HB3	1:J:58:GLN:NE2	2.18	0.57
1:J:144:ALA:HA	1:J:147:GLU:HB3	1.86	0.57
1:M:158:MET:HB2	1:M:166:ALA:HB1	1.87	0.57
1:T:56:LEU:HG	1:T:60:HIS:CE1	2.38	0.57
1:U:17:GLU:HG3	1:U:73:GLN:OE1	2.05	0.57
1:U:33:VAL:O	1:U:37:MET:HG3	2.04	0.57
1:C:87:LYS:HD3	1:X:82:LEU:O	2.04	0.57
1:D:71:LYS:HD2	1:D:71:LYS:C	2.30	0.57
1:O:6:SER:OG	1:O:77:GLY:HA2	2.04	0.57
1:O:134:GLU:OE1	1:Q:131:ASP:HB2	2.04	0.57
1:Q:72:LEU:O	1:Q:76:ARG:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:121:ALA:HB2	1:U:129:LEU:HD22	1.86	0.57
1:A:72:LEU:O	1:A:75:GLN:N	2.37	0.57
1:C:128:HIS:CD2	1:Q:142:VAL:HG11	2.39	0.57
1:F:68:LYS:HE3	1:F:132:PHE:CZ	2.40	0.57
1:M:113:SER:O	1:M:117:LEU:N	2.38	0.57
1:M:155:LEU:C	1:M:157:LYS:N	2.61	0.57
1:Q:12:TYR:CD1	1:Q:76:ARG:HG2	2.40	0.57
1:V:29:TYR:O	1:V:33:VAL:HG23	2.04	0.57
1:X:55:PHE:HZ	1:X:100:MET:HG2	1.69	0.57
1:A:158:MET:SD	1:A:170:PHE:HD2	2.28	0.57
1:F:87:LYS:NZ	1:F:88:PRO:O	2.37	0.57
1:J:154:ASN:O	1:J:158:MET:N	2.26	0.57
1:V:121:ALA:HB1	1:V:126:ASP:O	2.05	0.57
1:K:37:MET:HE2	1:K:93:TRP:CZ3	2.40	0.57
1:M:107:GLU:OE1	1:M:141:GLN:NE2	2.38	0.57
1:Q:21:ASN:ND2	1:Q:81:PHE:H	2.02	0.57
1:X:42:ASP:HA	1:X:49:LYS:HE3	1.87	0.57
1:X:50:ASN:HB3	1:X:175:LEU:CB	2.34	0.57
1:Q:63:ARG:HG3	1:Q:64:GLU:OE2	2.05	0.57
1:J:97:LEU:HD22	1:J:161:PRO:HD3	1.86	0.57
1:M:87:LYS:NZ	1:M:88:PRO:O	2.38	0.57
1:F:25:ASN:O	1:F:29:TYR:N	2.33	0.56
1:G:116:GLU:O	1:G:120:LEU:N	2.37	0.56
1:I:61:GLU:O	1:I:65:HIS:NE2	2.38	0.56
1:P:50:ASN:HA	1:P:53:LYS:CE	2.35	0.56
1:T:73:GLN:HG2	1:T:80:ILE:HG13	1.87	0.56
1:A:142:VAL:HA	1:A:145:ILE:HG12	1.86	0.56
1:Q:104:LEU:HD11	1:Q:145:ILE:HG23	1.87	0.56
1:C:21:ASN:ND2	1:C:81:PHE:O	2.33	0.56
1:C:79:ARG:HG3	1:X:43:ARG:HH11	1.71	0.56
1:C:85:ILE:HD11	1:X:32:TYR:CE1	2.40	0.56
1:D:110:VAL:HB	1:D:141:GLN:HE22	1.70	0.56
1:E:73:GLN:HG3	1:E:80:ILE:HG12	1.86	0.56
1:F:155:LEU:HA	1:F:158:MET:HE3	1.86	0.56
1:J:114:LEU:HD22	1:J:133:ILE:HG23	1.87	0.56
1:T:45:ASP:O	1:U:157:LYS:NZ	2.39	0.56
1:V:31:SER:O	1:V:59:SER:OG	2.23	0.56
1:X:27:GLU:HB2	1:X:66:ALA:HB2	1.86	0.56
1:E:90:CYS:HB2	1:E:93:TRP:CZ3	2.41	0.56
1:A:73:GLN:HG3	1:A:78:GLY:O	2.04	0.56
1:H:67:GLU:HA	1:H:70:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:ASP:HB3	1:M:120:LEU:HD21	1.86	0.56
1:N:92:ASP:C	1:N:94:GLU:H	2.14	0.56
1:S:9:ARG:NH2	1:S:12:TYR:O	2.37	0.56
1:V:94:GLU:CG	1:V:98:ASN:HD22	2.19	0.56
1:I:43:ARG:NH1	1:N:79:ARG:HD3	2.21	0.56
1:J:54:TYR:O	1:J:58:GLN:NE2	2.36	0.56
1:C:104:LEU:HD11	1:C:145:ILE:HG23	1.87	0.56
1:D:129:LEU:O	1:D:133:ILE:HB	2.06	0.56
1:F:111:ASN:HD22	1:F:141:GLN:HG2	1.70	0.56
1:J:149:GLY:O	1:U:7:GLN:NE2	2.38	0.56
1:K:112:GLN:HB2	1:R:10:GLN:NE2	2.19	0.56
1:L:92:ASP:OD1	1:L:94:GLU:N	2.28	0.56
1:P:73:GLN:O	1:P:78:GLY:N	2.37	0.56
1:T:43:ARG:NH2	1:T:45:ASP:OD2	2.36	0.56
1:X:131:ASP:HA	1:X:134:GLU:HB3	1.86	0.56
1:E:14:GLN:HA	1:E:17:GLU:HG2	1.87	0.56
1:J:47:ALA:O	1:J:48:LEU:HD23	2.05	0.56
1:I:72:LEU:O	1:I:76:ARG:N	2.38	0.56
1:N:10:GLN:O	1:N:76:ARG:NH2	2.39	0.56
1:U:30:ALA:HB1	1:U:106:LEU:HD21	1.87	0.56
1:D:147:GLU:HG2	1:D:151:HIS:CE1	2.41	0.56
1:L:137:TYR:O	1:L:141:GLN:HG2	2.06	0.56
1:D:34:TYR:CE1	1:D:58:GLN:HB2	2.41	0.55
1:D:76:ARG:HH11	1:D:76:ARG:HA	1.71	0.55
1:D:90:CYS:HB2	1:D:93:TRP:CE2	2.41	0.55
1:E:29:TYR:O	1:E:33:VAL:HG23	2.06	0.55
1:F:133:ILE:HG23	1:F:137:TYR:HB2	1.87	0.55
1:I:150:ASP:HA	1:I:153:THR:HB	1.87	0.55
1:K:104:LEU:HA	1:K:148:LEU:HD13	1.88	0.55
1:O:112:GLN:O	1:O:115:LEU:N	2.36	0.55
1:P:35:LEU:HD12	1:P:38:SER:HB3	1.87	0.55
1:D:65:HIS:HE1	1:D:140:GLU:HG3	1.69	0.55
1:K:13:HIS:CD2	1:K:124:LYS:HD2	2.42	0.55
1:L:92:ASP:OD1	1:L:93:TRP:N	2.39	0.55
1:Q:90:CYS:HB2	1:Q:93:TRP:CZ3	2.41	0.55
1:Q:153:THR:OG1	1:X:44:ASP:O	2.17	0.55
1:T:40:TYR:CZ	1:T:46:VAL:HG21	2.42	0.55
1:A:160:ALA:HB2	1:A:166:ALA:HB3	1.89	0.55
1:B:58:GLN:O	1:B:62:GLU:HG2	2.07	0.55
1:B:73:GLN:HG2	1:B:80:ILE:HG13	1.89	0.55
1:D:65:HIS:O	1:D:137:TYR:OH	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ILE:O	1:F:149:GLY:N	2.39	0.55
1:H:43:ARG:NE	1:R:79:ARG:HE	2.03	0.55
1:A:34:TYR:CE2	1:A:58:GLN:HB3	2.40	0.55
1:C:6:SER:HB3	1:C:9:ARG:HB2	1.88	0.55
1:D:68:LYS:HB3	1:D:132:PHE:CZ	2.41	0.55
1:G:56:LEU:HG	1:G:60:HIS:HE1	1.71	0.55
1:M:10:GLN:O	1:M:76:ARG:NH2	2.40	0.55
1:N:134:GLU:HA	1:N:138:LEU:HB2	1.87	0.55
1:R:15:ASP:HB3	1:R:120:LEU:HD21	1.87	0.55
1:O:151:HIS:CG	1:O:170:PHE:HZ	2.23	0.55
1:T:25:ASN:ND2	1:T:84:ASP:O	2.39	0.55
1:W:40:TYR:CG	1:W:93:TRP:HD1	2.25	0.55
1:I:90:CYS:HB2	1:I:93:TRP:CZ3	2.42	0.55
1:P:107:GLU:HG3	1:P:148:LEU:HD22	1.87	0.55
1:X:41:PHE:HB3	1:X:48:LEU:O	2.05	0.55
1:C:19:ALA:HA	1:C:22:ARG:HB3	1.88	0.55
1:H:71:LYS:HG3	1:H:75:GLN:NE2	2.21	0.55
1:I:43:ARG:HH12	1:N:79:ARG:HD3	1.72	0.55
1:M:5:THR:OG1	1:M:6:SER:N	2.40	0.55
1:U:29:TYR:CE2	1:U:86:LYS:HB3	2.41	0.55
1:G:84:ASP:OD1	1:U:87:LYS:N	2.34	0.55
1:K:20:ILE:O	1:K:24:ILE:N	2.40	0.55
1:N:62:GLU:HA	1:N:65:HIS:HB2	1.89	0.55
1:O:127:PRO:HA	1:O:130:CYS:HB2	1.88	0.55
1:P:25:ASN:O	1:P:29:TYR:N	2.40	0.55
1:Q:169:LEU:HB3	1:Q:173:HIS:CE1	2.42	0.55
1:U:17:GLU:HA	1:U:20:ILE:HD12	1.88	0.55
1:U:53:LYS:CD	1:U:53:LYS:C	2.75	0.55
1:U:68:LYS:HD2	1:U:68:LYS:N	2.21	0.55
1:W:35:LEU:C	1:W:37:MET:H	2.14	0.55
1:M:65:HIS:O	1:M:137:TYR:OH	2.23	0.55
1:N:142:VAL:HG21	1:W:128:HIS:CD2	2.42	0.55
1:P:142:VAL:HG21	1:X:128:HIS:CD2	2.41	0.55
1:X:41:PHE:HZ	1:X:96:GLY:HA2	1.71	0.55
1:C:32:TYR:CZ	1:X:85:ILE:HD11	2.42	0.55
1:C:119:LYS:HG3	1:C:120:LEU:N	2.22	0.55
1:F:22:ARG:HD2	1:F:22:ARG:N	2.22	0.55
1:J:98:ASN:O	1:J:102:CYS:N	2.35	0.55
1:K:41:PHE:HA	1:K:46:VAL:HG11	1.89	0.55
1:R:43:ARG:NH2	1:R:45:ASP:OD2	2.32	0.55
1:T:76:ARG:NH2	1:T:126:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:ASN:HB3	1:K:175:LEU:HB3	1.87	0.54
1:K:147:GLU:HA	1:K:150:ASP:HB2	1.89	0.54
1:C:43:ARG:HG2	1:X:79:ARG:HH12	1.72	0.54
1:R:34:TYR:O	1:R:38:SER:N	2.40	0.54
1:V:9:ARG:HD2	1:V:12:TYR:HB3	1.89	0.54
1:V:89:ASP:OD1	1:V:90:CYS:N	2.40	0.54
1:B:32:TYR:CE2	1:B:87:LYS:HA	2.42	0.54
1:I:162:GLU:H	1:I:162:GLU:CD	2.15	0.54
1:J:12:TYR:OH	1:J:17:GLU:HA	2.07	0.54
1:R:61:GLU:O	1:R:65:HIS:N	2.33	0.54
1:T:31:SER:HB2	1:T:62:GLU:HB2	1.89	0.54
1:X:71:LYS:O	1:X:75:GLN:HG3	2.06	0.54
1:A:23:GLN:OE1	1:A:113:SER:OG	2.19	0.54
1:K:71:LYS:O	1:K:75:GLN:HG3	2.07	0.54
1:V:41:PHE:HA	1:V:46:VAL:HG11	1.88	0.54
1:F:171:ASP:O	1:F:175:LEU:HB2	2.08	0.54
1:J:51:PHE:O	1:J:54:TYR:HB3	2.08	0.54
1:N:43:ARG:HB2	1:N:46:VAL:CG2	2.38	0.54
1:Q:14:GLN:HA	1:Q:17:GLU:HG2	1.89	0.54
1:U:8:VAL:O	1:U:10:GLN:N	2.41	0.54
1:X:167:GLU:O	1:X:171:ASP:HB2	2.07	0.54
1:C:85:ILE:N	1:X:85:ILE:O	2.38	0.54
1:F:21:ASN:HB2	1:F:22:ARG:NH1	2.22	0.54
1:H:9:ARG:HH21	1:H:12:TYR:C	2.15	0.54
1:O:106:LEU:O	1:O:110:VAL:HG23	2.08	0.54
1:P:151:HIS:CD2	1:P:170:PHE:HZ	2.26	0.54
1:R:16:SER:O	1:R:19:ALA:N	2.41	0.54
1:R:119:LYS:HE2	1:R:119:LYS:HA	1.88	0.54
1:U:40:TYR:O	1:U:46:VAL:HG21	2.07	0.54
1:C:85:ILE:O	1:X:85:ILE:N	2.38	0.54
1:F:158:MET:HA	1:O:165:LEU:N	2.23	0.54
1:G:70:MET:HG3	1:U:39:TYR:CE2	2.43	0.54
1:L:154:ASN:O	1:L:158:MET:N	2.37	0.54
1:M:154:ASN:O	1:M:158:MET:HG3	2.07	0.54
1:P:74:ASN:HD21	1:P:80:ILE:HD11	1.72	0.54
1:Q:68:LYS:HB2	1:Q:137:TYR:OH	2.07	0.54
1:Q:121:ALA:O	1:Q:125:ASN:N	2.41	0.54
1:R:12:TYR:HE2	1:R:78:GLY:HA3	1.73	0.54
1:R:29:TYR:O	1:R:33:VAL:HG23	2.07	0.54
1:T:34:TYR:HD2	1:T:59:SER:HA	1.72	0.54
1:V:49:LYS:O	1:V:52:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:97:LEU:HD22	1:V:161:PRO:HD3	1.90	0.54
1:X:97:LEU:HA	1:X:155:LEU:HD23	1.90	0.54
1:B:63:ARG:O	1:B:67:GLU:HG3	2.07	0.54
1:D:59:SER:O	1:D:62:GLU:HB3	2.07	0.54
1:R:13:HIS:HB3	1:R:16:SER:OG	2.08	0.54
1:U:66:ALA:O	1:U:70:MET:HG3	2.08	0.54
1:H:9:ARG:CZ	1:H:12:TYR:HB3	2.38	0.54
1:I:92:ASP:OD1	1:I:94:GLU:N	2.24	0.54
1:M:72:LEU:HA	1:M:75:GLN:HB2	1.90	0.54
1:R:102:CYS:O	1:R:106:LEU:N	2.32	0.54
1:R:127:PRO:O	1:R:131:ASP:N	2.38	0.54
1:T:9:ARG:HG3	1:T:76:ARG:O	2.08	0.54
1:W:66:ALA:O	1:W:70:MET:HG3	2.08	0.54
1:D:168:TYR:O	1:D:172:LYS:HG2	2.08	0.53
1:P:9:ARG:HB2	1:P:77:GLY:HA3	1.90	0.53
1:S:61:GLU:O	1:S:64:GLU:HG3	2.09	0.53
1:W:70:MET:HE3	1:W:80:ILE:HD13	1.91	0.53
1:C:32:TYR:CE2	1:X:85:ILE:HD11	2.43	0.53
1:C:108:LYS:HE2	1:O:10:GLN:OE1	2.07	0.53
1:D:11:ASN:OD1	1:D:126:ASP:HA	2.09	0.53
1:D:142:VAL:HG21	1:P:128:HIS:CD2	2.42	0.53
1:E:131:ASP:HB2	1:T:134:GLU:HB3	1.90	0.53
1:G:21:ASN:CG	1:G:73:GLN:HE22	2.16	0.53
1:K:161:PRO:C	1:K:163:SER:H	2.17	0.53
1:P:112:GLN:HA	1:P:115:LEU:HD12	1.90	0.53
1:Q:32:TYR:HE2	1:Q:87:LYS:HA	1.74	0.53
1:W:37:MET:O	1:W:41:PHE:HD2	1.91	0.53
1:W:130:CYS:O	1:W:133:ILE:HB	2.09	0.53
1:D:143:LYS:HE2	1:P:75:GLN:NE2	2.22	0.53
1:J:118:HIS:CD2	1:U:127:PRO:HB3	2.44	0.53
1:O:29:TYR:O	1:O:33:VAL:HG23	2.08	0.53
1:O:144:ALA:O	1:O:148:LEU:HG	2.08	0.53
1:V:47:ALA:O	1:V:49:LYS:HD2	2.09	0.53
1:D:111:ASN:N	1:D:141:GLN:HE22	2.05	0.53
1:L:33:VAL:O	1:L:36:SER:OG	2.24	0.53
1:R:158:MET:HB3	1:U:165:LEU:HD12	1.89	0.53
1:B:104:LEU:HA	1:B:148:LEU:HD13	1.90	0.53
1:E:24:ILE:HG23	1:E:66:ALA:HB1	1.90	0.53
1:F:9:ARG:HG2	1:F:76:ARG:O	2.09	0.53
1:H:64:GLU:HA	1:H:67:GLU:OE1	2.08	0.53
1:L:20:ILE:HD13	1:L:117:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:ASP:OD1	1:N:92:ASP:N	2.41	0.53
1:A:111:ASN:HD22	1:M:10:GLN:NE2	2.05	0.53
1:A:128:HIS:CD2	1:V:139:ASN:HD22	2.27	0.53
1:C:72:LEU:HD22	1:C:132:PHE:CE2	2.43	0.53
1:D:107:GLU:OE1	1:D:141:GLN:HG2	2.08	0.53
1:G:38:SER:OG	1:G:52:ALA:O	2.27	0.53
1:G:172:LYS:HD3	1:G:173:HIS:CD2	2.44	0.53
1:L:119:LYS:HG2	1:L:123:PHE:CE2	2.43	0.53
1:N:12:TYR:OH	1:N:17:GLU:HA	2.08	0.53
1:O:155:LEU:HB3	1:O:160:ALA:HB3	1.89	0.53
1:T:76:ARG:HH22	1:T:126:ASP:CG	2.15	0.53
1:A:18:ALA:O	1:A:22:ARG:HG2	2.09	0.53
1:B:44:ASP:OD1	1:B:44:ASP:N	2.41	0.53
1:B:168:TYR:OH	1:O:173:HIS:HB2	2.09	0.53
1:F:113:SER:HA	1:F:116:GLU:HB3	1.90	0.53
1:F:171:ASP:OD1	1:F:172:LYS:HD2	2.09	0.53
1:K:139:ASN:HA	1:R:128:HIS:CD2	2.44	0.53
1:Q:107:GLU:OE1	1:Q:141:GLN:NE2	2.41	0.53
1:W:43:ARG:HH21	1:W:45:ASP:CG	2.12	0.53
1:X:73:GLN:HG2	1:X:80:ILE:HG12	1.90	0.53
1:X:161:PRO:HD2	1:X:162:GLU:OE2	2.08	0.53
1:B:26:LEU:O	1:B:29:TYR:HB3	2.09	0.53
1:D:112:GLN:HB2	1:P:10:GLN:HE22	1.74	0.53
1:E:62:GLU:OE2	1:E:65:HIS:ND1	2.42	0.53
1:S:64:GLU:O	1:S:65:HIS:C	2.52	0.53
1:X:92:ASP:O	1:X:94:GLU:N	2.30	0.53
1:M:61:GLU:O	1:M:65:HIS:ND1	2.42	0.53
1:O:6:SER:HB2	1:O:79:ARG:NH1	2.23	0.53
1:P:34:TYR:CD1	1:P:58:GLN:HB2	2.44	0.53
1:T:35:LEU:C	1:T:37:MET:H	2.15	0.53
1:U:53:LYS:O	1:U:53:LYS:HD3	2.07	0.53
1:J:27:GLU:OE1	1:J:65:HIS:HB3	2.09	0.53
1:T:47:ALA:HB1	1:U:150:ASP:HB3	1.92	0.53
1:W:43:ARG:O	1:W:47:ALA:N	2.39	0.53
1:A:41:PHE:HZ	1:A:96:GLY:HA2	1.75	0.52
1:D:70:MET:HE1	1:V:35:LEU:HG	1.91	0.52
1:E:27:GLU:HB2	1:E:66:ALA:HB2	1.90	0.52
1:I:166:ALA:O	1:I:170:PHE:N	2.36	0.52
1:R:97:LEU:N	1:R:167:GLU:OE1	2.38	0.52
1:S:159:GLY:O	1:S:162:GLU:HG2	2.08	0.52
1:U:46:VAL:HG23	1:U:47:ALA:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ARG:HH12	1:T:60:HIS:CE1	2.28	0.52
1:G:76:ARG:NH1	1:G:126:ASP:OD2	2.35	0.52
1:M:41:PHE:HA	1:M:46:VAL:HG11	1.90	0.52
1:N:134:GLU:HB3	1:W:131:ASP:CG	2.33	0.52
1:R:51:PHE:CE2	1:R:96:GLY:HA3	2.44	0.52
1:A:90:CYS:HB2	1:A:93:TRP:CZ3	2.44	0.52
1:B:72:LEU:HA	1:B:75:GLN:HB2	1.92	0.52
1:K:27:GLU:HG2	1:K:65:HIS:HB3	1.91	0.52
1:M:42:ASP:HA	1:M:49:LYS:NZ	2.23	0.52
1:M:108:LYS:NZ	1:V:9:ARG:O	2.42	0.52
1:R:40:TYR:CB	1:R:93:TRP:HD1	2.22	0.52
1:U:112:GLN:HA	1:U:115:LEU:HB2	1.90	0.52
1:X:73:GLN:HG2	1:X:80:ILE:CG1	2.39	0.52
1:B:32:TYR:HE2	1:B:87:LYS:HA	1.75	0.52
1:E:74:ASN:HB3	1:S:43:ARG:HA	1.91	0.52
1:I:85:ILE:HD11	1:N:32:TYR:CE1	2.44	0.52
1:J:144:ALA:O	1:J:147:GLU:N	2.43	0.52
1:K:142:VAL:HG21	1:R:128:HIS:CD2	2.45	0.52
1:N:138:LEU:HD13	1:W:128:HIS:HA	1.92	0.52
1:P:171:ASP:HA	1:P:175:LEU:HD12	1.91	0.52
1:V:41:PHE:HD1	1:V:46:VAL:HG11	1.74	0.52
1:B:7:GLN:NE2	1:W:149:GLY:O	2.43	0.52
1:B:48:LEU:HD23	1:B:51:PHE:CD2	2.44	0.52
1:N:9:ARG:NH2	1:N:17:GLU:OE2	2.38	0.52
1:N:27:GLU:HB2	1:N:66:ALA:HB2	1.91	0.52
1:N:40:TYR:C	1:N:42:ASP:H	2.16	0.52
1:X:24:ILE:HG21	1:X:70:MET:CE	2.38	0.52
1:B:50:ASN:ND2	1:B:175:LEU:O	2.43	0.52
1:E:174:THR:HG1	1:N:168:TYR:HH	1.52	0.52
1:F:9:ARG:HG2	1:F:77:GLY:HA3	1.91	0.52
1:H:156:ARG:O	1:H:158:MET:N	2.43	0.52
1:M:111:ASN:HA	1:M:114:LEU:HD12	1.90	0.52
1:W:172:LYS:HB2	1:W:173:HIS:CE1	2.45	0.52
1:X:34:TYR:CE2	1:X:58:GLN:HB3	2.45	0.52
1:B:90:CYS:HB2	1:B:93:TRP:CH2	2.45	0.52
1:D:143:LYS:HA	1:D:146:LYS:HB3	1.92	0.52
1:I:86:LYS:HD3	1:N:84:ASP:CG	2.35	0.52
1:J:41:PHE:HZ	1:J:96:GLY:HA2	1.75	0.52
1:O:29:TYR:OH	1:O:88:PRO:HA	2.10	0.52
1:O:56:LEU:HD12	1:O:59:SER:HB3	1.92	0.52
1:C:69:LEU:HD21	1:C:137:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:HB3	1:D:48:LEU:O	2.10	0.52
1:F:128:HIS:NE2	1:U:139:ASN:HA	2.24	0.52
1:H:48:LEU:HD22	1:H:171:ASP:HB3	1.91	0.52
1:I:43:ARG:HB3	1:N:79:ARG:NH2	2.25	0.52
1:L:32:TYR:CE1	1:M:85:ILE:HD11	2.44	0.52
1:M:133:ILE:HG22	1:M:138:LEU:CG	2.35	0.52
1:O:102:CYS:O	1:O:106:LEU:N	2.41	0.52
1:V:121:ALA:HB2	1:V:129:LEU:HD23	1.92	0.52
1:C:90:CYS:HB2	1:C:93:TRP:CZ3	2.45	0.52
1:G:106:LEU:O	1:G:110:VAL:HG23	2.09	0.52
1:I:34:TYR:HD1	1:I:55:PHE:HD2	1.57	0.52
1:O:44:ASP:OD1	1:O:44:ASP:C	2.52	0.52
1:R:23:GLN:NE2	1:R:26:LEU:HB3	2.25	0.52
1:R:137:TYR:O	1:R:138:LEU:C	2.52	0.52
1:E:140:GLU:HA	1:E:143:LYS:HE3	1.92	0.52
1:F:32:TYR:CE1	1:T:82:LEU:HD13	2.45	0.52
1:F:92:ASP:OD1	1:F:93:TRP:N	2.43	0.52
1:G:131:ASP:OD1	1:G:135:THR:OG1	2.27	0.52
1:L:84:ASP:OD1	1:M:87:LYS:N	2.26	0.52
1:P:115:LEU:HB3	1:P:119:LYS:HZ3	1.73	0.52
1:Q:12:TYR:HE2	1:Q:17:GLU:HB3	1.75	0.52
1:A:104:LEU:O	1:A:108:LYS:N	2.32	0.51
1:J:53:LYS:O	1:J:57:HIS:HB2	2.11	0.51
1:J:103:ALA:O	1:J:106:LEU:HB3	2.10	0.51
1:Q:139:ASN:OD1	1:Q:139:ASN:O	2.28	0.51
1:V:48:LEU:O	1:V:51:PHE:HB2	2.09	0.51
1:A:39:TYR:CG	1:W:70:MET:HE2	2.44	0.51
1:B:83:GLN:O	1:Q:32:TYR:OH	2.24	0.51
1:B:139:ASN:O	1:B:143:LYS:HG3	2.09	0.51
1:C:56:LEU:HA	1:C:59:SER:HB3	1.92	0.51
1:D:53:LYS:O	1:D:57:HIS:N	2.33	0.51
1:L:115:LEU:O	1:L:118:HIS:N	2.42	0.51
1:M:41:PHE:HB3	1:M:48:LEU:O	2.10	0.51
1:P:23:GLN:O	1:P:27:GLU:N	2.31	0.51
1:X:94:GLU:OE1	1:X:98:ASN:ND2	2.42	0.51
1:X:150:ASP:O	1:X:153:THR:N	2.40	0.51
1:A:168:TYR:HD2	1:A:169:LEU:HD23	1.75	0.51
1:M:65:HIS:HD2	1:M:137:TYR:CE1	2.26	0.51
1:M:155:LEU:O	1:M:157:LYS:N	2.43	0.51
1:X:51:PHE:HE2	1:X:96:GLY:HA3	1.75	0.51
1:B:42:ASP:HB3	1:Q:74:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HA	1:C:75:GLN:HB2	1.92	0.51
1:D:53:LYS:NZ	1:D:57:HIS:HB2	2.26	0.51
1:F:36:SER:HB2	1:F:93:TRP:HZ2	1.76	0.51
1:G:104:LEU:HD11	1:G:145:ILE:HG23	1.92	0.51
1:H:63:ARG:O	1:H:67:GLU:HG3	2.10	0.51
1:U:116:GLU:HA	1:U:119:LYS:HD2	1.92	0.51
1:A:113:SER:O	1:A:116:GLU:HB2	2.10	0.51
1:E:161:PRO:HB3	1:E:167:GLU:OE2	2.11	0.51
1:F:159:GLY:O	1:F:163:SER:HB3	2.11	0.51
1:M:9:ARG:HE	1:M:12:TYR:HB3	1.76	0.51
1:P:71:LYS:O	1:P:75:GLN:N	2.43	0.51
1:S:92:ASP:OD1	1:S:94:GLU:N	2.37	0.51
1:D:64:GLU:O	1:D:68:LYS:HG3	2.11	0.51
1:D:170:PHE:O	1:D:172:LYS:N	2.43	0.51
1:G:18:ALA:O	1:G:22:ARG:HG3	2.11	0.51
1:O:149:GLY:O	1:O:152:VAL:HB	2.11	0.51
1:T:29:TYR:OH	1:T:88:PRO:HA	2.09	0.51
1:T:154:ASN:O	1:T:158:MET:HB2	2.11	0.51
1:D:128:HIS:NE2	1:X:142:VAL:HG21	2.25	0.51
1:J:155:LEU:HA	1:J:158:MET:HB2	1.92	0.51
1:L:6:SER:HB3	1:L:9:ARG:HG3	1.91	0.51
1:M:106:LEU:O	1:M:110:VAL:N	2.39	0.51
1:P:171:ASP:O	1:P:175:LEU:HB2	2.10	0.51
1:R:56:LEU:O	1:R:60:HIS:ND1	2.41	0.51
1:R:168:TYR:OH	1:S:174:THR:OG1	2.25	0.51
1:H:145:ILE:HG22	1:L:8:VAL:HG23	1.92	0.51
1:I:174:THR:O	1:I:175:LEU:HD23	2.11	0.51
1:J:138:LEU:O	1:J:142:VAL:HG23	2.09	0.51
1:K:112:GLN:HB2	1:R:10:GLN:HE21	1.74	0.51
1:N:108:LYS:O	1:W:10:GLN:NE2	2.44	0.51
1:U:78:GLY:C	1:U:79:ARG:HD3	2.35	0.51
1:X:171:ASP:O	1:X:175:LEU:HB2	2.11	0.51
1:J:49:LYS:O	1:J:52:ALA:HB3	2.11	0.51
1:P:146:LYS:HG2	1:X:75:GLN:HG2	1.92	0.51
1:Q:168:TYR:OH	1:W:173:HIS:HB2	2.11	0.51
1:B:8:VAL:HG12	1:W:145:ILE:HG22	1.93	0.51
1:D:79:ARG:NH1	1:V:43:ARG:HG2	2.25	0.51
1:F:33:VAL:C	1:F:35:LEU:H	2.19	0.51
1:N:66:ALA:O	1:N:69:LEU:N	2.43	0.51
1:T:12:TYR:OH	1:T:20:ILE:HG13	2.10	0.51
1:T:131:ASP:HA	1:T:134:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:44:ASP:OD1	1:X:44:ASP:N	2.44	0.51
1:B:97:LEU:HD11	1:B:152:VAL:HG13	1.93	0.50
1:C:93:TRP:O	1:C:95:SER:N	2.43	0.50
1:I:72:LEU:HA	1:I:75:GLN:HB2	1.94	0.50
1:N:68:LYS:HB3	1:N:137:TYR:OH	2.11	0.50
1:N:90:CYS:HB2	1:N:93:TRP:CZ3	2.46	0.50
1:O:21:ASN:HD21	1:O:80:ILE:HA	1.76	0.50
1:Q:33:VAL:HG22	1:Q:88:PRO:HG3	1.92	0.50
1:D:119:LYS:HA	1:D:122:THR:OG1	2.10	0.50
1:E:139:ASN:O	1:E:143:LYS:HG3	2.12	0.50
1:G:13:HIS:HB2	1:G:124:LYS:HB3	1.93	0.50
1:R:128:HIS:O	1:R:132:PHE:HB2	2.11	0.50
1:U:93:TRP:O	1:U:95:SER:N	2.45	0.50
1:X:59:SER:O	1:X:59:SER:OG	2.28	0.50
1:M:96:GLY:O	1:M:99:ALA:HB3	2.11	0.50
1:R:43:ARG:HB2	1:R:46:VAL:HG22	1.93	0.50
1:T:105:HIS:HA	1:T:108:LYS:HZ3	1.76	0.50
1:V:153:THR:HG21	1:W:45:ASP:C	2.37	0.50
1:X:37:MET:HG2	1:X:93:TRP:CE2	2.46	0.50
1:K:128:HIS:O	1:K:131:ASP:N	2.44	0.50
1:O:24:ILE:HD11	1:O:69:LEU:HB2	1.93	0.50
1:R:95:SER:OG	1:R:161:PRO:HG3	2.11	0.50
1:W:33:VAL:O	1:W:37:MET:HG3	2.10	0.50
1:D:25:ASN:ND2	1:D:84:ASP:O	2.36	0.50
1:J:58:GLN:CD	1:J:58:GLN:N	2.69	0.50
1:J:62:GLU:OE2	1:J:65:HIS:ND1	2.45	0.50
1:K:17:GLU:CG	1:K:73:GLN:HE22	2.17	0.50
1:P:165:LEU:O	1:P:169:LEU:HG	2.11	0.50
1:Q:10:GLN:O	1:Q:12:TYR:N	2.44	0.50
1:B:37:MET:O	1:B:40:TYR:HB3	2.12	0.50
1:C:12:TYR:HB2	1:C:76:ARG:NH2	2.26	0.50
1:D:67:GLU:O	1:D:70:MET:N	2.45	0.50
1:J:116:GLU:O	1:J:119:LYS:HG2	2.11	0.50
1:M:34:TYR:OH	1:M:107:GLU:OE2	2.21	0.50
1:P:58:GLN:O	1:P:62:GLU:N	2.40	0.50
1:Q:32:TYR:CE2	1:Q:87:LYS:HA	2.46	0.50
1:T:43:ARG:O	1:T:47:ALA:N	2.45	0.50
1:T:171:ASP:HA	1:T:175:LEU:HD12	1.93	0.50
1:B:126:ASP:OD1	1:B:129:LEU:HB3	2.12	0.50
1:F:43:ARG:HG2	1:T:74:ASN:CG	2.36	0.50
1:F:93:TRP:O	1:F:95:SER:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ASP:OD2	1:G:128:HIS:HB3	2.12	0.50
1:H:6:SER:HB2	1:H:79:ARG:HH22	1.77	0.50
1:I:167:GLU:O	1:I:171:ASP:N	2.44	0.50
1:K:67:GLU:O	1:K:69:LEU:N	2.35	0.50
1:O:6:SER:HB2	1:O:79:ARG:HH12	1.76	0.50
1:S:168:TYR:OH	1:T:173:HIS:HB2	2.12	0.50
1:T:56:LEU:O	1:T:59:SER:HB3	2.12	0.50
1:U:104:LEU:N	1:U:148:LEU:HD13	2.27	0.50
1:D:142:VAL:HG12	1:P:75:GLN:HG2	1.93	0.50
1:H:50:ASN:HB3	1:H:175:LEU:O	2.12	0.50
1:Q:169:LEU:O	1:Q:172:LYS:N	2.45	0.50
1:S:51:PHE:O	1:S:54:TYR:HB3	2.11	0.50
1:V:121:ALA:O	1:V:126:ASP:N	2.42	0.50
1:A:119:LYS:O	1:A:122:THR:N	2.43	0.50
1:B:158:MET:HG2	1:I:165:LEU:HD12	1.93	0.50
1:D:158:MET:CE	1:D:169:LEU:HB2	2.38	0.50
1:F:71:LYS:O	1:F:75:GLN:HG3	2.12	0.50
1:H:59:SER:OG	1:R:63:ARG:NH2	2.45	0.50
1:J:117:LEU:O	1:J:118:HIS:C	2.55	0.50
1:K:147:GLU:O	1:K:150:ASP:HB2	2.12	0.50
1:M:29:TYR:O	1:M:33:VAL:HG23	2.11	0.50
1:V:157:LYS:HE3	1:W:164:GLY:HA2	1.94	0.50
1:W:32:TYR:CE2	1:W:88:PRO:HD3	2.46	0.50
1:D:131:ASP:CB	1:X:134:GLU:HG3	2.42	0.49
1:F:9:ARG:CG	1:F:77:GLY:HA3	2.42	0.49
1:L:70:MET:HB3	1:M:39:TYR:CD2	2.47	0.49
1:P:94:GLU:OE1	1:P:98:ASN:ND2	2.41	0.49
1:P:132:PHE:HD2	1:P:133:ILE:HD13	1.77	0.49
1:D:51:PHE:N	1:D:171:ASP:OD1	2.44	0.49
1:H:6:SER:OG	1:R:44:ASP:OD2	2.30	0.49
1:H:57:HIS:O	1:H:61:GLU:HG2	2.12	0.49
1:O:131:ASP:HA	1:O:134:GLU:CD	2.37	0.49
1:P:31:SER:OG	1:P:59:SER:O	2.30	0.49
1:T:30:ALA:HA	1:T:106:LEU:HD21	1.93	0.49
1:A:90:CYS:HB2	1:A:93:TRP:CH2	2.47	0.49
1:F:55:PHE:HA	1:F:58:GLN:HG2	1.94	0.49
1:J:49:LYS:HE3	1:J:53:LYS:NZ	2.26	0.49
1:J:153:THR:O	1:J:156:ARG:HB2	2.12	0.49
1:P:50:ASN:N	1:P:171:ASP:OD1	2.45	0.49
1:W:72:LEU:O	1:W:75:GLN:HB2	2.13	0.49
1:C:32:TYR:CZ	1:X:82:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:LEU:HD13	1:D:148:LEU:HB3	1.94	0.49
1:E:143:LYS:O	1:E:146:LYS:HB3	2.12	0.49
1:I:138:LEU:HB3	1:T:128:HIS:HB2	1.95	0.49
1:J:84:ASP:HA	1:O:85:ILE:O	2.13	0.49
1:N:46:VAL:HG23	1:N:47:ALA:H	1.77	0.49
1:N:129:LEU:O	1:N:133:ILE:HG12	2.13	0.49
1:P:117:LEU:O	1:P:121:ALA:N	2.36	0.49
1:R:98:ASN:HA	1:R:101:GLU:CD	2.37	0.49
1:S:72:LEU:HA	1:S:75:GLN:OE1	2.13	0.49
1:V:11:ASN:OD1	1:V:126:ASP:HA	2.13	0.49
1:A:76:ARG:HB3	1:A:76:ARG:CZ	2.42	0.49
1:K:63:ARG:HH21	1:P:35:LEU:HD22	1.76	0.49
1:K:79:ARG:NE	1:P:43:ARG:HG2	2.27	0.49
1:L:50:ASN:HB2	1:L:171:ASP:CG	2.37	0.49
1:M:18:ALA:HA	1:M:21:ASN:HB2	1.94	0.49
1:Q:40:TYR:O	1:Q:43:ARG:HB2	2.13	0.49
1:R:77:GLY:O	1:R:79:ARG:NH1	2.46	0.49
1:X:50:ASN:HB2	1:X:171:ASP:CG	2.36	0.49
1:D:155:LEU:HB3	1:D:160:ALA:HB3	1.94	0.49
1:F:12:TYR:CE2	1:F:17:GLU:HB3	2.48	0.49
1:H:32:TYR:OH	1:R:82:LEU:HB3	2.13	0.49
1:H:71:LYS:O	1:H:75:GLN:HG3	2.13	0.49
1:I:131:ASP:OD1	1:I:135:THR:OG1	2.27	0.49
1:J:16:SER:O	1:J:20:ILE:HG12	2.12	0.49
1:K:145:ILE:HA	1:K:148:LEU:HB2	1.93	0.49
1:O:43:ARG:HB2	1:O:46:VAL:CG2	2.42	0.49
1:O:69:LEU:HD22	1:O:137:TYR:OH	2.12	0.49
1:A:128:HIS:O	1:A:131:ASP:HB3	2.12	0.49
1:E:168:TYR:HD1	1:E:169:LEU:HD23	1.77	0.49
1:M:13:HIS:ND1	1:M:15:ASP:OD2	2.45	0.49
1:M:50:ASN:ND2	1:M:171:ASP:O	2.29	0.49
1:T:25:ASN:HA	1:T:28:LEU:HD12	1.94	0.49
1:U:156:ARG:HA	1:U:160:ALA:HB3	1.94	0.49
1:X:96:GLY:HA2	1:X:99:ALA:HB3	1.94	0.49
1:C:8:VAL:HB	1:Q:145:ILE:HG22	1.95	0.49
1:D:5:THR:OG1	1:D:6:SER:N	2.37	0.49
1:H:71:LYS:HG3	1:H:75:GLN:HE21	1.77	0.49
1:K:67:GLU:C	1:K:69:LEU:H	2.18	0.49
1:V:158:MET:O	1:V:166:ALA:HB2	2.13	0.49
1:B:19:ALA:O	1:B:22:ARG:HB2	2.13	0.49
1:C:12:TYR:HE1	1:C:129:LEU:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:GLU:OE1	1:G:156:ARG:NH2	2.46	0.49
1:I:48:LEU:HD22	1:I:171:ASP:CG	2.38	0.49
1:I:71:LYS:O	1:I:75:GLN:HG3	2.13	0.49
1:J:114:LEU:HD22	1:J:133:ILE:HG21	1.95	0.49
1:S:14:GLN:HA	1:S:17:GLU:HB3	1.95	0.49
1:T:153:THR:HA	1:T:156:ARG:CG	2.42	0.49
1:X:41:PHE:CD1	1:X:48:LEU:HB2	2.48	0.49
1:A:153:THR:O	1:A:156:ARG:HB2	2.13	0.49
1:D:159:GLY:O	1:D:163:SER:N	2.27	0.49
1:I:50:ASN:ND2	1:I:171:ASP:O	2.40	0.49
1:M:111:ASN:OD1	1:M:115:LEU:HD13	2.13	0.49
1:N:138:LEU:HD13	1:W:128:HIS:CA	2.43	0.49
1:U:50:ASN:HB2	1:U:171:ASP:OD1	2.12	0.49
1:V:62:GLU:CD	1:V:141:GLN:HE21	2.20	0.49
1:G:107:GLU:OE2	1:G:144:ALA:HB1	2.13	0.48
1:L:71:LYS:O	1:L:75:GLN:HG3	2.13	0.48
1:Q:41:PHE:HE2	1:Q:55:PHE:CE2	2.30	0.48
1:X:136:HIS:HB2	1:X:137:TYR:CE1	2.48	0.48
1:A:106:LEU:O	1:A:110:VAL:HG23	2.13	0.48
1:E:160:ALA:HB2	1:E:166:ALA:HB3	1.95	0.48
1:G:27:GLU:OE2	1:G:65:HIS:HB2	2.13	0.48
1:G:67:GLU:HA	1:G:70:MET:SD	2.53	0.48
1:H:139:ASN:OD1	1:H:143:LYS:HE2	2.13	0.48
1:L:131:ASP:HA	1:L:134:GLU:HB2	1.95	0.48
1:P:115:LEU:O	1:P:118:HIS:N	2.46	0.48
1:P:134:GLU:HB3	1:X:131:ASP:CG	2.37	0.48
1:R:56:LEU:O	1:R:59:SER:HB3	2.13	0.48
1:R:145:ILE:H	1:R:145:ILE:HD12	1.78	0.48
1:U:34:TYR:CD1	1:U:37:MET:HE2	2.48	0.48
1:A:7:GLN:NE2	1:W:44:ASP:OD2	2.43	0.48
1:A:160:ALA:HB1	1:A:161:PRO:HA	1.95	0.48
1:B:20:ILE:O	1:B:24:ILE:HG13	2.13	0.48
1:D:71:LYS:HE3	1:D:71:LYS:HB3	1.67	0.48
1:E:40:TYR:O	1:E:43:ARG:HB2	2.13	0.48
1:F:6:SER:H	1:F:79:ARG:HH21	1.60	0.48
1:H:164:GLY:O	1:H:168:TYR:N	2.43	0.48
1:M:38:SER:HA	1:M:55:PHE:HB2	1.95	0.48
1:N:34:TYR:HD1	1:N:37:MET:HE2	1.77	0.48
1:P:34:TYR:CE1	1:P:58:GLN:HG3	2.49	0.48
1:T:16:SER:C	1:T:20:ILE:HG12	2.38	0.48
1:W:64:GLU:O	1:W:68:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:TYR:HB3	1:G:55:PHE:O	2.13	0.48
1:L:21:ASN:ND2	1:L:80:ILE:HA	2.28	0.48
1:Q:165:LEU:HD12	1:W:158:MET:HB3	1.94	0.48
1:U:29:TYR:CD2	1:U:86:LYS:HB3	2.48	0.48
1:A:146:LYS:HE3	1:M:74:ASN:O	2.12	0.48
1:B:42:ASP:OD1	1:Q:71:LYS:HE2	2.13	0.48
1:D:112:GLN:O	1:D:115:LEU:N	2.45	0.48
1:F:29:TYR:OH	1:F:89:ASP:OD1	2.32	0.48
1:F:128:HIS:CE1	1:U:142:VAL:HG11	2.48	0.48
1:G:31:SER:OG	1:G:63:ARG:N	2.47	0.48
1:G:43:ARG:HB3	1:G:45:ASP:OD1	2.14	0.48
1:G:50:ASN:HB2	1:G:171:ASP:CG	2.39	0.48
1:G:56:LEU:HD12	1:G:56:LEU:HA	1.73	0.48
1:M:90:CYS:HB2	1:M:93:TRP:CZ3	2.48	0.48
1:V:13:HIS:HB3	1:V:16:SER:H	1.77	0.48
1:X:138:LEU:O	1:X:142:VAL:HG23	2.14	0.48
1:A:55:PHE:CZ	1:A:100:MET:SD	3.07	0.48
1:B:74:ASN:O	1:B:76:ARG:N	2.46	0.48
1:D:16:SER:O	1:D:20:ILE:HG12	2.14	0.48
1:N:116:GLU:HA	1:N:119:LYS:HE2	1.95	0.48
1:N:137:TYR:O	1:N:141:GLN:HG2	2.13	0.48
1:O:9:ARG:HB2	1:O:77:GLY:HA3	1.96	0.48
1:P:40:TYR:HB2	1:P:93:TRP:HD1	1.77	0.48
1:B:41:PHE:HB3	1:B:48:LEU:O	2.14	0.48
1:B:43:ARG:HB2	1:B:46:VAL:HG23	1.95	0.48
1:D:165:LEU:O	1:D:169:LEU:HG	2.13	0.48
1:J:6:SER:HB3	1:J:9:ARG:HB3	1.96	0.48
1:N:142:VAL:HG21	1:W:128:HIS:NE2	2.28	0.48
1:X:33:VAL:O	1:X:37:MET:HG3	2.13	0.48
1:X:164:GLY:O	1:X:167:GLU:HG3	2.14	0.48
1:A:27:GLU:OE1	1:A:65:HIS:HB3	2.14	0.48
1:C:43:ARG:HG2	1:X:79:ARG:NH1	2.28	0.48
1:E:32:TYR:CE1	1:S:85:ILE:HD11	2.49	0.48
1:G:76:ARG:HH12	1:G:126:ASP:CG	2.19	0.48
1:I:145:ILE:HG22	1:T:8:VAL:HG12	1.96	0.48
1:L:123:PHE:C	1:L:125:ASN:H	2.22	0.48
1:R:172:LYS:HD3	1:R:172:LYS:HA	1.61	0.48
1:U:67:GLU:C	1:U:68:LYS:HD2	2.39	0.48
1:V:65:HIS:O	1:V:137:TYR:OH	2.20	0.48
1:X:131:ASP:O	1:X:135:THR:HG22	2.14	0.48
1:F:38:SER:OG	1:F:56:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:170:PHE:CE2	1:K:175:LEU:HD21	2.49	0.48
1:N:38:SER:OG	1:N:56:LEU:HB2	2.14	0.48
1:O:9:ARG:HA	1:O:76:ARG:O	2.14	0.48
1:Q:120:LEU:HG	1:Q:124:LYS:HG2	1.96	0.48
1:X:170:PHE:CZ	1:X:174:THR:HG21	2.49	0.48
1:A:119:LYS:HD2	1:M:125:ASN:HB3	1.95	0.48
1:E:158:MET:HG2	1:N:165:LEU:HD12	1.95	0.48
1:F:48:LEU:O	1:F:51:PHE:HB2	2.14	0.48
1:F:164:GLY:HA3	1:I:157:LYS:HZ2	1.78	0.48
1:G:29:TYR:O	1:G:33:VAL:HG23	2.14	0.48
1:H:128:HIS:CE1	1:S:142:VAL:HG21	2.49	0.48
1:J:6:SER:HB2	1:J:79:ARG:HH22	1.79	0.48
1:N:138:LEU:HA	1:N:138:LEU:HD23	1.37	0.48
1:P:18:ALA:O	1:P:22:ARG:HG3	2.14	0.48
1:P:34:TYR:HE1	1:P:58:GLN:HG3	1.79	0.48
1:Q:38:SER:OG	1:Q:38:SER:O	2.31	0.48
1:Q:50:ASN:HB2	1:Q:171:ASP:CG	2.38	0.48
1:Q:73:GLN:HG3	1:Q:78:GLY:O	2.14	0.48
1:Q:158:MET:HE2	1:Q:166:ALA:HB1	1.95	0.48
1:R:68:LYS:HG3	1:R:137:TYR:OH	2.13	0.48
1:S:69:LEU:HD23	1:S:132:PHE:HE2	1.79	0.48
1:U:69:LEU:O	1:U:72:LEU:HB3	2.14	0.48
1:U:158:MET:HE1	1:U:169:LEU:HB2	1.94	0.48
1:X:24:ILE:HD13	1:X:70:MET:HG2	1.96	0.48
1:F:11:ASN:ND2	1:U:112:GLN:HE22	2.12	0.47
1:H:64:GLU:HA	1:H:67:GLU:HG3	1.96	0.47
1:L:40:TYR:HA	1:L:43:ARG:HD3	1.96	0.47
1:O:43:ARG:O	1:O:47:ALA:N	2.46	0.47
1:Q:121:ALA:HA	1:Q:124:LYS:HB2	1.96	0.47
1:T:169:LEU:O	1:T:172:LYS:N	2.46	0.47
1:U:73:GLN:OE1	1:U:78:GLY:HA3	2.13	0.47
1:C:63:ARG:HH21	1:X:60:HIS:HD2	1.62	0.47
1:C:111:ASN:O	1:C:115:LEU:N	2.46	0.47
1:G:138:LEU:HD13	1:K:128:HIS:HB2	1.95	0.47
1:J:5:THR:HG22	1:J:6:SER:N	2.27	0.47
1:Q:38:SER:OG	1:Q:56:LEU:HB2	2.14	0.47
1:U:46:VAL:HG23	1:U:47:ALA:N	2.29	0.47
1:A:12:TYR:HB2	1:A:76:ARG:HH22	1.80	0.47
1:E:39:TYR:CD1	1:S:70:MET:HE2	2.49	0.47
1:G:131:ASP:HB2	1:R:134:GLU:CD	2.39	0.47
1:I:34:TYR:OH	1:I:107:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:ASN:O	1:J:28:LEU:HB2	2.14	0.47
1:L:104:LEU:HD11	1:L:145:ILE:HG23	1.96	0.47
1:M:130:CYS:O	1:M:134:GLU:HG3	2.14	0.47
1:P:58:GLN:HA	1:P:61:GLU:HB2	1.97	0.47
1:R:154:ASN:O	1:R:158:MET:N	2.33	0.47
1:S:62:GLU:OE1	1:S:62:GLU:N	2.47	0.47
1:D:23:GLN:HE21	1:D:117:LEU:HD23	1.79	0.47
1:E:10:GLN:HE22	1:T:108:LYS:HB3	1.80	0.47
1:F:40:TYR:OH	1:F:94:GLU:N	2.48	0.47
1:G:19:ALA:HA	1:G:22:ARG:HG3	1.95	0.47
1:J:92:ASP:O	1:J:94:GLU:HG3	2.14	0.47
1:O:172:LYS:HB3	1:O:173:HIS:HD2	1.79	0.47
1:P:158:MET:HE1	1:P:170:PHE:HB2	1.95	0.47
1:Q:71:LYS:O	1:Q:75:GLN:N	2.38	0.47
1:Q:146:LYS:HZ2	1:X:44:ASP:HB3	1.80	0.47
1:S:56:LEU:O	1:S:59:SER:HB3	2.14	0.47
1:T:18:ALA:O	1:T:19:ALA:C	2.56	0.47
1:U:53:LYS:O	1:U:57:HIS:HB2	2.15	0.47
1:U:136:HIS:O	1:U:140:GLU:HB2	2.15	0.47
1:A:41:PHE:CZ	1:A:96:GLY:HA2	2.49	0.47
1:A:157:LYS:HD3	1:L:164:GLY:CA	2.44	0.47
1:D:79:ARG:HH11	1:V:43:ARG:HG2	1.80	0.47
1:F:139:ASN:OD1	1:F:143:LYS:NZ	2.43	0.47
1:G:141:GLN:O	1:G:145:ILE:HD12	2.14	0.47
1:H:43:ARG:NH1	1:H:92:ASP:OD2	2.48	0.47
1:H:87:LYS:HD2	1:H:87:LYS:C	2.39	0.47
1:I:48:LEU:HD23	1:I:48:LEU:HA	1.53	0.47
1:J:87:LYS:HB3	1:O:83:GLN:C	2.39	0.47
1:K:21:ASN:HD21	1:K:80:ILE:HA	1.79	0.47
1:Q:44:ASP:HA	1:W:150:ASP:OD1	2.15	0.47
1:U:60:HIS:O	1:U:64:GLU:HG3	2.14	0.47
1:A:44:ASP:HB3	1:N:146:LYS:HD2	1.95	0.47
1:A:76:ARG:C	1:A:78:GLY:H	2.23	0.47
1:C:153:THR:HG21	1:J:45:ASP:C	2.40	0.47
1:D:44:ASP:OD2	1:V:7:GLN:HG2	2.14	0.47
1:M:51:PHE:HD2	1:M:55:PHE:CE2	2.32	0.47
1:M:60:HIS:O	1:M:64:GLU:HG2	2.14	0.47
1:P:106:LEU:HD23	1:P:107:GLU:N	2.30	0.47
1:T:123:PHE:C	1:T:125:ASN:H	2.23	0.47
1:T:169:LEU:O	1:T:173:HIS:N	2.41	0.47
1:V:121:ALA:HB2	1:V:129:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:HA	1:A:116:GLU:HB2	1.96	0.47
1:A:150:ASP:OD1	1:L:44:ASP:HA	2.15	0.47
1:H:6:SER:HB2	1:H:79:ARG:NH2	2.29	0.47
1:K:137:TYR:O	1:K:140:GLU:N	2.42	0.47
1:L:21:ASN:HD21	1:L:80:ILE:HA	1.80	0.47
1:L:39:TYR:HA	1:L:42:ASP:HB2	1.97	0.47
1:M:107:GLU:O	1:M:111:ASN:N	2.37	0.47
1:T:76:ARG:C	1:T:78:GLY:N	2.73	0.47
1:C:63:ARG:CZ	1:X:63:ARG:HD3	2.45	0.47
1:J:41:PHE:HD2	1:J:48:LEU:HB2	1.80	0.47
1:J:97:LEU:O	1:J:101:GLU:N	2.35	0.47
1:P:43:ARG:HB3	1:P:45:ASP:OD1	2.14	0.47
1:Q:48:LEU:HD13	1:Q:51:PHE:CD2	2.50	0.47
1:R:105:HIS:O	1:R:108:LYS:HB2	2.15	0.47
1:U:58:GLN:HA	1:U:61:GLU:HG2	1.97	0.47
1:X:41:PHE:CE1	1:X:48:LEU:HD12	2.50	0.47
1:D:114:LEU:HD23	1:D:114:LEU:HA	1.64	0.47
1:E:22:ARG:NH1	1:E:22:ARG:HB2	2.30	0.47
1:F:86:LYS:HA	1:T:84:ASP:OD2	2.15	0.47
1:G:35:LEU:HG	1:U:70:MET:HE1	1.97	0.47
1:G:173:HIS:HB3	1:P:172:LYS:HG2	1.96	0.47
1:I:70:MET:HE1	1:N:35:LEU:HG	1.97	0.47
1:K:63:ARG:HH11	1:P:63:ARG:HH11	1.62	0.47
1:L:98:ASN:O	1:L:101:GLU:HB2	2.15	0.47
1:P:21:ASN:HD21	1:P:73:GLN:NE2	2.13	0.47
1:R:45:ASP:OD1	1:R:45:ASP:N	2.47	0.47
1:X:12:TYR:HB2	1:X:76:ARG:NE	2.23	0.47
1:C:128:HIS:NE2	1:Q:142:VAL:HG21	2.30	0.47
1:D:41:PHE:HB2	1:D:52:ALA:HB2	1.96	0.47
1:D:53:LYS:HZ2	1:D:57:HIS:HB2	1.80	0.47
1:L:142:VAL:HG21	1:S:128:HIS:CD2	2.49	0.47
1:M:33:VAL:O	1:M:37:MET:HG3	2.15	0.47
1:N:56:LEU:O	1:N:60:HIS:ND1	2.37	0.47
1:O:146:LYS:HE2	1:Q:74:ASN:O	2.15	0.47
1:Q:42:ASP:OD1	1:Q:49:LYS:HE3	2.14	0.47
1:T:62:GLU:O	1:T:66:ALA:N	2.45	0.47
1:V:73:GLN:HG3	1:V:78:GLY:C	2.40	0.47
1:A:39:TYR:CD2	1:W:70:MET:HE2	2.50	0.46
1:D:41:PHE:CZ	1:D:51:PHE:HD2	2.33	0.46
1:D:169:LEU:O	1:K:168:TYR:OH	2.20	0.46
1:E:64:GLU:OE2	1:E:68:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ARG:HH22	1:U:59:SER:HG	1.57	0.46
1:G:141:GLN:C	1:G:144:ALA:H	2.23	0.46
1:H:23:GLN:O	1:H:24:ILE:C	2.58	0.46
1:I:27:GLU:HG2	1:I:65:HIS:CB	2.42	0.46
1:J:52:ALA:O	1:J:55:PHE:N	2.47	0.46
1:N:53:LYS:NZ	1:N:56:LEU:HD23	2.30	0.46
1:O:136:HIS:HB2	1:O:137:TYR:CD2	2.50	0.46
1:P:131:ASP:HA	1:P:134:GLU:OE1	2.15	0.46
1:R:173:HIS:HB2	1:U:168:TYR:OH	2.15	0.46
1:E:76:ARG:NH2	1:E:126:ASP:OD1	2.44	0.46
1:G:34:TYR:O	1:G:38:SER:HB2	2.15	0.46
1:I:27:GLU:CG	1:I:65:HIS:HB2	2.45	0.46
1:I:41:PHE:HA	1:I:46:VAL:HG11	1.95	0.46
1:I:83:GLN:HA	1:N:87:LYS:HE2	1.96	0.46
1:K:64:GLU:O	1:K:68:LYS:HB2	2.15	0.46
1:K:84:ASP:O	1:K:86:LYS:HD2	2.15	0.46
1:Q:38:SER:HB2	1:Q:56:LEU:N	2.31	0.46
1:Q:45:ASP:HA	1:W:153:THR:HG21	1.97	0.46
1:Q:58:GLN:O	1:Q:62:GLU:HG2	2.15	0.46
1:S:141:GLN:O	1:S:144:ALA:HB3	2.16	0.46
1:U:41:PHE:HB3	1:U:48:LEU:O	2.15	0.46
1:V:9:ARG:CD	1:V:12:TYR:HB3	2.45	0.46
1:A:87:LYS:HD2	1:W:82:LEU:O	2.16	0.46
1:C:34:TYR:HA	1:C:37:MET:HE3	1.97	0.46
1:C:104:LEU:O	1:C:108:LYS:HG3	2.15	0.46
1:G:97:LEU:HD23	1:G:161:PRO:HG3	1.96	0.46
1:G:150:ASP:OD2	1:P:44:ASP:HA	2.16	0.46
1:G:155:LEU:HD11	1:G:170:PHE:CD1	2.49	0.46
1:H:48:LEU:HD22	1:H:171:ASP:CB	2.45	0.46
1:I:157:LYS:HG3	1:I:157:LYS:O	2.15	0.46
1:I:168:TYR:O	1:I:172:LYS:HG2	2.15	0.46
1:P:129:LEU:O	1:P:133:ILE:HG12	2.15	0.46
1:R:62:GLU:O	1:R:65:HIS:HB2	2.16	0.46
1:B:147:GLU:HG2	1:B:151:HIS:NE2	2.31	0.46
1:C:63:ARG:HH21	1:X:60:HIS:CD2	2.34	0.46
1:D:142:VAL:HG11	1:P:128:HIS:CE1	2.51	0.46
1:D:150:ASP:HA	1:K:47:ALA:HB2	1.96	0.46
1:K:50:ASN:HB2	1:K:171:ASP:OD1	2.16	0.46
1:K:121:ALA:HB2	1:K:129:LEU:HD22	1.97	0.46
1:L:70:MET:O	1:L:74:ASN:ND2	2.48	0.46
1:L:152:VAL:HG12	1:L:156:ARG:NH1	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:TYR:C	1:N:42:ASP:N	2.74	0.46
1:Q:9:ARG:NE	1:Q:12:TYR:HB3	2.30	0.46
1:R:127:PRO:O	1:R:130:CYS:N	2.49	0.46
1:B:87:LYS:HD2	1:Q:82:LEU:O	2.16	0.46
1:C:64:GLU:HA	1:C:67:GLU:HG3	1.97	0.46
1:G:74:ASN:O	1:R:146:LYS:HE2	2.15	0.46
1:H:45:ASP:CG	1:R:79:ARG:HH21	2.24	0.46
1:J:66:ALA:O	1:J:69:LEU:HB2	2.15	0.46
1:Q:19:ALA:O	1:Q:23:GLN:N	2.41	0.46
1:S:78:GLY:O	1:S:79:ARG:NH1	2.49	0.46
1:T:28:LEU:HD13	1:T:85:ILE:HD11	1.97	0.46
1:U:45:ASP:OD1	1:U:45:ASP:N	2.49	0.46
1:U:90:CYS:HB3	1:U:92:ASP:O	2.16	0.46
1:V:135:THR:OG1	1:V:136:HIS:ND1	2.43	0.46
1:D:111:ASN:H	1:D:141:GLN:HE22	1.64	0.46
1:G:85:ILE:HB	1:U:85:ILE:HB	1.97	0.46
1:H:118:HIS:O	1:H:118:HIS:ND1	2.48	0.46
1:U:143:LYS:O	1:U:146:LYS:N	2.48	0.46
1:B:67:GLU:HA	1:B:70:MET:CE	2.41	0.46
1:C:84:ASP:CG	1:X:86:LYS:HG2	2.41	0.46
1:H:66:ALA:HA	1:H:69:LEU:HD12	1.97	0.46
1:I:86:LYS:HA	1:N:84:ASP:OD1	2.16	0.46
1:N:54:TYR:O	1:N:58:GLN:HG2	2.15	0.46
1:O:114:LEU:HB2	1:O:138:LEU:HD21	1.97	0.46
1:P:112:GLN:HG2	1:X:10:GLN:HE21	1.80	0.46
1:Q:47:ALA:HA	1:Q:49:LYS:NZ	2.31	0.46
1:Q:146:LYS:HZ2	1:X:44:ASP:CB	2.29	0.46
1:U:114:LEU:HD13	1:U:137:TYR:HB3	1.98	0.46
1:C:65:HIS:O	1:C:69:LEU:HG	2.16	0.46
1:D:29:TYR:OH	1:D:88:PRO:HA	2.15	0.46
1:F:60:HIS:CD2	1:T:63:ARG:NH2	2.83	0.46
1:F:63:ARG:HH12	1:T:60:HIS:CD2	2.34	0.46
1:G:154:ASN:ND2	1:P:47:ALA:O	2.49	0.46
1:H:9:ARG:HG2	1:H:10:GLN:N	2.31	0.46
1:H:108:LYS:O	1:H:112:GLN:N	2.44	0.46
1:K:32:TYR:OH	1:P:83:GLN:O	2.31	0.46
1:M:53:LYS:HB3	1:M:53:LYS:HE2	1.71	0.46
1:P:16:SER:O	1:P:20:ILE:HG12	2.15	0.46
1:P:35:LEU:O	1:P:39:TYR:HD2	1.99	0.46
1:P:58:GLN:O	1:P:61:GLU:N	2.48	0.46
1:S:38:SER:OG	1:S:56:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:112:GLN:O	1:T:115:LEU:HB2	2.15	0.46
1:X:33:VAL:HG11	1:X:106:LEU:HD22	1.97	0.46
1:A:33:VAL:HG22	1:A:37:MET:HE2	1.97	0.46
1:C:68:LYS:NZ	1:C:136:HIS:HB3	2.31	0.46
1:D:90:CYS:HB2	1:D:93:TRP:CD2	2.51	0.46
1:E:112:GLN:HA	1:E:115:LEU:HD12	1.96	0.46
1:H:142:VAL:HG21	1:L:128:HIS:CD2	2.51	0.46
1:J:14:GLN:N	1:J:14:GLN:OE1	2.48	0.46
1:K:21:ASN:CG	1:K:81:PHE:H	2.24	0.46
1:O:39:TYR:O	1:O:42:ASP:HB3	2.16	0.46
1:Q:147:GLU:O	1:Q:150:ASP:HB2	2.16	0.46
1:R:57:HIS:O	1:R:58:GLN:C	2.59	0.46
1:T:13:HIS:CG	1:T:14:GLN:H	2.34	0.46
1:V:10:GLN:C	1:V:12:TYR:N	2.73	0.46
1:A:43:ARG:NH2	1:A:45:ASP:OD2	2.49	0.46
1:B:50:ASN:HB2	1:B:171:ASP:OD2	2.15	0.46
1:C:70:MET:HE1	1:X:35:LEU:HG	1.97	0.46
1:F:49:LYS:O	1:F:52:ALA:HB3	2.16	0.46
1:L:85:ILE:HB	1:M:85:ILE:HB	1.98	0.46
1:R:5:THR:OG1	1:R:6:SER:N	2.47	0.46
1:A:74:ASN:O	1:V:146:LYS:NZ	2.43	0.45
1:G:37:MET:HG2	1:G:93:TRP:CG	2.51	0.45
1:I:32:TYR:OH	1:N:82:LEU:HB3	2.16	0.45
1:I:148:LEU:HD23	1:I:148:LEU:HA	1.76	0.45
1:I:149:GLY:O	1:I:152:VAL:HB	2.16	0.45
1:N:118:HIS:O	1:N:122:THR:HG23	2.16	0.45
1:R:73:GLN:HG2	1:R:80:ILE:HG13	1.98	0.45
1:X:110:VAL:O	1:X:114:LEU:HG	2.16	0.45
1:B:158:MET:HE2	1:B:166:ALA:HA	1.98	0.45
1:C:45:ASP:OD1	1:C:45:ASP:N	2.47	0.45
1:D:91:ASP:OD2	1:V:81:PHE:HA	2.16	0.45
1:I:146:LYS:HD3	1:T:75:GLN:HA	1.97	0.45
1:M:148:LEU:O	1:M:151:HIS:N	2.42	0.45
1:O:51:PHE:HD1	1:O:55:PHE:HE2	1.64	0.45
1:P:44:ASP:C	1:P:46:VAL:H	2.25	0.45
1:P:137:TYR:O	1:P:141:GLN:HG2	2.16	0.45
1:R:40:TYR:CE2	1:R:93:TRP:HB2	2.52	0.45
1:V:133:ILE:HA	1:V:137:TYR:HB2	1.99	0.45
1:W:133:ILE:HG22	1:W:138:LEU:HD13	1.97	0.45
1:C:60:HIS:HA	1:C:63:ARG:HB3	1.98	0.45
1:D:156:ARG:O	1:D:159:GLY:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:HIS:CD2	1:T:63:ARG:HH21	2.34	0.45
1:F:111:ASN:HD22	1:F:141:GLN:CB	2.29	0.45
1:I:165:LEU:O	1:I:169:LEU:HG	2.16	0.45
1:J:48:LEU:HD11	1:J:167:GLU:HG3	1.97	0.45
1:L:79:ARG:C	1:L:80:ILE:HG13	2.41	0.45
1:M:148:LEU:C	1:M:151:HIS:H	2.23	0.45
1:M:154:ASN:O	1:M:157:LYS:HB3	2.17	0.45
1:N:119:LYS:O	1:N:122:THR:OG1	2.33	0.45
1:S:151:HIS:O	1:S:155:LEU:HG	2.17	0.45
1:T:104:LEU:O	1:T:108:LYS:HG3	2.16	0.45
1:T:171:ASP:O	1:T:175:LEU:HB2	2.16	0.45
1:V:121:ALA:CB	1:V:129:LEU:HB3	2.47	0.45
1:X:34:TYR:CE2	1:X:62:GLU:HG3	2.45	0.45
1:X:39:TYR:O	1:X:42:ASP:HB3	2.16	0.45
1:B:172:LYS:C	1:B:174:THR:H	2.23	0.45
1:C:61:GLU:HG3	1:C:62:GLU:OE1	2.16	0.45
1:L:79:ARG:HD3	1:L:79:ARG:HA	1.49	0.45
1:P:150:ASP:C	1:P:152:VAL:H	2.24	0.45
1:Q:41:PHE:CG	1:Q:51:PHE:HB3	2.52	0.45
1:R:62:GLU:HA	1:R:65:HIS:ND1	2.32	0.45
1:T:164:GLY:HA3	1:U:157:LYS:O	2.16	0.45
1:V:17:GLU:O	1:V:21:ASN:ND2	2.50	0.45
1:W:154:ASN:O	1:W:158:MET:N	2.49	0.45
1:A:20:ILE:O	1:A:24:ILE:N	2.41	0.45
1:B:114:LEU:C	1:B:116:GLU:N	2.74	0.45
1:B:170:PHE:CZ	1:B:174:THR:HG21	2.51	0.45
1:C:33:VAL:HA	1:C:88:PRO:HG3	1.99	0.45
1:D:61:GLU:O	1:D:64:GLU:HG2	2.16	0.45
1:E:19:ALA:HA	1:E:22:ARG:HH22	1.81	0.45
1:H:40:TYR:O	1:H:46:VAL:HG21	2.17	0.45
1:K:54:TYR:O	1:K:58:GLN:HG2	2.16	0.45
1:K:69:LEU:O	1:K:72:LEU:HB3	2.17	0.45
1:O:104:LEU:HD23	1:O:108:LYS:HG3	1.98	0.45
1:P:17:GLU:OE1	1:P:78:GLY:HA2	2.17	0.45
1:R:64:GLU:O	1:R:68:LYS:HG2	2.17	0.45
1:R:143:LYS:O	1:R:146:LYS:HB3	2.16	0.45
1:S:33:VAL:O	1:S:37:MET:HG3	2.17	0.45
1:A:145:ILE:HG13	1:A:146:LYS:H	1.81	0.45
1:C:131:ASP:HA	1:C:134:GLU:CD	2.41	0.45
1:G:36:SER:HB2	1:U:82:LEU:HD12	1.98	0.45
1:K:16:SER:O	1:K:20:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:155:LEU:HD21	1:W:170:PHE:CG	2.51	0.45
1:C:40:TYR:O	1:C:43:ARG:HB2	2.17	0.45
1:E:65:HIS:C	1:E:137:TYR:HH	2.22	0.45
1:I:93:TRP:HZ3	1:I:102:CYS:SG	2.40	0.45
1:J:36:SER:OG	1:J:93:TRP:NE1	2.49	0.45
1:J:41:PHE:CD2	1:J:48:LEU:HB2	2.51	0.45
1:K:6:SER:OG	1:K:7:GLN:N	2.47	0.45
1:L:39:TYR:HB3	1:M:80:ILE:HD12	1.98	0.45
1:M:40:TYR:CD2	1:M:93:TRP:HD1	2.35	0.45
1:O:45:ASP:N	1:O:45:ASP:OD1	2.48	0.45
1:O:119:LYS:HA	1:O:122:THR:HG22	1.98	0.45
1:S:129:LEU:O	1:S:133:ILE:HG12	2.16	0.45
1:V:120:LEU:HD12	1:V:120:LEU:HA	1.66	0.45
1:W:9:ARG:NH2	1:W:12:TYR:O	2.47	0.45
1:B:134:GLU:HB3	1:N:131:ASP:HB2	1.98	0.45
1:C:34:TYR:CG	1:C:58:GLN:HB2	2.51	0.45
1:F:37:MET:HE1	1:F:103:ALA:HB2	1.98	0.45
1:G:118:HIS:CE1	1:G:134:GLU:HG3	2.44	0.45
1:H:43:ARG:HB2	1:H:46:VAL:HG22	1.98	0.45
1:I:24:ILE:HG12	1:I:69:LEU:HB2	1.99	0.45
1:I:94:GLU:N	1:I:94:GLU:OE1	2.50	0.45
1:L:8:VAL:HG13	1:L:77:GLY:HA3	1.99	0.45
1:M:40:TYR:O	1:M:43:ARG:HD3	2.17	0.45
1:O:43:ARG:HB2	1:O:46:VAL:HG23	1.98	0.45
1:P:8:VAL:HG23	1:P:77:GLY:HA2	1.98	0.45
1:Q:73:GLN:NE2	1:Q:78:GLY:HA3	2.32	0.45
1:Q:139:ASN:O	1:Q:143:LYS:HD3	2.17	0.45
1:T:50:ASN:O	1:T:175:LEU:HD13	2.16	0.45
1:V:7:GLN:HG3	1:V:8:VAL:HG13	1.99	0.45
1:B:44:ASP:O	1:O:153:THR:OG1	2.31	0.45
1:C:25:ASN:ND2	1:C:83:GLN:HG3	2.32	0.45
1:D:121:ALA:HB2	1:D:129:LEU:HD23	1.98	0.45
1:F:42:ASP:OD1	1:T:71:LYS:NZ	2.26	0.45
1:J:82:LEU:HD13	1:O:32:TYR:CE1	2.52	0.45
1:K:29:TYR:HD1	1:K:86:LYS:O	2.00	0.45
1:K:131:ASP:OD1	1:K:134:GLU:HB2	2.17	0.45
1:L:60:HIS:O	1:L:64:GLU:HG2	2.17	0.45
1:L:68:LYS:HB2	1:L:68:LYS:HE3	1.70	0.45
1:N:50:ASN:HB2	1:N:171:ASP:CG	2.42	0.45
1:N:139:ASN:O	1:N:143:LYS:HG3	2.17	0.45
1:Q:146:LYS:HZ2	1:X:44:ASP:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD11	1:A:128:HIS:NE2	2.32	0.45
1:A:83:GLN:O	1:W:32:TYR:OH	2.21	0.45
1:B:40:TYR:O	1:B:46:VAL:HG21	2.17	0.45
1:E:23:GLN:O	1:E:26:LEU:N	2.50	0.45
1:E:44:ASP:OD2	1:S:6:SER:OG	2.35	0.45
1:F:41:PHE:HZ	1:F:96:GLY:HA2	1.82	0.45
1:G:51:PHE:CZ	1:G:170:PHE:HD1	2.35	0.45
1:G:72:LEU:HD13	1:G:132:PHE:CE2	2.52	0.45
1:I:87:LYS:N	1:N:84:ASP:OD1	2.37	0.45
1:J:32:TYR:CD2	1:J:88:PRO:HD3	2.52	0.45
1:Q:119:LYS:O	1:Q:122:THR:HB	2.17	0.45
1:W:101:GLU:OE1	1:W:156:ARG:NH2	2.50	0.45
1:F:6:SER:H	1:F:79:ARG:NH2	2.16	0.44
1:L:138:LEU:HA	1:L:138:LEU:HD23	1.65	0.44
1:P:165:LEU:HD12	1:P:168:TYR:HB3	1.98	0.44
1:X:72:LEU:HD12	1:X:132:PHE:CE2	2.51	0.44
1:B:40:TYR:O	1:B:43:ARG:HD3	2.17	0.44
1:F:37:MET:HG2	1:F:93:TRP:CG	2.52	0.44
1:F:49:LYS:HE3	1:F:49:LYS:HB2	1.69	0.44
1:F:128:HIS:HD2	1:U:138:LEU:HB3	1.83	0.44
1:H:133:ILE:HG23	1:H:137:TYR:HB2	2.00	0.44
1:J:23:GLN:O	1:J:27:GLU:HG2	2.17	0.44
1:M:132:PHE:HD2	1:M:133:ILE:HD13	1.82	0.44
1:P:49:LYS:C	1:P:53:LYS:NZ	2.75	0.44
1:Q:10:GLN:C	1:Q:12:TYR:H	2.25	0.44
1:U:80:ILE:C	1:U:81:PHE:HD1	2.26	0.44
1:X:150:ASP:O	1:X:151:HIS:C	2.60	0.44
1:A:168:TYR:OH	1:N:173:HIS:HB2	2.17	0.44
1:C:146:LYS:NZ	1:C:150:ASP:OD2	2.44	0.44
1:G:108:LYS:NZ	1:K:10:GLN:HB2	2.32	0.44
1:H:48:LEU:CD2	1:H:168:TYR:HA	2.44	0.44
1:H:153:THR:OG1	1:M:44:ASP:O	2.27	0.44
1:H:165:LEU:HD12	1:K:158:MET:HG2	1.97	0.44
1:J:17:GLU:C	1:J:73:GLN:HE22	2.22	0.44
1:J:23:GLN:O	1:J:24:ILE:C	2.60	0.44
1:J:168:TYR:O	1:J:171:ASP:HB3	2.17	0.44
1:R:32:TYR:CD2	1:R:88:PRO:HD3	2.52	0.44
1:T:69:LEU:HD23	1:T:69:LEU:HA	1.54	0.44
1:T:110:VAL:O	1:T:113:SER:N	2.51	0.44
1:V:49:LYS:O	1:V:51:PHE:N	2.51	0.44
1:X:73:GLN:HG3	1:X:78:GLY:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HD3	1:L:164:GLY:HA3	2.00	0.44
1:C:20:ILE:O	1:C:24:ILE:HG13	2.17	0.44
1:D:13:HIS:HD2	1:D:15:ASP:HB2	1.79	0.44
1:D:68:LYS:HE3	1:D:132:PHE:CZ	2.52	0.44
1:D:168:TYR:HD1	1:D:169:LEU:HD23	1.82	0.44
1:H:152:VAL:C	1:H:154:ASN:N	2.76	0.44
1:Q:62:GLU:OE2	1:Q:65:HIS:ND1	2.51	0.44
1:U:58:GLN:O	1:U:62:GLU:HG2	2.18	0.44
1:V:44:ASP:HB3	1:X:146:LYS:NZ	2.33	0.44
1:V:68:LYS:HB2	1:V:137:TYR:OH	2.17	0.44
1:A:37:MET:O	1:A:40:TYR:HB3	2.18	0.44
1:C:43:ARG:HH21	1:C:45:ASP:CG	2.23	0.44
1:D:47:ALA:O	1:D:48:LEU:HD22	2.17	0.44
1:F:43:ARG:C	1:F:45:ASP:H	2.25	0.44
1:H:42:ASP:HB3	1:R:74:ASN:OD1	2.17	0.44
1:H:152:VAL:O	1:H:154:ASN:N	2.50	0.44
1:J:69:LEU:HA	1:J:69:LEU:HD23	1.67	0.44
1:M:66:ALA:O	1:M:70:MET:HG3	2.18	0.44
1:M:107:GLU:HA	1:M:110:VAL:HB	2.00	0.44
1:N:35:LEU:HA	1:N:35:LEU:HD12	1.72	0.44
1:R:112:GLN:HA	1:R:115:LEU:HD12	1.98	0.44
1:T:50:ASN:HB2	1:T:171:ASP:OD1	2.18	0.44
1:U:158:MET:HE2	1:U:166:ALA:HB1	1.99	0.44
1:V:149:GLY:HA2	1:V:152:VAL:HB	1.99	0.44
1:W:116:GLU:HA	1:W:119:LYS:HB3	1.99	0.44
1:X:27:GLU:CB	1:X:66:ALA:HB2	2.47	0.44
1:A:67:GLU:HA	1:A:70:MET:CE	2.47	0.44
1:C:28:LEU:HD21	1:C:66:ALA:HB2	2.00	0.44
1:C:32:TYR:OH	1:X:82:LEU:HD22	2.17	0.44
1:F:21:ASN:OD1	1:F:73:GLN:NE2	2.51	0.44
1:F:116:GLU:HG2	1:F:117:LEU:HD12	1.99	0.44
1:I:54:TYR:CD2	1:I:175:LEU:HD22	2.53	0.44
1:T:76:ARG:HH12	1:T:129:LEU:HD13	1.81	0.44
1:V:73:GLN:HG3	1:V:78:GLY:HA3	2.00	0.44
1:V:100:MET:SD	1:V:148:LEU:HD22	2.58	0.44
1:A:74:ASN:C	1:A:76:ARG:H	2.25	0.44
1:E:126:ASP:O	1:E:129:LEU:HB3	2.17	0.44
1:Q:54:TYR:OH	1:Q:147:GLU:OE2	2.24	0.44
1:S:152:VAL:O	1:S:156:ARG:HG3	2.17	0.44
1:T:76:ARG:O	1:T:78:GLY:N	2.50	0.44
1:V:31:SER:O	1:V:35:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:111:ASN:O	1:W:112:GLN:C	2.58	0.44
1:A:119:LYS:O	1:A:122:THR:HB	2.18	0.44
1:C:69:LEU:HA	1:C:72:LEU:HB3	1.99	0.44
1:D:45:ASP:OD1	1:D:45:ASP:N	2.51	0.44
1:F:48:LEU:O	1:F:51:PHE:N	2.50	0.44
1:F:92:ASP:OD1	1:F:94:GLU:N	2.40	0.44
1:H:73:GLN:OE1	1:H:78:GLY:HA3	2.18	0.44
1:K:40:TYR:CD2	1:K:93:TRP:HB2	2.53	0.44
1:K:41:PHE:HZ	1:K:96:GLY:HA2	1.83	0.44
1:L:66:ALA:O	1:L:69:LEU:N	2.51	0.44
1:P:83:GLN:HG3	1:P:84:ASP:H	1.83	0.44
1:Q:158:MET:HB3	1:Q:166:ALA:HB1	1.99	0.44
1:S:45:ASP:OD1	1:S:46:VAL:HG23	2.17	0.44
1:W:43:ARG:HB3	1:W:45:ASP:OD1	2.17	0.44
1:A:93:TRP:O	1:A:95:SER:N	2.51	0.44
1:C:45:ASP:C	1:P:153:THR:HG21	2.43	0.44
1:C:165:LEU:HB2	1:P:158:MET:O	2.18	0.44
1:D:39:TYR:OH	1:V:67:GLU:O	2.24	0.44
1:D:51:PHE:HD1	1:D:175:LEU:HD12	1.83	0.44
1:D:167:GLU:OE2	1:M:157:LYS:HE2	2.18	0.44
1:J:34:TYR:CE1	1:J:58:GLN:HB2	2.53	0.44
1:J:70:MET:HG2	1:J:80:ILE:HD13	2.00	0.44
1:K:63:ARG:NH1	1:P:63:ARG:HD3	2.33	0.44
1:L:50:ASN:HB2	1:L:171:ASP:OD1	2.18	0.44
1:O:96:GLY:O	1:O:99:ALA:HB3	2.18	0.44
1:P:58:GLN:O	1:P:62:GLU:HG2	2.17	0.44
1:R:110:VAL:O	1:R:113:SER:HB3	2.18	0.44
1:S:50:ASN:HB2	1:S:171:ASP:CG	2.42	0.44
1:U:96:GLY:O	1:U:99:ALA:HB3	2.18	0.44
1:W:34:TYR:HB3	1:W:55:PHE:O	2.18	0.44
1:B:41:PHE:HA	1:B:46:VAL:HG11	2.00	0.43
1:E:60:HIS:CD2	1:S:63:ARG:HH21	2.36	0.43
1:F:111:ASN:CB	1:F:141:GLN:HG2	2.38	0.43
1:H:155:LEU:HD23	1:H:155:LEU:HA	1.65	0.43
1:K:93:TRP:O	1:K:95:SER:N	2.51	0.43
1:L:44:ASP:OD1	1:L:45:ASP:N	2.50	0.43
1:M:26:LEU:HD21	1:M:110:VAL:HA	2.00	0.43
1:P:171:ASP:OD2	1:P:172:LYS:NZ	2.40	0.43
1:X:61:GLU:O	1:X:65:HIS:N	2.43	0.43
1:D:87:LYS:HE2	1:V:82:LEU:O	2.18	0.43
1:G:41:PHE:HD1	1:G:46:VAL:HG11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:VAL:O	1:H:37:MET:HG3	2.18	0.43
1:K:130:CYS:O	1:K:134:GLU:HG3	2.18	0.43
1:N:97:LEU:HD11	1:N:156:ARG:HG3	2.00	0.43
1:P:140:GLU:HG3	1:P:141:GLN:NE2	2.32	0.43
1:V:24:ILE:HD13	1:V:70:MET:HG2	2.00	0.43
1:V:117:LEU:O	1:V:118:HIS:C	2.61	0.43
1:D:29:TYR:O	1:D:32:TYR:N	2.50	0.43
1:D:73:GLN:O	1:D:78:GLY:N	2.49	0.43
1:F:37:MET:O	1:F:39:TYR:N	2.51	0.43
1:G:74:ASN:HB3	1:U:43:ARG:HA	2.00	0.43
1:H:32:TYR:HD2	1:H:85:ILE:HG22	1.83	0.43
1:I:20:ILE:HA	1:I:20:ILE:HD13	1.82	0.43
1:J:95:SER:OG	1:J:96:GLY:N	2.50	0.43
1:P:120:LEU:HA	1:P:123:PHE:HB2	1.99	0.43
1:Q:72:LEU:HA	1:Q:75:GLN:HB2	1.98	0.43
1:Q:82:LEU:HD23	1:Q:82:LEU:HA	1.83	0.43
1:S:87:LYS:HE3	1:S:87:LYS:HB2	1.85	0.43
1:W:66:ALA:O	1:W:69:LEU:HB2	2.19	0.43
1:W:97:LEU:O	1:W:101:GLU:HG3	2.18	0.43
1:X:136:HIS:HB2	1:X:137:TYR:CD1	2.53	0.43
1:D:140:GLU:OE1	1:D:141:GLN:HG3	2.17	0.43
1:G:34:TYR:CZ	1:G:58:GLN:HB3	2.52	0.43
1:G:117:LEU:O	1:G:121:ALA:N	2.43	0.43
1:I:33:VAL:HG22	1:I:88:PRO:HB3	1.99	0.43
1:M:20:ILE:HD13	1:M:20:ILE:HA	1.79	0.43
1:M:160:ALA:HA	1:M:161:PRO:HA	1.66	0.43
1:R:14:GLN:O	1:R:17:GLU:HG2	2.17	0.43
1:S:174:THR:HG22	1:S:175:LEU:HD12	1.99	0.43
1:U:67:GLU:HA	1:U:70:MET:SD	2.58	0.43
1:U:140:GLU:O	1:U:141:GLN:HG2	2.18	0.43
1:U:146:LYS:HD2	1:U:146:LYS:HA	1.72	0.43
1:X:153:THR:O	1:X:157:LYS:N	2.48	0.43
1:A:76:ARG:O	1:A:78:GLY:N	2.49	0.43
1:C:28:LEU:O	1:C:31:SER:N	2.51	0.43
1:C:150:ASP:OD1	1:J:44:ASP:HA	2.19	0.43
1:D:83:GLN:HA	1:V:87:LYS:HB3	2.01	0.43
1:F:13:HIS:HB3	1:F:16:SER:H	1.83	0.43
1:F:106:LEU:HD12	1:F:106:LEU:HA	1.83	0.43
1:G:32:TYR:CE2	1:G:87:LYS:HA	2.54	0.43
1:H:9:ARG:HA	1:H:76:ARG:O	2.18	0.43
1:H:154:ASN:O	1:H:158:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:LEU:O	1:J:75:GLN:HB2	2.18	0.43
1:K:20:ILE:O	1:K:23:GLN:N	2.51	0.43
1:N:45:ASP:OD1	1:N:45:ASP:N	2.51	0.43
1:N:50:ASN:HB2	1:N:171:ASP:OD1	2.18	0.43
1:T:106:LEU:O	1:T:110:VAL:HG23	2.17	0.43
1:V:104:LEU:HD12	1:V:104:LEU:HA	1.86	0.43
1:W:37:MET:O	1:W:41:PHE:CD2	2.70	0.43
1:X:18:ALA:O	1:X:22:ARG:HG3	2.19	0.43
1:X:134:GLU:HA	1:X:138:LEU:CD1	2.48	0.43
1:C:152:VAL:O	1:C:155:LEU:HB2	2.18	0.43
1:D:44:ASP:OD1	1:D:44:ASP:N	2.50	0.43
1:E:24:ILE:HG12	1:E:69:LEU:HB2	2.01	0.43
1:J:102:CYS:O	1:J:105:HIS:HB3	2.19	0.43
1:K:111:ASN:C	1:K:111:ASN:OD1	2.62	0.43
1:L:146:LYS:HA	1:S:8:VAL:HG11	2.00	0.43
1:O:51:PHE:N	1:O:171:ASP:OD1	2.42	0.43
1:T:35:LEU:C	1:T:37:MET:N	2.77	0.43
1:A:67:GLU:HA	1:A:70:MET:HE2	2.00	0.43
1:A:119:LYS:C	1:A:122:THR:H	2.26	0.43
1:B:85:ILE:HB	1:Q:85:ILE:HB	2.01	0.43
1:D:95:SER:O	1:D:98:ASN:N	2.52	0.43
1:D:150:ASP:OD2	1:K:47:ALA:HA	2.18	0.43
1:H:120:LEU:O	1:H:124:LYS:N	2.34	0.43
1:K:50:ASN:HB2	1:K:171:ASP:CG	2.44	0.43
1:M:134:GLU:HB3	1:V:131:ASP:OD2	2.19	0.43
1:P:41:PHE:HA	1:P:46:VAL:HG11	2.00	0.43
1:P:120:LEU:HA	1:P:123:PHE:CB	2.49	0.43
1:Q:124:LYS:HA	1:Q:124:LYS:HD3	1.54	0.43
1:U:34:TYR:HA	1:U:37:MET:HE2	2.00	0.43
1:V:19:ALA:O	1:V:23:GLN:N	2.45	0.43
1:V:34:TYR:HB3	1:V:55:PHE:O	2.19	0.43
1:D:31:SER:HB2	1:D:62:GLU:HG2	2.01	0.43
1:F:19:ALA:O	1:F:22:ARG:HB2	2.19	0.43
1:F:36:SER:HB2	1:F:93:TRP:CZ2	2.52	0.43
1:F:54:TYR:O	1:F:58:GLN:HG2	2.19	0.43
1:H:43:ARG:HB3	1:H:45:ASP:OD1	2.19	0.43
1:H:60:HIS:O	1:H:63:ARG:HB3	2.18	0.43
1:I:73:GLN:NE2	1:I:79:ARG:O	2.52	0.43
1:K:25:ASN:HA	1:K:28:LEU:HD12	2.00	0.43
1:K:161:PRO:O	1:K:163:SER:N	2.50	0.43
1:L:39:TYR:CE2	1:M:70:MET:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:92:ASP:OD1	1:L:92:ASP:C	2.61	0.43
1:N:39:TYR:HA	1:N:42:ASP:HB2	2.00	0.43
1:V:106:LEU:HD22	1:V:107:GLU:HG2	2.01	0.43
1:W:50:ASN:HB2	1:W:171:ASP:CG	2.44	0.43
1:X:48:LEU:HD11	1:X:167:GLU:OE1	2.17	0.43
1:A:85:ILE:HD11	1:W:32:TYR:CE1	2.54	0.43
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.83	0.43
1:H:25:ASN:ND2	1:H:83:GLN:HB3	2.34	0.43
1:J:97:LEU:O	1:J:101:GLU:HB2	2.19	0.43
1:M:169:LEU:O	1:M:173:HIS:HB2	2.18	0.43
1:P:35:LEU:HD12	1:P:35:LEU:HA	1.79	0.43
1:E:37:MET:HA	1:E:93:TRP:CD1	2.54	0.43
1:F:100:MET:HE1	1:F:151:HIS:ND1	2.34	0.43
1:O:60:HIS:O	1:O:63:ARG:HB3	2.18	0.43
1:R:154:ASN:ND2	1:U:47:ALA:HB1	2.34	0.43
1:V:93:TRP:HB3	1:V:99:ALA:HB2	2.01	0.43
1:W:56:LEU:HA	1:W:59:SER:HB3	2.00	0.43
1:X:53:LYS:O	1:X:57:HIS:N	2.38	0.43
1:X:73:GLN:HE21	1:X:78:GLY:C	2.26	0.43
1:B:55:PHE:CZ	1:B:100:MET:SD	3.12	0.42
1:B:172:LYS:HD3	1:O:173:HIS:ND1	2.33	0.42
1:F:87:LYS:HE2	1:F:87:LYS:HB2	1.80	0.42
1:G:168:TYR:OH	1:J:174:THR:OG1	2.12	0.42
1:H:97:LEU:HD12	1:H:160:ALA:HB3	2.01	0.42
1:I:9:ARG:CG	1:I:12:TYR:HB3	2.48	0.42
1:L:6:SER:OG	1:L:8:VAL:HG12	2.19	0.42
1:L:168:TYR:CZ	1:L:172:LYS:HE3	2.53	0.42
1:N:160:ALA:HA	1:N:161:PRO:HA	1.75	0.42
1:O:114:LEU:CB	1:O:138:LEU:HD21	2.48	0.42
1:O:145:ILE:O	1:O:149:GLY:N	2.40	0.42
1:P:112:GLN:O	1:P:116:GLU:HG3	2.19	0.42
1:R:16:SER:O	1:R:20:ILE:HG12	2.19	0.42
1:B:72:LEU:HD12	1:B:132:PHE:CD2	2.55	0.42
1:B:155:LEU:HA	1:B:158:MET:HB2	2.00	0.42
1:C:139:ASN:HA	1:O:128:HIS:HD2	1.82	0.42
1:D:73:GLN:HG3	1:D:78:GLY:C	2.45	0.42
1:E:106:LEU:O	1:E:110:VAL:HG23	2.19	0.42
1:F:19:ALA:HB1	1:F:117:LEU:HG	2.01	0.42
1:F:93:TRP:O	1:F:98:ASN:ND2	2.53	0.42
1:G:71:LYS:O	1:G:75:GLN:HG3	2.19	0.42
1:J:102:CYS:O	1:J:106:LEU:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:LYS:HE3	1:L:119:LYS:HB3	1.76	0.42
1:M:51:PHE:HD2	1:M:55:PHE:HE2	1.67	0.42
1:P:111:ASN:HB3	1:X:10:GLN:HE22	1.81	0.42
1:Q:16:SER:O	1:Q:20:ILE:HG12	2.19	0.42
1:V:66:ALA:O	1:V:70:MET:N	2.50	0.42
1:X:166:ALA:C	1:X:168:TYR:N	2.76	0.42
1:B:41:PHE:HB2	1:B:52:ALA:HB2	2.01	0.42
1:G:20:ILE:C	1:G:22:ARG:N	2.77	0.42
1:G:136:HIS:HB2	1:G:137:TYR:CD1	2.54	0.42
1:H:72:LEU:C	1:H:72:LEU:HD23	2.44	0.42
1:K:41:PHE:HB3	1:K:48:LEU:O	2.19	0.42
1:L:62:GLU:OE1	1:L:65:HIS:CE1	2.72	0.42
1:M:97:LEU:HD12	1:M:160:ALA:HB1	2.01	0.42
1:R:40:TYR:CD2	1:R:93:TRP:HB2	2.54	0.42
1:T:13:HIS:CG	1:T:14:GLN:N	2.86	0.42
1:U:127:PRO:O	1:U:130:CYS:HB2	2.18	0.42
1:U:160:ALA:HB1	1:U:161:PRO:HA	2.01	0.42
1:V:43:ARG:O	1:V:47:ALA:N	2.48	0.42
1:V:62:GLU:O	1:V:65:HIS:HB2	2.19	0.42
1:C:19:ALA:O	1:C:23:GLN:N	2.51	0.42
1:C:160:ALA:HA	1:C:161:PRO:HA	1.79	0.42
1:E:9:ARG:HG3	1:E:12:TYR:HB3	2.01	0.42
1:F:106:LEU:O	1:F:110:VAL:HG23	2.18	0.42
1:L:107:GLU:HA	1:L:110:VAL:HB	2.00	0.42
1:M:137:TYR:C	1:M:139:ASN:H	2.27	0.42
1:O:56:LEU:HA	1:O:59:SER:HB3	2.01	0.42
1:U:97:LEU:HG	1:U:101:GLU:OE2	2.20	0.42
1:V:10:GLN:C	1:V:12:TYR:H	2.27	0.42
1:A:19:ALA:O	1:A:23:GLN:HB2	2.20	0.42
1:C:157:LYS:HD2	1:C:157:LYS:HA	1.60	0.42
1:D:62:GLU:HA	1:D:65:HIS:HD2	1.83	0.42
1:F:138:LEU:HD23	1:F:138:LEU:HA	1.85	0.42
1:F:164:GLY:HA3	1:I:157:LYS:NZ	2.34	0.42
1:H:31:SER:OG	1:H:59:SER:O	2.31	0.42
1:J:115:LEU:C	1:J:118:HIS:HB3	2.42	0.42
1:K:145:ILE:HG22	1:R:8:VAL:HG12	2.02	0.42
1:L:125:ASN:HD22	1:L:125:ASN:HA	1.69	0.42
1:Q:139:ASN:O	1:Q:142:VAL:HG22	2.19	0.42
1:R:118:HIS:O	1:R:122:THR:OG1	2.30	0.42
1:W:106:LEU:O	1:W:110:VAL:HG23	2.20	0.42
1:C:85:ILE:HD11	1:X:32:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:PHE:N	1:E:123:PHE:CD1	2.87	0.42
1:J:16:SER:O	1:J:19:ALA:N	2.52	0.42
1:K:8:VAL:HG23	1:K:76:ARG:C	2.45	0.42
1:M:111:ASN:HA	1:M:114:LEU:CD1	2.50	0.42
1:N:155:LEU:HD23	1:N:155:LEU:HA	1.67	0.42
1:R:66:ALA:HA	1:R:69:LEU:CD1	2.44	0.42
1:S:72:LEU:HD13	1:S:132:PHE:CD2	2.55	0.42
1:V:66:ALA:O	1:V:69:LEU:N	2.51	0.42
1:V:92:ASP:C	1:V:94:GLU:H	2.28	0.42
1:X:35:LEU:HD12	1:X:35:LEU:HA	1.59	0.42
1:A:140:GLU:HA	1:A:143:LYS:HE3	2.01	0.42
1:C:100:MET:HB3	1:C:152:VAL:HG22	2.02	0.42
1:F:13:HIS:O	1:F:16:SER:HB2	2.20	0.42
1:F:26:LEU:HD12	1:F:26:LEU:HA	1.69	0.42
1:G:111:ASN:HA	1:G:114:LEU:HD12	2.00	0.42
1:I:11:ASN:ND2	1:I:125:ASN:O	2.52	0.42
1:I:84:ASP:H	1:N:87:LYS:HE2	1.84	0.42
1:M:37:MET:HE2	1:M:37:MET:HB3	1.90	0.42
1:N:12:TYR:HB2	1:N:76:ARG:NH2	2.34	0.42
1:T:86:LYS:HG3	1:T:87:LYS:N	2.34	0.42
1:B:143:LYS:HE3	1:B:143:LYS:HB2	1.69	0.42
1:E:7:GLN:HG3	1:E:8:VAL:HG13	2.02	0.42
1:F:13:HIS:CE1	1:F:124:LYS:HD2	2.55	0.42
1:G:111:ASN:O	1:G:114:LEU:HB2	2.19	0.42
1:K:6:SER:HB3	1:K:9:ARG:HG3	2.01	0.42
1:N:92:ASP:C	1:N:94:GLU:N	2.78	0.42
1:P:17:GLU:CD	1:P:78:GLY:HA2	2.44	0.42
1:R:64:GLU:C	1:R:68:LYS:HZ3	2.27	0.42
1:W:58:GLN:O	1:W:62:GLU:HG2	2.19	0.42
1:X:43:ARG:O	1:X:47:ALA:N	2.51	0.42
1:E:9:ARG:NE	1:E:12:TYR:O	2.41	0.42
1:F:56:LEU:HD12	1:F:56:LEU:HA	1.84	0.42
1:G:24:ILE:O	1:G:28:LEU:HD12	2.20	0.42
1:G:60:HIS:O	1:G:64:GLU:HB2	2.19	0.42
1:G:168:TYR:O	1:G:171:ASP:N	2.48	0.42
1:K:87:LYS:HG2	1:P:84:ASP:OD1	2.20	0.42
1:K:146:LYS:HD3	1:R:75:GLN:HA	2.02	0.42
1:L:30:ALA:C	1:L:32:TYR:N	2.78	0.42
1:O:120:LEU:O	1:O:123:PHE:HB2	2.19	0.42
1:O:173:HIS:CD2	1:O:173:HIS:N	2.87	0.42
1:U:118:HIS:ND1	1:U:118:HIS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:150:ASP:OD1	1:U:150:ASP:N	2.48	0.42
1:W:57:HIS:CD2	1:W:61:GLU:HG2	2.54	0.42
1:A:168:TYR:O	1:A:172:LYS:HG2	2.19	0.42
1:A:169:LEU:HD21	1:N:169:LEU:HD13	2.01	0.42
1:C:21:ASN:HD21	1:C:81:PHE:C	2.24	0.42
1:H:28:LEU:HB3	1:H:85:ILE:HD11	2.02	0.42
1:H:43:ARG:HG2	1:R:79:ARG:NE	2.35	0.42
1:H:62:GLU:HA	1:H:65:HIS:ND1	2.35	0.42
1:H:92:ASP:O	1:H:94:GLU:N	2.49	0.42
1:L:41:PHE:HA	1:L:46:VAL:CG1	2.45	0.42
1:M:41:PHE:HA	1:M:46:VAL:CG1	2.50	0.42
1:M:48:LEU:HD23	1:M:48:LEU:HA	1.89	0.42
1:N:92:ASP:O	1:N:94:GLU:N	2.50	0.42
1:S:44:ASP:OD1	1:S:44:ASP:N	2.53	0.42
1:S:131:ASP:HA	1:S:134:GLU:HB2	2.01	0.42
1:V:12:TYR:CZ	1:V:17:GLU:HB2	2.55	0.42
1:V:80:ILE:O	1:V:80:ILE:HG13	2.20	0.42
1:A:32:TYR:O	1:A:35:LEU:HB3	2.20	0.41
1:B:156:ARG:C	1:B:158:MET:H	2.27	0.41
1:C:144:ALA:O	1:C:148:LEU:HG	2.20	0.41
1:D:9:ARG:O	1:X:108:LYS:NZ	2.53	0.41
1:F:158:MET:HE1	1:F:170:PHE:CD1	2.55	0.41
1:G:141:GLN:O	1:G:145:ILE:N	2.47	0.41
1:H:134:GLU:HB3	1:L:131:ASP:CG	2.44	0.41
1:I:93:TRP:O	1:I:95:SER:N	2.53	0.41
1:I:137:TYR:O	1:I:141:GLN:HG2	2.20	0.41
1:J:123:PHE:CD2	1:J:124:LYS:HE3	2.55	0.41
1:N:40:TYR:O	1:N:42:ASP:N	2.53	0.41
1:P:37:MET:C	1:P:39:TYR:H	2.27	0.41
1:P:140:GLU:HG3	1:P:141:GLN:HE21	1.83	0.41
1:W:132:PHE:CZ	1:W:137:TYR:HE1	2.38	0.41
1:X:34:TYR:HB3	1:X:59:SER:HB2	2.02	0.41
1:X:48:LEU:CD1	1:X:167:GLU:HB2	2.50	0.41
1:B:56:LEU:HD21	1:Q:67:GLU:OE2	2.19	0.41
1:D:75:GLN:O	1:D:76:ARG:HD2	2.20	0.41
1:D:112:GLN:HG2	1:D:116:GLU:OE1	2.20	0.41
1:F:165:LEU:HD12	1:F:165:LEU:HA	1.90	0.41
1:H:14:GLN:O	1:H:17:GLU:HB3	2.20	0.41
1:H:106:LEU:O	1:H:110:VAL:HG23	2.20	0.41
1:J:34:TYR:HB3	1:J:55:PHE:O	2.19	0.41
1:Q:27:GLU:HB3	1:Q:66:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:ASP:HA	1:Q:127:PRO:HD3	1.91	0.41
1:Q:127:PRO:HD2	1:Q:128:HIS:H	1.85	0.41
1:U:73:GLN:HG3	1:U:78:GLY:C	2.45	0.41
1:W:50:ASN:HB3	1:W:175:LEU:HB2	2.02	0.41
1:B:74:ASN:O	1:B:75:GLN:C	2.63	0.41
1:C:108:LYS:HB3	1:O:10:GLN:OE1	2.20	0.41
1:C:154:ASN:O	1:C:158:MET:HG3	2.21	0.41
1:G:20:ILE:C	1:G:22:ARG:H	2.28	0.41
1:G:173:HIS:CD2	1:P:173:HIS:NE2	2.89	0.41
1:L:107:GLU:O	1:L:111:ASN:N	2.30	0.41
1:L:111:ASN:HD22	1:S:10:GLN:CD	2.28	0.41
1:O:140:GLU:OE1	1:O:140:GLU:N	2.53	0.41
1:P:52:ALA:O	1:P:56:LEU:HB2	2.21	0.41
1:P:125:ASN:O	1:P:127:PRO:HD3	2.20	0.41
1:T:40:TYR:HD1	1:T:43:ARG:HH11	1.67	0.41
1:T:110:VAL:HG12	1:T:114:LEU:CD1	2.51	0.41
1:T:129:LEU:O	1:T:133:ILE:HG13	2.20	0.41
1:E:32:TYR:CE2	1:E:87:LYS:HA	2.55	0.41
1:E:161:PRO:C	1:E:163:SER:H	2.29	0.41
1:F:32:TYR:HE1	1:T:82:LEU:HD13	1.85	0.41
1:G:28:LEU:HD22	1:G:85:ILE:HD11	2.03	0.41
1:I:138:LEU:HD13	1:T:128:HIS:N	2.35	0.41
1:J:23:GLN:HG3	1:J:117:LEU:CD1	2.48	0.41
1:M:49:LYS:O	1:M:51:PHE:N	2.54	0.41
1:M:131:ASP:N	1:M:134:GLU:OE1	2.53	0.41
1:P:93:TRP:O	1:P:95:SER:N	2.52	0.41
1:R:50:ASN:HD22	1:R:171:ASP:CG	2.23	0.41
1:W:41:PHE:HB3	1:W:48:LEU:O	2.20	0.41
1:X:55:PHE:CZ	1:X:100:MET:HG2	2.53	0.41
1:C:111:ASN:HB3	1:O:10:GLN:NE2	2.36	0.41
1:F:39:TYR:CD2	1:T:70:MET:HE2	2.56	0.41
1:H:115:LEU:O	1:H:119:LYS:N	2.47	0.41
1:Q:7:GLN:H	1:Q:7:GLN:HG2	1.68	0.41
1:Q:37:MET:C	1:Q:39:TYR:H	2.28	0.41
1:T:158:MET:HE2	1:T:166:ALA:O	2.20	0.41
1:U:83:GLN:HG2	1:U:84:ASP:O	2.20	0.41
1:X:33:VAL:HG22	1:X:88:PRO:HG3	2.03	0.41
1:E:100:MET:SD	1:E:151:HIS:HB3	2.61	0.41
1:G:100:MET:CB	1:G:152:VAL:HG12	2.48	0.41
1:J:8:VAL:O	1:J:9:ARG:C	2.63	0.41
1:J:50:ASN:O	1:J:54:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:TYR:O	1:J:138:LEU:C	2.63	0.41
1:K:50:ASN:ND2	1:K:175:LEU:O	2.53	0.41
1:L:38:SER:HA	1:L:52:ALA:HA	2.03	0.41
1:T:112:GLN:NE2	1:T:115:LEU:HB2	2.36	0.41
1:U:83:GLN:CG	1:U:84:ASP:N	2.84	0.41
1:U:116:GLU:HA	1:U:119:LYS:CD	2.50	0.41
1:W:155:LEU:HA	1:W:155:LEU:HD23	1.83	0.41
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.94	0.41
1:H:7:GLN:NE2	1:S:149:GLY:O	2.54	0.41
1:K:160:ALA:HB1	1:K:161:PRO:HA	2.03	0.41
1:M:149:GLY:O	1:M:153:THR:OG1	2.38	0.41
1:N:56:LEU:HG	1:N:60:HIS:HE1	1.86	0.41
1:P:68:LYS:HE2	1:P:136:HIS:CD2	2.56	0.41
1:V:120:LEU:C	1:V:122:THR:N	2.79	0.41
1:B:97:LEU:O	1:B:101:GLU:HG3	2.20	0.41
1:C:23:GLN:HG3	1:C:117:LEU:HD13	2.03	0.41
1:D:121:ALA:HB1	1:D:126:ASP:HB3	2.02	0.41
1:D:142:VAL:HG21	1:P:128:HIS:NE2	2.35	0.41
1:G:56:LEU:O	1:G:60:HIS:ND1	2.40	0.41
1:I:43:ARG:NH1	1:N:79:ARG:CD	2.83	0.41
1:I:92:ASP:OD1	1:I:93:TRP:N	2.53	0.41
1:M:45:ASP:N	1:M:45:ASP:OD1	2.42	0.41
1:O:155:LEU:HB3	1:O:160:ALA:CB	2.51	0.41
1:S:152:VAL:H	1:S:152:VAL:HG23	1.59	0.41
1:A:160:ALA:HA	1:A:163:SER:H	1.86	0.41
1:C:20:ILE:HD13	1:C:20:ILE:HA	1.84	0.41
1:D:68:LYS:HB3	1:D:68:LYS:HE3	1.87	0.41
1:F:13:HIS:CG	1:F:15:ASP:HB2	2.55	0.41
1:F:33:VAL:HG22	1:F:88:PRO:HB3	2.01	0.41
1:F:35:LEU:HA	1:F:35:LEU:HD12	1.62	0.41
1:F:97:LEU:HD21	1:F:156:ARG:HG2	2.03	0.41
1:G:149:GLY:O	1:G:152:VAL:HG22	2.20	0.41
1:H:156:ARG:C	1:H:158:MET:N	2.76	0.41
1:I:20:ILE:HD13	1:I:117:LEU:HD11	2.03	0.41
1:I:37:MET:HG2	1:I:93:TRP:CE2	2.56	0.41
1:I:66:ALA:O	1:I:70:MET:HG3	2.21	0.41
1:K:67:GLU:C	1:K:69:LEU:N	2.79	0.41
1:M:100:MET:HB2	1:M:152:VAL:HG22	2.03	0.41
1:M:114:LEU:HA	1:M:117:LEU:HD12	2.02	0.41
1:M:118:HIS:O	1:M:122:THR:HG23	2.21	0.41
1:N:43:ARG:HB3	1:N:45:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:115:LEU:HD13	1:N:115:LEU:HA	1.91	0.41
1:P:70:MET:HB3	1:P:80:ILE:HD13	2.02	0.41
1:R:165:LEU:HD22	1:S:158:MET:HA	2.03	0.41
1:S:12:TYR:HB2	1:S:76:ARG:NH2	2.36	0.41
1:S:51:PHE:CE1	1:S:175:LEU:HD22	2.56	0.41
1:T:48:LEU:HA	1:T:48:LEU:HD23	1.75	0.41
1:U:16:SER:HA	1:U:120:LEU:HD21	2.01	0.41
1:U:20:ILE:C	1:U:22:ARG:H	2.29	0.41
1:U:23:GLN:HE22	1:U:110:VAL:HG13	1.85	0.41
1:U:55:PHE:C	1:U:57:HIS:N	2.77	0.41
1:V:49:LYS:C	1:V:51:PHE:N	2.79	0.41
1:X:162:GLU:CD	1:X:162:GLU:H	2.29	0.41
1:A:11:ASN:ND2	1:A:125:ASN:O	2.47	0.41
1:C:85:ILE:HB	1:X:85:ILE:HD12	2.03	0.41
1:D:47:ALA:HB2	1:M:150:ASP:OD1	2.21	0.41
1:D:113:SER:HA	1:D:116:GLU:HB2	2.03	0.41
1:D:139:ASN:HA	1:D:142:VAL:HB	2.03	0.41
1:F:47:ALA:HA	1:I:150:ASP:OD2	2.21	0.41
1:H:120:LEU:O	1:H:123:PHE:N	2.54	0.41
1:J:116:GLU:HA	1:J:119:LYS:HE3	2.02	0.41
1:K:85:ILE:N	1:P:85:ILE:O	2.52	0.41
1:O:21:ASN:ND2	1:O:81:PHE:H	2.18	0.41
1:U:55:PHE:C	1:U:57:HIS:H	2.29	0.41
1:V:114:LEU:HD23	1:V:117:LEU:HD22	2.03	0.41
1:W:118:HIS:NE2	1:W:130:CYS:HB3	2.37	0.41
1:X:146:LYS:HD2	1:X:146:LYS:HA	1.94	0.41
1:B:92:ASP:OD1	1:B:93:TRP:N	2.54	0.40
1:D:39:TYR:HH	1:V:71:LYS:HB2	1.85	0.40
1:E:111:ASN:HB3	1:I:10:GLN:NE2	2.33	0.40
1:E:126:ASP:HB3	1:E:129:LEU:HB3	2.03	0.40
1:F:24:ILE:HD13	1:F:70:MET:HG2	2.03	0.40
1:G:141:GLN:HA	1:G:144:ALA:HB3	2.03	0.40
1:H:84:ASP:OD1	1:R:87:LYS:N	2.54	0.40
1:O:12:TYR:CE1	1:O:76:ARG:HD3	2.56	0.40
1:Q:92:ASP:OD1	1:Q:93:TRP:N	2.54	0.40
1:W:49:LYS:HA	1:W:52:ALA:HB3	2.03	0.40
1:C:60:HIS:O	1:C:63:ARG:HB3	2.22	0.40
1:C:120:LEU:O	1:C:123:PHE:HB2	2.22	0.40
1:C:123:PHE:C	1:C:125:ASN:H	2.29	0.40
1:D:47:ALA:C	1:D:48:LEU:HD22	2.47	0.40
1:F:5:THR:HA	1:F:79:ARG:NH2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:GLU:O	1:F:65:HIS:HB2	2.21	0.40
1:H:33:VAL:HG11	1:H:106:LEU:HD22	2.04	0.40
1:I:27:GLU:OE2	1:I:62:GLU:OE1	2.40	0.40
1:J:57:HIS:O	1:J:61:GLU:N	2.41	0.40
1:J:93:TRP:O	1:J:94:GLU:HB2	2.20	0.40
1:K:90:CYS:HB2	1:K:93:TRP:CZ3	2.56	0.40
1:L:116:GLU:HA	1:L:119:LYS:HE3	2.03	0.40
1:M:116:GLU:O	1:M:119:LYS:HG2	2.21	0.40
1:M:134:GLU:OE2	1:V:131:ASP:HB2	2.21	0.40
1:O:72:LEU:HD23	1:O:72:LEU:C	2.47	0.40
1:O:116:GLU:OE1	1:O:116:GLU:N	2.43	0.40
1:P:140:GLU:OE2	1:P:144:ALA:HB2	2.21	0.40
1:P:151:HIS:HD2	1:P:170:PHE:HZ	1.67	0.40
1:X:116:GLU:HA	1:X:119:LYS:HB3	2.03	0.40
1:A:12:TYR:CB	1:A:76:ARG:HH22	2.35	0.40
1:B:32:TYR:OH	1:Q:83:GLN:O	2.34	0.40
1:C:82:LEU:HD12	1:X:36:SER:HB2	2.02	0.40
1:C:157:LYS:O	1:J:164:GLY:HA3	2.21	0.40
1:L:81:PHE:HD1	1:L:81:PHE:HA	1.76	0.40
1:L:94:GLU:HB3	1:L:95:SER:H	1.63	0.40
1:R:155:LEU:HD13	1:R:167:GLU:HG2	2.03	0.40
1:U:114:LEU:HD23	1:U:114:LEU:HA	1.88	0.40
1:X:82:LEU:HA	1:X:82:LEU:HD23	1.82	0.40
1:D:169:LEU:HD13	1:K:169:LEU:HD11	2.03	0.40
1:G:173:HIS:NE2	1:P:173:HIS:NE2	2.69	0.40
1:J:9:ARG:HH11	1:J:9:ARG:HD2	1.76	0.40
1:L:15:ASP:O	1:L:19:ALA:N	2.54	0.40
1:M:40:TYR:HA	1:M:43:ARG:HD3	2.02	0.40
1:M:97:LEU:HD21	1:M:156:ARG:HG2	2.04	0.40
1:M:130:CYS:O	1:M:134:GLU:N	2.35	0.40
1:N:107:GLU:O	1:N:111:ASN:HB2	2.21	0.40
1:O:15:ASP:O	1:O:19:ALA:N	2.54	0.40
1:P:118:HIS:HA	1:P:121:ALA:HB3	2.02	0.40
1:Q:10:GLN:C	1:Q:12:TYR:N	2.78	0.40
1:Q:168:TYR:CD2	1:Q:169:LEU:HD23	2.52	0.40
1:R:58:GLN:NE2	1:R:58:GLN:HA	2.36	0.40
1:T:76:ARG:HA	1:T:76:ARG:HD2	1.67	0.40
1:V:171:ASP:O	1:V:176:GLY:N	2.54	0.40
1:D:155:LEU:O	1:D:158:MET:HB2	2.21	0.40
1:E:161:PRO:C	1:E:163:SER:N	2.79	0.40
1:H:24:ILE:HG22	1:H:28:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:ARG:NE	1:N:43:ARG:CZ	2.84	0.40
1:M:106:LEU:O	1:M:107:GLU:C	2.65	0.40
1:P:76:ARG:HD2	1:P:76:ARG:HA	1.86	0.40
1:Q:37:MET:O	1:Q:39:TYR:N	2.54	0.40
1:Q:108:LYS:O	1:Q:111:ASN:HB3	2.21	0.40
1:T:32:TYR:CE2	1:T:88:PRO:HD3	2.57	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:M:124:LYS:NZ	1:O:123:PHE:O[3_545]	2.14	0.06

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	170/183 (93%)	144 (85%)	23 (14%)	3 (2%)	6	8
1	B	170/183 (93%)	149 (88%)	18 (11%)	3 (2%)	6	8
1	C	170/183 (93%)	148 (87%)	20 (12%)	2 (1%)	10	14
1	D	170/183 (93%)	144 (85%)	24 (14%)	2 (1%)	10	14
1	E	170/183 (93%)	154 (91%)	13 (8%)	3 (2%)	6	8
1	F	170/183 (93%)	144 (85%)	22 (13%)	4 (2%)	4	4
1	G	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	4	4
1	H	170/183 (93%)	144 (85%)	17 (10%)	9 (5%)	1	0
1	I	170/183 (93%)	145 (85%)	18 (11%)	7 (4%)	2	1
1	J	170/183 (93%)	145 (85%)	21 (12%)	4 (2%)	4	4
1	K	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	10	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	170/183 (93%)	148 (87%)	18 (11%)	4 (2%)	4	4
1	M	170/183 (93%)	153 (90%)	15 (9%)	2 (1%)	10	14
1	N	170/183 (93%)	153 (90%)	14 (8%)	3 (2%)	6	8
1	O	170/183 (93%)	146 (86%)	21 (12%)	3 (2%)	6	8
1	P	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	4	4
1	Q	170/183 (93%)	138 (81%)	26 (15%)	6 (4%)	3	2
1	R	170/183 (93%)	134 (79%)	28 (16%)	8 (5%)	2	1
1	S	170/183 (93%)	151 (89%)	18 (11%)	1 (1%)	21	28
1	T	170/183 (93%)	139 (82%)	27 (16%)	4 (2%)	4	4
1	U	170/183 (93%)	143 (84%)	22 (13%)	5 (3%)	3	3
1	V	170/183 (93%)	135 (79%)	30 (18%)	5 (3%)	3	3
1	W	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	10	14
1	X	170/183 (93%)	144 (85%)	23 (14%)	3 (2%)	6	8
All	All	4080/4392 (93%)	3473 (85%)	514 (13%)	93 (2%)	5	5

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	B	115	LEU
1	I	21	ASN
1	K	68	LYS
1	N	158	MET
1	P	49	LYS
1	R	99	ALA
1	S	144	ALA
1	T	9	ARG
1	U	94	GLU
1	V	49	LYS
1	V	99	ALA
1	X	94	GLU
1	X	167	GLU
1	D	171	ASP
1	F	167	GLU
1	G	89	ASP
1	G	94	GLU
1	H	94	GLU

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Mol	Chain	Res	Type
1	J	52	ALA
1	J	118	HIS
1	L	31	SER
1	P	11	ASN
1	Q	94	GLU
1	R	16	SER
1	R	100	MET
1	T	152	VAL
1	V	94	GLU
1	X	93	TRP
1	D	38	SER
1	E	94	GLU
1	G	125	ASN
1	H	156	ARG
1	I	15	ASP
1	I	94	GLU
1	J	171	ASP
1	K	94	GLU
1	L	94	GLU
1	N	41	PHE
1	Q	11	ASN
1	Q	38	SER
1	Q	128	HIS
1	R	47	ALA
1	R	138	LEU
1	W	104	LEU
1	B	94	GLU
1	C	20	ILE
1	C	166	ALA
1	E	9	ARG
1	E	65	HIS
1	F	159	GLY
1	H	103	ALA
1	H	161	PRO
1	H	162	GLU
1	L	116	GLU
1	M	139	ASN
1	N	93	TRP
1	O	152	VAL
1	O	157	LYS
1	P	147	GLU
1	Q	75	GLN

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Mol	Chain	Res	Type
1	R	43	ARG
1	R	59	SER
1	V	48	LEU
1	V	100	MET
1	W	106	LEU
1	A	127	PRO
1	B	164	GLY
1	F	94	GLU
1	G	73	GLN
1	H	153	THR
1	H	157	LYS
1	H	165	LEU
1	I	22	ARG
1	L	16	SER
1	M	138	LEU
1	Q	47	ALA
1	R	112	GLN
1	U	9	ARG
1	U	38	SER
1	U	88	PRO
1	H	83	GLN
1	I	125	ASN
1	J	94	GLU
1	O	145	ILE
1	T	16	SER
1	T	77	GLY
1	U	130	CYS
1	I	152	VAL
1	P	159	GLY
1	I	164	GLY
1	A	77	GLY
1	F	161	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	153/163 (94%)	153 (100%)	0	100	100
1	B	153/163 (94%)	153 (100%)	0	100	100
1	C	153/163 (94%)	153 (100%)	0	100	100
1	D	153/163 (94%)	153 (100%)	0	100	100
1	E	153/163 (94%)	152 (99%)	1 (1%)	76	84
1	F	153/163 (94%)	153 (100%)	0	100	100
1	G	153/163 (94%)	153 (100%)	0	100	100
1	H	153/163 (94%)	153 (100%)	0	100	100
1	I	153/163 (94%)	153 (100%)	0	100	100
1	J	153/163 (94%)	153 (100%)	0	100	100
1	K	153/163 (94%)	153 (100%)	0	100	100
1	L	153/163 (94%)	153 (100%)	0	100	100
1	M	153/163 (94%)	153 (100%)	0	100	100
1	N	153/163 (94%)	153 (100%)	0	100	100
1	O	152/163 (93%)	152 (100%)	0	100	100
1	P	153/163 (94%)	153 (100%)	0	100	100
1	Q	153/163 (94%)	153 (100%)	0	100	100
1	R	153/163 (94%)	153 (100%)	0	100	100
1	S	153/163 (94%)	153 (100%)	0	100	100
1	T	153/163 (94%)	153 (100%)	0	100	100
1	U	153/163 (94%)	153 (100%)	0	100	100
1	V	153/163 (94%)	152 (99%)	1 (1%)	76	84
1	W	153/163 (94%)	153 (100%)	0	100	100
1	X	153/163 (94%)	153 (100%)	0	100	100
All	All	3671/3912 (94%)	3669 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	123	PHE
1	V	140	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	74	ASN
1	A	98	ASN
1	A	118	HIS
1	B	60	HIS
1	B	112	GLN
1	B	139	ASN
1	C	21	ASN
1	C	25	ASN
1	C	65	HIS
1	C	73	GLN
1	C	98	ASN
1	D	7	GLN
1	D	23	GLN
1	D	60	HIS
1	D	65	HIS
1	E	25	ASN
1	E	109	ASN
1	E	154	ASN
1	F	10	GLN
1	F	11	ASN
1	F	14	GLN
1	F	65	HIS
1	F	73	GLN
1	F	75	GLN
1	F	109	ASN
1	F	111	ASN
1	G	73	GLN
1	G	118	HIS
1	G	173	HIS
1	H	7	GLN
1	H	21	ASN
1	H	57	HIS
1	H	58	GLN
1	H	98	ASN
1	H	105	HIS
1	H	173	HIS
1	I	7	GLN
1	I	75	GLN
1	I	125	ASN
1	J	25	ASN
1	J	111	ASN
1	K	14	GLN

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Mol	Chain	Res	Type
1	K	21	ASN
1	K	50	ASN
1	K	57	HIS
1	K	58	GLN
1	K	60	HIS
1	K	112	GLN
1	K	173	HIS
1	L	111	ASN
1	L	118	HIS
1	L	125	ASN
1	L	136	HIS
1	M	10	GLN
1	M	25	ASN
1	M	112	GLN
1	N	23	GLN
1	N	58	GLN
1	O	13	HIS
1	O	60	HIS
1	O	173	HIS
1	P	10	GLN
1	P	74	ASN
1	P	125	ASN
1	P	136	HIS
1	P	139	ASN
1	Q	7	GLN
1	Q	10	GLN
1	Q	73	GLN
1	Q	74	ASN
1	Q	154	ASN
1	R	111	ASN
1	R	128	HIS
1	S	109	ASN
1	S	141	GLN
1	T	11	ASN
1	T	73	GLN
1	T	118	HIS
1	T	141	GLN
1	U	21	ASN
1	U	50	ASN
1	U	98	ASN
1	U	141	GLN
1	V	50	ASN

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Mol	Chain	Res	Type
1	V	74	ASN
1	V	98	ASN
1	V	118	HIS
1	V	139	ASN
1	W	73	GLN
1	W	105	HIS
1	W	109	ASN
1	X	7	GLN
1	X	14	GLN
1	X	60	HIS
1	X	73	GLN
1	X	128	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	172/183 (93%)	1.31	27 (15%)	5 4	26, 49, 65, 73	0
1	B	172/183 (93%)	1.00	17 (9%)	13 13	21, 41, 59, 75	0
1	C	172/183 (93%)	2.25	95 (55%)	0 0	41, 60, 77, 90	0
1	D	172/183 (93%)	2.18	97 (56%)	0 0	43, 61, 73, 83	0
1	E	172/183 (93%)	1.28	34 (19%)	3 2	28, 51, 68, 80	0
1	F	172/183 (93%)	2.18	87 (50%)	0 0	42, 61, 73, 83	0
1	G	172/183 (93%)	2.23	90 (52%)	0 0	46, 61, 77, 94	0
1	H	172/183 (93%)	1.62	51 (29%)	1 1	28, 55, 70, 84	0
1	I	172/183 (93%)	1.52	44 (25%)	1 1	29, 55, 71, 78	0
1	J	172/183 (93%)	1.89	77 (44%)	0 0	40, 56, 72, 83	0
1	K	172/183 (93%)	1.95	79 (45%)	0 0	44, 60, 73, 90	0
1	L	172/183 (93%)	1.03	13 (7%)	20 19	26, 40, 60, 72	0
1	M	172/183 (93%)	1.61	54 (31%)	1 0	31, 53, 71, 81	0
1	N	172/183 (93%)	1.06	21 (12%)	8 8	27, 43, 63, 80	0
1	O	172/183 (93%)	1.97	81 (47%)	0 0	38, 59, 72, 84	0
1	P	172/183 (93%)	2.10	84 (48%)	0 0	43, 59, 75, 92	0
1	Q	172/183 (93%)	1.25	24 (13%)	6 6	26, 48, 66, 81	0
1	R	172/183 (93%)	1.85	69 (40%)	0 0	39, 58, 72, 89	0
1	S	172/183 (93%)	1.12	26 (15%)	5 5	24, 48, 65, 78	0
1	T	172/183 (93%)	2.00	76 (44%)	0 0	44, 57, 73, 85	0
1	U	172/183 (93%)	2.16	89 (51%)	0 0	43, 57, 72, 94	0
1	V	172/183 (93%)	1.96	89 (51%)	0 0	40, 57, 71, 82	0
1	W	172/183 (93%)	1.06	14 (8%)	18 18	27, 42, 61, 82	0
1	X	172/183 (93%)	2.18	90 (52%)	0 0	41, 60, 73, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4128/4392 (93%)	1.70	1428 (34%) 1 0	21, 55, 72, 94	0

All (1428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	24	ILE	7.4
1	X	30	ALA	7.2
1	C	132	PHE	6.9
1	K	129	LEU	6.7
1	C	67	GLU	6.4
1	D	99	ALA	6.4
1	P	81	PHE	6.0
1	F	8	VAL	5.7
1	F	133	ILE	5.7
1	P	8	VAL	5.6
1	U	88	PRO	5.6
1	K	89	ASP	5.4
1	U	24	ILE	5.4
1	C	70	MET	5.3
1	G	154	ASN	5.2
1	G	104	LEU	5.2
1	T	85	ILE	5.2
1	G	30	ALA	5.2
1	P	93	TRP	5.1
1	J	157	LYS	5.1
1	F	142	VAL	5.1
1	R	34	TYR	5.1
1	U	99	ALA	5.1
1	O	8	VAL	5.0
1	U	120	LEU	5.0
1	M	152	VAL	4.9
1	O	93	TRP	4.8
1	X	138	LEU	4.8
1	O	85	ILE	4.8
1	X	27	GLU	4.8
1	I	169	LEU	4.8
1	P	88	PRO	4.7
1	F	24	ILE	4.7
1	D	100	MET	4.7
1	P	176	GLY	4.7
1	S	176	GLY	4.7
1	G	119	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	102	CYS	4.6
1	C	38	SER	4.6
1	C	133	ILE	4.6
1	F	127	PRO	4.6
1	H	150	ASP	4.6
1	P	129	LEU	4.6
1	T	155	LEU	4.6
1	U	161	PRO	4.5
1	F	46	VAL	4.5
1	F	175	LEU	4.5
1	T	102	CYS	4.5
1	S	165	LEU	4.5
1	X	34	TYR	4.4
1	G	85	ILE	4.4
1	T	99	ALA	4.4
1	C	107	GLU	4.4
1	H	170	PHE	4.4
1	G	138	LEU	4.4
1	X	26	LEU	4.4
1	G	93	TRP	4.4
1	U	114	LEU	4.4
1	P	127	PRO	4.4
1	O	76	ARG	4.4
1	D	103	ALA	4.4
1	H	48	LEU	4.4
1	K	176	GLY	4.3
1	V	142	VAL	4.3
1	R	170	PHE	4.3
1	G	176	GLY	4.3
1	D	152	VAL	4.3
1	S	34	TYR	4.3
1	G	134	GLU	4.3
1	J	10	GLN	4.3
1	X	33	VAL	4.3
1	P	41	PHE	4.3
1	K	169	LEU	4.3
1	B	176	GLY	4.3
1	H	176	GLY	4.3
1	I	81	PHE	4.3
1	P	75	GLN	4.2
1	F	129	LEU	4.2
1	P	6	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	U	100	MET	4.2
1	J	165	LEU	4.2
1	C	103	ALA	4.2
1	H	96	GLY	4.2
1	V	122	THR	4.1
1	P	148	LEU	4.1
1	C	56	LEU	4.1
1	F	104	LEU	4.1
1	G	26	LEU	4.1
1	J	158	MET	4.1
1	V	81	PHE	4.1
1	U	93	TRP	4.1
1	J	32	TYR	4.1
1	T	39	TYR	4.1
1	C	135	THR	4.1
1	T	169	LEU	4.1
1	U	103	ALA	4.1
1	G	16	SER	4.1
1	O	91	ASP	4.1
1	O	150	ASP	4.0
1	D	49	LYS	4.0
1	X	110	VAL	4.0
1	X	176	GLY	4.0
1	J	74	ASN	4.0
1	C	91	ASP	4.0
1	U	158	MET	4.0
1	J	12	TYR	4.0
1	H	90	CYS	3.9
1	O	133	ILE	3.9
1	G	5	THR	3.9
1	T	46	VAL	3.9
1	V	152	VAL	3.9
1	O	125	ASN	3.9
1	H	164	GLY	3.9
1	G	15	ASP	3.9
1	C	168	TYR	3.9
1	K	37	MET	3.9
1	D	91	ASP	3.9
1	D	97	LEU	3.9
1	G	112	GLN	3.9
1	C	32	TYR	3.9
1	O	104	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	170	PHE	3.8
1	X	32	TYR	3.8
1	W	78	GLY	3.8
1	D	145	ILE	3.8
1	C	102	CYS	3.8
1	G	123	PHE	3.8
1	P	128	HIS	3.8
1	V	104	LEU	3.8
1	X	37	MET	3.8
1	K	132	PHE	3.8
1	V	76	ARG	3.8
1	D	133	ILE	3.8
1	D	129	LEU	3.8
1	L	131	ASP	3.8
1	X	134	GLU	3.8
1	D	132	PHE	3.8
1	H	132	PHE	3.8
1	T	77	GLY	3.8
1	C	120	LEU	3.8
1	X	31	SER	3.7
1	K	96	GLY	3.7
1	F	72	LEU	3.7
1	F	115	LEU	3.7
1	X	69	LEU	3.7
1	C	49	LYS	3.7
1	X	142	VAL	3.7
1	X	61	GLU	3.7
1	C	24	ILE	3.7
1	D	35	LEU	3.7
1	F	139	ASN	3.7
1	E	91	ASP	3.7
1	X	12	TYR	3.7
1	X	88	PRO	3.7
1	J	49	LYS	3.7
1	P	5	THR	3.7
1	E	81	PHE	3.7
1	F	41	PHE	3.7
1	H	165	LEU	3.7
1	V	80	ILE	3.7
1	N	171	ASP	3.7
1	V	150	ASP	3.7
1	G	29	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	110	VAL	3.7
1	Q	152	VAL	3.7
1	U	81	PHE	3.7
1	V	123	PHE	3.7
1	O	139	ASN	3.7
1	K	40	TYR	3.7
1	U	167	GLU	3.6
1	G	81	PHE	3.6
1	V	132	PHE	3.6
1	C	148	LEU	3.6
1	T	100	MET	3.6
1	P	45	ASP	3.6
1	G	34	TYR	3.6
1	O	167	GLU	3.6
1	U	55	PHE	3.6
1	X	81	PHE	3.6
1	V	93	TRP	3.6
1	C	158	MET	3.6
1	D	138	LEU	3.6
1	F	176	GLY	3.6
1	G	165	LEU	3.6
1	U	145	ILE	3.6
1	P	90	CYS	3.6
1	P	64	GLU	3.6
1	U	71	LYS	3.6
1	F	138	LEU	3.6
1	O	176	GLY	3.6
1	P	164	GLY	3.6
1	X	103	ALA	3.6
1	D	51	PHE	3.6
1	O	24	ILE	3.6
1	O	137	TYR	3.5
1	K	70	MET	3.5
1	K	158	MET	3.5
1	O	66	ALA	3.5
1	P	169	LEU	3.5
1	C	161	PRO	3.5
1	C	60	HIS	3.5
1	C	119	LYS	3.5
1	R	64	GLU	3.5
1	C	155	LEU	3.5
1	D	148	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	120	LEU	3.5
1	U	35	LEU	3.5
1	X	106	LEU	3.5
1	C	96	GLY	3.5
1	U	25	ASN	3.5
1	O	5	THR	3.5
1	R	152	VAL	3.5
1	F	137	TYR	3.5
1	I	72	LEU	3.5
1	P	149	GLY	3.5
1	X	24	ILE	3.5
1	X	55	PHE	3.5
1	S	119	LYS	3.5
1	G	111	ASN	3.5
1	M	148	LEU	3.5
1	R	165	LEU	3.5
1	T	103	ALA	3.5
1	S	158	MET	3.4
1	D	135	THR	3.4
1	U	122	THR	3.4
1	X	8	VAL	3.4
1	G	155	LEU	3.4
1	G	88	PRO	3.4
1	K	145	ILE	3.4
1	X	16	SER	3.4
1	B	150	ASP	3.4
1	P	110	VAL	3.4
1	G	72	LEU	3.4
1	O	32	TYR	3.4
1	V	16	SER	3.4
1	C	63	ARG	3.4
1	M	101	GLU	3.4
1	F	42	ASP	3.4
1	I	158	MET	3.4
1	D	119	LYS	3.4
1	K	97	LEU	3.4
1	T	104	LEU	3.4
1	X	28	LEU	3.4
1	V	145	ILE	3.4
1	J	54	TYR	3.4
1	C	98	ASN	3.4
1	O	138	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	T	165	LEU	3.4
1	X	129	LEU	3.4
1	I	176	GLY	3.4
1	G	18	ALA	3.4
1	G	133	ILE	3.4
1	C	123	PHE	3.3
1	G	41	PHE	3.3
1	T	137	TYR	3.3
1	V	32	TYR	3.3
1	C	21	ASN	3.3
1	T	50	ASN	3.3
1	V	139	ASN	3.3
1	G	169	LEU	3.3
1	D	60	HIS	3.3
1	D	118	HIS	3.3
1	O	65	HIS	3.3
1	R	63	ARG	3.3
1	F	85	ILE	3.3
1	N	123	PHE	3.3
1	F	91	ASP	3.3
1	X	92	ASP	3.3
1	X	139	ASN	3.3
1	G	28	LEU	3.3
1	I	138	LEU	3.3
1	M	138	LEU	3.3
1	D	122	THR	3.3
1	C	65	HIS	3.3
1	T	61	GLU	3.3
1	T	159	GLY	3.3
1	C	144	ALA	3.3
1	P	47	ALA	3.3
1	V	100	MET	3.3
1	K	54	TYR	3.3
1	N	84	ASP	3.3
1	T	34	TYR	3.3
1	P	74	ASN	3.3
1	K	155	LEU	3.3
1	G	105	HIS	3.3
1	K	142	VAL	3.3
1	J	166	ALA	3.3
1	X	80	ILE	3.3
1	I	36	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	132	PHE	3.3
1	P	51	PHE	3.3
1	G	84	ASP	3.3
1	F	34	TYR	3.3
1	O	168	TYR	3.3
1	I	104	LEU	3.3
1	K	88	PRO	3.3
1	R	120	LEU	3.3
1	T	164	GLY	3.3
1	K	52	ALA	3.3
1	H	41	PHE	3.2
1	K	55	PHE	3.2
1	H	91	ASP	3.2
1	T	44	ASP	3.2
1	U	91	ASP	3.2
1	C	35	LEU	3.2
1	X	35	LEU	3.2
1	U	152	VAL	3.2
1	G	157	LYS	3.2
1	U	163	SER	3.2
1	F	50	ASN	3.2
1	D	48	LEU	3.2
1	R	12	TYR	3.2
1	R	117	LEU	3.2
1	J	164	GLY	3.2
1	T	144	ALA	3.2
1	G	51	PHE	3.2
1	L	81	PHE	3.2
1	W	91	ASP	3.2
1	U	151	HIS	3.2
1	K	143	LYS	3.2
1	S	157	LYS	3.2
1	A	5	THR	3.2
1	M	122	THR	3.2
1	V	133	ILE	3.2
1	A	55	PHE	3.2
1	C	97	LEU	3.2
1	D	67	GLU	3.2
1	F	161	PRO	3.2
1	Q	127	PRO	3.2
1	T	158	MET	3.2
1	U	29	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	U	142	VAL	3.2
1	B	5	THR	3.2
1	D	153	THR	3.2
1	M	5	THR	3.2
1	F	160	ALA	3.1
1	G	14	GLN	3.1
1	P	170	PHE	3.1
1	O	62	GLU	3.1
1	A	138	LEU	3.1
1	X	111	ASN	3.1
1	D	176	GLY	3.1
1	G	137	TYR	3.1
1	F	80	ILE	3.1
1	X	145	ILE	3.1
1	D	58	GLN	3.1
1	E	75	GLN	3.1
1	P	172	LYS	3.1
1	T	81	PHE	3.1
1	U	140	GLU	3.1
1	J	100	MET	3.1
1	V	118	HIS	3.1
1	F	165	LEU	3.1
1	V	35	LEU	3.1
1	L	139	ASN	3.1
1	G	39	TYR	3.1
1	H	54	TYR	3.1
1	H	85	ILE	3.1
1	I	137	TYR	3.1
1	O	100	MET	3.1
1	R	161	PRO	3.1
1	O	155	LEU	3.1
1	U	165	LEU	3.1
1	F	125	ASN	3.1
1	F	96	GLY	3.1
1	A	133	ILE	3.1
1	G	54	TYR	3.1
1	T	32	TYR	3.1
1	G	66	ALA	3.1
1	U	19	ALA	3.1
1	D	140	GLU	3.1
1	M	90	CYS	3.1
1	D	28	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	92	ASP	3.1
1	O	148	LEU	3.1
1	R	114	LEU	3.1
1	U	48	LEU	3.1
1	V	131	ASP	3.1
1	X	41	PHE	3.1
1	E	109	ASN	3.1
1	J	133	ILE	3.1
1	K	85	ILE	3.1
1	C	157	LYS	3.0
1	U	157	LYS	3.0
1	K	65	HIS	3.0
1	C	138	LEU	3.0
1	G	106	LEU	3.0
1	J	56	LEU	3.0
1	O	117	LEU	3.0
1	U	115	LEU	3.0
1	E	76	ARG	3.0
1	S	96	GLY	3.0
1	F	66	ALA	3.0
1	P	34	TYR	3.0
1	I	117	LEU	3.0
1	T	35	LEU	3.0
1	F	81	PHE	3.0
1	N	91	ASP	3.0
1	Q	123	PHE	3.0
1	R	51	PHE	3.0
1	V	51	PHE	3.0
1	F	111	ASN	3.0
1	T	139	ASN	3.0
1	D	20	ILE	3.0
1	P	46	VAL	3.0
1	R	5	THR	3.0
1	O	19	ALA	3.0
1	S	40	TYR	3.0
1	X	40	TYR	3.0
1	A	127	PRO	3.0
1	O	88	PRO	3.0
1	P	161	PRO	3.0
1	O	175	LEU	3.0
1	X	120	LEU	3.0
1	J	51	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	95	SER	3.0
1	G	142	VAL	3.0
1	U	133	ILE	3.0
1	F	37	MET	3.0
1	D	128	HIS	3.0
1	E	18	ALA	3.0
1	H	40	TYR	3.0
1	J	175	LEU	3.0
1	S	175	LEU	3.0
1	T	28	LEU	3.0
1	D	81	PHE	3.0
1	U	44	ASP	3.0
1	U	139	ASN	3.0
1	C	73	GLN	3.0
1	V	77	GLY	3.0
1	X	10	GLN	3.0
1	H	46	VAL	2.9
1	E	19	ALA	2.9
1	H	93	TRP	2.9
1	M	118	HIS	2.9
1	U	39	TYR	2.9
1	X	108	LYS	2.9
1	D	123	PHE	2.9
1	F	132	PHE	2.9
1	F	16	SER	2.9
1	J	95	SER	2.9
1	O	6	SER	2.9
1	D	130	CYS	2.9
1	G	96	GLY	2.9
1	K	164	GLY	2.9
1	V	75	GLN	2.9
1	N	85	ILE	2.9
1	U	85	ILE	2.9
1	K	151	HIS	2.9
1	F	63	ARG	2.9
1	G	144	ALA	2.9
1	J	63	ARG	2.9
1	C	106	LEU	2.9
1	U	148	LEU	2.9
1	U	137	TYR	2.9
1	O	41	PHE	2.9
1	V	41	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	51	PHE	2.9
1	H	38	SER	2.9
1	U	70	MET	2.9
1	V	176	GLY	2.9
1	C	90	CYS	2.9
1	C	105	HIS	2.9
1	S	46	VAL	2.9
1	C	122	THR	2.9
1	D	104	LEU	2.9
1	H	97	LEU	2.9
1	P	35	LEU	2.9
1	X	82	LEU	2.9
1	M	93	TRP	2.9
1	X	93	TRP	2.9
1	C	54	TYR	2.9
1	H	42	ASP	2.9
1	Q	116	GLU	2.9
1	R	163	SER	2.9
1	U	78	GLY	2.9
1	P	49	LYS	2.9
1	T	49	LYS	2.9
1	G	160	ALA	2.9
1	R	103	ALA	2.9
1	E	120	LEU	2.9
1	V	115	LEU	2.9
1	A	93	TRP	2.9
1	F	93	TRP	2.9
1	C	39	TYR	2.9
1	C	141	GLN	2.9
1	D	83	GLN	2.9
1	D	137	TYR	2.9
1	L	39	TYR	2.9
1	T	73	GLN	2.9
1	U	123	PHE	2.9
1	G	94	GLU	2.9
1	P	96	GLY	2.9
1	D	125	ASN	2.8
1	G	63	ARG	2.8
1	J	127	PRO	2.8
1	U	30	ALA	2.8
1	X	121	ALA	2.8
1	X	160	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	117	LEU	2.8
1	A	10	GLN	2.8
1	D	167	GLU	2.8
1	J	170	PHE	2.8
1	K	34	TYR	2.8
1	O	157	LYS	2.8
1	M	80	ILE	2.8
1	X	20	ILE	2.8
1	C	142	VAL	2.8
1	J	152	VAL	2.8
1	C	99	ALA	2.8
1	P	130	CYS	2.8
1	U	82	LEU	2.8
1	U	102	CYS	2.8
1	E	131	ASP	2.8
1	F	94	GLU	2.8
1	F	171	ASP	2.8
1	U	131	ASP	2.8
1	B	157	LYS	2.8
1	D	53	LYS	2.8
1	J	132	PHE	2.8
1	U	119	LYS	2.8
1	W	93	TRP	2.8
1	V	137	TYR	2.8
1	D	139	ASN	2.8
1	G	20	ILE	2.8
1	O	74	ASN	2.8
1	J	110	VAL	2.8
1	F	97	LEU	2.8
1	F	114	LEU	2.8
1	G	166	ALA	2.8
1	V	5	THR	2.8
1	J	129	LEU	2.8
1	U	90	CYS	2.8
1	X	143	LYS	2.8
1	I	13	HIS	2.8
1	R	132	PHE	2.8
1	X	164	GLY	2.8
1	F	40	TYR	2.8
1	H	32	TYR	2.8
1	I	154	ASN	2.8
1	D	56	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	155	LEU	2.8
1	M	106	LEU	2.8
1	O	122	THR	2.8
1	P	56	LEU	2.8
1	T	120	LEU	2.8
1	U	97	LEU	2.8
1	V	69	LEU	2.8
1	P	167	GLU	2.8
1	I	150	ASP	2.8
1	K	42	ASP	2.8
1	G	13	HIS	2.8
1	M	151	HIS	2.8
1	X	123	PHE	2.8
1	R	133	ILE	2.7
1	D	34	TYR	2.7
1	F	29	TYR	2.7
1	K	125	ASN	2.7
1	T	168	TYR	2.7
1	P	36	SER	2.7
1	C	26	LEU	2.7
1	J	69	LEU	2.7
1	U	169	LEU	2.7
1	K	66	ALA	2.7
1	K	99	ALA	2.7
1	F	49	LYS	2.7
1	C	167	GLU	2.7
1	R	107	GLU	2.7
1	J	130	CYS	2.7
1	M	102	CYS	2.7
1	M	136	HIS	2.7
1	X	126	ASP	2.7
1	C	145	ILE	2.7
1	H	50	ASN	2.7
1	Q	139	ASN	2.7
1	C	152	VAL	2.7
1	F	31	SER	2.7
1	F	168	TYR	2.7
1	R	32	TYR	2.7
1	V	12	TYR	2.7
1	K	117	LEU	2.7
1	M	48	LEU	2.7
1	R	97	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	T	175	LEU	2.7
1	B	158	MET	2.7
1	C	121	ALA	2.7
1	D	47	ALA	2.7
1	D	144	ALA	2.7
1	E	157	LYS	2.7
1	J	172	LYS	2.7
1	M	119	LYS	2.7
1	P	160	ALA	2.7
1	R	99	ALA	2.7
1	R	166	ALA	2.7
1	V	63	ARG	2.7
1	D	107	GLU	2.7
1	R	60	HIS	2.7
1	C	77	GLY	2.7
1	M	170	PHE	2.7
1	Q	85	ILE	2.7
1	K	25	ASN	2.7
1	D	39	TYR	2.7
1	H	49	LYS	2.7
1	K	46	VAL	2.7
1	K	32	TYR	2.7
1	M	104	LEU	2.7
1	R	48	LEU	2.7
1	V	49	LYS	2.7
1	X	155	LEU	2.7
1	X	172	LYS	2.7
1	M	121	ALA	2.7
1	P	52	ALA	2.7
1	R	66	ALA	2.7
1	X	135	THR	2.7
1	I	134	GLU	2.7
1	R	150	ASP	2.7
1	D	96	GLY	2.7
1	R	90	CYS	2.7
1	F	123	PHE	2.7
1	H	81	PHE	2.7
1	N	81	PHE	2.7
1	E	127	PRO	2.7
1	T	145	ILE	2.7
1	I	139	ASN	2.7
1	C	28	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	37	MET	2.7
1	M	97	LEU	2.7
1	R	35	LEU	2.7
1	R	82	LEU	2.7
1	V	46	VAL	2.7
1	P	32	TYR	2.7
1	R	167	GLU	2.7
1	X	39	TYR	2.7
1	B	99	ALA	2.7
1	C	30	ALA	2.7
1	F	19	ALA	2.7
1	G	99	ALA	2.7
1	K	5	THR	2.7
1	S	166	ALA	2.7
1	X	52	ALA	2.7
1	R	75	GLN	2.7
1	G	92	ASP	2.6
1	T	92	ASP	2.6
1	A	81	PHE	2.6
1	O	130	CYS	2.6
1	W	161	PRO	2.6
1	G	25	ASN	2.6
1	G	33	VAL	2.6
1	O	114	LEU	2.6
1	P	142	VAL	2.6
1	Q	48	LEU	2.6
1	U	104	LEU	2.6
1	G	95	SER	2.6
1	T	38	SER	2.6
1	C	34	TYR	2.6
1	D	121	ALA	2.6
1	M	166	ALA	2.6
1	P	137	TYR	2.6
1	R	144	ALA	2.6
1	X	122	THR	2.6
1	L	42	ASP	2.6
1	D	172	LYS	2.6
1	F	119	LYS	2.6
1	T	176	GLY	2.6
1	H	43	ARG	2.6
1	C	117	LEU	2.6
1	G	117	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	139	ASN	2.6
1	M	169	LEU	2.6
1	R	125	ASN	2.6
1	A	134	GLU	2.6
1	P	16	SER	2.6
1	E	122	THR	2.6
1	T	5	THR	2.6
1	X	141	GLN	2.6
1	A	137	TYR	2.6
1	C	128	HIS	2.6
1	E	118	HIS	2.6
1	G	12	TYR	2.6
1	J	65	HIS	2.6
1	J	151	HIS	2.6
1	V	13	HIS	2.6
1	P	143	LYS	2.6
1	F	92	ASP	2.6
1	M	149	GLY	2.6
1	R	78	GLY	2.6
1	S	91	ASP	2.6
1	H	20	ILE	2.6
1	J	85	ILE	2.6
1	K	63	ARG	2.6
1	O	80	ILE	2.6
1	P	63	ARG	2.6
1	M	158	MET	2.6
1	P	145	ILE	2.6
1	R	37	MET	2.6
1	D	26	LEU	2.6
1	D	106	LEU	2.6
1	O	26	LEU	2.6
1	V	28	LEU	2.6
1	X	117	LEU	2.6
1	F	11	ASN	2.6
1	O	163	SER	2.6
1	T	23	GLN	2.6
1	U	141	GLN	2.6
1	T	166	ALA	2.6
1	F	105	HIS	2.6
1	G	60	HIS	2.6
1	M	13	HIS	2.6
1	O	128	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	12	TYR	2.6
1	K	137	TYR	2.6
1	J	124	LYS	2.6
1	K	71	LYS	2.6
1	C	76	ARG	2.6
1	K	92	ASP	2.6
1	V	88	PRO	2.6
1	X	85	ILE	2.6
1	K	81	PHE	2.6
1	P	132	PHE	2.6
1	T	170	PHE	2.6
1	D	101	GLU	2.6
1	J	48	LEU	2.6
1	J	162	GLU	2.6
1	L	62	GLU	2.6
1	J	111	ASN	2.6
1	F	75	GLN	2.6
1	G	8	VAL	2.6
1	G	83	GLN	2.6
1	I	152	VAL	2.6
1	R	8	VAL	2.6
1	P	38	SER	2.6
1	V	99	ALA	2.6
1	P	68	LYS	2.6
1	X	156	ARG	2.5
1	G	164	GLY	2.5
1	R	89	ASP	2.5
1	T	70	MET	2.5
1	E	133	ILE	2.5
1	H	51	PHE	2.5
1	M	123	PHE	2.5
1	P	48	LEU	2.5
1	A	141	GLN	2.5
1	K	139	ASN	2.5
1	B	53	LYS	2.5
1	G	19	ALA	2.5
1	K	157	LYS	2.5
1	X	130	CYS	2.5
1	Q	5	THR	2.5
1	D	168	TYR	2.5
1	H	39	TYR	2.5
1	O	54	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	70	MET	2.5
1	E	161	PRO	2.5
1	G	91	ASP	2.5
1	H	80	ILE	2.5
1	J	93	TRP	2.5
1	P	126	ASP	2.5
1	R	93	TRP	2.5
1	R	134	GLU	2.5
1	T	134	GLU	2.5
1	U	27	GLU	2.5
1	J	138	LEU	2.5
1	M	81	PHE	2.5
1	T	41	PHE	2.5
1	H	83	GLN	2.5
1	C	109	ASN	2.5
1	G	57	HIS	2.5
1	H	60	HIS	2.5
1	I	110	VAL	2.5
1	J	8	VAL	2.5
1	K	110	VAL	2.5
1	O	11	ASN	2.5
1	Q	8	VAL	2.5
1	Q	157	LYS	2.5
1	X	13	HIS	2.5
1	F	52	ALA	2.5
1	O	18	ALA	2.5
1	S	47	ALA	2.5
1	X	99	ALA	2.5
1	E	5	THR	2.5
1	F	90	CYS	2.5
1	J	122	THR	2.5
1	N	5	THR	2.5
1	T	63	ARG	2.5
1	D	54	TYR	2.5
1	K	29	TYR	2.5
1	P	168	TYR	2.5
1	V	29	TYR	2.5
1	X	29	TYR	2.5
1	M	91	ASP	2.5
1	U	92	ASP	2.5
1	G	24	ILE	2.5
1	K	133	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	51	PHE	2.5
1	C	115	LEU	2.5
1	M	114	LEU	2.5
1	O	97	LEU	2.5
1	V	169	LEU	2.5
1	X	170	PHE	2.5
1	C	53	LYS	2.5
1	M	57	HIS	2.5
1	O	105	HIS	2.5
1	D	156	ARG	2.5
1	K	144	ALA	2.5
1	T	30	ALA	2.5
1	W	47	ALA	2.5
1	D	37	MET	2.5
1	G	40	TYR	2.5
1	P	92	ASP	2.5
1	Q	44	ASP	2.5
1	U	15	ASP	2.5
1	A	49	LYS	2.5
1	F	169	LEU	2.5
1	G	68	LYS	2.5
1	K	104	LEU	2.5
1	L	82	LEU	2.5
1	Q	138	LEU	2.5
1	S	170	PHE	2.5
1	E	13	HIS	2.5
1	R	57	HIS	2.5
1	U	105	HIS	2.5
1	O	111	ASN	2.5
1	V	110	VAL	2.5
1	M	47	ALA	2.5
1	U	144	ALA	2.5
1	D	70	MET	2.5
1	Q	6	SER	2.5
1	S	5	THR	2.5
1	T	174	THR	2.5
1	N	176	GLY	2.4
1	F	150	ASP	2.4
1	F	157	LYS	2.4
1	I	42	ASP	2.4
1	P	131	ASP	2.4
1	P	133	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	145	ILE	2.4
1	V	39	TYR	2.4
1	X	53	LYS	2.4
1	J	72	LEU	2.4
1	V	112	GLN	2.4
1	C	118	HIS	2.4
1	O	81	PHE	2.4
1	V	57	HIS	2.4
1	W	51	PHE	2.4
1	R	74	ASN	2.4
1	X	125	ASN	2.4
1	J	121	ALA	2.4
1	H	5	THR	2.4
1	C	88	PRO	2.4
1	S	147	GLU	2.4
1	W	162	GLU	2.4
1	E	68	LYS	2.4
1	J	90	CYS	2.4
1	O	78	GLY	2.4
1	P	53	LYS	2.4
1	R	71	LYS	2.4
1	V	87	LYS	2.4
1	V	130	CYS	2.4
1	X	68	LYS	2.4
1	A	45	ASP	2.4
1	G	89	ASP	2.4
1	Q	133	ILE	2.4
1	V	15	ASP	2.4
1	D	10	GLN	2.4
1	E	12	TYR	2.4
1	F	23	GLN	2.4
1	J	29	TYR	2.4
1	K	112	GLN	2.4
1	M	155	LEU	2.4
1	O	112	GLN	2.4
1	T	138	LEU	2.4
1	T	141	GLN	2.4
1	R	128	HIS	2.4
1	P	76	ARG	2.4
1	U	66	ALA	2.4
1	U	160	ALA	2.4
1	H	153	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	5	THR	2.4
1	F	59	SER	2.4
1	H	167	GLU	2.4
1	N	95	SER	2.4
1	M	124	LYS	2.4
1	U	172	LYS	2.4
1	V	86	LYS	2.4
1	A	126	ASP	2.4
1	D	150	ASP	2.4
1	I	133	ILE	2.4
1	O	126	ASP	2.4
1	P	85	ILE	2.4
1	F	26	LEU	2.4
1	H	104	LEU	2.4
1	T	26	LEU	2.4
1	T	148	LEU	2.4
1	U	56	LEU	2.4
1	U	106	LEU	2.4
1	V	97	LEU	2.4
1	J	9	ARG	2.4
1	G	32	TYR	2.4
1	K	12	TYR	2.4
1	M	137	TYR	2.4
1	U	168	TYR	2.4
1	A	100	MET	2.4
1	A	152	VAL	2.4
1	K	152	VAL	2.4
1	R	33	VAL	2.4
1	T	33	VAL	2.4
1	K	103	ALA	2.4
1	X	18	ALA	2.4
1	C	68	LYS	2.4
1	D	64	GLU	2.4
1	G	49	LYS	2.4
1	K	122	THR	2.4
1	M	161	PRO	2.4
1	E	6	SER	2.4
1	K	159	GLY	2.4
1	P	159	GLY	2.4
1	T	24	ILE	2.4
1	B	91	ASP	2.4
1	E	92	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	136	HIS	2.4
1	G	97	LEU	2.4
1	I	57	HIS	2.4
1	J	118	HIS	2.4
1	J	169	LEU	2.4
1	K	45	ASP	2.4
1	Q	63	ARG	2.4
1	R	155	LEU	2.4
1	U	117	LEU	2.4
1	V	22	ARG	2.4
1	V	120	LEU	2.4
1	E	90	CYS	2.4
1	E	123	PHE	2.4
1	I	123	PHE	2.4
1	S	41	PHE	2.4
1	S	168	TYR	2.4
1	U	132	PHE	2.4
1	H	109	ASN	2.4
1	O	109	ASN	2.4
1	A	19	ALA	2.4
1	D	157	LYS	2.4
1	O	49	LYS	2.4
1	R	49	LYS	2.4
1	T	121	ALA	2.4
1	U	87	LYS	2.4
1	D	62	GLU	2.4
1	F	140	GLU	2.4
1	I	93	TRP	2.4
1	I	147	GLU	2.4
1	O	61	GLU	2.4
1	P	162	GLU	2.4
1	V	27	GLU	2.4
1	C	36	SER	2.3
1	H	31	SER	2.3
1	N	6	SER	2.3
1	L	176	GLY	2.3
1	D	63	ARG	2.3
1	A	129	LEU	2.3
1	C	20	ILE	2.3
1	J	80	ILE	2.3
1	K	80	ILE	2.3
1	R	80	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	126	ASP	2.3
1	N	92	ASP	2.3
1	O	48	LEU	2.3
1	O	129	LEU	2.3
1	R	129	LEU	2.3
1	X	104	LEU	2.3
1	S	37	MET	2.3
1	P	54	TYR	2.3
1	R	81	PHE	2.3
1	F	110	VAL	2.3
1	F	152	VAL	2.3
1	M	110	VAL	2.3
1	P	139	ASN	2.3
1	V	74	ASN	2.3
1	B	47	ALA	2.3
1	F	103	ALA	2.3
1	F	134	GLU	2.3
1	K	64	GLU	2.3
1	I	127	PRO	2.3
1	K	93	TRP	2.3
1	C	163	SER	2.3
1	I	22	ARG	2.3
1	O	31	SER	2.3
1	U	38	SER	2.3
1	R	77	GLY	2.3
1	C	80	ILE	2.3
1	C	165	LEU	2.3
1	D	82	LEU	2.3
1	E	105	HIS	2.3
1	G	48	LEU	2.3
1	J	128	HIS	2.3
1	R	73	GLN	2.3
1	P	82	LEU	2.3
1	V	20	ILE	2.3
1	E	89	ASP	2.3
1	P	91	ASP	2.3
1	A	41	PHE	2.3
1	C	71	LYS	2.3
1	G	90	CYS	2.3
1	J	41	PHE	2.3
1	L	49	LYS	2.3
1	O	68	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	124	LYS	2.3
1	P	157	LYS	2.3
1	Q	90	CYS	2.3
1	W	90	CYS	2.3
1	C	110	VAL	2.3
1	K	39	TYR	2.3
1	E	134	GLU	2.3
1	U	147	GLU	2.3
1	D	50	ASN	2.3
1	N	25	ASN	2.3
1	T	25	ASN	2.3
1	A	18	ALA	2.3
1	C	52	ALA	2.3
1	G	52	ALA	2.3
1	K	161	PRO	2.3
1	L	88	PRO	2.3
1	M	103	ALA	2.3
1	P	166	ALA	2.3
1	X	161	PRO	2.3
1	U	5	THR	2.3
1	H	163	SER	2.3
1	S	93	TRP	2.3
1	J	73	GLN	2.3
1	F	20	ILE	2.3
1	S	169	LEU	2.3
1	U	129	LEU	2.3
1	C	100	MET	2.3
1	J	91	ASP	2.3
1	K	91	ASP	2.3
1	K	150	ASP	2.3
1	P	146	LYS	2.3
1	V	124	LYS	2.3
1	X	157	LYS	2.3
1	D	55	PHE	2.3
1	J	123	PHE	2.3
1	E	152	VAL	2.3
1	I	130	CYS	2.3
1	N	102	CYS	2.3
1	R	46	VAL	2.3
1	R	67	GLU	2.3
1	J	40	TYR	2.3
1	T	152	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	25	ASN	2.3
1	G	161	PRO	2.3
1	I	125	ASN	2.3
1	V	103	ALA	2.3
1	X	109	ASN	2.3
1	I	156	ARG	2.3
1	O	63	ARG	2.3
1	M	159	GLY	2.3
1	P	163	SER	2.3
1	V	105	HIS	2.3
1	X	57	HIS	2.3
1	X	163	SER	2.3
1	B	165	LEU	2.3
1	I	28	LEU	2.3
1	J	26	LEU	2.3
1	J	114	LEU	2.3
1	K	138	LEU	2.3
1	K	165	LEU	2.3
1	O	69	LEU	2.3
1	P	175	LEU	2.3
1	T	48	LEU	2.3
1	V	26	LEU	2.3
1	X	72	LEU	2.3
1	H	84	ASP	2.3
1	X	84	ASP	2.3
1	C	55	PHE	2.3
1	N	167	GLU	2.3
1	V	167	GLU	2.3
1	O	110	VAL	2.3
1	F	39	TYR	2.3
1	F	166	ALA	2.2
1	J	50	ASN	2.2
1	O	25	ASN	2.2
1	Q	125	ASN	2.2
1	D	5	THR	2.2
1	F	153	THR	2.2
1	G	77	GLY	2.2
1	H	173	HIS	2.2
1	P	7	GLN	2.2
1	T	60	HIS	2.2
1	W	176	GLY	2.2
1	F	68	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	26	LEU	2.2
1	H	56	LEU	2.2
1	H	133	ILE	2.2
1	I	85	ILE	2.2
1	M	145	ILE	2.2
1	V	68	LYS	2.2
1	W	82	LEU	2.2
1	C	44	ASP	2.2
1	K	44	ASP	2.2
1	X	42	ASP	2.2
1	T	94	GLU	2.2
1	V	55	PHE	2.2
1	O	142	VAL	2.2
1	P	33	VAL	2.2
1	Q	142	VAL	2.2
1	G	109	ASN	2.2
1	G	125	ASN	2.2
1	O	98	ASN	2.2
1	T	52	ALA	2.2
1	V	98	ASN	2.2
1	F	54	TYR	2.2
1	O	12	TYR	2.2
1	R	39	TYR	2.2
1	U	32	TYR	2.2
1	C	5	THR	2.2
1	G	153	THR	2.2
1	U	58	GLN	2.2
1	U	65	HIS	2.2
1	F	56	LEU	2.2
1	F	82	LEU	2.2
1	K	148	LEU	2.2
1	M	37	MET	2.2
1	T	124	LYS	2.2
1	T	117	LEU	2.2
1	D	85	ILE	2.2
1	R	36	SER	2.2
1	L	91	ASP	2.2
1	R	116	GLU	2.2
1	V	116	GLU	2.2
1	W	81	PHE	2.2
1	B	152	VAL	2.2
1	K	127	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	30	ALA	2.2
1	C	172	LYS	2.2
1	D	173	HIS	2.2
1	F	13	HIS	2.2
1	B	100	MET	2.2
1	G	130	CYS	2.2
1	J	75	GLN	2.2
1	L	32	TYR	2.2
1	U	128	HIS	2.2
1	V	10	GLN	2.2
1	V	40	TYR	2.2
1	C	169	LEU	2.2
1	J	28	LEU	2.2
1	J	176	GLY	2.2
1	O	158	MET	2.2
1	R	138	LEU	2.2
1	T	114	LEU	2.2
1	V	165	LEU	2.2
1	Q	80	ILE	2.2
1	V	24	ILE	2.2
1	N	38	SER	2.2
1	X	6	SER	2.2
1	J	44	ASP	2.2
1	K	126	ASP	2.2
1	E	64	GLU	2.2
1	G	64	GLU	2.2
1	J	116	GLU	2.2
1	K	107	GLU	2.2
1	P	134	GLU	2.2
1	U	64	GLU	2.2
1	V	140	GLU	2.2
1	A	123	PHE	2.2
1	D	88	PRO	2.2
1	J	55	PHE	2.2
1	K	170	PHE	2.2
1	M	88	PRO	2.2
1	T	55	PHE	2.2
1	T	123	PHE	2.2
1	U	170	PHE	2.2
1	A	142	VAL	2.2
1	D	110	VAL	2.2
1	E	8	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	119	LYS	2.2
1	I	172	LYS	2.2
1	I	11	ASN	2.2
1	M	139	ASN	2.2
1	F	100	MET	2.2
1	H	141	GLN	2.2
1	Q	128	HIS	2.2
1	R	136	HIS	2.2
1	U	57	HIS	2.2
1	C	69	LEU	2.2
1	C	104	LEU	2.2
1	D	40	TYR	2.2
1	D	77	GLY	2.2
1	F	12	TYR	2.2
1	I	29	TYR	2.2
1	M	129	LEU	2.2
1	N	56	LEU	2.2
1	P	106	LEU	2.2
1	X	56	LEU	2.2
1	X	115	LEU	2.2
1	B	92	ASP	2.2
1	K	62	GLU	2.2
1	O	44	ASP	2.2
1	P	89	ASP	2.2
1	T	91	ASP	2.2
1	T	147	GLU	2.2
1	U	62	GLU	2.2
1	X	91	ASP	2.2
1	M	9	ARG	2.2
1	V	127	PRO	2.2
1	G	124	LYS	2.2
1	H	53	LYS	2.2
1	I	51	PHE	2.2
1	U	146	LYS	2.2
1	C	46	VAL	2.1
1	D	33	VAL	2.1
1	H	33	VAL	2.1
1	H	110	VAL	2.1
1	C	160	ALA	2.1
1	D	105	HIS	2.1
1	R	19	ALA	2.1
1	T	160	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	173	HIS	2.1
1	V	66	ALA	2.1
1	X	58	GLN	2.1
1	C	48	LEU	2.1
1	D	114	LEU	2.1
1	G	56	LEU	2.1
1	K	120	LEU	2.1
1	L	114	LEU	2.1
1	M	175	LEU	2.1
1	O	120	LEU	2.1
1	U	176	GLY	2.1
1	V	96	GLY	2.1
1	F	32	TYR	2.1
1	M	54	TYR	2.1
1	N	32	TYR	2.1
1	D	90	CYS	2.1
1	K	61	GLU	2.1
1	V	61	GLU	2.1
1	V	62	GLU	2.1
1	V	94	GLU	2.1
1	V	95	SER	2.1
1	C	87	LYS	2.1
1	F	172	LYS	2.1
1	O	172	LYS	2.1
1	V	143	LYS	2.1
1	F	55	PHE	2.1
1	J	81	PHE	2.1
1	K	41	PHE	2.1
1	T	51	PHE	2.1
1	I	33	VAL	2.1
1	J	57	HIS	2.1
1	J	105	HIS	2.1
1	K	8	VAL	2.1
1	M	46	VAL	2.1
1	V	8	VAL	2.1
1	K	141	GLN	2.1
1	X	70	MET	2.1
1	D	66	ALA	2.1
1	F	18	ALA	2.1
1	I	66	ALA	2.1
1	J	160	ALA	2.1
1	P	99	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	47	ALA	2.1
1	D	120	LEU	2.1
1	D	149	GLY	2.1
1	J	106	LEU	2.1
1	N	122	THR	2.1
1	P	26	LEU	2.1
1	P	72	LEU	2.1
1	U	155	LEU	2.1
1	F	156	ARG	2.1
1	G	147	GLU	2.1
1	K	147	GLU	2.1
1	N	29	TYR	2.1
1	S	39	TYR	2.1
1	T	12	TYR	2.1
1	F	130	CYS	2.1
1	O	90	CYS	2.1
1	V	90	CYS	2.1
1	W	130	CYS	2.1
1	B	171	ASP	2.1
1	D	36	SER	2.1
1	G	113	SER	2.1
1	K	146	LYS	2.1
1	U	124	LYS	2.1
1	M	127	PRO	2.1
1	S	88	PRO	2.1
1	B	55	PHE	2.1
1	G	55	PHE	2.1
1	I	100	MET	2.1
1	K	60	HIS	2.1
1	R	158	MET	2.1
1	V	70	MET	2.1
1	G	7	GLN	2.1
1	H	58	GLN	2.1
1	R	142	VAL	2.1
1	S	58	GLN	2.1
1	A	121	ALA	2.1
1	F	30	ALA	2.1
1	J	99	ALA	2.1
1	O	52	ALA	2.1
1	V	144	ALA	2.1
1	J	11	ASN	2.1
1	T	21	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	111	ASN	2.1
1	O	56	LEU	2.1
1	T	69	LEU	2.1
1	T	97	LEU	2.1
1	F	135	THR	2.1
1	X	78	GLY	2.1
1	P	22	ARG	2.1
1	C	85	ILE	2.1
1	E	20	ILE	2.1
1	E	145	ILE	2.1
1	F	167	GLU	2.1
1	P	24	ILE	2.1
1	R	20	ILE	2.1
1	R	24	ILE	2.1
1	U	20	ILE	2.1
1	V	85	ILE	2.1
1	J	168	TYR	2.1
1	O	34	TYR	2.1
1	A	102	CYS	2.1
1	C	16	SER	2.1
1	C	92	ASP	2.1
1	O	36	SER	2.1
1	O	59	SER	2.1
1	Q	16	SER	2.1
1	R	131	ASP	2.1
1	U	84	ASP	2.1
1	V	119	LYS	2.1
1	W	49	LYS	2.1
1	J	6	SER	2.1
1	K	16	SER	2.1
1	B	88	PRO	2.1
1	N	88	PRO	2.1
1	R	127	PRO	2.1
1	B	105	HIS	2.1
1	P	123	PHE	2.1
1	I	99	ALA	2.1
1	U	166	ALA	2.1
1	I	98	ASN	2.1
1	I	43	ARG	2.1
1	O	165	LEU	2.1
1	P	138	LEU	2.1
1	U	138	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	5	THR	2.1
1	O	140	GLU	2.1
1	P	174	THR	2.1
1	U	135	THR	2.1
1	X	17	GLU	2.1
1	S	24	ILE	2.1
1	H	172	LYS	2.1
1	N	157	LYS	2.1
1	W	157	LYS	2.1
1	A	12	TYR	2.1
1	J	34	TYR	2.1
1	J	92	ASP	2.1
1	A	13	HIS	2.1
1	O	60	HIS	2.1
1	R	105	HIS	2.1
1	T	105	HIS	2.1
1	U	136	HIS	2.1
1	V	7	GLN	2.0
1	D	142	VAL	2.0
1	G	152	VAL	2.0
1	H	152	VAL	2.0
1	I	132	PHE	2.0
1	J	33	VAL	2.0
1	T	8	VAL	2.0
1	X	46	VAL	2.0
1	U	47	ALA	2.0
1	X	79	ARG	2.0
1	D	11	ASN	2.0
1	D	117	LEU	2.0
1	D	165	LEU	2.0
1	G	175	LEU	2.0
1	H	82	LEU	2.0
1	P	11	ASN	2.0
1	R	28	LEU	2.0
1	V	106	LEU	2.0
1	X	165	LEU	2.0
1	C	62	GLU	2.0
1	M	167	GLU	2.0
1	C	93	TRP	2.0
1	M	176	GLY	2.0
1	F	5	THR	2.0
1	K	68	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	20	ILE	2.0
1	V	135	THR	2.0
1	V	153	THR	2.0
1	C	137	TYR	2.0
1	E	150	ASP	2.0
1	T	42	ASP	2.0
1	J	88	PRO	2.0
1	C	37	MET	2.0
1	D	95	SER	2.0
1	O	127	PRO	2.0
1	X	59	SER	2.0
1	O	151	HIS	2.0
1	X	173	HIS	2.0
1	F	58	GLN	2.0
1	V	58	GLN	2.0
1	D	8	VAL	2.0
1	D	41	PHE	2.0
1	J	46	VAL	2.0
1	U	110	VAL	2.0
1	C	27	GLU	2.0
1	C	175	LEU	2.0
1	D	69	LEU	2.0
1	D	115	LEU	2.0
1	E	66	ALA	2.0
1	K	94	GLU	2.0
1	M	115	LEU	2.0
1	P	114	LEU	2.0
1	Q	134	GLU	2.0
1	U	175	LEU	2.0
1	X	140	GLU	2.0
1	M	77	GLY	2.0
1	Q	109	ASN	2.0
1	R	109	ASN	2.0
1	I	80	ILE	2.0
1	M	133	ILE	2.0
1	X	5	THR	2.0
1	Q	93	TRP	2.0
1	D	44	ASP	2.0
1	I	91	ASP	2.0
1	S	89	ASP	2.0
1	V	92	ASP	2.0
1	C	31	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	136	HIS	2.0
1	G	65	HIS	2.0
1	O	39	TYR	2.0
1	O	95	SER	2.0
1	T	95	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](#)

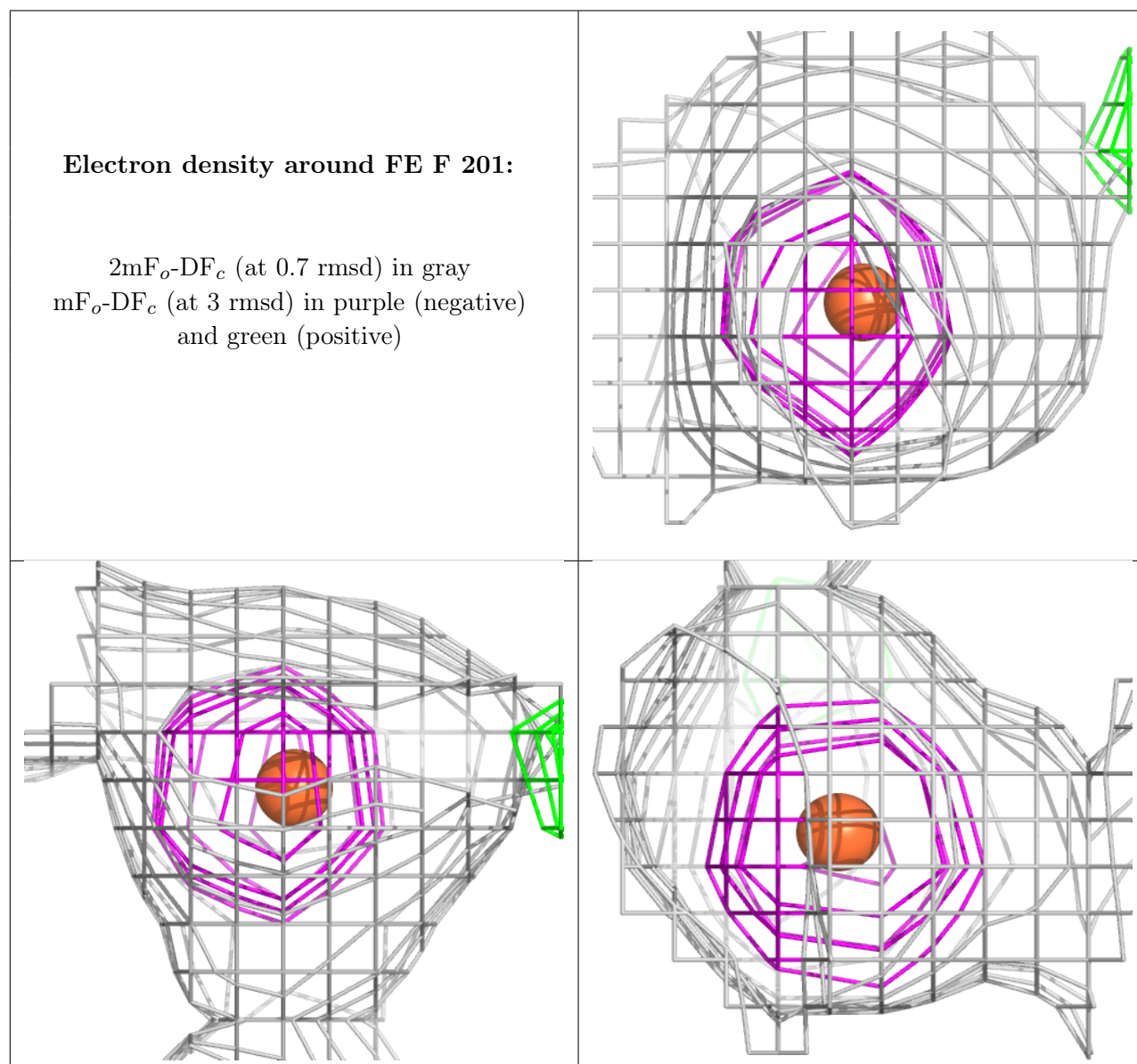
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

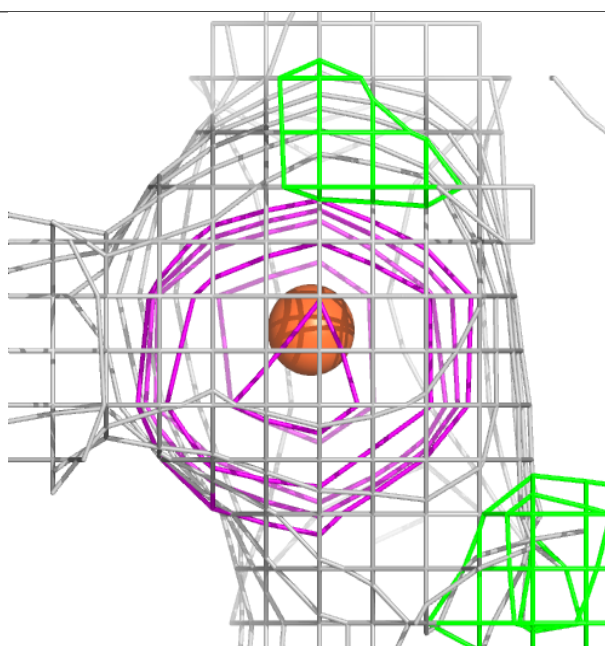
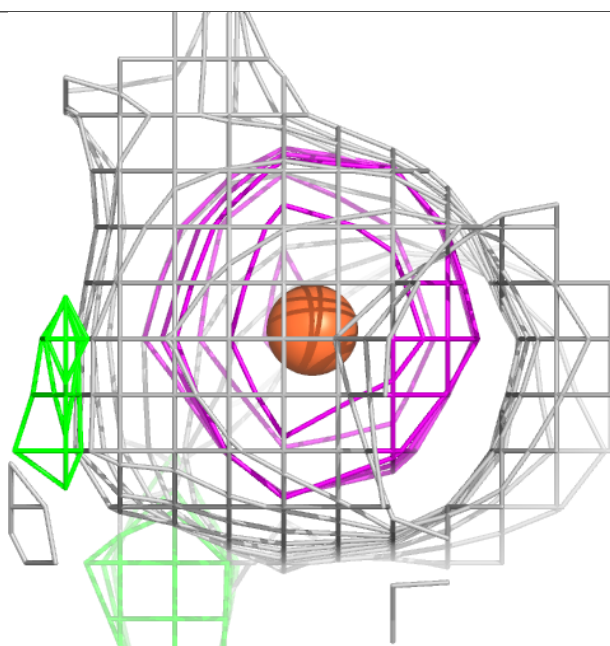
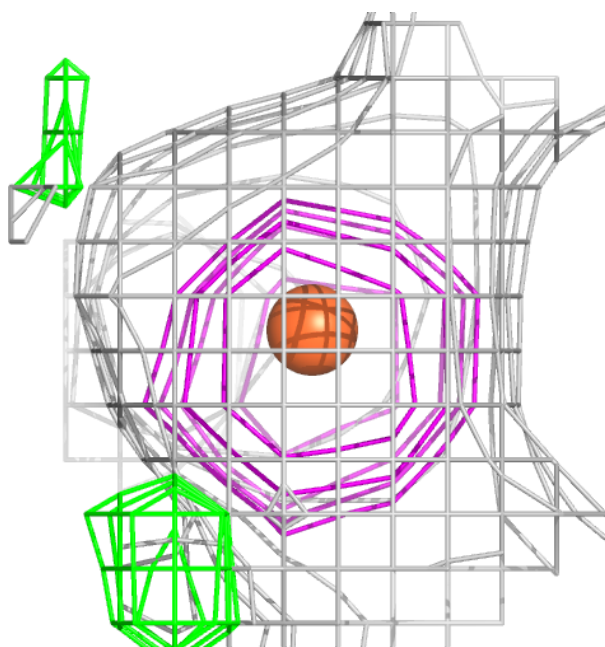
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	F	201	1/1	0.96	0.16	30,30,30,30	0
2	FE	B	202	1/1	0.97	0.18	30,30,30,30	0
2	FE	D	201	1/1	0.97	0.18	30,30,30,30	0
2	FE	B	201	1/1	0.97	0.08	30,30,30,30	0
2	FE	H	201	1/1	0.97	0.13	30,30,30,30	0
2	FE	P	202	1/1	0.97	0.18	30,30,30,30	0
2	FE	Q	201	1/1	0.97	0.16	30,30,30,30	0
2	FE	L	201	1/1	0.98	0.17	30,30,30,30	0
2	FE	P	201	1/1	0.98	0.22	30,30,30,30	0
2	FE	G	201	1/1	0.98	0.16	30,30,30,30	0
2	FE	E	201	1/1	0.98	0.16	30,30,30,30	0
2	FE	S	202	1/1	0.98	0.18	30,30,30,30	0
2	FE	W	201	1/1	0.98	0.11	30,30,30,30	0
2	FE	I	201	1/1	0.99	0.13	30,30,30,30	0
2	FE	E	202	1/1	0.99	0.17	30,30,30,30	0
2	FE	M	201	1/1	0.99	0.11	30,30,30,30	0
2	FE	A	201	1/1	0.99	0.16	30,30,30,30	0
2	FE	S	201	1/1	1.00	0.15	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



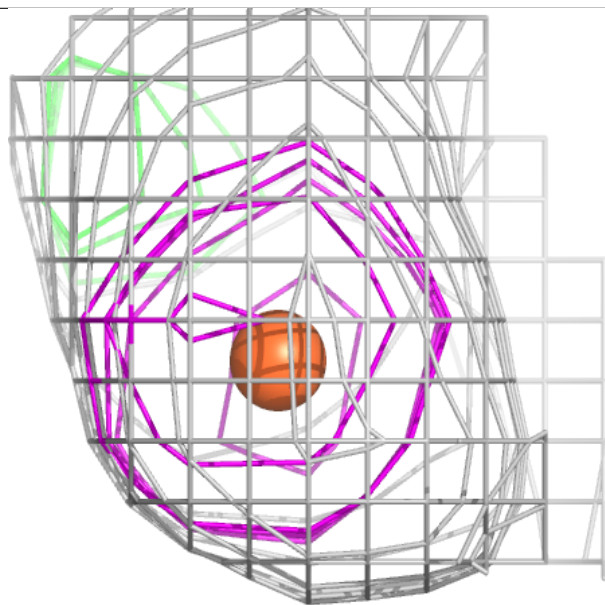
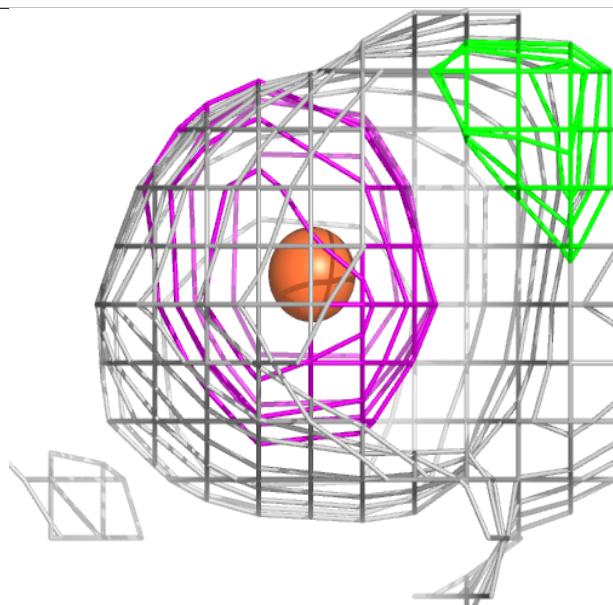
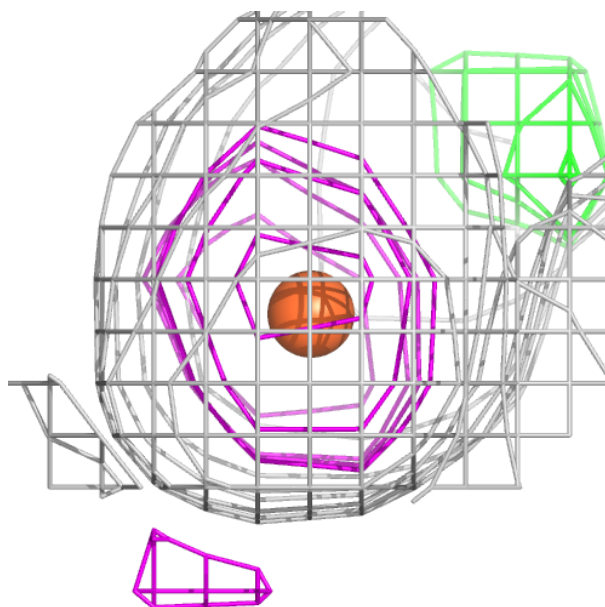
Electron density around FE B 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



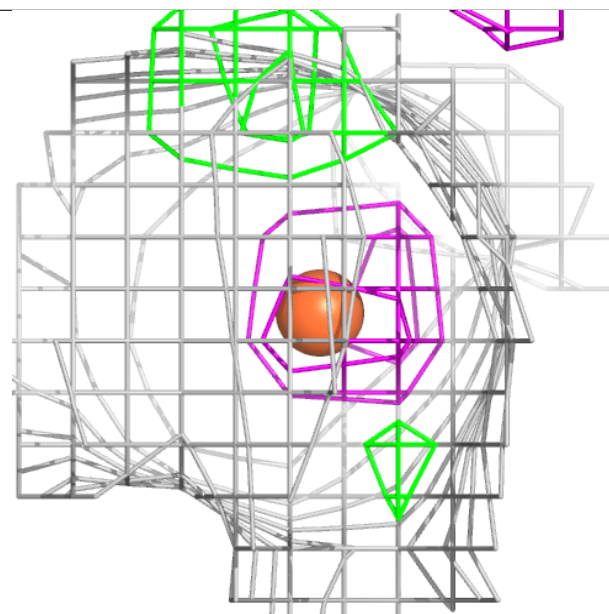
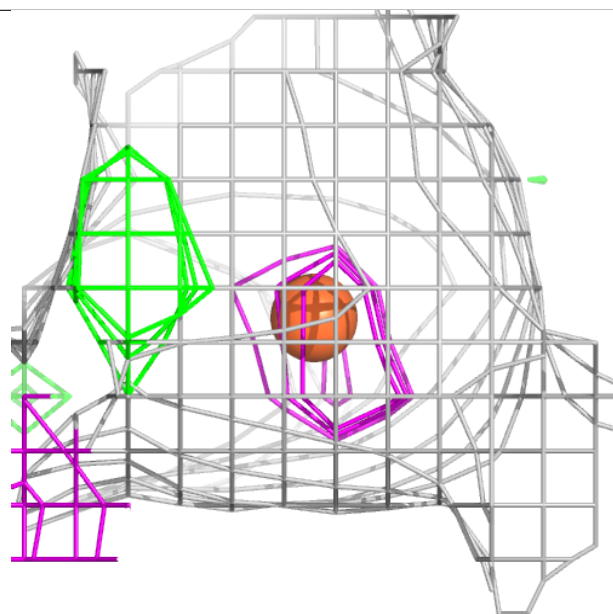
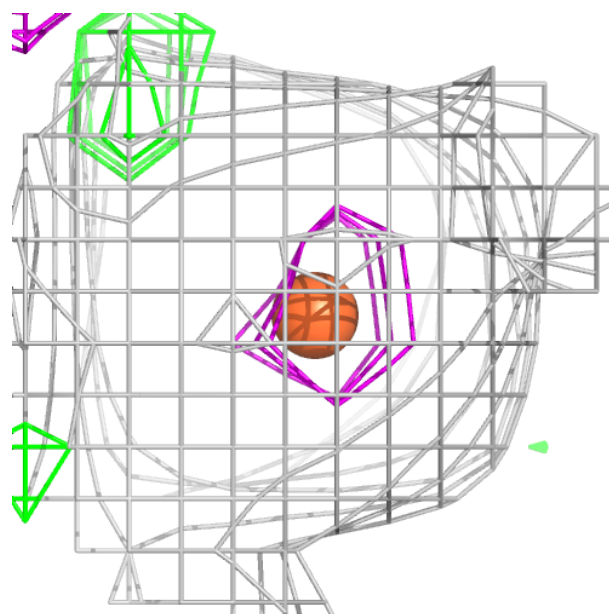
Electron density around FE D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



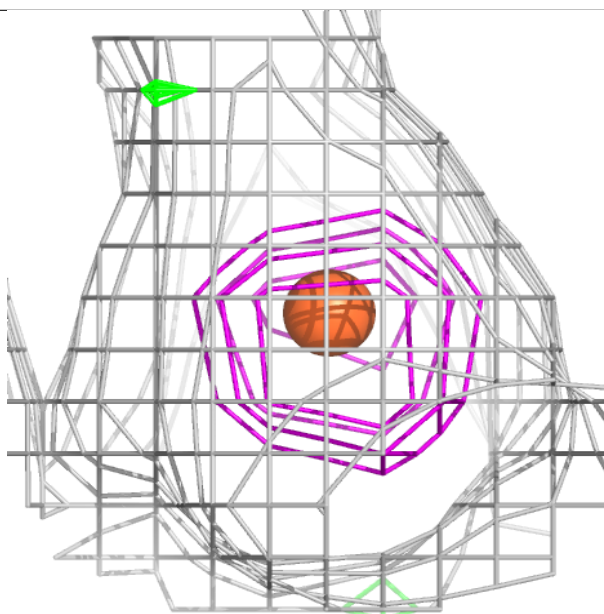
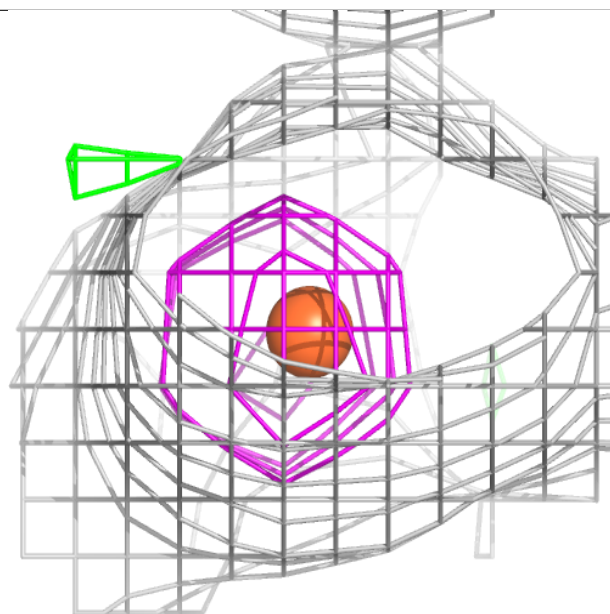
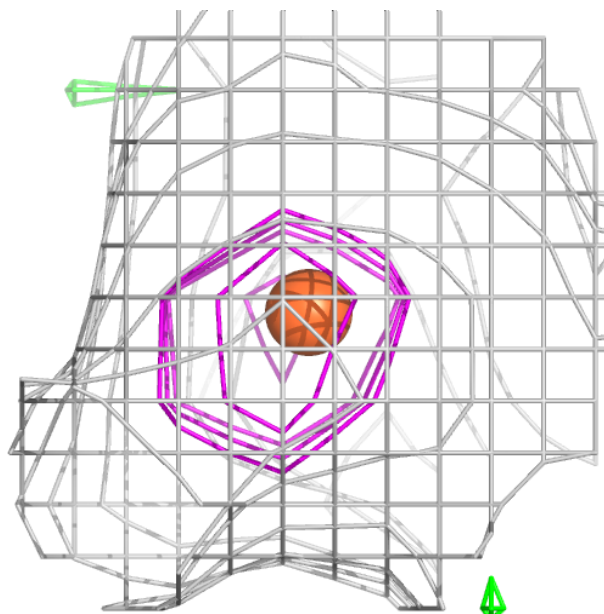
Electron density around FE B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



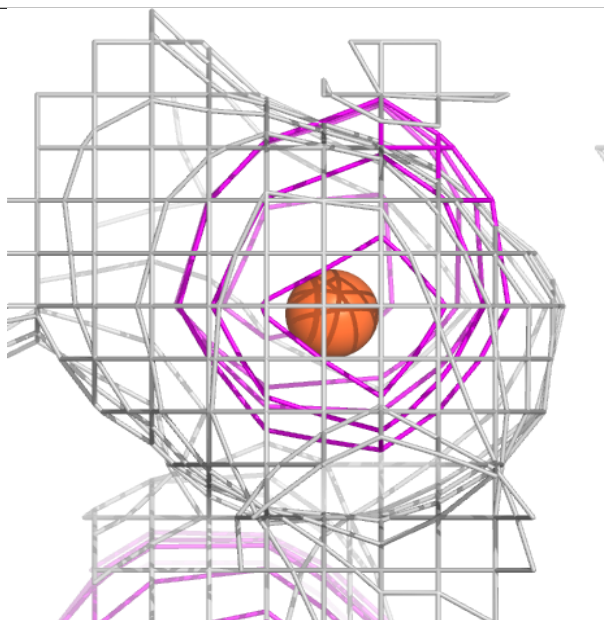
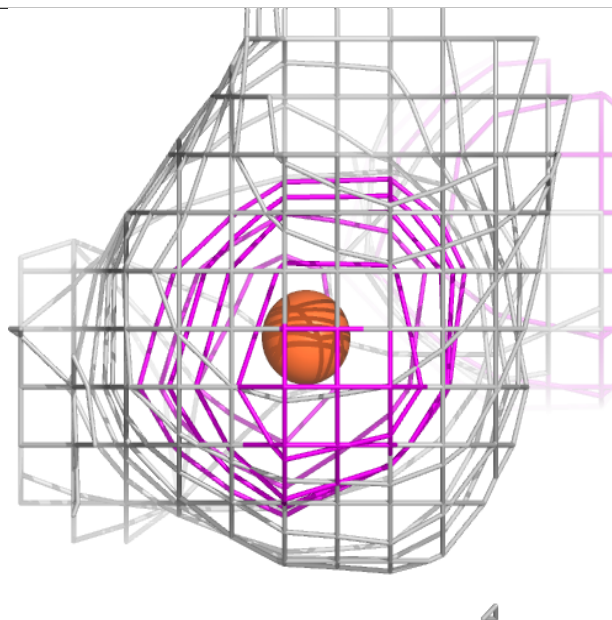
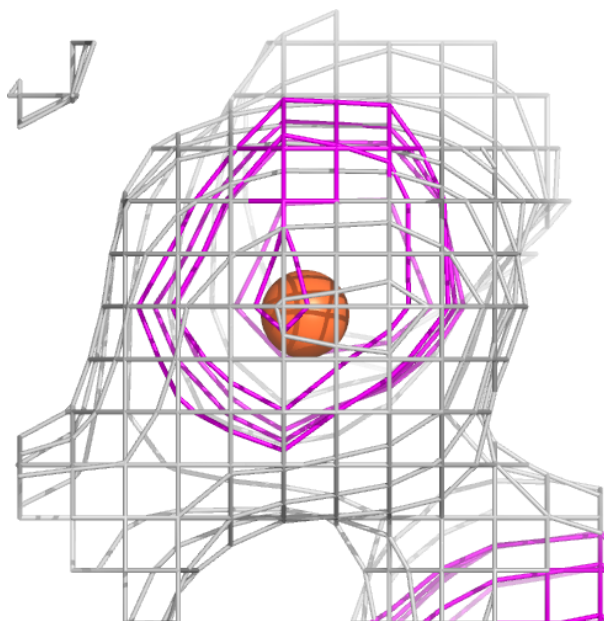
Electron density around FE H 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



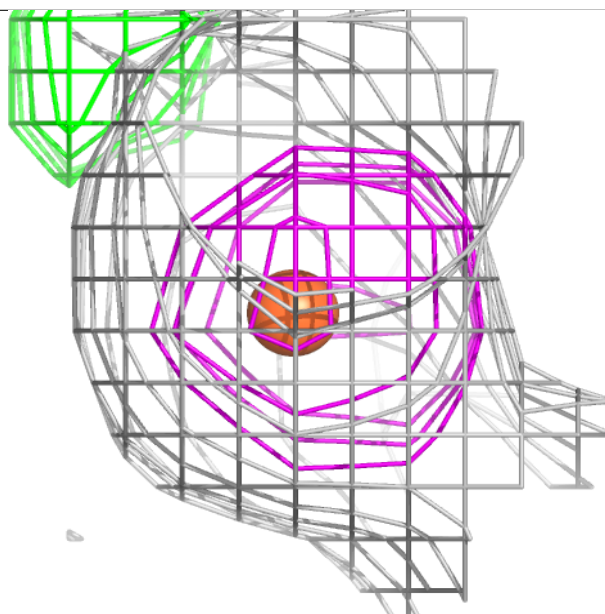
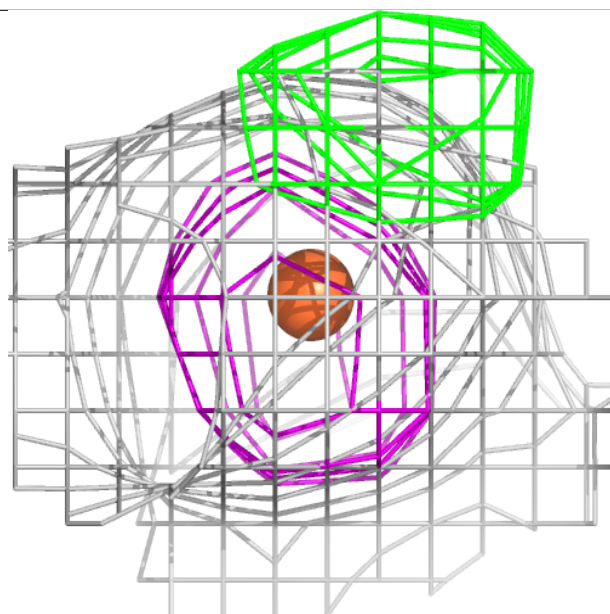
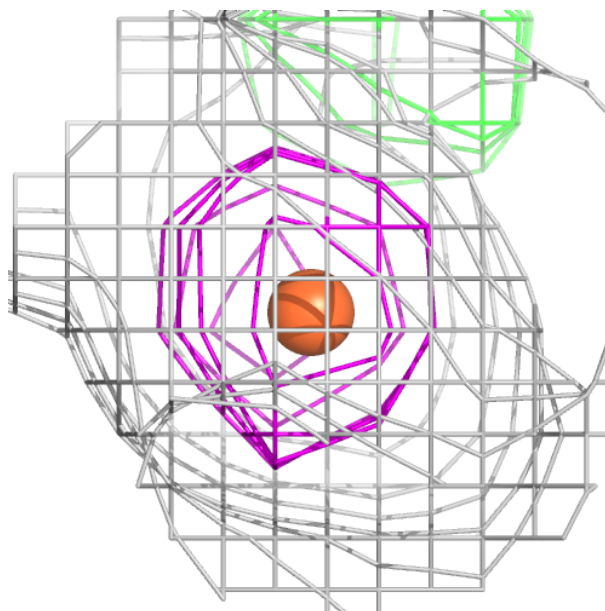
Electron density around FE P 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



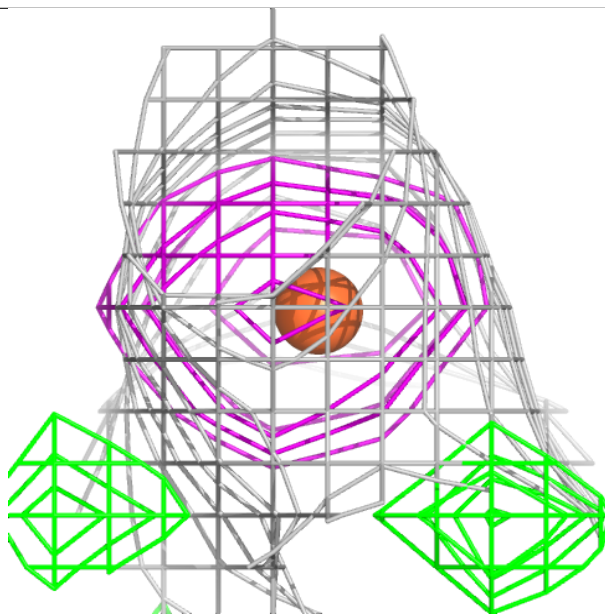
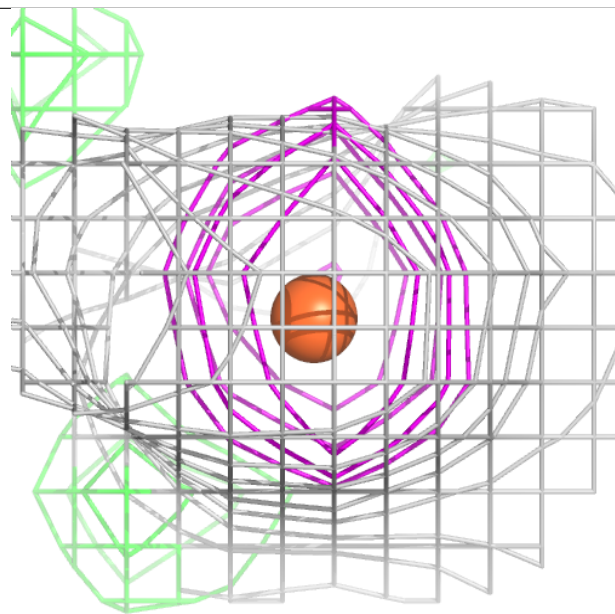
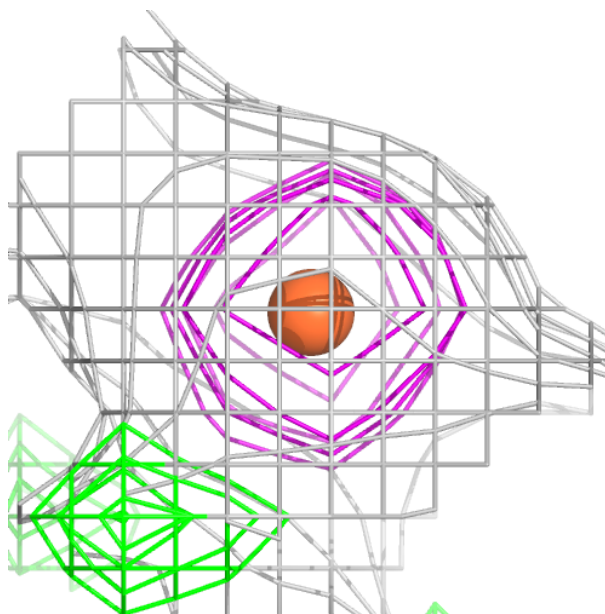
Electron density around FE Q 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



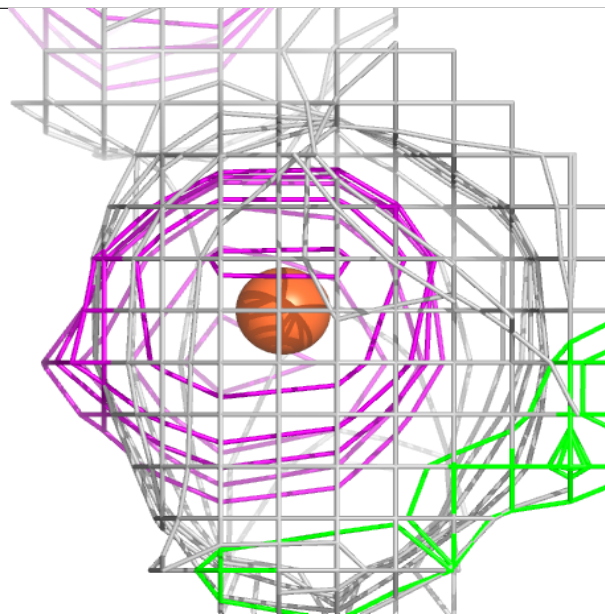
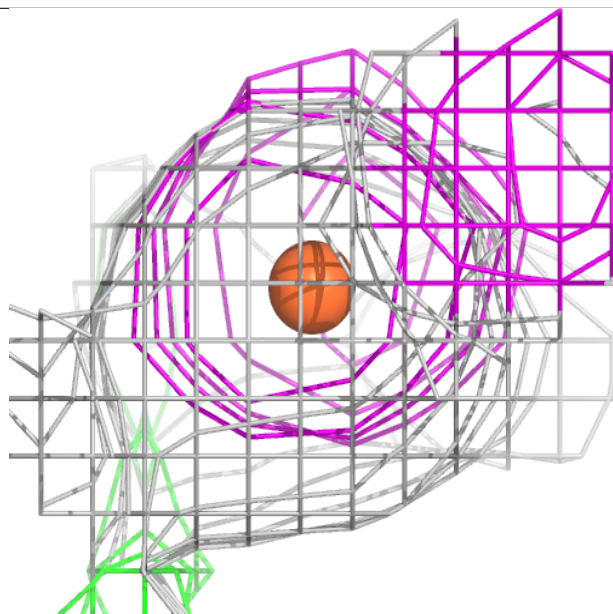
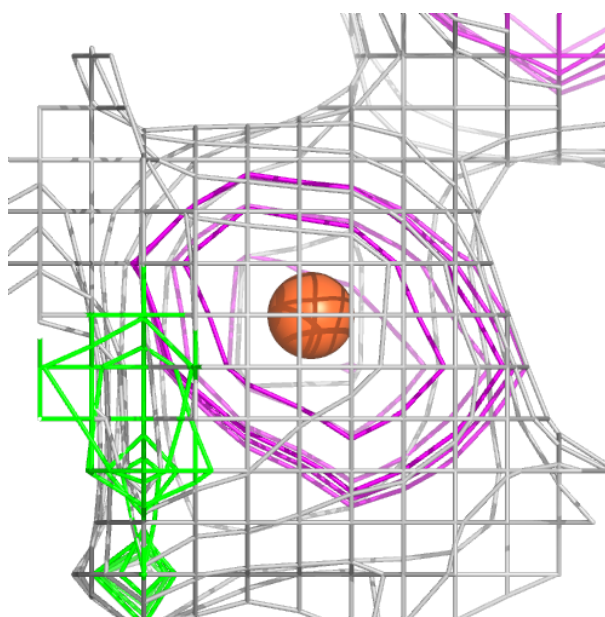
Electron density around FE L 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



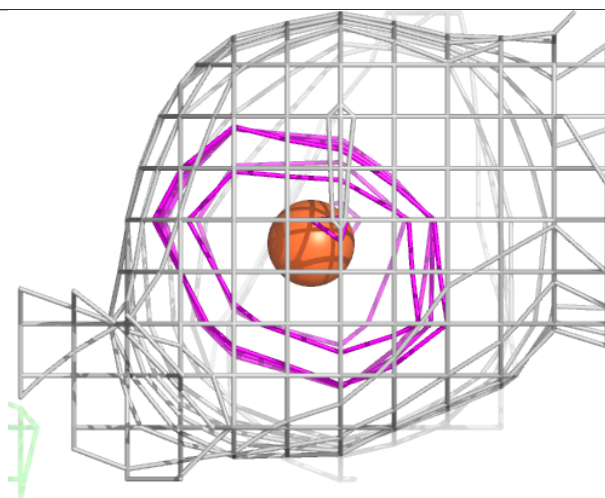
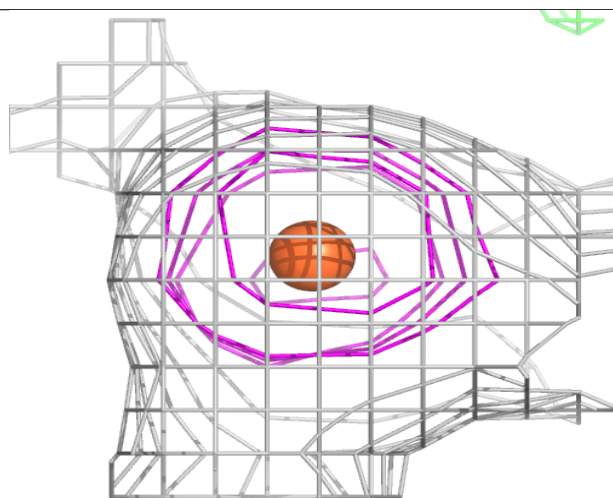
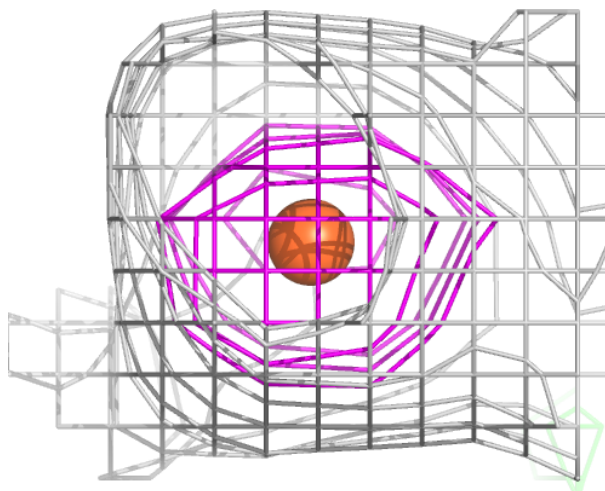
Electron density around FE P 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



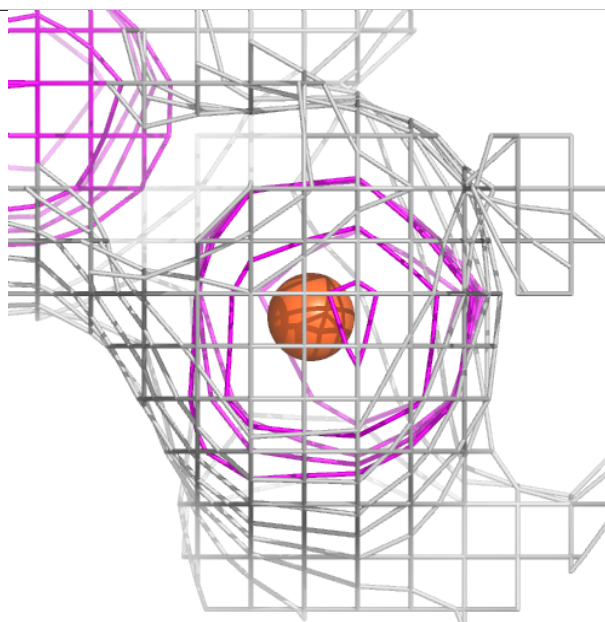
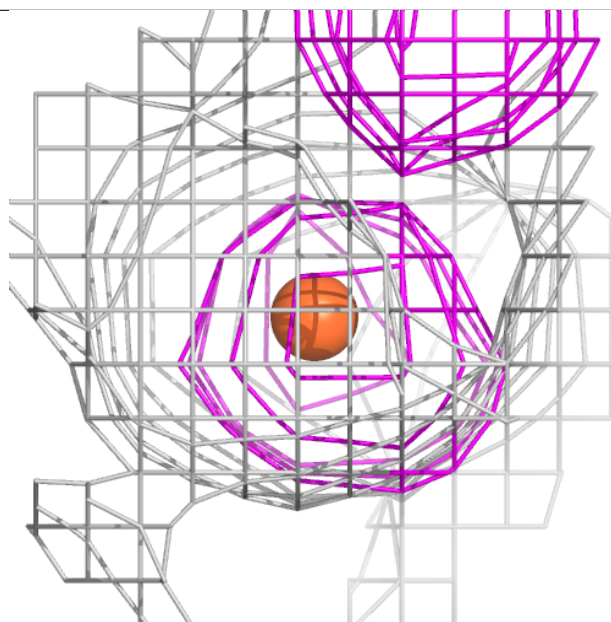
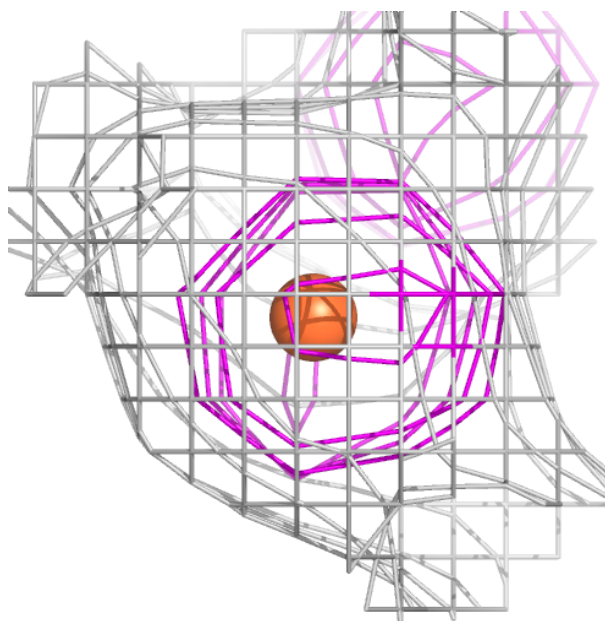
Electron density around FE G 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



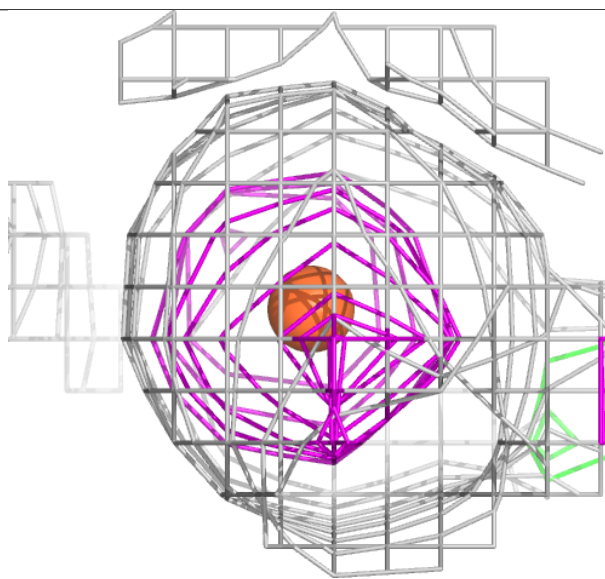
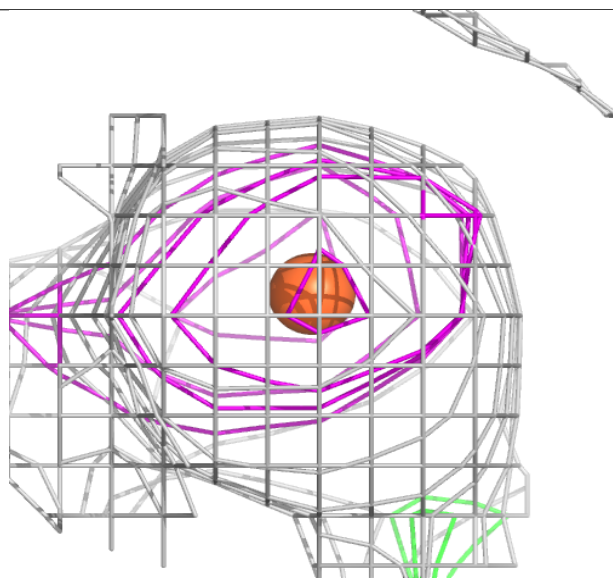
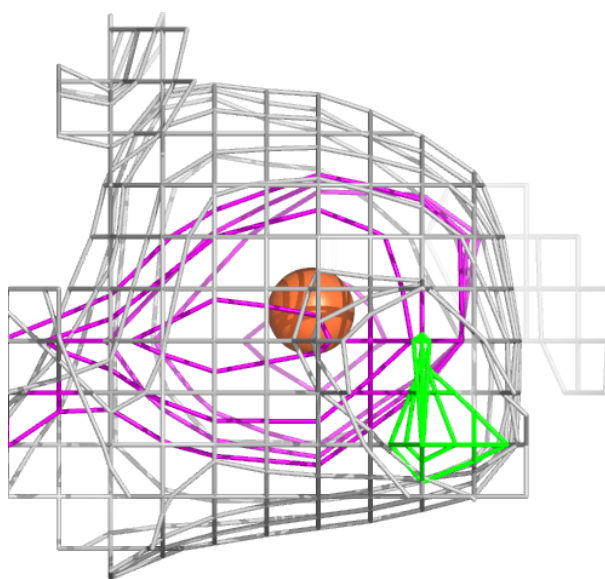
Electron density around FE E 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



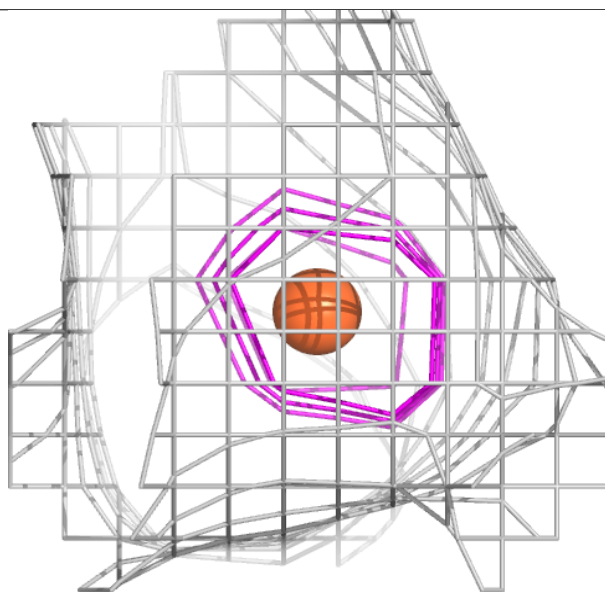
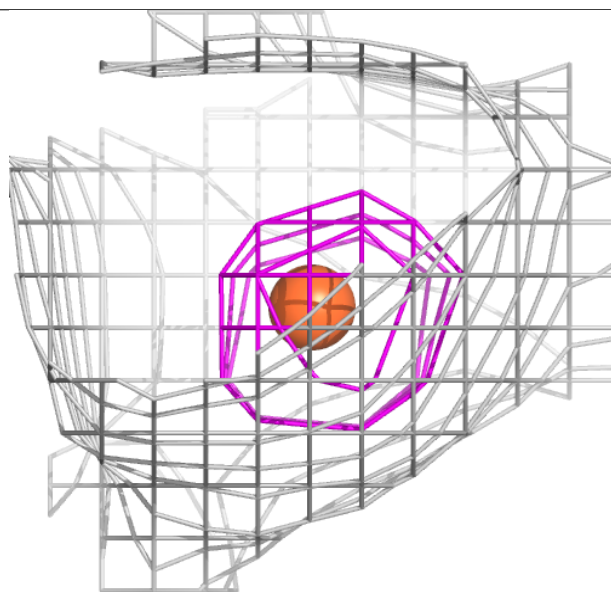
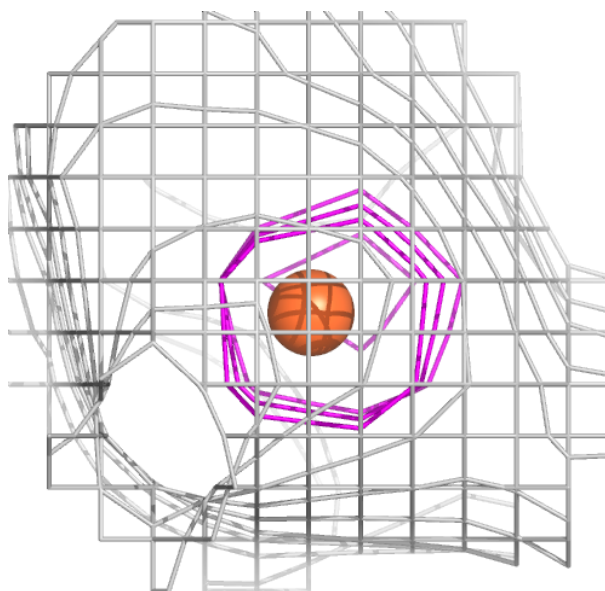
Electron density around FE S 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



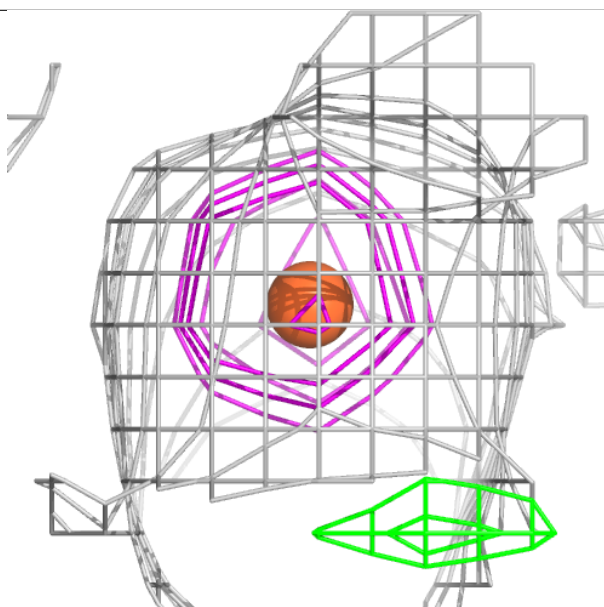
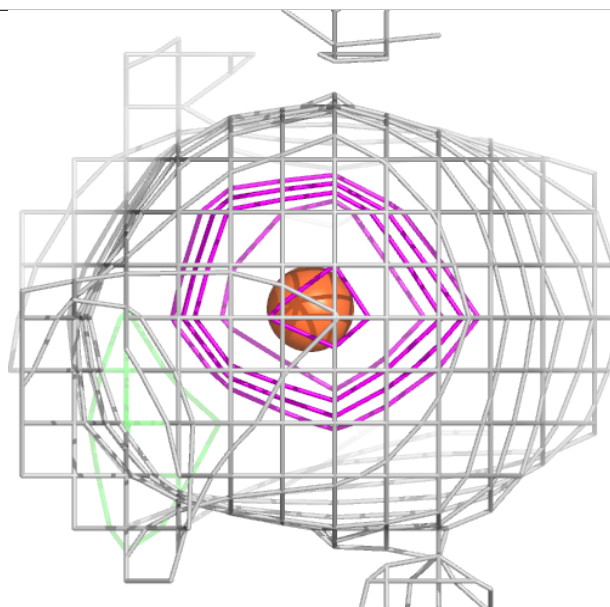
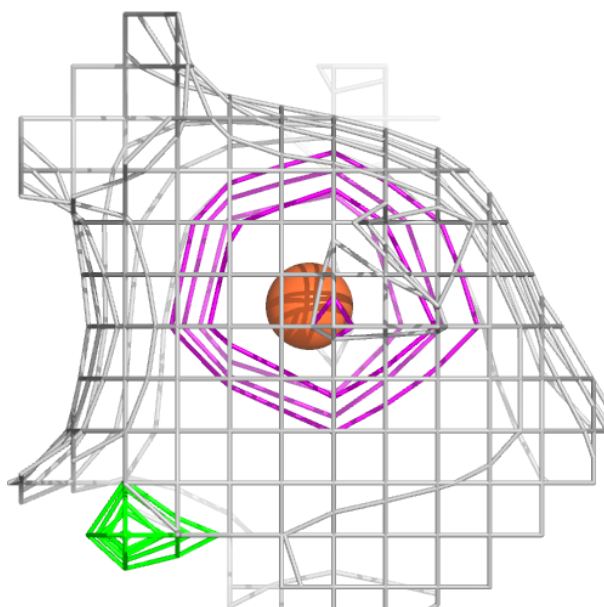
Electron density around FE W 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



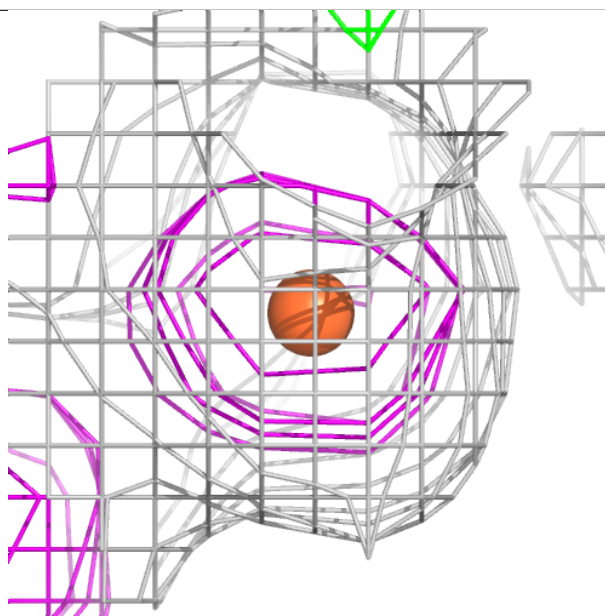
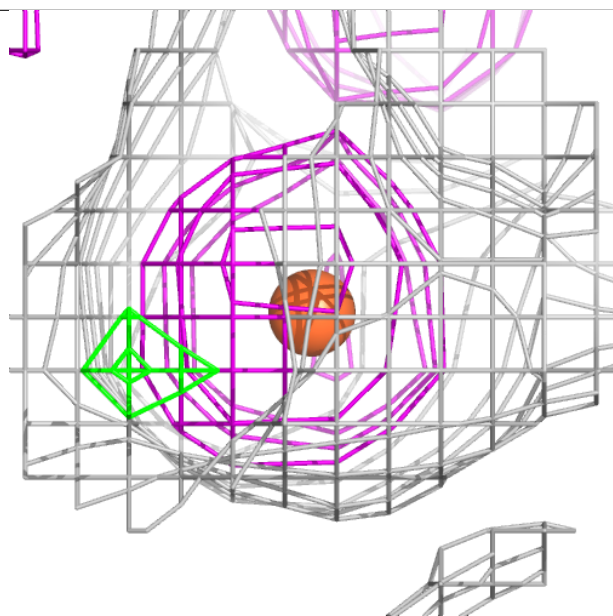
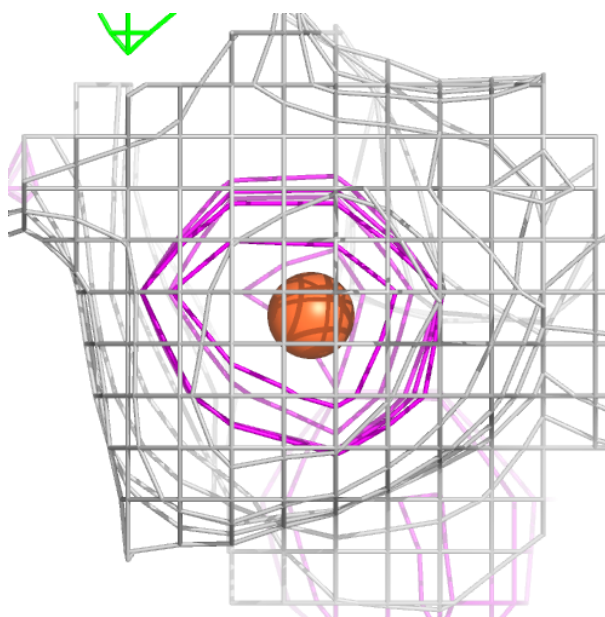
Electron density around FE I 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



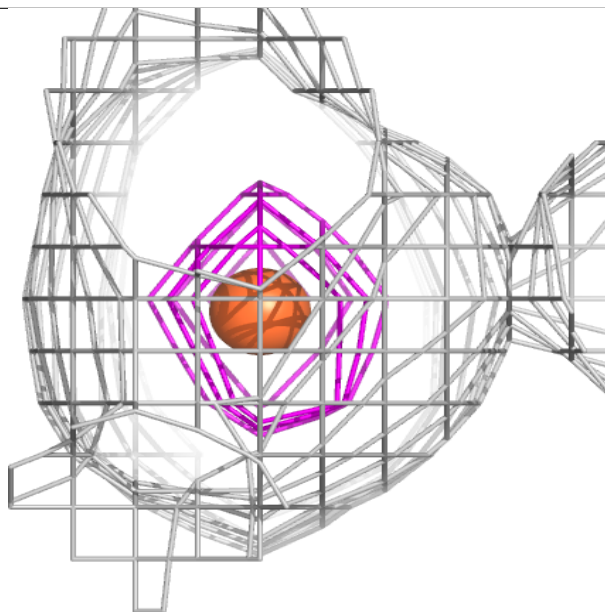
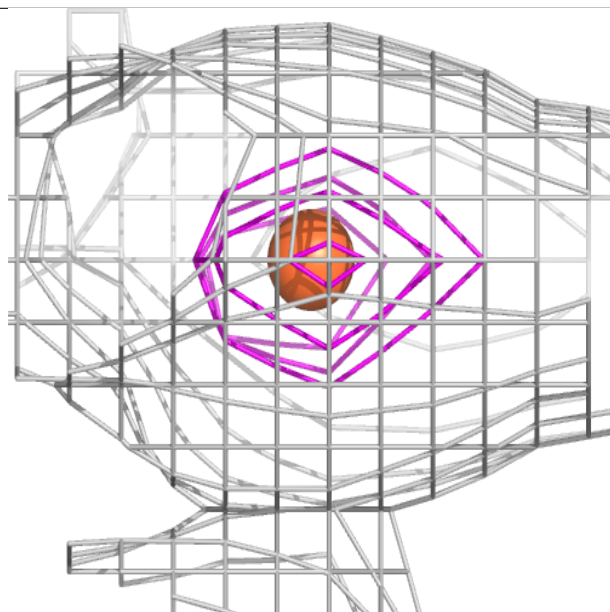
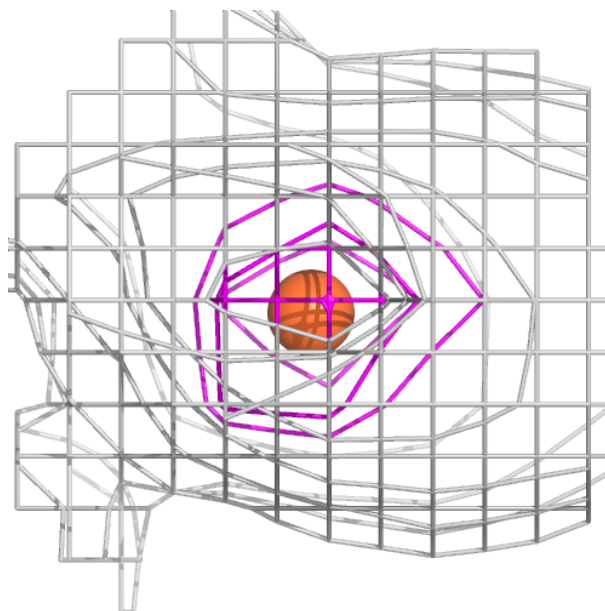
Electron density around FE E 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



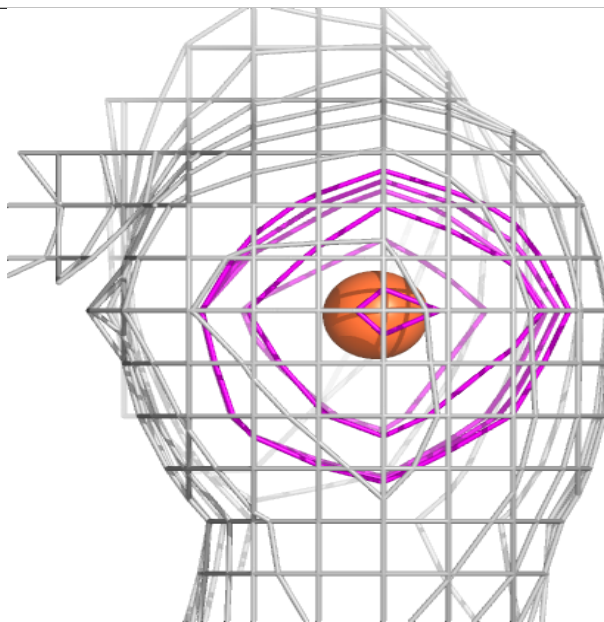
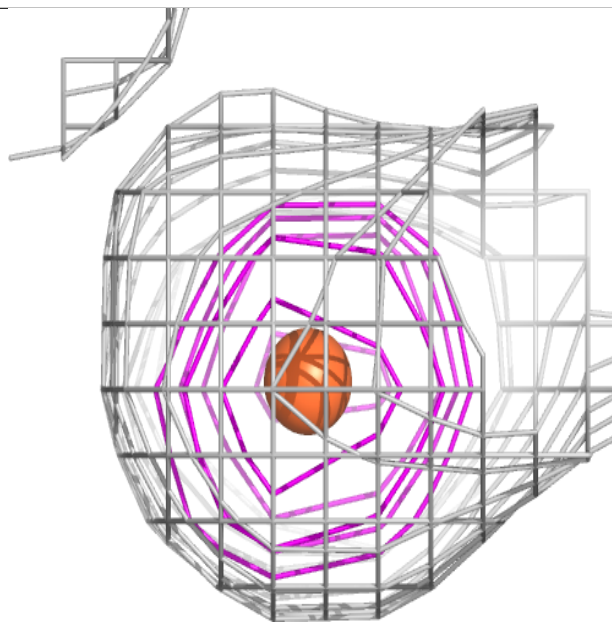
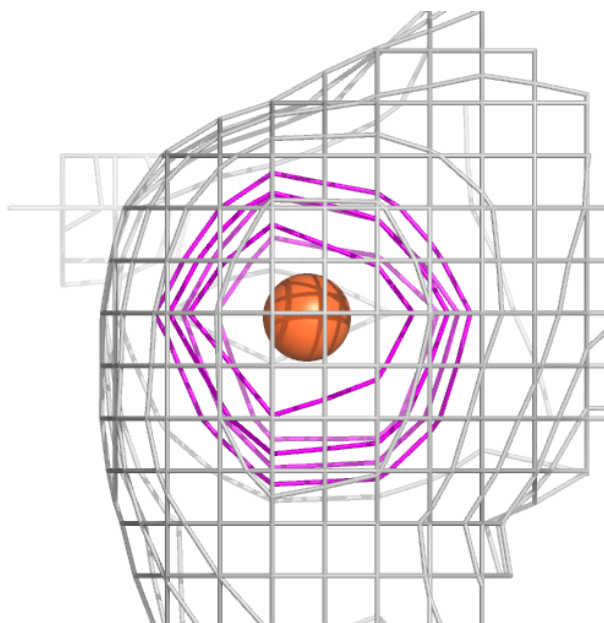
Electron density around FE M 201:

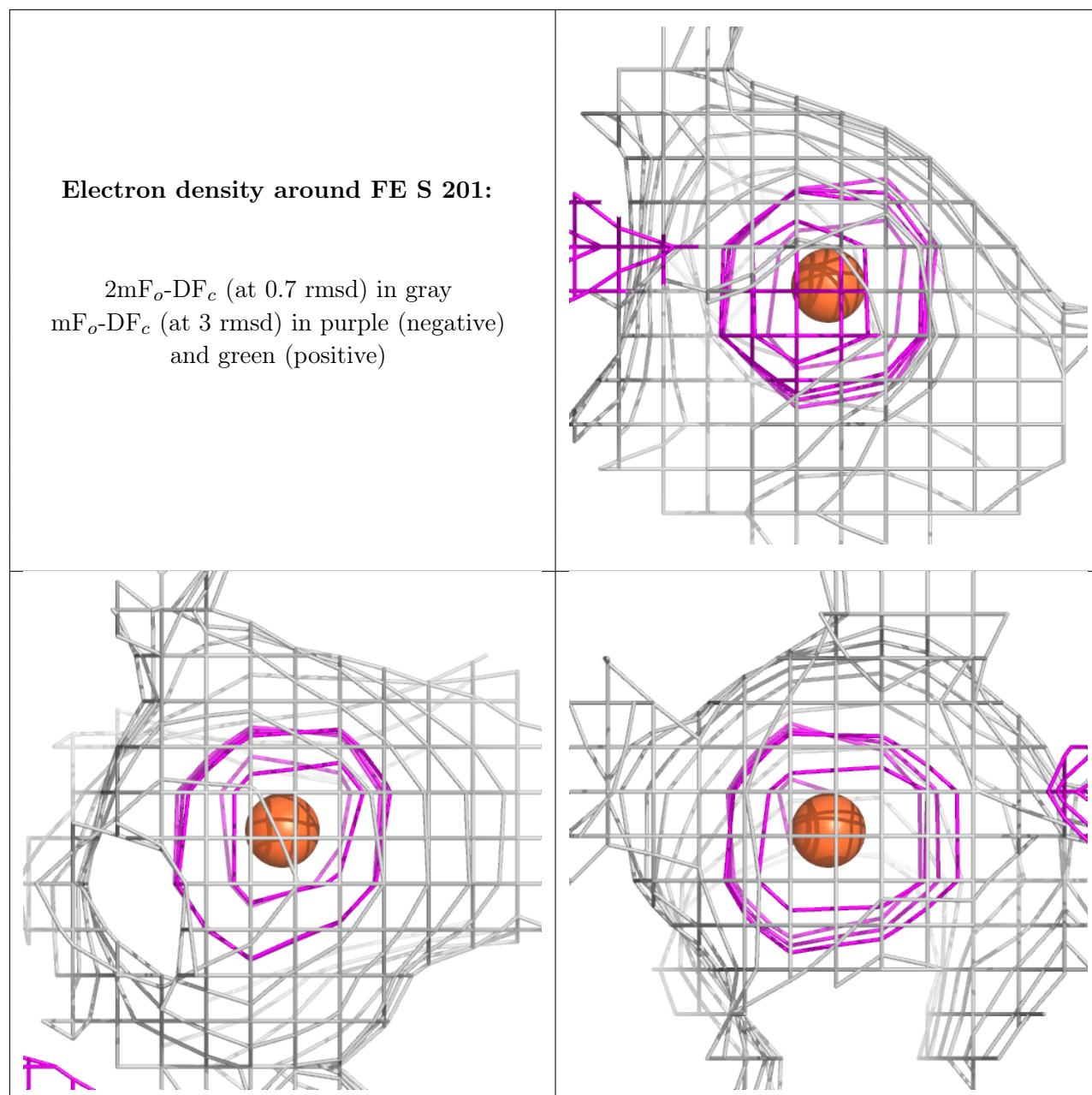
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.