Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2024 – 08:18 PM JST

PDB ID	:	8JAI
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:

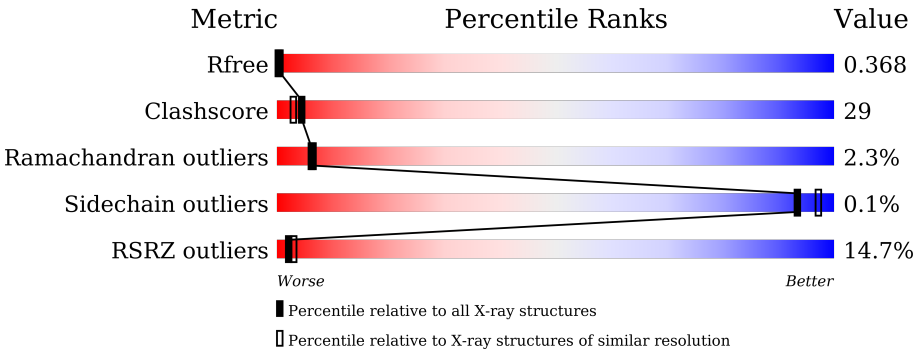
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 <=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	7% 48% 45% · 6%
1	B	183	3% 48% 46% · 6%
1	C	183	19% 42% 51% · 6%
1	D	183	20% 33% 60% · 6%
1	E	183	4% 51% 42% · 6%
1	F	183	22% 36% 56% · 6%

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Mol	Chain	Length	Quality of chain
1	G	183	25% 40% 52% 6%
1	H	183	11% 39% 50% 6%
1	I	183	8% 47% 43% 6%
1	J	183	22% 39% 52% 6%
1	K	183	18% 46% 47% 6%
1	L	183	3% 46% 46% 6%
1	M	183	14% 35% 56% 6%
1	N	183	7% 50% 42% 6%
1	O	183	19% 44% 49% 6%
1	P	183	24% 36% 56% 6%
1	Q	183	5% 38% 54% 6%
1	R	183	15% 36% 54% 6%
1	S	183	9% 57% 36% 6%
1	T	183	18% 44% 49% 6%
1	U	183	22% 37% 54% 6%
1	V	183	13% 45% 45% 6%
1	W	183	4% 51% 42% 6%
1	X	183	19% 42% 50% 6%

2 Entry composition (i)

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 (three-letter code: 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.

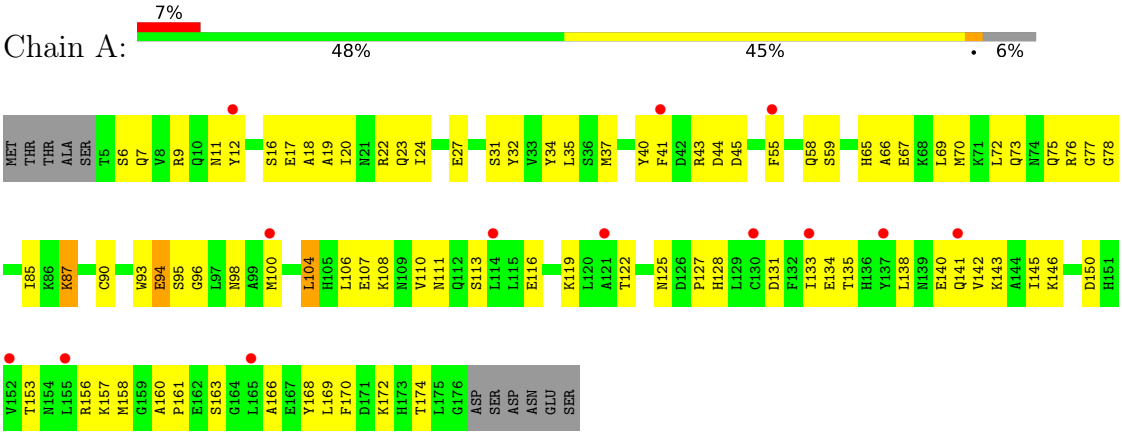
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0

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.

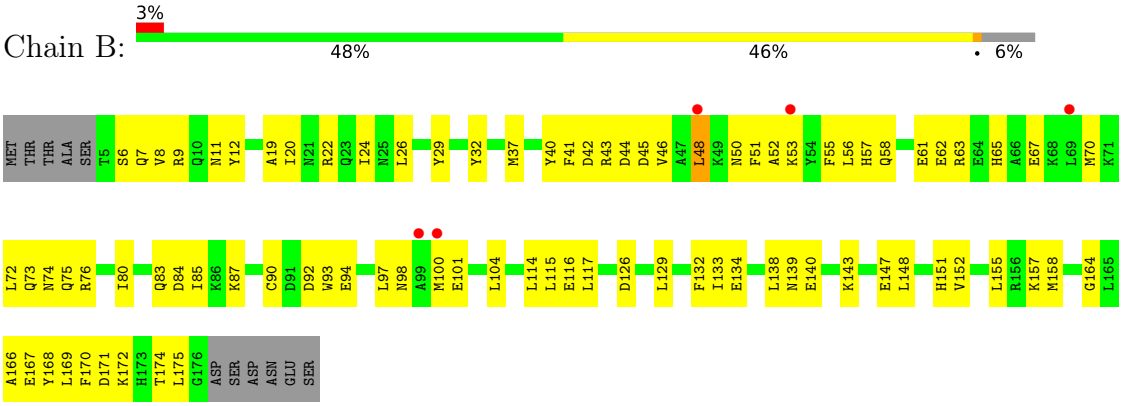
• Molecule 1: Ferritin heavy chain

Chain A:



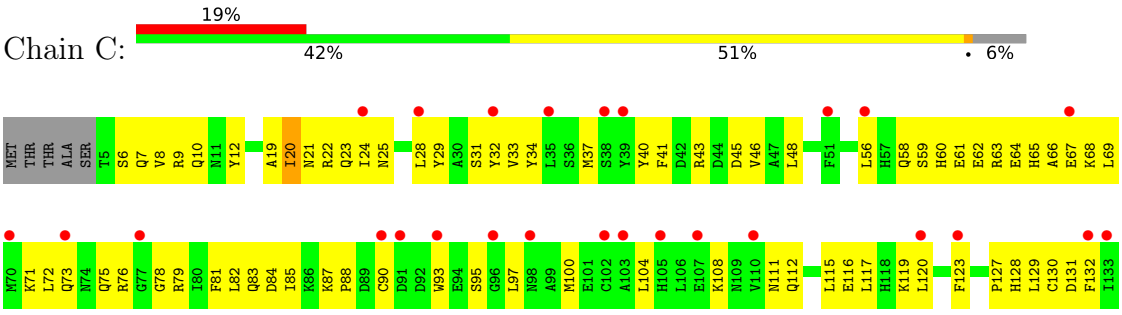
• Molecule 1: Ferritin heavy chain

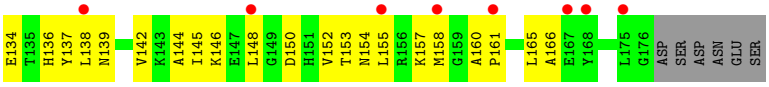
Chain B:



• Molecule 1: Ferritin heavy chain

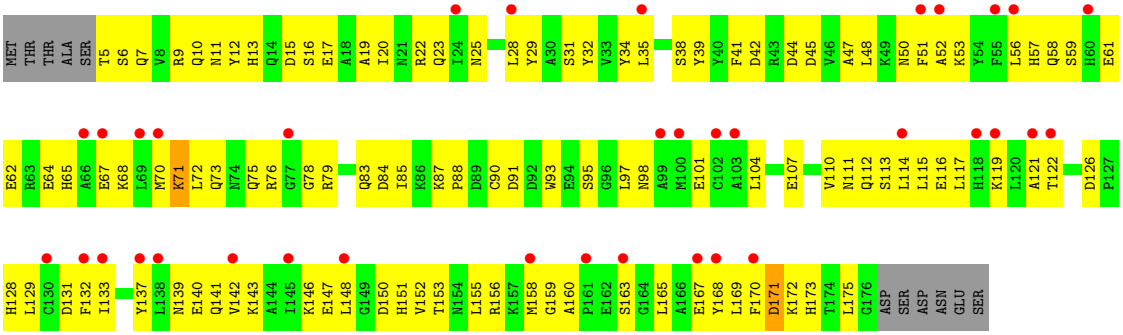
Chain C:





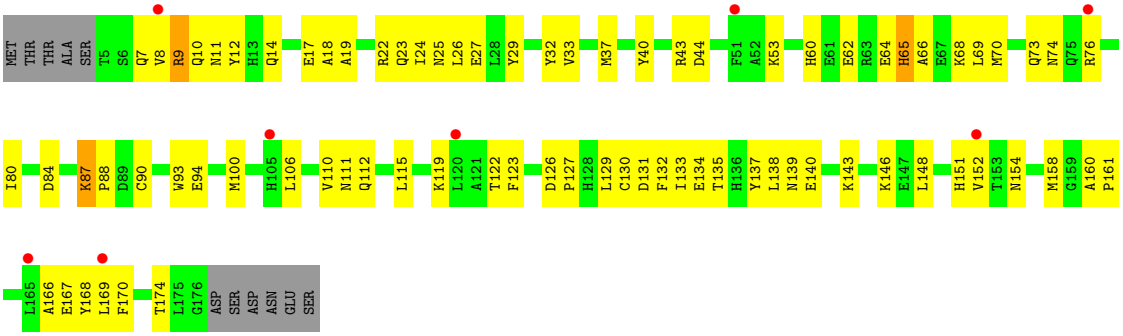
• Molecule 1: Ferritin heavy chain

Chain D:



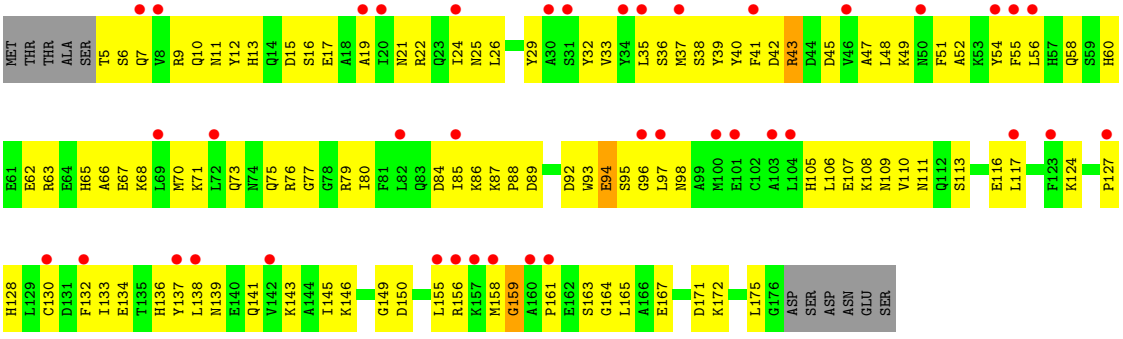
• Molecule 1: Ferritin heavy chain

Chain E:



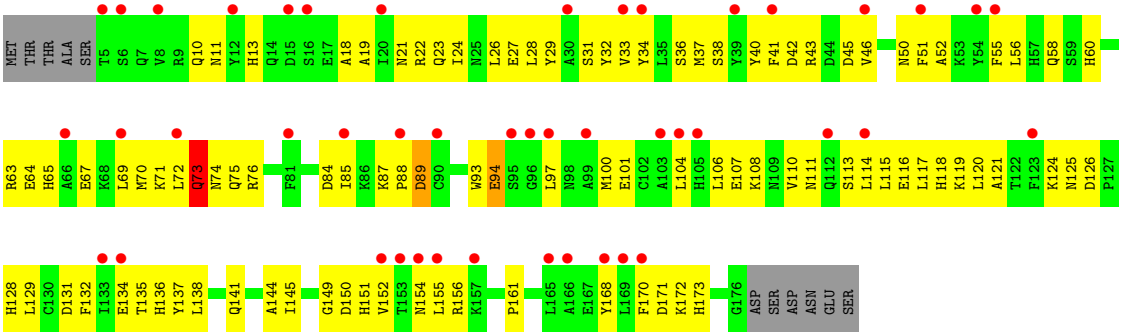
• Molecule 1: Ferritin heavy chain

Chain F:



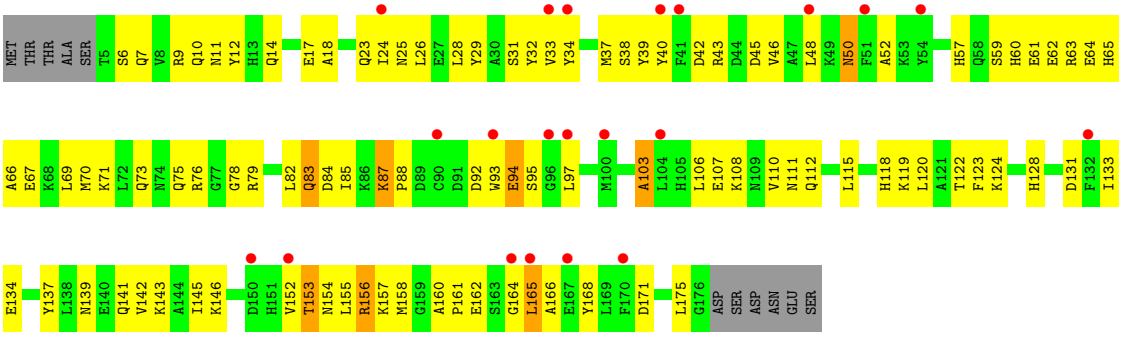
• Molecule 1: Ferritin heavy chain

Chain G:



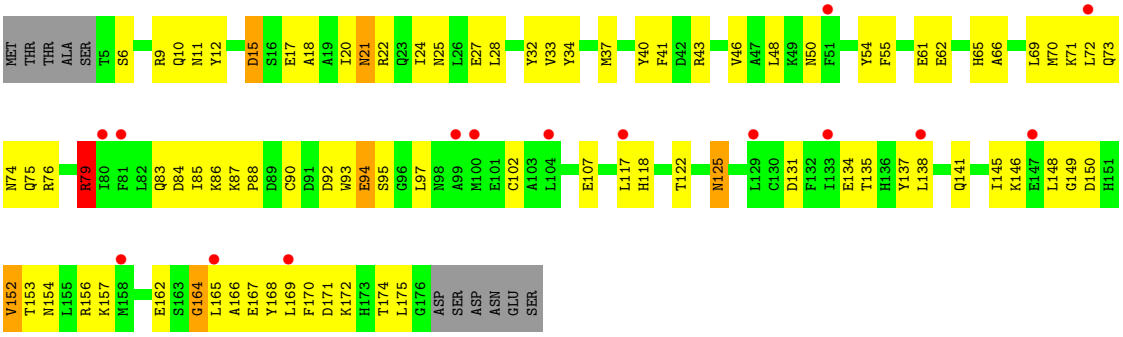
• Molecule 1: Ferritin heavy chain

Chain H:



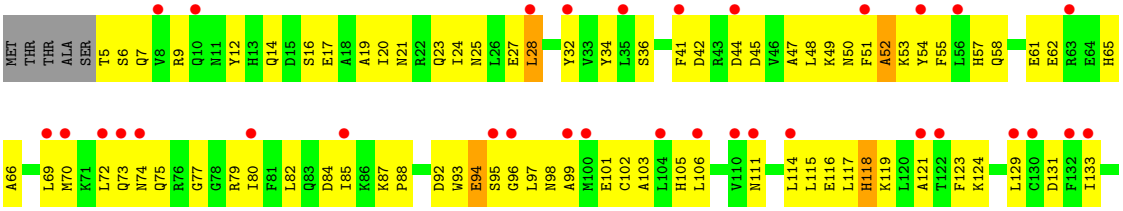
• Molecule 1: Ferritin heavy chain

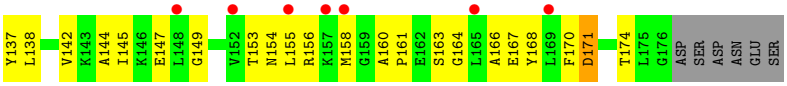
Chain I:



• Molecule 1: Ferritin heavy chain

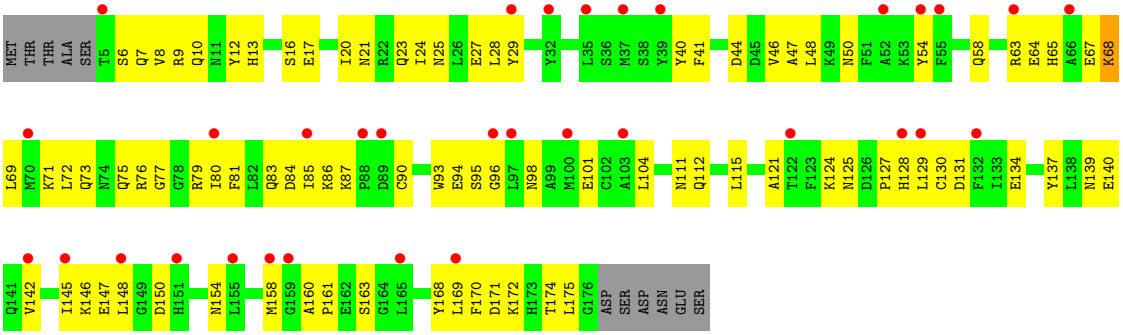
Chain J:





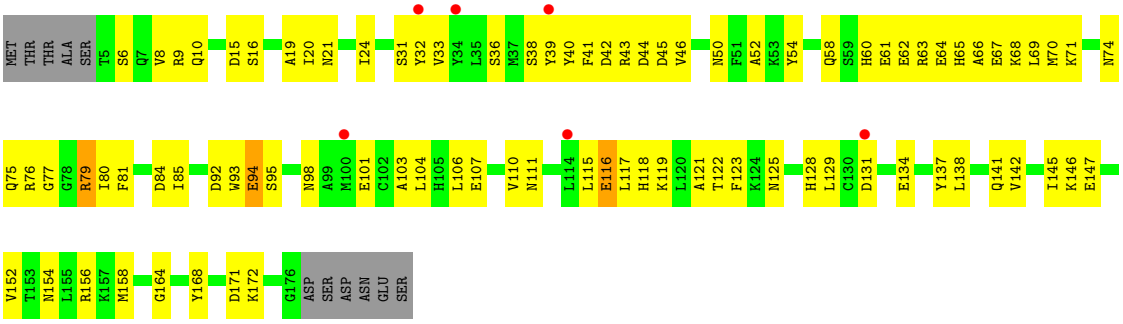
• Molecule 1: Ferritin heavy chain

Chain K:



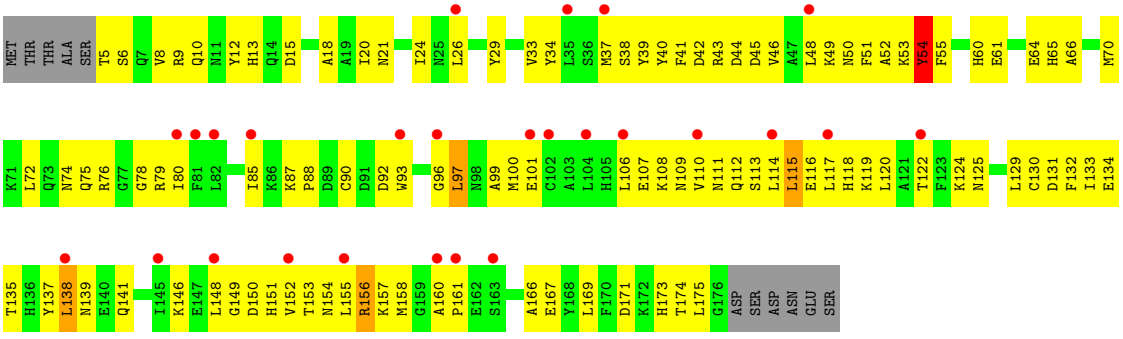
• Molecule 1: Ferritin heavy chain

Chain L:



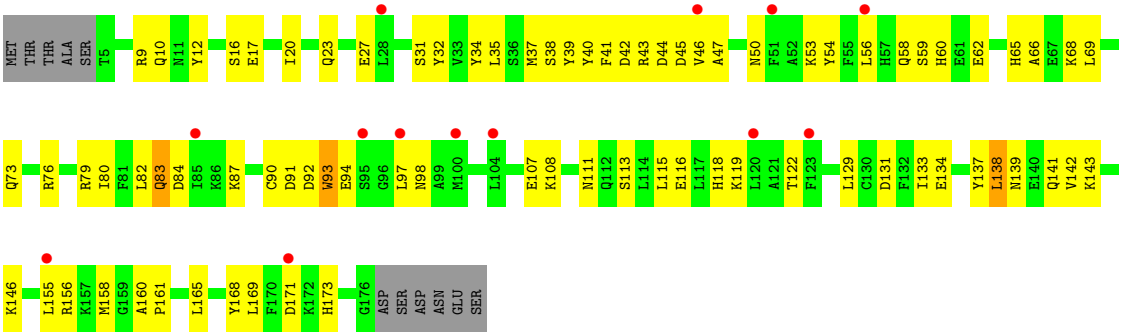
• Molecule 1: Ferritin heavy chain

Chain M:



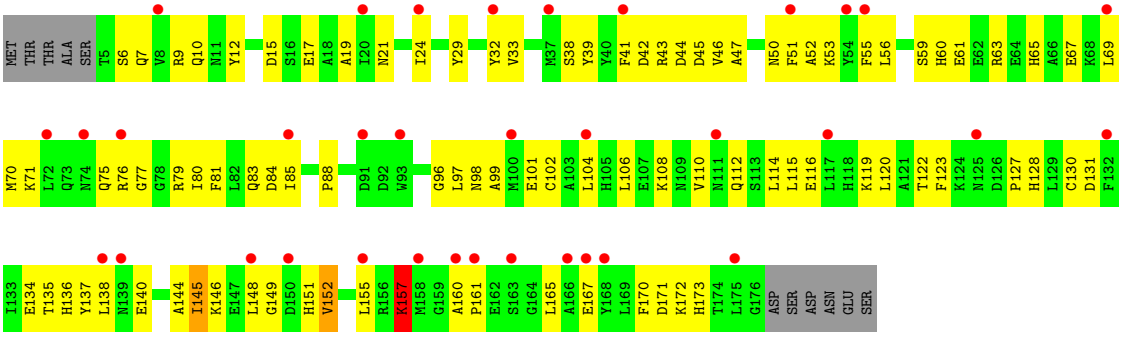
• Molecule 1: Ferritin heavy chain

Chain N:



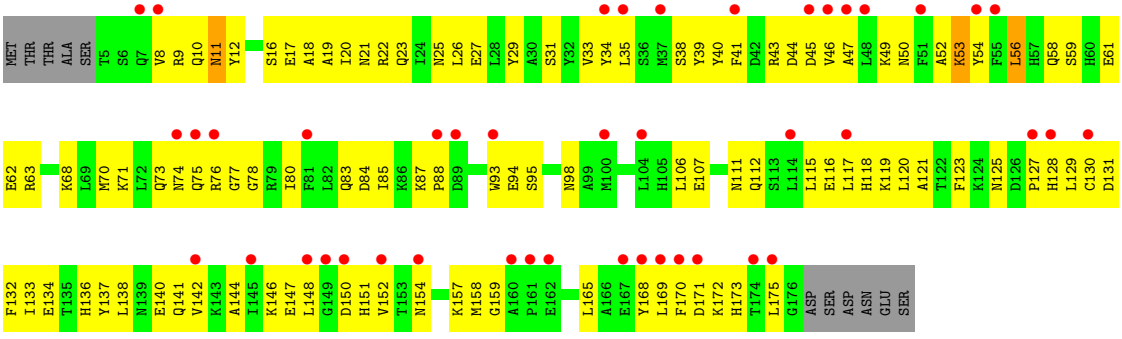
• Molecule 1: Ferritin heavy chain

Chain O:



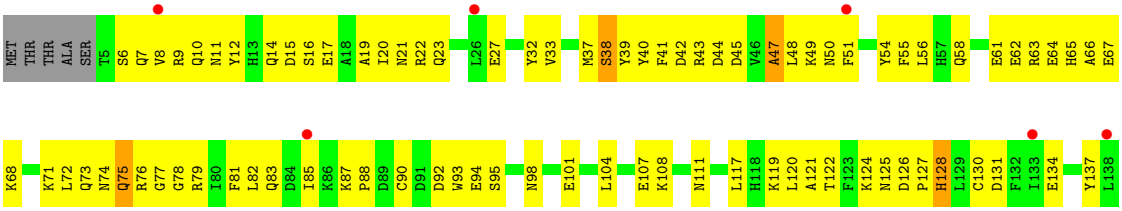
• Molecule 1: Ferritin heavy chain

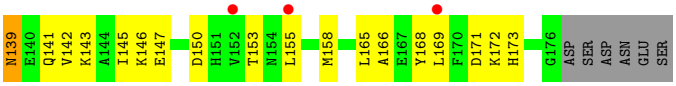
Chain P:



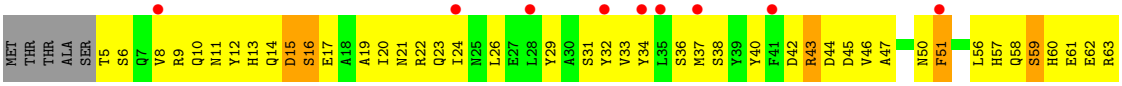
• Molecule 1: Ferritin heavy chain

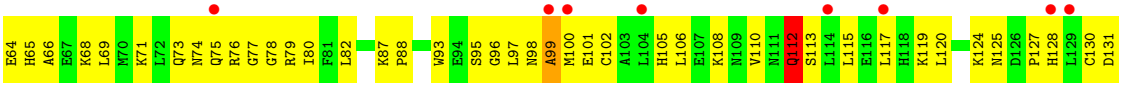
Chain Q:

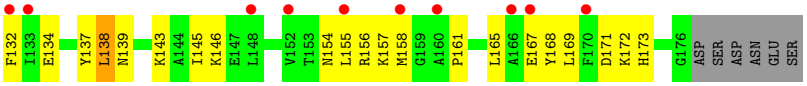




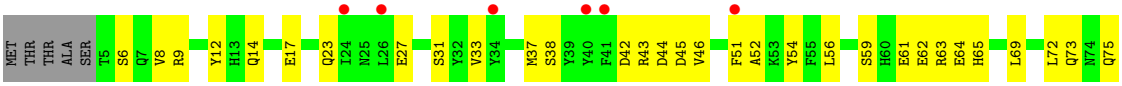
• Molecule 1: Ferritin heavy chain

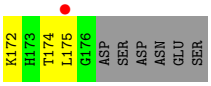




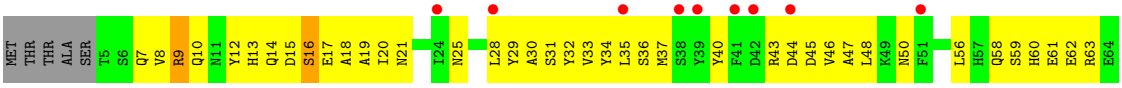


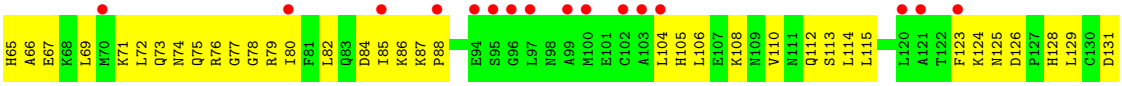
• Molecule 1: Ferritin heavy chain

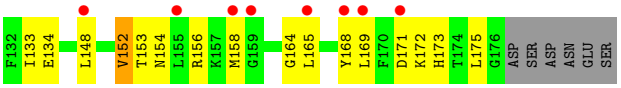




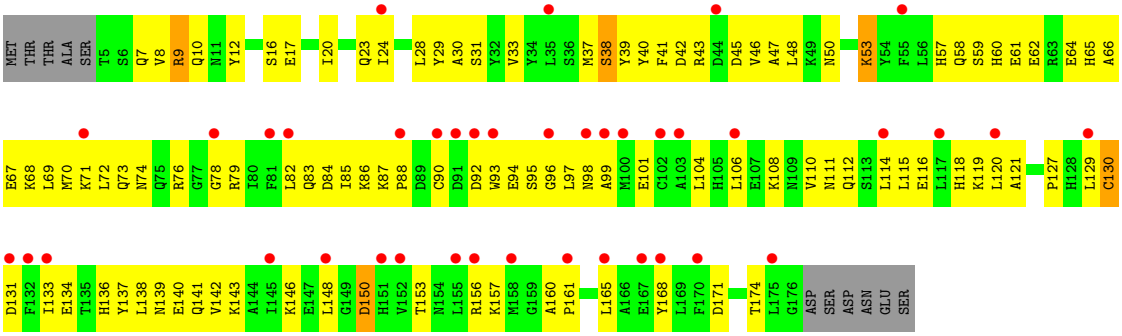
• Molecule 1: Ferritin heavy chain





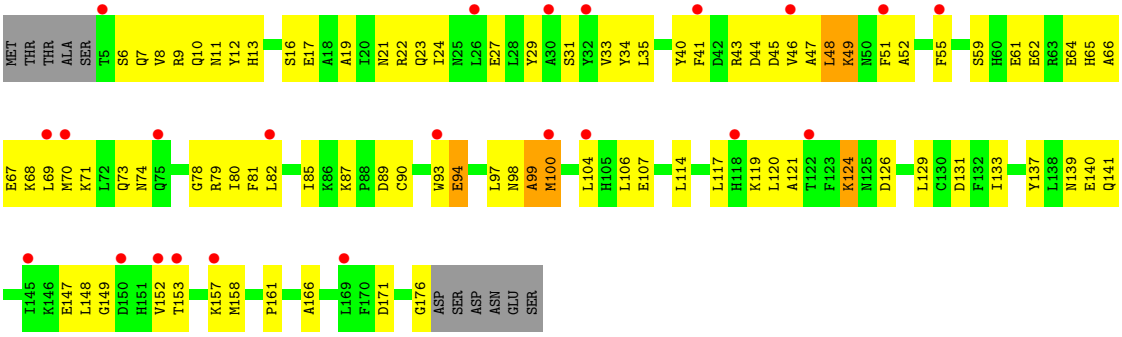


• Molecule 1: Ferritin heavy chain



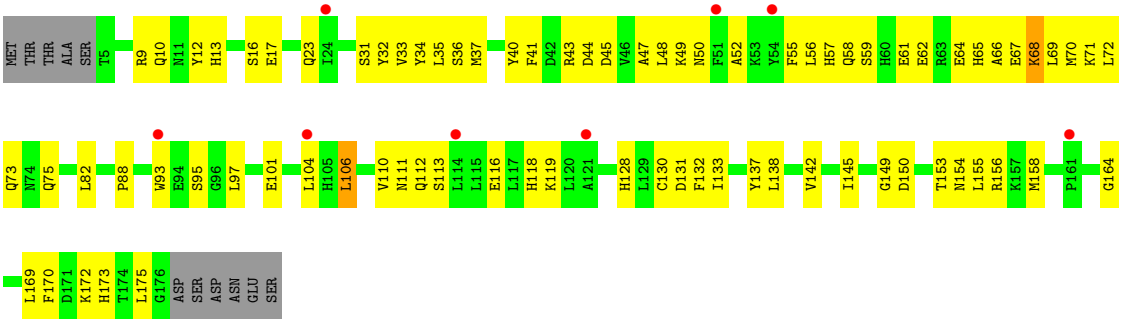
• Molecule 1: Ferritin heavy chain

Chain V:



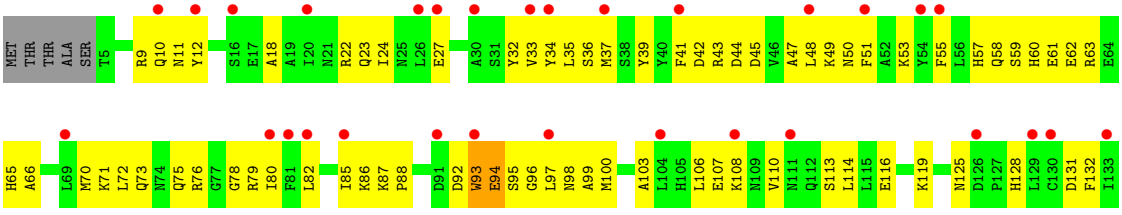
• Molecule 1: Ferritin heavy chain

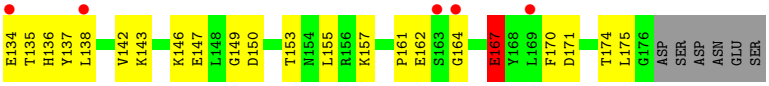
Chain W:



• Molecule 1: Ferritin heavy chain

Chain X:




E134
T135
H136
Y137
L138
V142
K143
K146
E147
L148
G149
D150
T153
N154
L155
R156
K157
P161
E162
S163
G164
E167
Y168
L169
F170
D171
T174
L175
G176
ASP
SER
ASP
ASN
GLU
SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.08 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.335 , 0.368 0.335 , 0.368	Depositor DCC
R_{free} test set	11628 reflections (5.03%)	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)	0.29 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.089 for -l,-k,-h 0.095 for -h,l,k	Xtriage
F_o,F_c correlation	0.81	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.55	0/1446	0.69	2/1947 (0.1%)
1	B	0.62	2/1446 (0.1%)	0.69	1/1947 (0.1%)
1	C	0.55	0/1446	0.67	0/1947
1	D	0.69	4/1446 (0.3%)	0.71	2/1947 (0.1%)
1	E	0.53	0/1446	0.66	0/1947
1	F	0.55	0/1446	0.70	1/1947 (0.1%)
1	G	0.52	0/1446	0.72	2/1947 (0.1%)
1	H	0.57	1/1446 (0.1%)	0.74	1/1947 (0.1%)
1	I	0.76	2/1446 (0.1%)	0.78	6/1947 (0.3%)
1	J	0.54	0/1446	0.68	1/1947 (0.1%)
1	K	0.50	0/1446	0.67	1/1947 (0.1%)
1	L	0.61	1/1446 (0.1%)	0.72	0/1947
1	M	0.69	3/1446 (0.2%)	0.87	7/1947 (0.4%)
1	N	0.60	1/1446 (0.1%)	0.68	2/1947 (0.1%)
1	O	0.60	2/1443 (0.1%)	0.67	0/1944
1	P	0.54	1/1446 (0.1%)	0.64	1/1947 (0.1%)
1	Q	0.55	0/1446	0.70	2/1947 (0.1%)
1	R	0.65	1/1446 (0.1%)	0.76	2/1947 (0.1%)
1	S	0.58	0/1446	0.72	2/1947 (0.1%)
1	T	0.55	0/1446	0.68	2/1947 (0.1%)
1	U	0.53	0/1446	0.75	3/1947 (0.2%)
1	V	0.63	1/1446 (0.1%)	0.73	1/1947 (0.1%)
1	W	0.65	1/1446 (0.1%)	0.67	0/1947
1	X	0.62	2/1446 (0.1%)	0.67	2/1947 (0.1%)
All	All	0.59	22/34701 (0.1%)	0.71	41/46725 (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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	79	ARG	NE-CZ	14.76	1.52	1.33
1	I	79	ARG	CZ-NH1	12.61	1.49	1.33
1	W	68	LYS	CE-NZ	12.52	1.80	1.49
1	X	167	GLU	CB-CG	10.26	1.71	1.52
1	R	112	GLN	CG-CD	9.96	1.74	1.51
1	D	17	GLU	CB-CG	9.44	1.70	1.52
1	M	54	TYR	CG-CD2	8.79	1.50	1.39
1	X	167	GLU	CD-OE2	8.09	1.34	1.25
1	O	157	LYS	CE-NZ	7.58	1.68	1.49
1	V	147	GLU	CB-CG	7.53	1.66	1.52
1	M	156	ARG	CG-CD	6.61	1.68	1.51
1	P	53	LYS	CE-NZ	6.36	1.65	1.49
1	L	79	ARG	CB-CG	-6.32	1.35	1.52
1	D	17	GLU	CG-CD	-5.95	1.43	1.51
1	B	53	LYS	CE-NZ	5.79	1.63	1.49
1	D	17	GLU	CD-OE2	5.78	1.32	1.25
1	O	167	GLU	CB-CG	5.47	1.62	1.52
1	N	83	GLN	CD-NE2	5.35	1.46	1.32
1	D	71	LYS	CD-CE	5.34	1.64	1.51
1	H	87	LYS	CD-CE	5.22	1.64	1.51
1	B	53	LYS	CD-CE	5.18	1.64	1.51
1	M	156	ARG	CZ-NH1	5.04	1.39	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	79	ARG	CG-CD-NE	12.76	138.60	111.80
1	M	156	ARG	NE-CZ-NH2	11.37	125.98	120.30
1	U	53	LYS	CD-CE-NZ	10.29	135.36	111.70
1	I	79	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	S	79	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	U	150	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	M	54	TYR	CD1-CG-CD2	-7.07	110.12	117.90
1	H	87	LYS	CD-CE-NZ	-7.04	95.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	54	TYR	CB-CG-CD1	6.78	125.06	121.00
1	M	97	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	N	83	GLN	CA-CB-CG	6.34	127.34	113.40
1	K	115	LEU	CB-CG-CD2	-6.33	100.24	111.00
1	V	119	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	G	69	LEU	CB-CG-CD2	-6.06	100.70	111.00
1	I	79	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	I	79	ARG	CD-NE-CZ	-5.99	115.21	123.60
1	S	114	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	17	GLU	OE1-CD-OE2	5.97	130.46	123.30
1	X	167	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	J	28	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	G	73	GLN	O-C-N	-5.87	113.31	122.70
1	M	115	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	A	104	LEU	CB-CG-CD2	-5.86	101.04	111.00
1	I	79	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	T	72	LEU	CB-CG-CD2	5.80	120.87	111.00
1	A	87	LYS	CD-CE-NZ	-5.75	98.47	111.70
1	M	156	ARG	CA-CB-CG	5.70	125.95	113.40
1	T	165	LEU	CA-CB-CG	5.64	128.28	115.30
1	Q	139	ASN	CB-CA-C	5.60	121.61	110.40
1	U	150	ASP	OD1-CG-OD2	5.53	133.80	123.30
1	R	156	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	Q	155	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	R	15	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	48	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	M	54	TYR	CG-CD1-CE1	5.24	125.49	121.30
1	X	167	GLU	CG-CD-OE1	-5.22	107.86	118.30
1	N	138	LEU	CA-CB-CG	-5.21	103.31	115.30
1	I	28	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	71	LYS	N-CA-CB	-5.18	101.27	110.60
1	P	56	LEU	CB-CG-CD2	5.13	119.73	111.00
1	F	43	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	74	0
1	B	1416	0	1362	78	0
1	C	1416	0	1362	98	0
1	D	1416	0	1362	120	0
1	E	1416	0	1362	63	0
1	F	1416	0	1362	109	0
1	G	1416	0	1362	100	0
1	H	1416	0	1362	93	0
1	I	1416	0	1362	87	0
1	J	1416	0	1362	103	0
1	K	1416	0	1362	86	0
1	L	1416	0	1362	75	0
1	M	1416	0	1362	112	1
1	N	1416	0	1362	83	0
1	O	1413	0	1355	98	1
1	P	1416	0	1361	108	0
1	Q	1416	0	1362	106	0
1	R	1416	0	1362	111	0
1	S	1416	0	1362	59	0
1	T	1416	0	1362	96	0
1	U	1416	0	1362	98	0
1	V	1416	0	1362	87	0
1	W	1416	0	1362	69	0
1	X	1416	0	1362	114	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1919	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 29.

All (1919) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:174:THR:HG1	1:I:168:TYR:HH	1.32	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:OD1	1:O:128:HIS:NE2	2.26	0.67
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:F:146:LYS:HZ3	1:J:74:ASN:HB3	1.60	0.67
1:U:38:SER:OG	1:U:39:TYR:N	2.28	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:A:145:ILE:HG13	1:A:146:LYS:N	2.10	0.67
1:W:64:GLU:HG2	1:W:68:LYS:NZ	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:156:ARG:HA	1:M:160:ALA:HB3	1.78	0.66
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:E:174:THR:HG1	1:N:168:TYR:HH	1.43	0.66
1:X:9:ARG:NH1	1:X:12:TYR:O	2.28	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: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: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:R:37:MET:CE	1:R:99:ALA:HB1	2.26	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:D:168:TYR:OH	1:M:174:THR:OG1	2.07	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
1:E:131:ASP:OD2	1:E:135:THR:OG1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:35:LEU:HD21	1:V:70:MET:HE1	1.80	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:T:33:VAL:O	1:T:36:SER:OG	2.12	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: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
1:F:10:GLN:NE2	1:U:108:LYS:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:28:LEU:O	1:U:31:SER:OG	2.14	0.63
1:V:40:TYR:OH	1:V:94:GLU:O	2.16	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:128:HIS:CE1	1:X:142:VAL:HG21	2.35	0.62
1:F:7:GLN:O	1:U:108:LYS:NZ	2.26	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: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:B:63:ARG:HH12	1:Q:63:ARG:HD2	1.65	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:M:155:LEU:C	1:M:157:LYS:H	2.01	0.61
1:G:128:HIS:ND1	1:G:129:LEU:HD12	2.15	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:101:GLU:OE2	1:D:156:ARG:NH2	2.33	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:W:64:GLU:HG2	1:W:68:LYS:HZ2	1.66	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:23:GLN:OE1	1:W:113:SER:OG	2.19	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:S:27:GLU:CD	1:S:65:HIS:HB3	2.22	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
1:U:139:ASN:O	1:U:143:LYS:NZ	2.35	0.59
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:R:168:TYR:HH	1:S:174:THR:HG1	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:98:ASN:HA	1:K:101:GLU:CD	2.23	0.59
1:T:29:TYR:OH	1:T:86:LYS:NZ	2.25	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: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: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:67:GLU:HA	1:B:70:MET:HE3	1.86	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:R:37:MET:HE3	1:R:99:ALA:HB1	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:T:76:ARG:C	1:T:78:GLY:H	2.07	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:F:67:GLU:HA	1:F:70:MET:HE2	1.86	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:54:TYR:HH	1:L:147:GLU:CD	2.07	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:D:170:PHE:C	1:D:172:LYS:H	2.08	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:D:169:LEU:O	1:K:168:TYR:OH	2.20	0.56
1:E:73:GLN:HG3	1:E:80:ILE:HG12	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:X:27:GLU:HB2	1:X:66:ALA:HB2	1.86	0.56
1:A:72:LEU:HA	1:A:75:GLN:CD	2.24	0.56
1:D:5:THR:OG1	1:D:6:SER:N	2.37	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:M:15:ASP:HB3	1:M:120:LEU:HD21	1.86	0.56
1:Q:146:LYS:HZ2	1:X:44:ASP:N	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:LYS:HZ2	1:D:57:HIS:HB2	1.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:146:LYS:HZ1	1:V:74:ASN:C	2.10	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:J:36:SER:HG	1:J:93:TRP:HE1	1.52	0.55
1:M:5:THR:OG1	1:M:6:SER:N	2.40	0.55
1:N:31:SER:O	1:N:59:SER:OG	2.20	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:68:LYS:HD2	1:U:68:LYS:N	2.21	0.55
1:H:67:GLU:HA	1:H:70:MET:HE3	1.89	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:Q:65:HIS:O	1:Q:137:TYR:OH	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:S:72:LEU:C	1:S:72:LEU:HD23	2.28	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:10:GLN:HE22	1:U:108:LYS:C	2.10	0.54
1:F:21:ASN:HB2	1:F:22:ARG:NH1	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:66:ALA:O	1:U:70:MET:HG3	2.08	0.54
1:B:50:ASN:HB2	1:B:171:ASP:CG	2.28	0.54
1:D:158:MET:CE	1:D:169:LEU:HB2	2.38	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:T:61:GLU:C	1:T:65:HIS:HD1	2.11	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: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: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:V:31:SER:O	1:V:59:SER:OG	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:M:155:LEU:C	1:M:157:LYS:N	2.61	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:174:THR:OG1	1:N:168:TYR:OH	2.20	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:D:71:LYS:HD2	1:D:71:LYS:C	2.30	0.52
1:L:40:TYR:OH	1:L:94:GLU:O	2.21	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:23:GLN:NE2	1:R:26:LEU:HB3	2.25	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: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:N:34:TYR:HD1	1:N:37:MET:HE2	1.74	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: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:N:92:ASP:C	1:N:94:GLU:H	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:153:THR:OG1	1:M:44:ASP:O	2.27	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:D:158:MET:HE1	1:D:169:LEU:HB2	1.91	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: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:B:67:GLU:HA	1:B:70:MET:CE	2.41	0.51
1:D:79:ARG:NH1	1:V:43:ARG:HG2	2.25	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
1:X:44:ASP:N	1:X:44:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:128:HIS:O	1:R:132:PHE:HB2	2.11	0.50
1:U:53:LYS:CD	1:U:53:LYS:C	2.75	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: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: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:W:35:LEU:C	1:W:37:MET:H	2.14	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:93:TRP:O	1:F:95:SER:N	2.42	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H:9:ARG:HH21	1:H:12:TYR:C	2.15	0.49
1:I:162:GLU:H	1:I:162:GLU:CD	2.15	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:77:GLY:O	1:R:79:ARG:NH1	2.46	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:H:71:LYS:HG3	1:H:75:GLN:HE21	1.77	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
1:G:101:GLU:OE1	1:G:156:ARG:NH2	2.46	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:G:21:ASN:CG	1:G:73:GLN:HE22	2.16	0.48
1:G:107:GLU:OE2	1:G:144:ALA:HB1	2.13	0.48
1:K:161:PRO:C	1:K:163:SER:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:P:34:TYR:CE1	1:P:58:GLN:HG3	2.49	0.48
1:W:64:GLU:O	1:W:68:LYS:HG3	2.13	0.48
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:T:35:LEU:C	1:T:37:MET:H	2.15	0.48
1:T:76:ARG:HH22	1:T:126:ASP:CG	2.15	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: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:W:43:ARG:HH21	1:W:45:ASP:CG	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:64:GLU:O	1:S:65:HIS:C	2.52	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:I:145:ILE:HG22	1:T:8:VAL:HG12	1.96	0.48
1:R:172:LYS:HD3	1:R:172:LYS:HA	1.61	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
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:155:LEU:HA	1:F:158:MET:HE3	1.95	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:134:GLU:HB3	1:W:131:ASP:CG	2.33	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:O	1:Q:38:SER:OG	2.31	0.48
1:Q:73:GLN:HG3	1:Q:78:GLY:O	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:34:TYR:OH	1:I:107:GLU:OE2	2.32	0.47
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:N:40:TYR:C	1:N:42:ASP:H	2.16	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:Q:71:LYS:O	1:Q:75:GLN:N	2.38	0.47
1:S:56:LEU:O	1:S:59:SER:HB3	2.14	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:I:48:LEU:HD23	1:I:48:LEU:HA	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:HB3	1:N:146:LYS:HD2	1.95	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: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
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:O:44:ASP:OD1	1:O:44:ASP:C	2.52	0.47
1:R:137:TYR:O	1:R:138:LEU:C	2.52	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:173:HIS:HB3	1:P:172:LYS:HG2	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:CZ	1:D:51:PHE:HD2	2.33	0.46
1:E:64:GLU:OE2	1:E:68:LYS:HE2	2.15	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:115:LEU:HB3	1:P:119:LYS:HZ3	1.78	0.46
1:P:131:ASP:HA	1:P:134:GLU:OE1	2.15	0.46
1:R:5:THR:OG1	1:R:6:SER:N	2.47	0.46
1:R:168:TYR:OH	1:S:174:THR:OG1	2.25	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: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:86:LYS:HD3	1:N:84:ASP:CG	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:66:ALA:O	1:J:69:LEU:HB2	2.15	0.46
1:K:6:SER:OG	1:K:7:GLN:N	2.47	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:78:GLY:C	1:U:79:ARG:HD3	2.35	0.46
1:U:90:CYS:HB3	1:U:92:ASP:O	2.16	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:F:33:VAL:C	1:F:35:LEU:H	2.19	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:U:114:LEU:HD13	1:U:137:TYR:HB3	1.98	0.46
1:B:50:ASN:HB2	1:B:171:ASP:OD2	2.15	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: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
1:T:105:HIS:HA	1:T:108:LYS:HZ3	1.80	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: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: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:T:13:HIS:CG	1:T:14:GLN:H	2.34	0.46
1:A:43:ARG:NH2	1:A:45:ASP:OD2	2.49	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:V:153:THR:HG21	1:W:45:ASP:C	2.37	0.46
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: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:J:58:GLN:CD	1:J:58:GLN:N	2.69	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: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:S:38:SER:OG	1:S:52:ALA:O	2.16	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:44:ASP:OD1	1:D:44:ASP:N	2.50	0.45
1:D:156:ARG:O	1:D:159:GLY:N	2.43	0.45
1:F:60:HIS:CD2	1:T:63:ARG:HH21	2.34	0.45
1:F:68:LYS:HZ3	1:F:136:HIS:CE1	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:M:154:ASN:O	1:M:157:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:24:ILE:HG21	1:X:70:MET:HE3	1.99	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:158:MET:HE2	1:B:166:ALA:HA	1.97	0.45
1:C:61:GLU:HG3	1:C:62:GLU:OE1	2.16	0.45
1:F:43:ARG:HG2	1:T:74:ASN:CG	2.36	0.45
1:F:66:ALA:O	1:F:70:MET:HE2	2.16	0.45
1:L:79:ARG:HD3	1:L:79:ARG:HA	1.49	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:70:MET:HB3	1:W:70:MET:HE2	1.66	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: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:G:63:ARG:HH22	1:U:59:SER:HG	1.57	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:X:50:ASN:HB2	1:X:171:ASP:CG	2.36	0.45
1:A:145:ILE:HG13	1:A:146:LYS:H	1.81	0.45
1:G:36:SER:HB2	1:U:82:LEU:HD12	1.98	0.45
1:J:117:LEU:O	1:J:118:HIS:C	2.55	0.45
1:K:16:SER:O	1:K:20:ILE:HG13	2.16	0.45
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:I:93:TRP:HZ3	1:I:102:CYS:SG	2.40	0.45
1:J:41:PHE:CD2	1:J:48:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:131:ASP:HA	1:O:134:GLU:CD	2.37	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: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: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:139:ASN:O	1:N:143:LYS:HG3	2.17	0.45
1:A:72:LEU:HD11	1:A:128:HIS:NE2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:50:ASN:HB2	1:L:171:ASP:CG	2.37	0.44
1:M:132:PHE:HD2	1:M:133:ILE:HD13	1.82	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:165:LEU:HD12	1:K:158:MET:HG2	1.97	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: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:J:158:MET:HE1	1:J:170:PHE:HB2	1.99	0.44
1:K:67:GLU:C	1:K:69:LEU:H	2.18	0.44
1:Q:62:GLU:OE2	1:Q:65:HIS:ND1	2.51	0.44
1:R:98:ASN:HA	1:R:101:GLU:CD	2.37	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:D:47:ALA:O	1:D:48:LEU:HD22	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:62:GLU:CD	1:V:141:GLN:HE21	2.20	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: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
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:P:134:GLU:HB3	1:X:131:ASP:CG	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:G:50:ASN:HB2	1:G:171:ASP:CG	2.39	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:VAL:HG22	1:I:88:PRO:HB3	1.99	0.43
1:I:48:LEU:HD22	1:I:171:ASP:CG	2.38	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:G:76:ARG:HH12	1:G:126:ASP:CG	2.19	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
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:L:123:PHE:C	1:L:125:ASN:H	2.22	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:U:67:GLU:C	1:U:68:LYS:HD2	2.39	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: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: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: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:M:134:GLU:HB3	1:V:131:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:ASN:HB2	1:Q:171:ASP:CG	2.38	0.43
1:Q:124:LYS:HA	1:Q:124:LYS:HD3	1.54	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
1:N:39:TYR:HA	1:N:42:ASP:HB2	2.00	0.43
1:T:13:HIS:CG	1:T:14:GLN:N	2.86	0.43
1:V:106:LEU:HD22	1:V:107:GLU:HG2	2.01	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:G:131:ASP:HB2	1:R:134:GLU:CD	2.39	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: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: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:42:ASP:OD1	1:T:71:LYS:NZ	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:18:ALA:O	1:T:19:ALA:C	2.56	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: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:H:87:LYS:HD2	1:H:87:LYS:C	2.39	0.42
1:J:87:LYS:HB3	1:O:83:GLN:C	2.39	0.42
1:J:102:CYS:O	1:J:106:LEU:N	2.43	0.42
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:T:76:ARG:C	1:T:78:GLY:N	2.73	0.42
1:V:66:ALA:O	1:V:70:MET:N	2.50	0.42
1:A:76:ARG:C	1:A:78:GLY:H	2.23	0.42
1:B:41:PHE:HB2	1:B:52:ALA:HB2	2.01	0.42
1:C:153:THR:HG21	1:J:45:ASP:C	2.40	0.42
1:D:170:PHE:C	1:D:172:LYS:N	2.73	0.42
1:G:136:HIS:HB2	1:G:137:TYR:CD1	2.54	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:123:PHE:C	1:T:125:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:107:GLU:HA	1:L:110:VAL:HB	2.00	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: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: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: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
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: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: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: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:A:70:MET:HB2	1:A:70:MET:HE3	1.90	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:S:44:ASP:N	1:S:44:ASP:OD1	2.53	0.42
1:V:73:GLN:HG3	1:V:78:GLY:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:GLN:C	1:G:144:ALA:H	2.23	0.42
1:G:168:TYR:O	1:G:171:ASP:N	2.48	0.42
1:H:23:GLN:O	1:H:24:ILE:C	2.58	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: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
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: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: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: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:G:141:GLN:O	1:G:145:ILE:N	2.47	0.41
1:H:45:ASP:CG	1:R:79:ARG:HH21	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:C	1:B:174:THR:H	2.23	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:N:40:TYR:C	1:N:42:ASP:N	2.74	0.41
1:Q:27:GLU:HB3	1:Q:66:ALA:HB2	2.01	0.41
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:W:50:ASN:HB3	1:W:175:LEU:HB2	2.02	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:173:HIS:CD2	1:P:173:HIS:NE2	2.89	0.41
1:J:93:TRP:O	1:J:94:GLU:HB2	2.20	0.41
1:L:107:GLU:O	1:L:111:ASN:N	2.30	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:V:10:GLN:C	1:V:12:TYR:N	2.73	0.41
1:E:32:TYR:CE2	1:E:87:LYS:HA	2.55	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: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:84:ASP:CG	1:X:86:LYS:HG2	2.41	0.41
1:C:111:ASN:HB3	1:O:10:GLN:NE2	2.36	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: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:X:37:MET:HE1	1:X:103:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:ASN:O	1:J:54:TYR:HB2	2.21	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:21:ASN:CG	1:K:81:PHE:H	2.24	0.41
1:K:160:ALA:HB1	1:K:161:PRO:HA	2.03	0.41
1:L:79:ARG:C	1:L:80:ILE:HG13	2.41	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:R:57:HIS:O	1:R:58:GLN:C	2.59	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:115:LEU:HD13	1:N:115:LEU:HA	1.91	0.41
1:P:44:ASP:C	1:P:46:VAL:H	2.25	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:16:SER:C	1:T:20:ILE:HG12	2.38	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:23:GLN:HE22	1:U:110:VAL:HG13	1.85	0.41
1:W:111:ASN:O	1:W:112:GLN:C	2.58	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:M:148:LEU:C	1:M:151:HIS:H	2.23	0.41
1:O:21:ASN:ND2	1:O:81:PHE:H	2.18	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: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:P:150:ASP:C	1:P:152:VAL:H	2.24	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:F:5:THR:HA	1:F:79:ARG:NH2	2.35	0.40
1:F:62:GLU:O	1:F:65:HIS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:Q:47:ALA:HA	1:Q:49:LYS:HZ2	1.85	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:B:114:LEU:C	1:B:116:GLU:N	2.74	0.40
1:C:82:LEU:HD12	1:X:36:SER:HB2	2.02	0.40
1:C:131:ASP:HA	1:C:134:GLU:CD	2.41	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: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:H:24:ILE:HG22	1:H:28:LEU:HD12	2.03	0.40
1:I:79:ARG:NE	1:N:43:ARG:CZ	2.84	0.40
1:P:76:ARG:HD2	1:P:76:ARG:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	8 10
1	B	170/183 (93%)	149 (88%)	18 (11%)	3 (2%)	8 10
1	C	170/183 (93%)	148 (87%)	20 (12%)	2 (1%)	13 17
1	D	170/183 (93%)	144 (85%)	24 (14%)	2 (1%)	13 17
1	E	170/183 (93%)	154 (91%)	13 (8%)	3 (2%)	8 10
1	F	170/183 (93%)	144 (85%)	22 (13%)	4 (2%)	6 6
1	G	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	6 6
1	H	170/183 (93%)	144 (85%)	17 (10%)	9 (5%)	2 1
1	I	170/183 (93%)	145 (85%)	18 (11%)	7 (4%)	3 2
1	J	170/183 (93%)	145 (85%)	21 (12%)	4 (2%)	6 6
1	K	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	13 17
1	L	170/183 (93%)	148 (87%)	18 (11%)	4 (2%)	6 6
1	M	170/183 (93%)	153 (90%)	15 (9%)	2 (1%)	13 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	170/183 (93%)	153 (90%)	14 (8%)	3 (2%)	8 10
1	O	170/183 (93%)	146 (86%)	21 (12%)	3 (2%)	8 10
1	P	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	6 6
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%)	25 33
1	T	170/183 (93%)	139 (82%)	27 (16%)	4 (2%)	6 6
1	U	170/183 (93%)	143 (84%)	22 (13%)	5 (3%)	4 4
1	V	170/183 (93%)	135 (79%)	30 (18%)	5 (3%)	4 4
1	W	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	13 17
1	X	170/183 (93%)	144 (85%)	23 (14%)	3 (2%)	8 10
All	All	4080/4392 (93%)	3473 (85%)	514 (13%)	93 (2%)	6 6

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
1	J	52	ALA
1	J	118	HIS
1	L	31	SER

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Mol	Chain	Res	Type
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
1	R	43	ARG
1	R	59	SER
1	V	48	LEU

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Mol	Chain	Res	Type
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 (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	84	90
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%)	152 (99%)	1 (1%)	84	90
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%)	152 (99%)	1 (1%)	84	90
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%)	153 (100%)	0	100	100
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%)	3668 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	LYS
1	M	54	TYR
1	R	51	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	50	ASN
1	B	112	GLN
1	C	73	GLN
1	C	98	ASN
1	D	7	GLN
1	D	23	GLN
1	D	65	HIS
1	D	98	ASN
1	D	139	ASN
1	D	141	GLN
1	F	11	ASN
1	F	73	GLN
1	F	105	HIS
1	F	111	ASN
1	G	73	GLN
1	G	118	HIS
1	H	57	HIS
1	H	105	HIS
1	H	173	HIS
1	I	11	ASN
1	I	125	ASN
1	J	10	GLN
1	J	111	ASN
1	K	14	GLN
1	K	21	ASN
1	K	50	ASN
1	K	173	HIS
1	L	111	ASN
1	L	125	ASN
1	M	10	GLN
1	M	112	GLN
1	N	23	GLN
1	N	58	GLN
1	O	21	ASN
1	O	173	HIS
1	P	10	GLN
1	P	125	ASN
1	Q	10	GLN
1	Q	73	GLN
1	Q	74	ASN
1	R	128	HIS
1	R	154	ASN

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Mol	Chain	Res	Type
1	S	57	HIS
1	S	109	ASN
1	T	23	GLN
1	T	118	HIS
1	V	74	ASN
1	V	98	ASN
1	V	139	ASN
1	W	23	GLN
1	W	105	HIS
1	W	109	ASN
1	X	60	HIS
1	X	73	GLN
1	X	136	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.73	13 (7%) 13 18	26, 49, 65, 73	0
1	B	172/183 (93%)	0.59	5 (2%) 51 61	21, 41, 59, 75	0
1	C	172/183 (93%)	1.25	34 (19%) 1 1	41, 60, 77, 90	0
1	D	172/183 (93%)	1.25	36 (20%) 1 1	43, 61, 73, 83	0
1	E	172/183 (93%)	0.60	8 (4%) 31 40	28, 51, 68, 80	0
1	F	172/183 (93%)	1.35	40 (23%) 0 0	42, 61, 73, 83	0
1	G	172/183 (93%)	1.35	45 (26%) 0 0	46, 61, 77, 94	0
1	H	172/183 (93%)	0.91	21 (12%) 4 6	28, 55, 70, 84	0
1	I	172/183 (93%)	0.82	15 (8%) 10 14	29, 55, 71, 78	0
1	J	172/183 (93%)	1.19	40 (23%) 0 0	40, 56, 72, 83	0
1	K	172/183 (93%)	1.12	33 (19%) 1 1	44, 60, 73, 90	0
1	L	172/183 (93%)	0.52	6 (3%) 44 53	26, 40, 60, 72	0
1	M	172/183 (93%)	1.00	26 (15%) 2 3	31, 53, 71, 81	0
1	N	172/183 (93%)	0.66	13 (7%) 13 18	27, 43, 63, 80	0
1	O	172/183 (93%)	1.12	35 (20%) 1 1	38, 59, 72, 84	0
1	P	172/183 (93%)	1.37	44 (25%) 0 0	43, 59, 75, 92	0
1	Q	172/183 (93%)	0.69	9 (5%) 27 34	26, 48, 66, 81	0
1	R	172/183 (93%)	1.04	27 (15%) 2 3	39, 58, 72, 89	0
1	S	172/183 (93%)	0.68	17 (9%) 7 10	24, 48, 65, 78	0
1	T	172/183 (93%)	1.15	33 (19%) 1 1	44, 57, 73, 85	0
1	U	172/183 (93%)	1.29	40 (23%) 0 0	43, 57, 72, 94	0
1	V	172/183 (93%)	1.05	23 (13%) 3 4	40, 57, 71, 82	0
1	W	172/183 (93%)	0.63	8 (4%) 31 40	27, 42, 61, 82	0
1	X	172/183 (93%)	1.08	35 (20%) 1 1	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%)	0.98	606 (14%) 2 3	21, 55, 72, 94	0

All (606) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	129	LEU	8.2
1	D	24	ILE	7.8
1	G	165	LEU	7.8
1	D	99	ALA	7.6
1	U	99	ALA	7.5
1	K	169	LEU	7.1
1	U	100	MET	6.9
1	F	96	GLY	6.8
1	V	152	VAL	6.5
1	P	81	PHE	6.3
1	G	169	LEU	6.2
1	S	165	LEU	6.2
1	G	104	LEU	6.1
1	T	155	LEU	6.1
1	G	30	ALA	6.0
1	I	169	LEU	6.0
1	X	129	LEU	6.0
1	U	103	ALA	5.8
1	P	148	LEU	5.7
1	K	158	MET	5.7
1	F	104	LEU	5.7
1	P	41	PHE	5.7
1	R	170	PHE	5.6
1	V	104	LEU	5.6
1	D	133	ILE	5.6
1	P	8	VAL	5.5
1	D	100	MET	5.5
1	U	35	LEU	5.4
1	X	30	ALA	5.4
1	C	132	PHE	5.3
1	O	163	SER	5.3
1	R	166	ALA	5.3
1	K	96	GLY	5.2
1	H	96	GLY	5.1
1	F	54	TYR	5.1
1	T	104	LEU	5.1
1	T	158	MET	5.1

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Mol	Chain	Res	Type	RSRZ
1	T	100	MET	5.0
1	H	165	LEU	5.0
1	M	152	VAL	5.0
1	D	56	LEU	4.9
1	U	93	TRP	4.9
1	F	8	VAL	4.9
1	P	169	LEU	4.8
1	U	114	LEU	4.8
1	P	88	PRO	4.8
1	G	157	LYS	4.8
1	U	88	PRO	4.8
1	T	85	ILE	4.7
1	F	72	LEU	4.7
1	F	46	VAL	4.7
1	G	154	ASN	4.7
1	U	165	LEU	4.6
1	P	93	TRP	4.6
1	C	161	PRO	4.6
1	P	161	PRO	4.6
1	R	51	PHE	4.6
1	T	99	ALA	4.6
1	C	158	MET	4.5
1	O	85	ILE	4.5
1	U	102	CYS	4.5
1	R	34	TYR	4.5
1	C	70	MET	4.5
1	O	93	TRP	4.4
1	C	96	GLY	4.4
1	F	97	LEU	4.4
1	T	35	LEU	4.4
1	U	91	ASP	4.3
1	O	167	GLU	4.3
1	U	167	GLU	4.3
1	J	169	LEU	4.3
1	T	39	TYR	4.3
1	T	97	LEU	4.2
1	O	117	LEU	4.2
1	Q	152	VAL	4.2
1	J	32	TYR	4.2
1	G	90	CYS	4.2
1	H	97	LEU	4.2
1	J	100	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	67	GLU	4.2
1	P	127	PRO	4.2
1	G	81	PHE	4.2
1	F	37	MET	4.2
1	K	70	MET	4.2
1	C	35	LEU	4.1
1	U	24	ILE	4.1
1	C	133	ILE	4.1
1	U	148	LEU	4.1
1	J	70	MET	4.1
1	C	148	LEU	4.0
1	S	169	LEU	4.0
1	P	55	PHE	4.0
1	R	167	GLU	4.0
1	U	155	LEU	4.0
1	T	169	LEU	4.0
1	G	112	GLN	4.0
1	D	138	LEU	3.9
1	V	145	ILE	3.9
1	I	100	MET	3.9
1	C	168	TYR	3.9
1	I	104	LEU	3.9
1	K	52	ALA	3.9
1	T	102	CYS	3.9
1	F	127	PRO	3.9
1	G	8	VAL	3.9
1	W	51	PHE	3.8
1	U	145	ILE	3.8
1	E	8	VAL	3.8
1	D	69	LEU	3.8
1	J	158	MET	3.8
1	C	24	ILE	3.8
1	X	97	LEU	3.8
1	F	20	ILE	3.8
1	P	47	ALA	3.8
1	K	55	PHE	3.8
1	K	80	ILE	3.8
1	O	160	ALA	3.8
1	A	133	ILE	3.7
1	G	15	ASP	3.7
1	S	166	ALA	3.7
1	O	76	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	167	GLU	3.7
1	O	100	MET	3.7
1	G	16	SER	3.7
1	S	175	LEU	3.7
1	M	148	LEU	3.6
1	M	155	LEU	3.6
1	X	26	LEU	3.6
1	K	54	TYR	3.6
1	R	133	ILE	3.6
1	F	138	LEU	3.6
1	C	51	PHE	3.6
1	J	155	LEU	3.6
1	R	104	LEU	3.6
1	P	75	GLN	3.6
1	G	155	LEU	3.5
1	K	155	LEU	3.5
1	F	41	PHE	3.5
1	V	93	TRP	3.5
1	J	96	GLY	3.5
1	R	117	LEU	3.5
1	U	151	HIS	3.5
1	W	161	PRO	3.5
1	G	96	GLY	3.5
1	T	96	GLY	3.5
1	G	54	TYR	3.5
1	H	41	PHE	3.5
1	C	91	ASP	3.5
1	E	152	VAL	3.5
1	H	132	PHE	3.5
1	Q	51	PHE	3.5
1	C	167	GLU	3.5
1	G	99	ALA	3.5
1	X	34	TYR	3.4
1	M	48	LEU	3.4
1	N	104	LEU	3.4
1	D	51	PHE	3.4
1	H	51	PHE	3.4
1	K	89	ASP	3.4
1	O	8	VAL	3.4
1	G	170	PHE	3.4
1	F	19	ALA	3.4
1	E	120	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	158	MET	3.4
1	V	150	ASP	3.4
1	G	133	ILE	3.4
1	D	137	TYR	3.4
1	I	117	LEU	3.4
1	D	163	SER	3.4
1	S	158	MET	3.4
1	V	46	VAL	3.4
1	D	170	PHE	3.4
1	C	38	SER	3.4
1	J	28	LEU	3.3
1	J	129	LEU	3.3
1	J	63	ARG	3.3
1	P	48	LEU	3.3
1	S	168	TYR	3.3
1	J	152	VAL	3.3
1	U	129	LEU	3.3
1	H	100	MET	3.3
1	P	149	GLY	3.3
1	S	41	PHE	3.3
1	S	96	GLY	3.3
1	J	35	LEU	3.3
1	J	133	ILE	3.3
1	V	51	PHE	3.3
1	R	155	LEU	3.2
1	T	165	LEU	3.2
1	X	138	LEU	3.2
1	H	170	PHE	3.2
1	P	170	PHE	3.2
1	T	38	SER	3.2
1	T	95	SER	3.2
1	X	20	ILE	3.2
1	G	88	PRO	3.2
1	F	55	PHE	3.2
1	X	51	PHE	3.2
1	C	98	ASN	3.2
1	J	54	TYR	3.2
1	F	85	ILE	3.2
1	O	20	ILE	3.2
1	C	155	LEU	3.2
1	F	160	ALA	3.2
1	C	105	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	159	GLY	3.2
1	C	103	ALA	3.1
1	K	148	LEU	3.2
1	K	165	LEU	3.2
1	P	167	GLU	3.1
1	U	161	PRO	3.1
1	P	34	TYR	3.1
1	P	54	TYR	3.1
1	U	96	GLY	3.1
1	P	128	HIS	3.1
1	P	117	LEU	3.1
1	D	35	LEU	3.1
1	M	93	TRP	3.1
1	X	12	TYR	3.1
1	O	55	PHE	3.1
1	M	138	LEU	3.1
1	W	114	LEU	3.1
1	J	41	PHE	3.1
1	V	41	PHE	3.1
1	J	157	LYS	3.1
1	D	132	PHE	3.1
1	I	133	ILE	3.1
1	J	51	PHE	3.1
1	O	161	PRO	3.1
1	T	70	MET	3.1
1	X	133	ILE	3.0
1	M	104	LEU	3.0
1	H	164	GLY	3.0
1	O	138	LEU	3.0
1	T	148	LEU	3.0
1	U	117	LEU	3.0
1	P	152	VAL	3.0
1	U	170	PHE	3.0
1	O	74	ASN	3.0
1	G	168	TYR	3.0
1	J	95	SER	3.0
1	V	30	ALA	3.0
1	B	100	MET	3.0
1	B	48	LEU	3.0
1	O	166	ALA	3.0
1	R	114	LEU	3.0
1	G	123	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	32	TYR	3.0
1	G	72	LEU	3.0
1	S	155	LEU	3.0
1	C	102	CYS	2.9
1	O	148	LEU	2.9
1	U	158	MET	2.9
1	S	24	ILE	2.9
1	F	35	LEU	2.9
1	P	160	ALA	2.9
1	K	97	LEU	2.9
1	H	54	TYR	2.9
1	O	132	PHE	2.9
1	R	152	VAL	2.9
1	X	81	PHE	2.9
1	T	88	PRO	2.9
1	K	5	THR	2.9
1	O	155	LEU	2.9
1	Q	155	LEU	2.9
1	X	33	VAL	2.8
1	D	145	ILE	2.8
1	U	81	PHE	2.8
1	U	133	ILE	2.8
1	G	105	HIS	2.8
1	F	31	SER	2.8
1	P	37	MET	2.8
1	T	159	GLY	2.8
1	G	51	PHE	2.8
1	D	102	CYS	2.8
1	V	55	PHE	2.8
1	M	122	THR	2.8
1	U	71	LYS	2.8
1	U	82	LEU	2.8
1	U	175	LEU	2.8
1	L	114	LEU	2.8
1	X	104	LEU	2.8
1	H	90	CYS	2.8
1	M	102	CYS	2.8
1	A	41	PHE	2.8
1	V	69	LEU	2.8
1	G	95	SER	2.8
1	D	161	PRO	2.8
1	S	34	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	V	75	GLN	2.8
1	J	132	PHE	2.8
1	Q	85	ILE	2.8
1	O	175	LEU	2.8
1	U	120	LEU	2.8
1	H	93	TRP	2.7
1	A	55	PHE	2.7
1	R	24	ILE	2.7
1	U	132	PHE	2.7
1	O	104	LEU	2.7
1	P	175	LEU	2.7
1	X	69	LEU	2.7
1	O	125	ASN	2.7
1	G	55	PHE	2.7
1	G	66	ALA	2.7
1	I	51	PHE	2.7
1	J	80	ILE	2.7
1	M	106	LEU	2.7
1	A	155	LEU	2.7
1	Q	138	LEU	2.7
1	X	16	SER	2.7
1	P	162	GLU	2.7
1	M	35	LEU	2.7
1	O	72	LEU	2.7
1	R	35	LEU	2.7
1	V	100	MET	2.7
1	D	148	LEU	2.7
1	T	28	LEU	2.7
1	F	137	TYR	2.7
1	U	152	VAL	2.7
1	C	107	GLU	2.7
1	C	120	LEU	2.7
1	F	117	LEU	2.7
1	F	156	ARG	2.7
1	X	111	ASN	2.7
1	H	150	ASP	2.7
1	T	120	LEU	2.6
1	M	161	PRO	2.6
1	K	63	ARG	2.6
1	C	110	VAL	2.6
1	T	103	ALA	2.6
1	A	114	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	106	LEU	2.6
1	P	35	LEU	2.6
1	I	81	PHE	2.6
1	P	145	ILE	2.6
1	R	129	LEU	2.6
1	R	148	LEU	2.6
1	V	169	LEU	2.6
1	D	168	TYR	2.6
1	G	166	ALA	2.6
1	H	33	VAL	2.6
1	P	89	ASP	2.6
1	O	158	MET	2.6
1	C	77	GLY	2.6
1	U	98	ASN	2.6
1	C	28	LEU	2.6
1	G	114	LEU	2.6
1	M	114	LEU	2.6
1	X	48	LEU	2.6
1	P	51	PHE	2.6
1	X	41	PHE	2.6
1	C	175	LEU	2.6
1	D	114	LEU	2.6
1	F	161	PRO	2.6
1	J	114	LEU	2.6
1	G	20	ILE	2.6
1	R	100	MET	2.6
1	K	39	TYR	2.6
1	V	32	TYR	2.6
1	D	130	CYS	2.6
1	R	160	ALA	2.6
1	B	69	LEU	2.6
1	P	168	TYR	2.6
1	X	134	GLU	2.6
1	F	69	LEU	2.5
1	J	165	LEU	2.5
1	P	7	GLN	2.5
1	A	100	MET	2.5
1	U	92	ASP	2.5
1	J	121	ALA	2.5
1	V	122	THR	2.5
1	R	28	LEU	2.5
1	O	41	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	2.5
1	H	34	TYR	2.5
1	L	34	TYR	2.5
1	P	104	LEU	2.5
1	V	70	MET	2.5
1	K	142	VAL	2.5
1	W	104	LEU	2.5
1	F	100	MET	2.5
1	K	37	MET	2.5
1	A	130	CYS	2.5
1	H	167	GLU	2.5
1	C	93	TRP	2.5
1	V	153	THR	2.5
1	M	117	LEU	2.5
1	R	8	VAL	2.5
1	U	78	GLY	2.5
1	K	151	HIS	2.5
1	V	118	HIS	2.5
1	K	85	ILE	2.5
1	R	75	GLN	2.5
1	U	44	ASP	2.5
1	A	152	VAL	2.5
1	O	32	TYR	2.5
1	X	163	SER	2.5
1	G	41	PHE	2.5
1	D	158	MET	2.5
1	N	100	MET	2.5
1	G	134	GLU	2.5
1	X	82	LEU	2.4
1	X	130	CYS	2.4
1	D	55	PHE	2.4
1	X	37	MET	2.4
1	P	154	ASN	2.4
1	C	138	LEU	2.4
1	I	72	LEU	2.4
1	U	55	PHE	2.4
1	M	160	ALA	2.4
1	P	174	THR	2.4
1	S	114	LEU	2.4
1	G	34	TYR	2.4
1	C	123	PHE	2.4
1	I	80	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	10	GLN	2.4
1	F	30	ALA	2.4
1	G	6	SER	2.4
1	S	26	LEU	2.4
1	P	45	ASP	2.4
1	H	152	VAL	2.4
1	T	80	ILE	2.4
1	R	132	PHE	2.4
1	P	46	VAL	2.4
1	F	158	MET	2.4
1	T	24	ILE	2.4
1	G	153	THR	2.4
1	J	130	CYS	2.4
1	F	56	LEU	2.4
1	H	104	LEU	2.4
1	P	114	LEU	2.4
1	X	10	GLN	2.4
1	F	50	ASN	2.4
1	O	54	TYR	2.4
1	I	99	ALA	2.4
1	J	122	THR	2.4
1	D	67	GLU	2.4
1	X	93	TRP	2.4
1	M	82	LEU	2.4
1	O	69	LEU	2.4
1	J	44	ASP	2.3
1	J	99	ALA	2.3
1	K	66	ALA	2.3
1	D	122	THR	2.3
1	V	5	THR	2.3
1	G	33	VAL	2.3
1	U	156	ARG	2.3
1	M	80	ILE	2.3
1	N	85	ILE	2.3
1	M	81	PHE	2.3
1	C	56	LEU	2.3
1	G	97	LEU	2.3
1	V	82	LEU	2.3
1	X	126	ASP	2.3
1	C	90	CYS	2.3
1	K	100	MET	2.3
1	U	90	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	40	TYR	2.3
1	D	77	GLY	2.3
1	I	138	LEU	2.3
1	I	165	LEU	2.3
1	W	93	TRP	2.3
1	F	130	CYS	2.3
1	F	132	PHE	2.3
1	M	96	GLY	2.3
1	X	27	GLU	2.3
1	C	39	TYR	2.3
1	C	73	GLN	2.3
1	U	106	LEU	2.3
1	X	169	LEU	2.3
1	J	8	VAL	2.3
1	B	53	LYS	2.3
1	D	103	ALA	2.3
1	M	163	SER	2.3
1	J	56	LEU	2.3
1	K	88	PRO	2.3
1	N	46	VAL	2.3
1	A	141	GLN	2.3
1	Q	133	ILE	2.3
1	D	66	ALA	2.3
1	N	171	ASP	2.3
1	O	91	ASP	2.3
1	K	128	HIS	2.3
1	N	28	LEU	2.3
1	N	120	LEU	2.3
1	O	168	TYR	2.3
1	X	54	TYR	2.3
1	F	142	VAL	2.2
1	G	152	VAL	2.2
1	P	142	VAL	2.2
1	O	37	MET	2.2
1	N	95	SER	2.2
1	O	150	ASP	2.2
1	K	145	ILE	2.2
1	X	55	PHE	2.2
1	S	97	LEU	2.2
1	J	110	VAL	2.2
1	L	100	MET	2.2
1	T	94	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	24	ILE	2.2
1	X	85	ILE	2.2
1	K	132	PHE	2.2
1	H	48	LEU	2.2
1	J	72	LEU	2.2
1	N	97	LEU	2.2
1	P	74	ASN	2.2
1	G	85	ILE	2.2
1	G	103	ALA	2.2
1	G	5	THR	2.2
1	S	51	PHE	2.2
1	A	165	LEU	2.2
1	F	82	LEU	2.2
1	I	129	LEU	2.2
1	N	56	LEU	2.2
1	O	139	ASN	2.2
1	P	171	ASP	2.2
1	F	103	ALA	2.2
1	I	147	GLU	2.2
1	G	69	LEU	2.2
1	J	69	LEU	2.2
1	J	148	LEU	2.2
1	G	39	TYR	2.2
1	T	168	TYR	2.2
1	K	122	THR	2.2
1	E	51	PHE	2.2
1	K	32	TYR	2.2
1	R	158	MET	2.2
1	J	74	ASN	2.2
1	F	157	LYS	2.1
1	V	157	LYS	2.1
1	O	111	ASN	2.1
1	D	28	LEU	2.1
1	E	165	LEU	2.1
1	K	35	LEU	2.1
1	F	7	GLN	2.1
1	E	105	HIS	2.1
1	D	70	MET	2.1
1	E	76	ARG	2.1
1	L	32	TYR	2.1
1	R	37	MET	2.1
1	G	46	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	51	PHE	2.1
1	T	123	PHE	2.1
1	N	155	LEU	2.1
1	B	99	ALA	2.1
1	F	34	TYR	2.1
1	K	29	TYR	2.1
1	L	39	TYR	2.1
1	M	110	VAL	2.1
1	W	54	TYR	2.1
1	T	41	PHE	2.1
1	J	104	LEU	2.1
1	M	26	LEU	2.1
1	Q	26	LEU	2.1
1	Q	169	LEU	2.1
1	X	108	LYS	2.1
1	F	123	PHE	2.1
1	M	101	GLU	2.1
1	S	104	LEU	2.1
1	T	171	ASP	2.1
1	F	101	GLU	2.1
1	Q	8	VAL	2.1
1	W	121	ALA	2.1
1	H	24	ILE	2.1
1	D	118	HIS	2.1
1	N	123	PHE	2.1
1	P	150	ASP	2.1
1	W	24	ILE	2.1
1	X	80	ILE	2.1
1	P	130	CYS	2.1
1	R	41	PHE	2.1
1	R	128	HIS	2.1
1	V	26	LEU	2.1
1	X	164	GLY	2.1
1	T	121	ALA	2.1
1	H	40	TYR	2.1
1	L	131	ASP	2.1
1	X	91	ASP	2.1
1	D	60	HIS	2.1
1	J	85	ILE	2.1
1	M	85	ILE	2.1
1	F	155	LEU	2.1
1	N	51	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	52	ALA	2.0
1	T	44	ASP	2.0
1	D	142	VAL	2.0
1	G	12	TYR	2.0
1	J	111	ASN	2.0
1	M	37	MET	2.0
1	U	131	ASP	2.0
1	A	12	TYR	2.0
1	A	137	TYR	2.0
1	O	24	ILE	2.0
1	O	51	PHE	2.0
1	P	76	ARG	2.0
1	U	168	TYR	2.0
1	P	100	MET	2.0
1	D	119	LYS	2.0
1	D	121	ALA	2.0
1	K	103	ALA	2.0
1	R	99	ALA	2.0
1	E	169	LEU	2.0
1	M	145	ILE	2.0
1	R	32	TYR	2.0
1	T	42	ASP	2.0
1	J	73	GLN	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 monosaccharides 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, 95^{th} 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.

Continued on next page...

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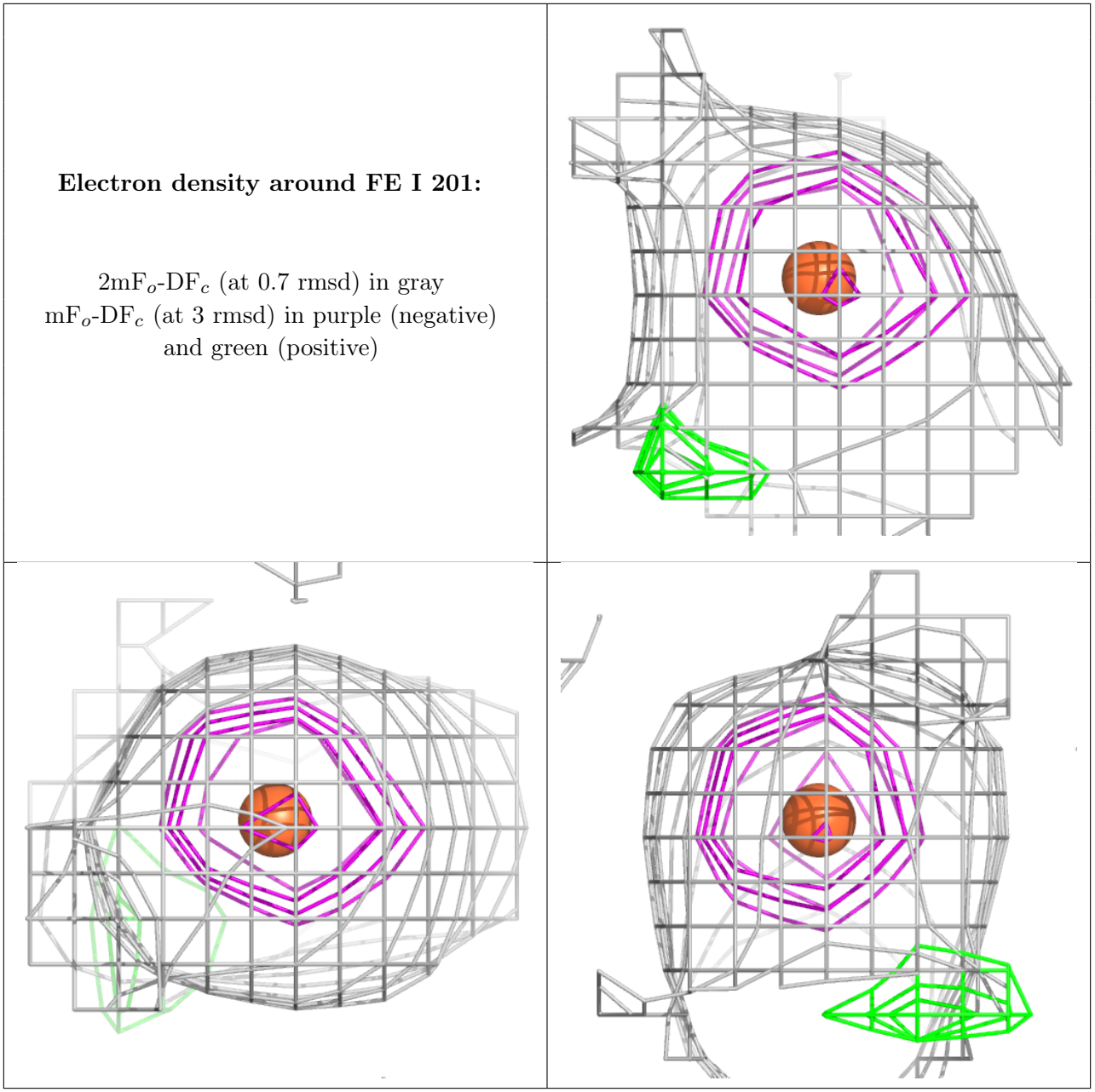
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	I	201	1/1	0.96	0.04	30,30,30,30	0
2	FE	D	201	1/1	0.97	0.07	30,30,30,30	0
2	FE	F	201	1/1	0.97	0.08	30,30,30,30	0
2	FE	G	201	1/1	0.97	0.06	30,30,30,30	0
2	FE	B	201	1/1	0.97	0.06	30,30,30,30	0
2	FE	P	201	1/1	0.97	0.10	30,30,30,30	0
2	FE	P	202	1/1	0.97	0.08	30,30,30,30	0
2	FE	W	201	1/1	0.97	0.04	30,30,30,30	0
2	FE	H	201	1/1	0.98	0.06	30,30,30,30	0
2	FE	B	202	1/1	0.98	0.07	30,30,30,30	0
2	FE	Q	201	1/1	0.98	0.04	30,30,30,30	0
2	FE	S	202	1/1	0.98	0.05	30,30,30,30	0
2	FE	L	201	1/1	0.98	0.09	30,30,30,30	0
2	FE	A	201	1/1	0.99	0.04	30,30,30,30	0
2	FE	E	201	1/1	0.99	0.08	30,30,30,30	0
2	FE	S	201	1/1	0.99	0.02	30,30,30,30	0
2	FE	M	201	1/1	0.99	0.02	30,30,30,30	0
2	FE	E	202	1/1	0.99	0.06	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.

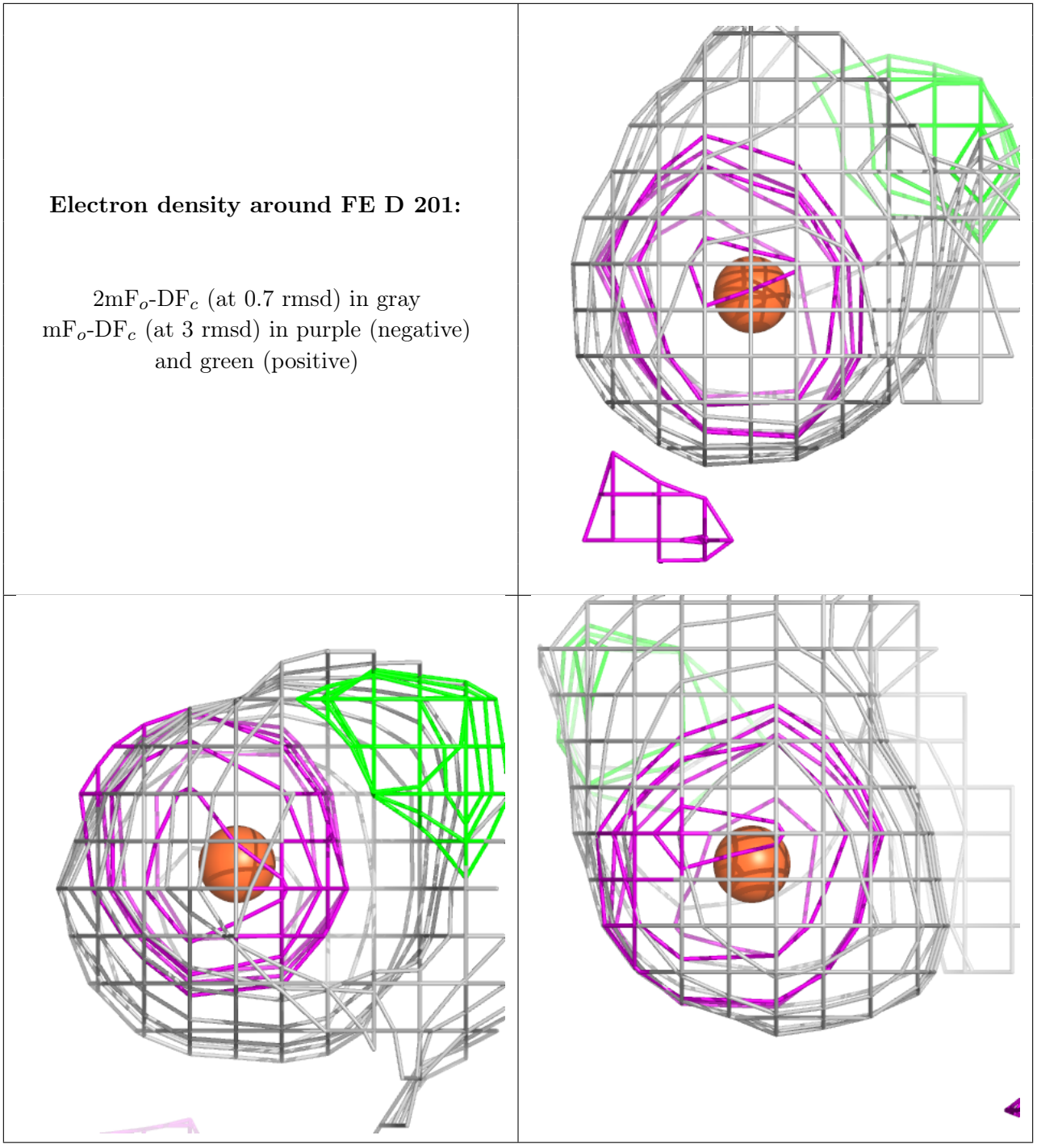
Electron density around FE I 201:

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



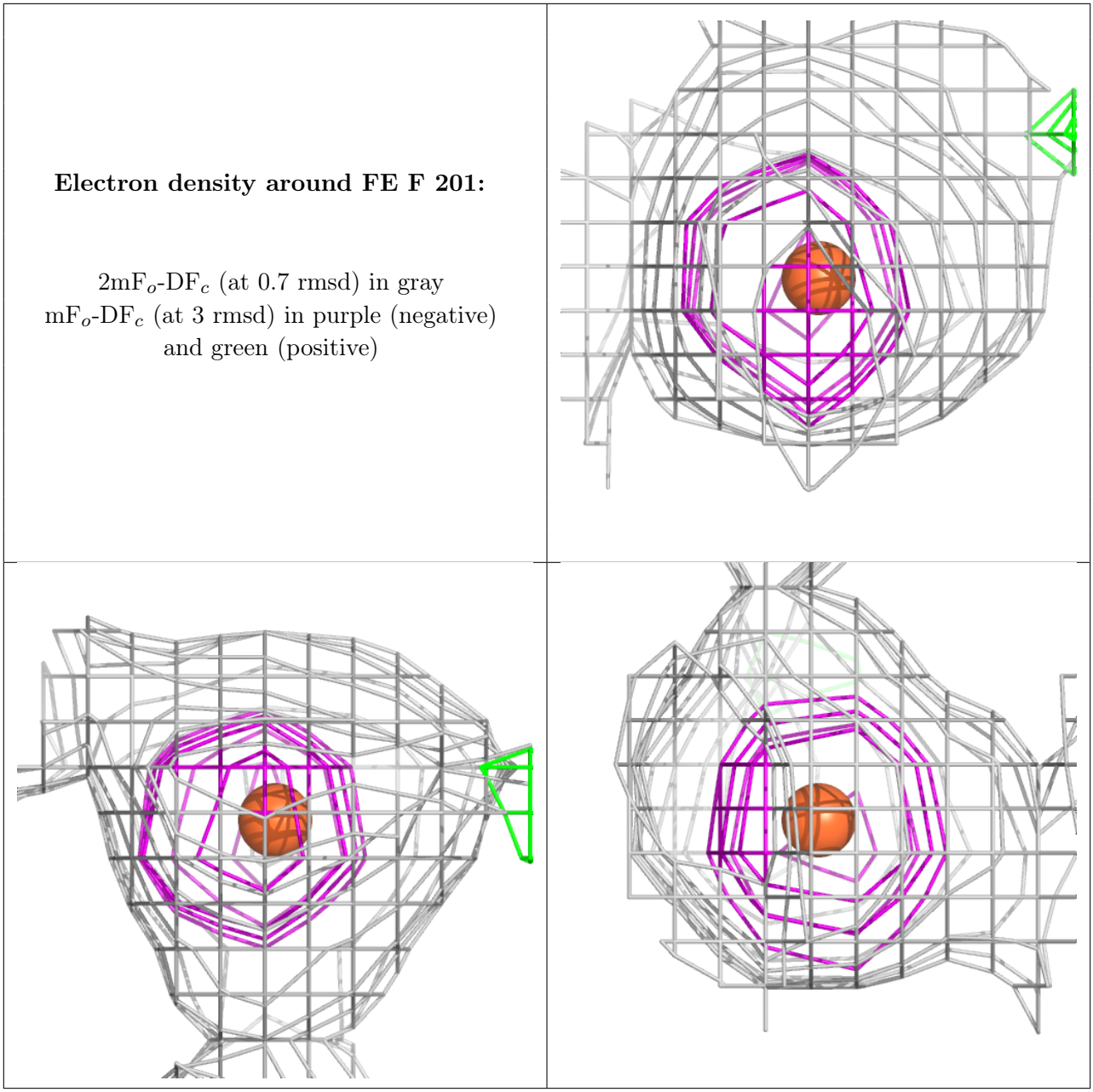
Electron density around FE D 201:

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



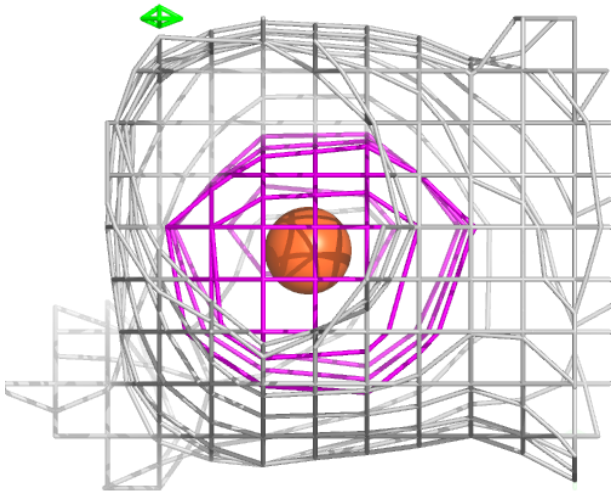
Electron density around FE F 201:

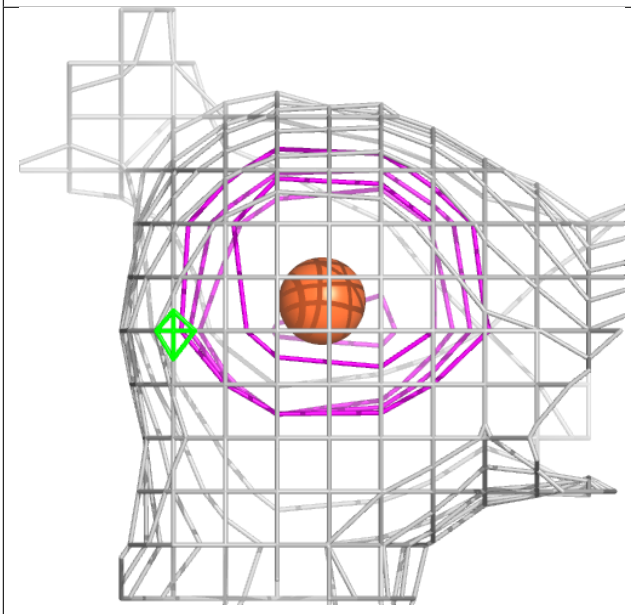
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

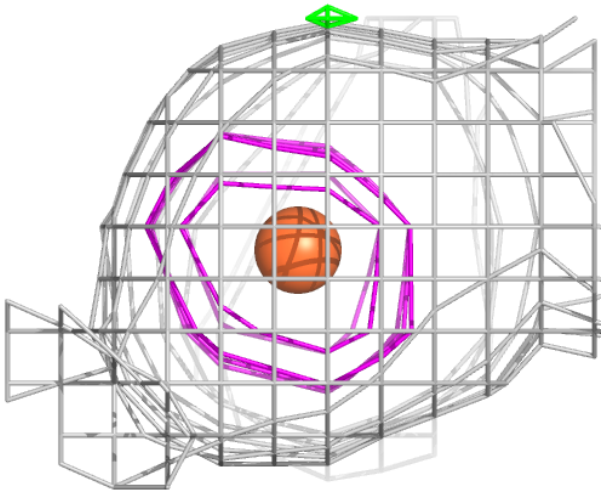


Electron density around FE G 201:

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

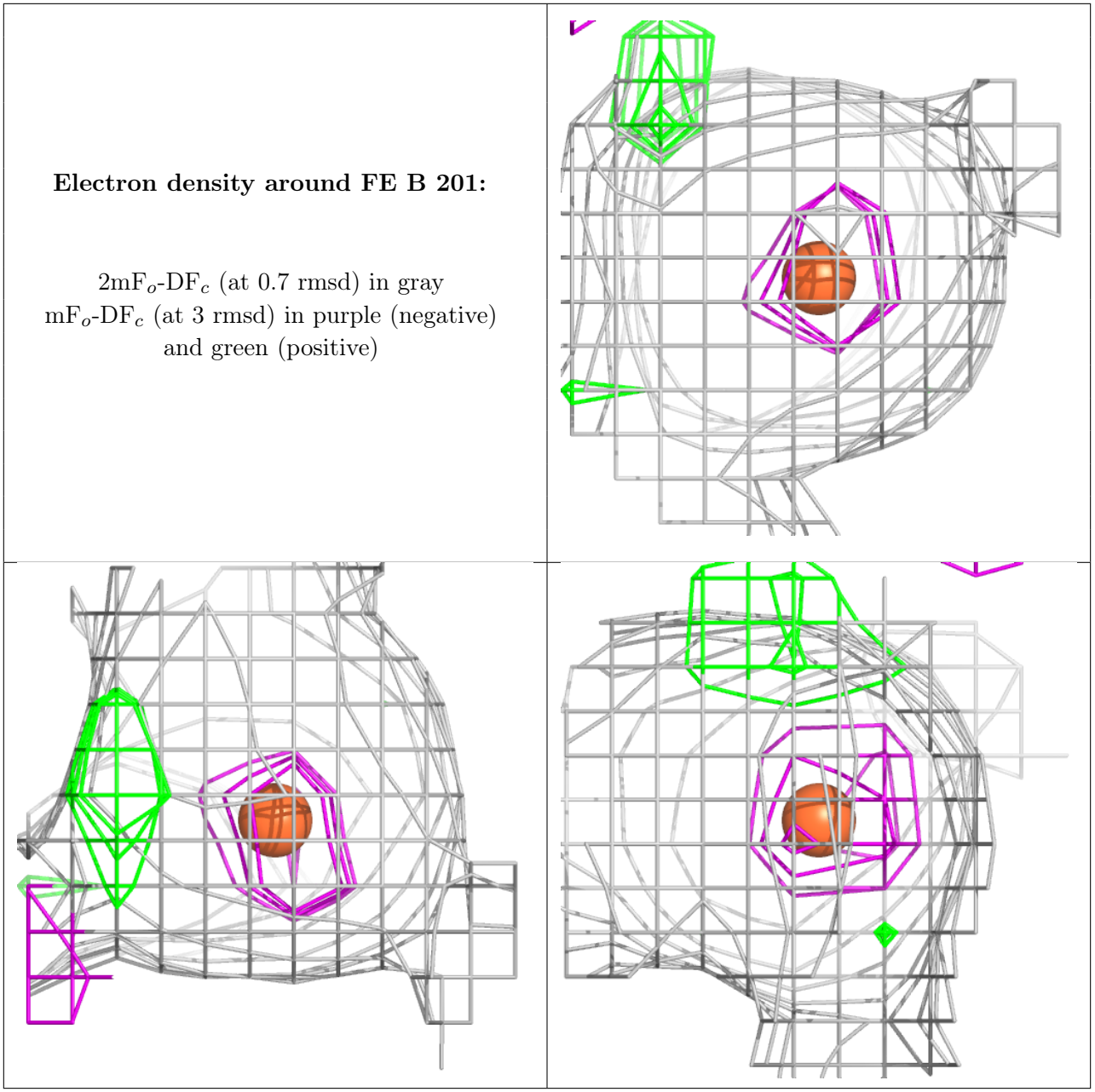






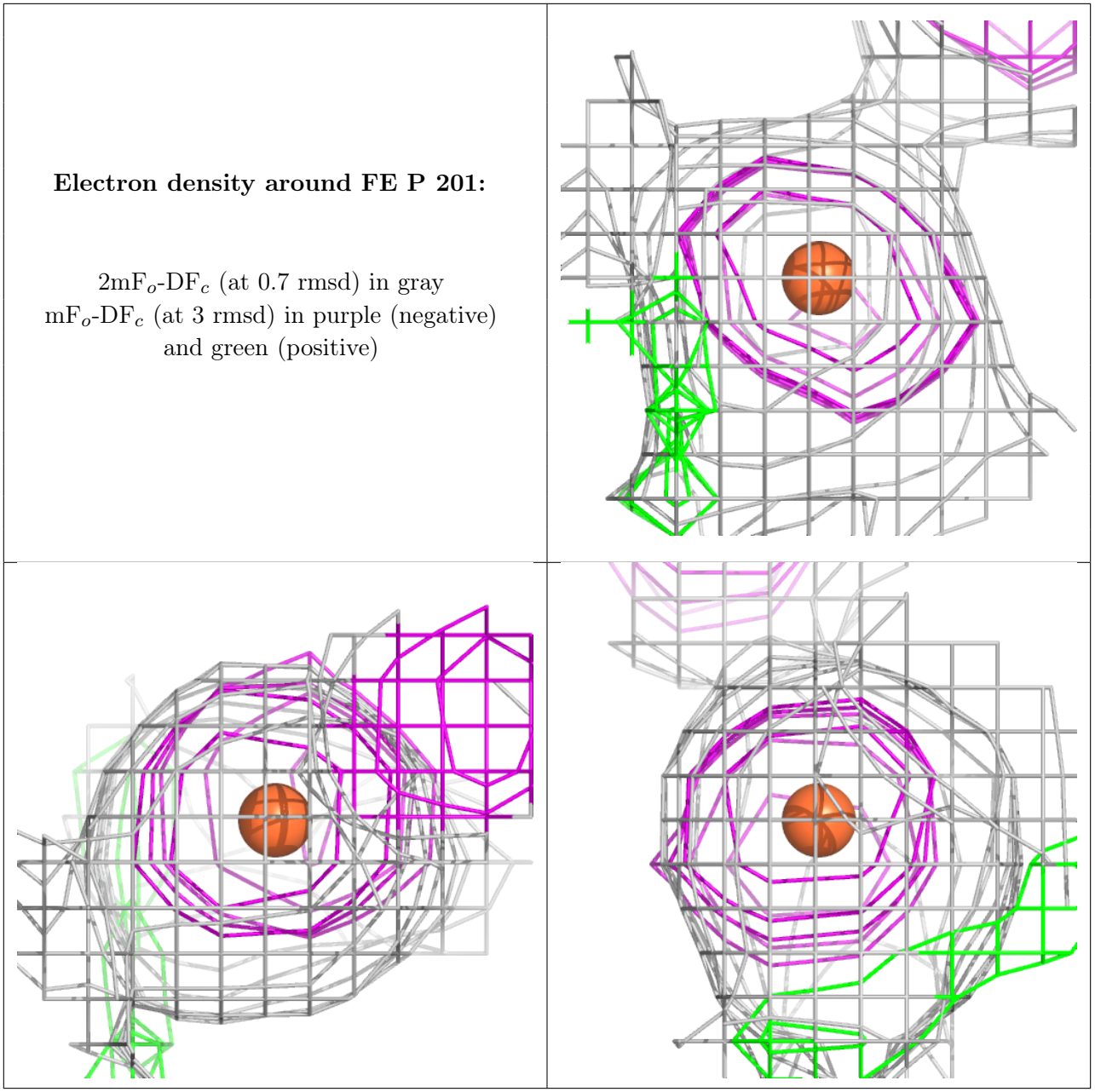
Electron density around FE B 201:

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



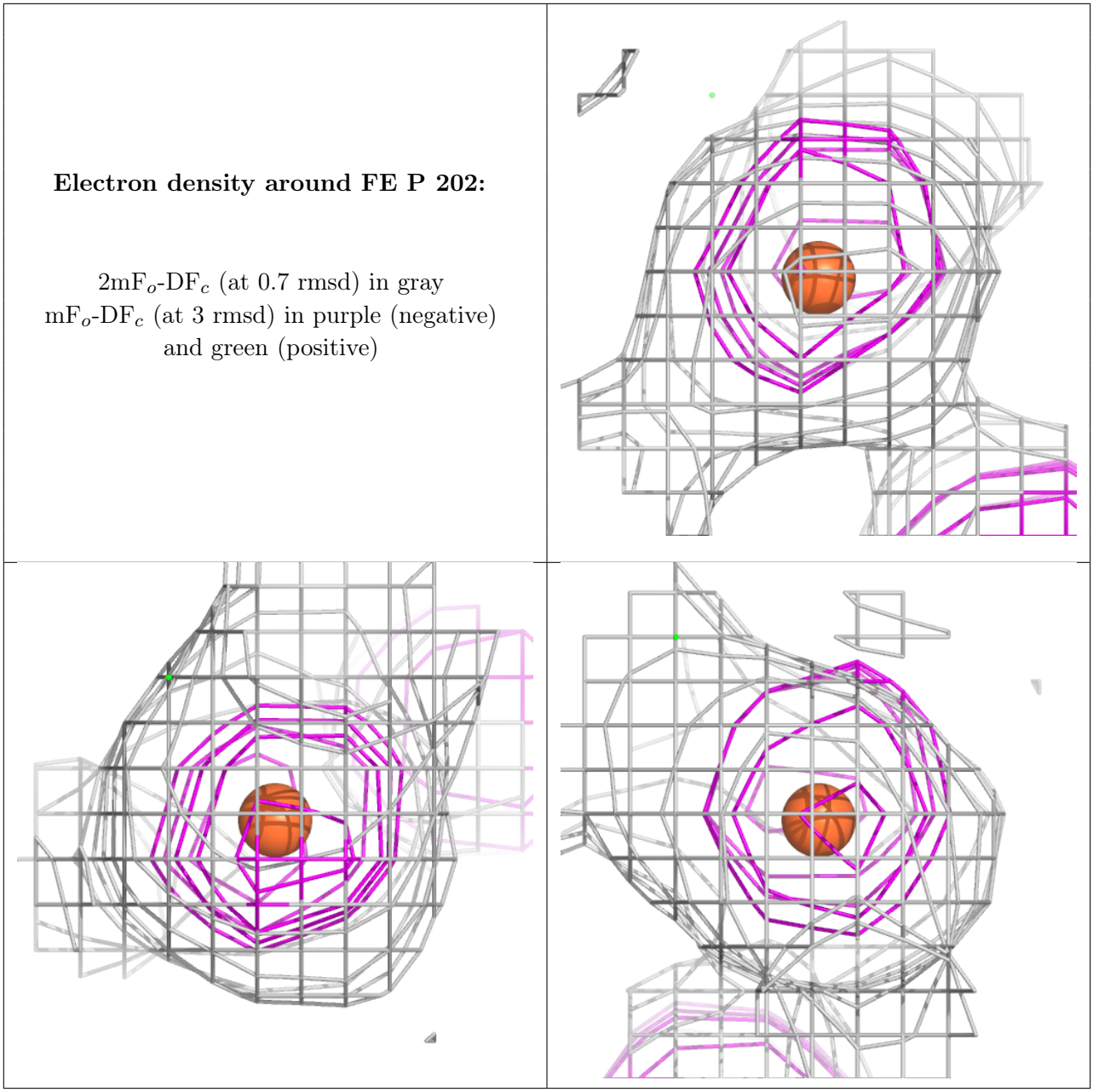
Electron density around FE P 201:

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



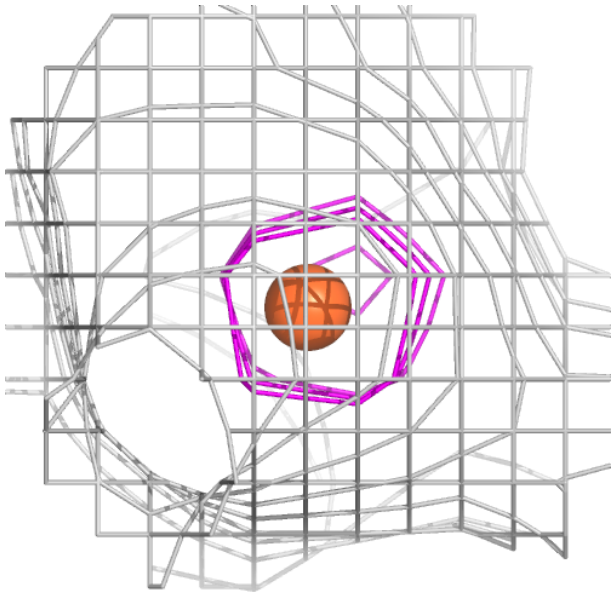
Electron density around FE P 202:

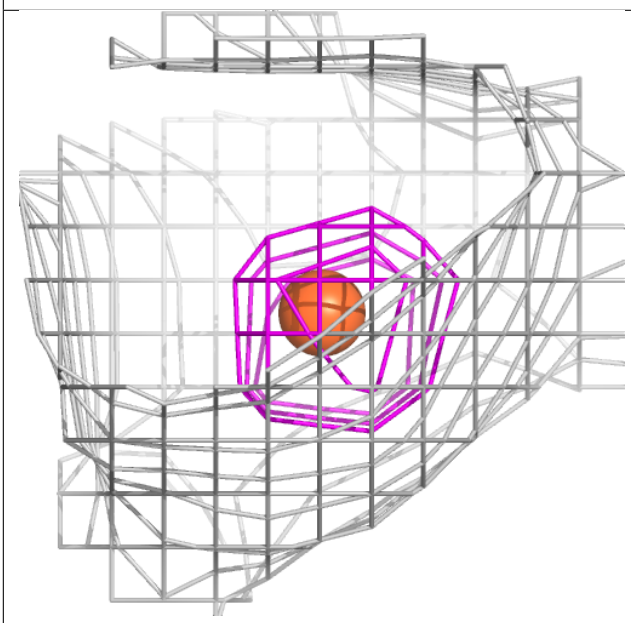
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

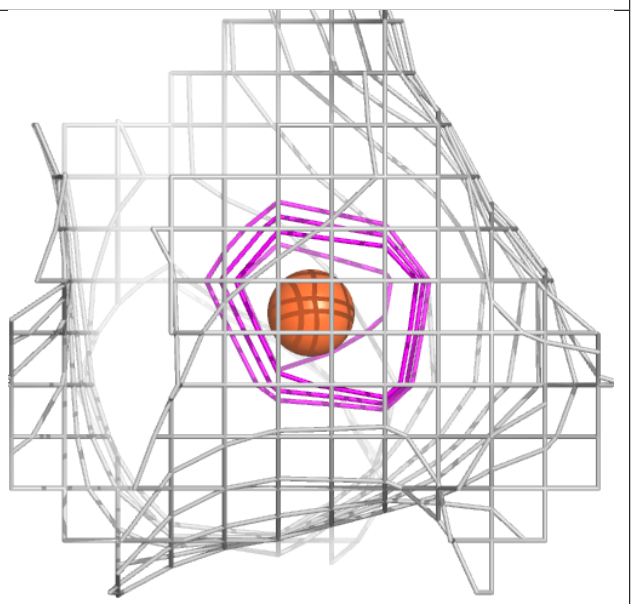


Electron density around FE W 201:

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

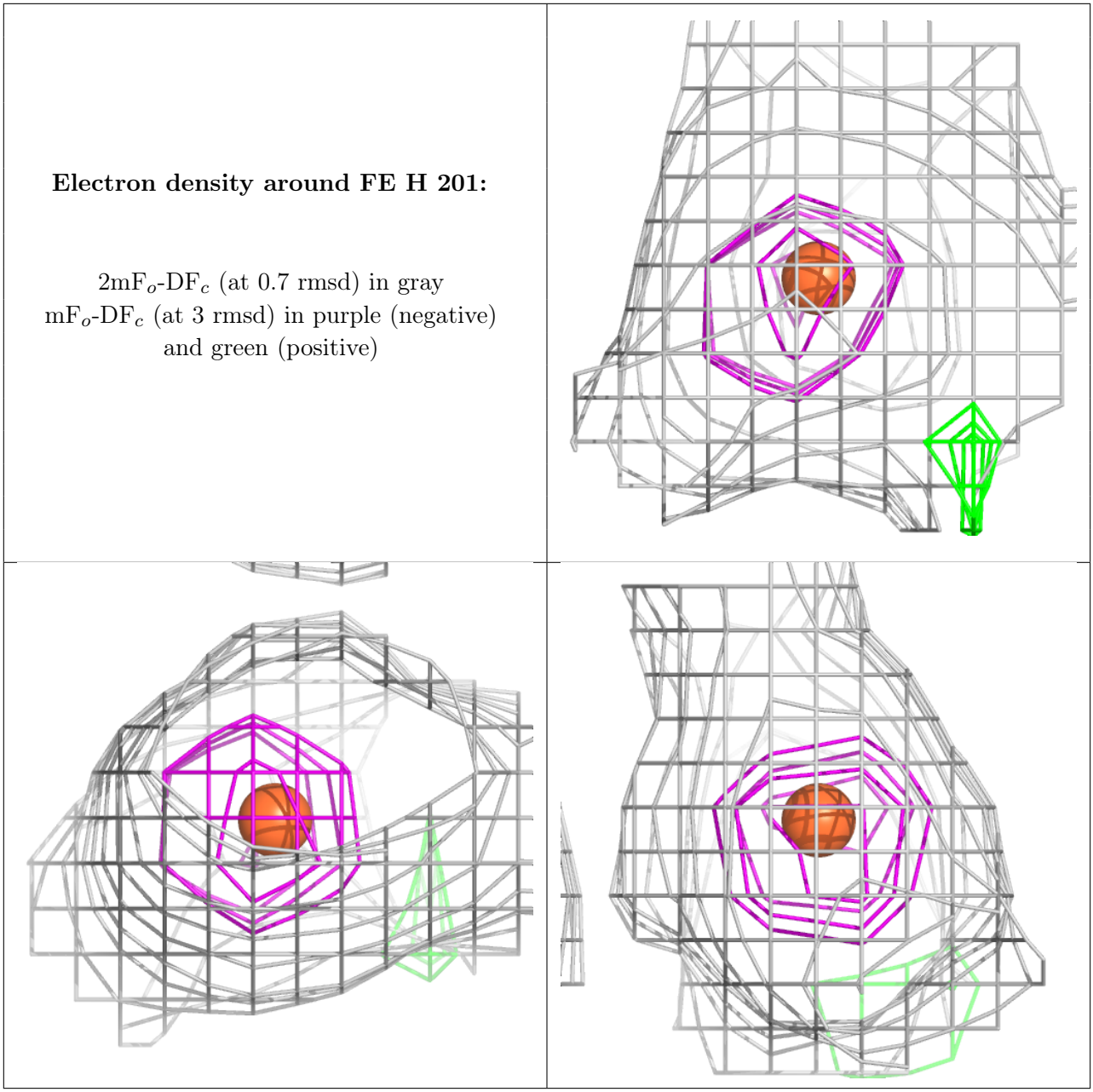






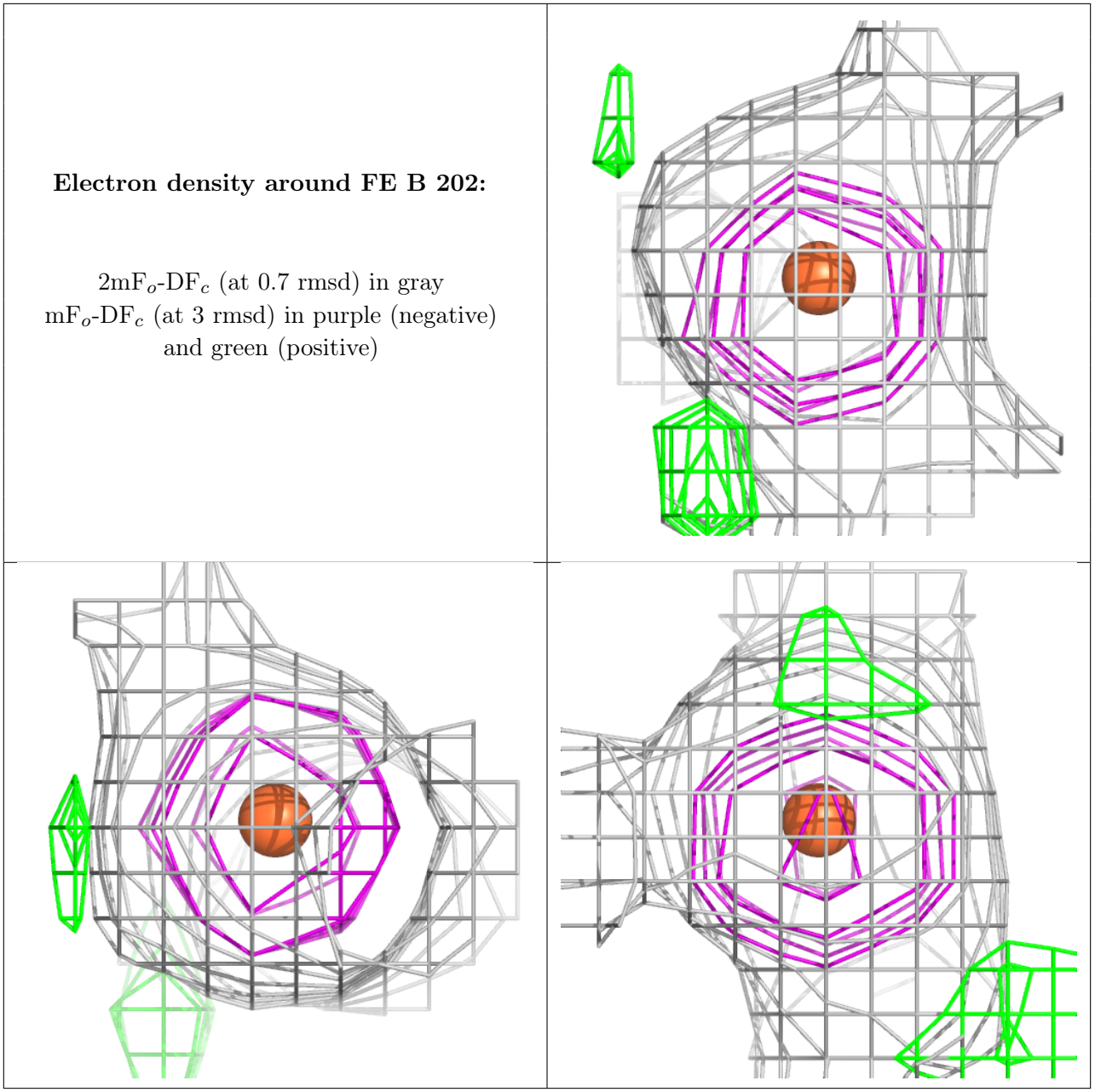
Electron density around FE H 201:

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



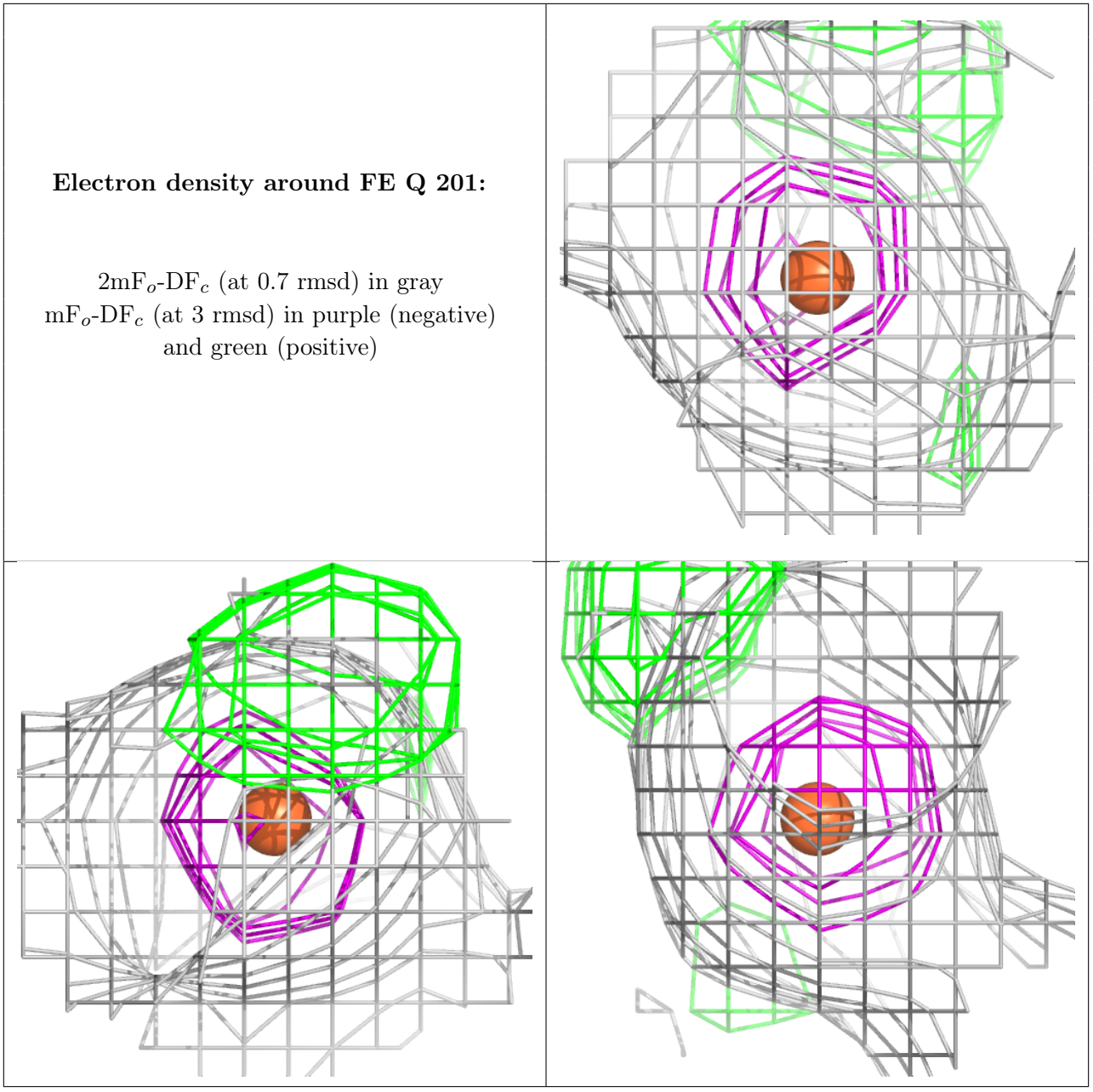
Electron density around FE B 202:

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



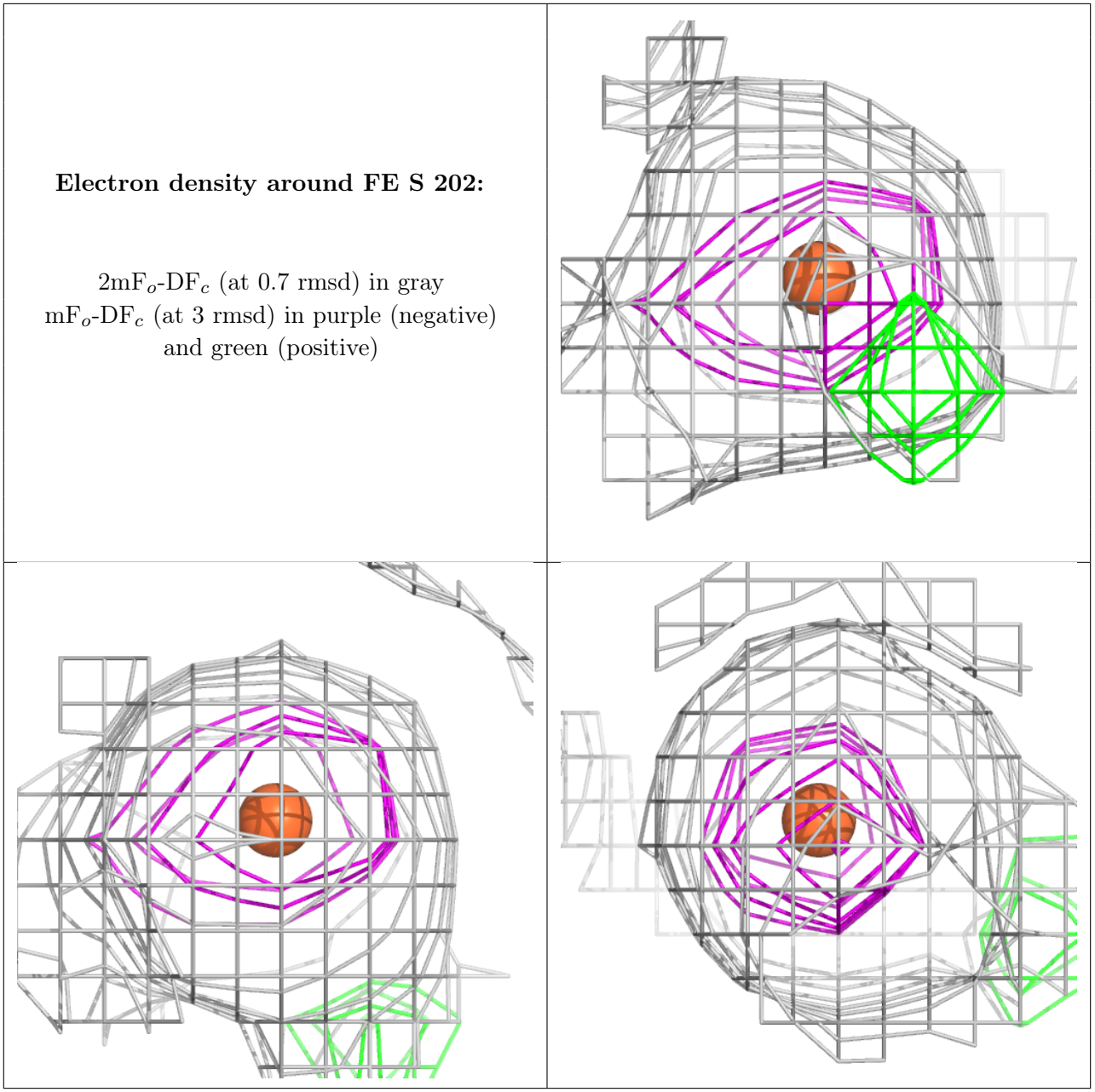
Electron density around FE Q 201:

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



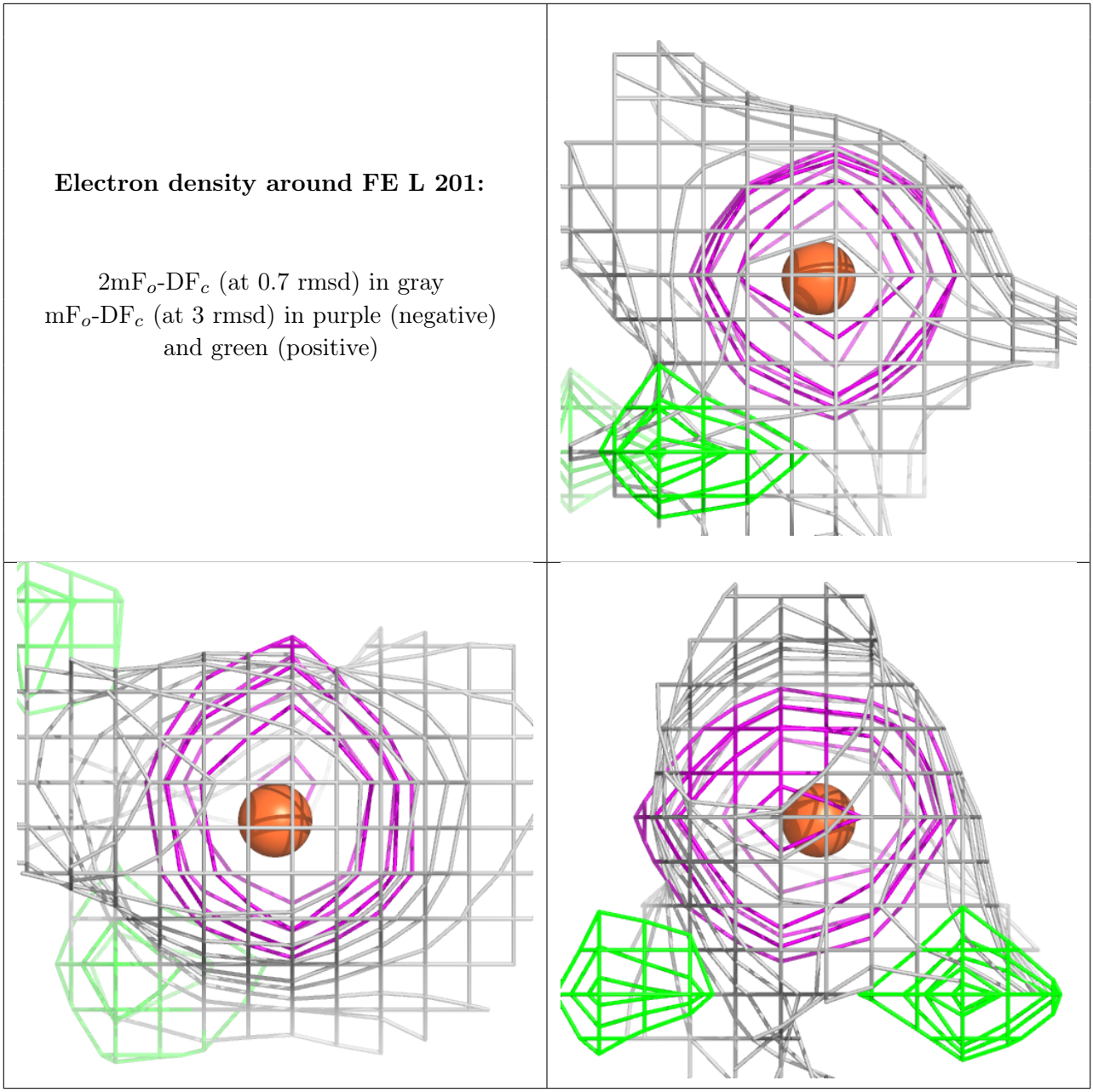
Electron density around FE S 202:

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



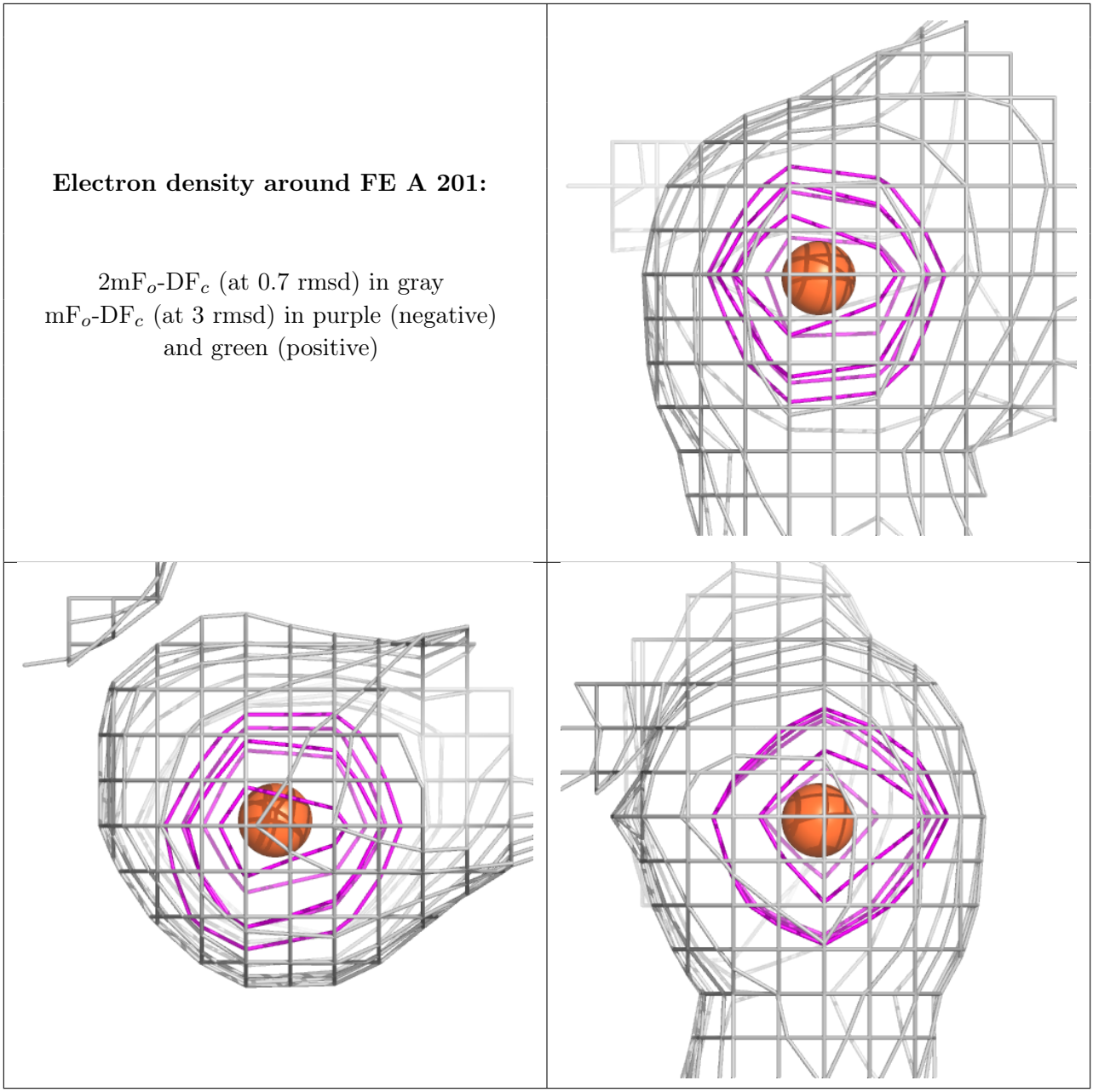
Electron density around FE L 201:

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



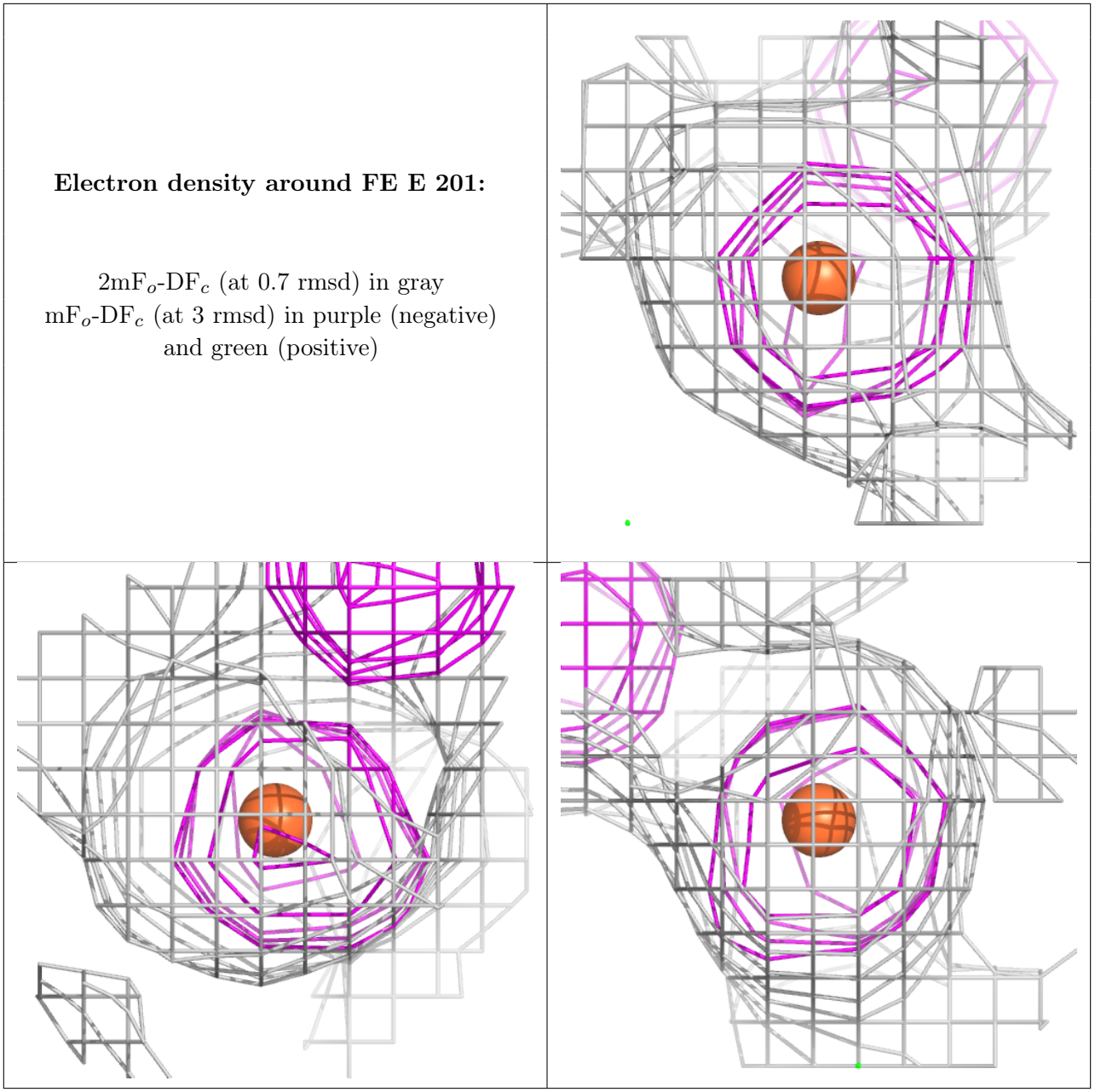
Electron density around FE A 201:

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



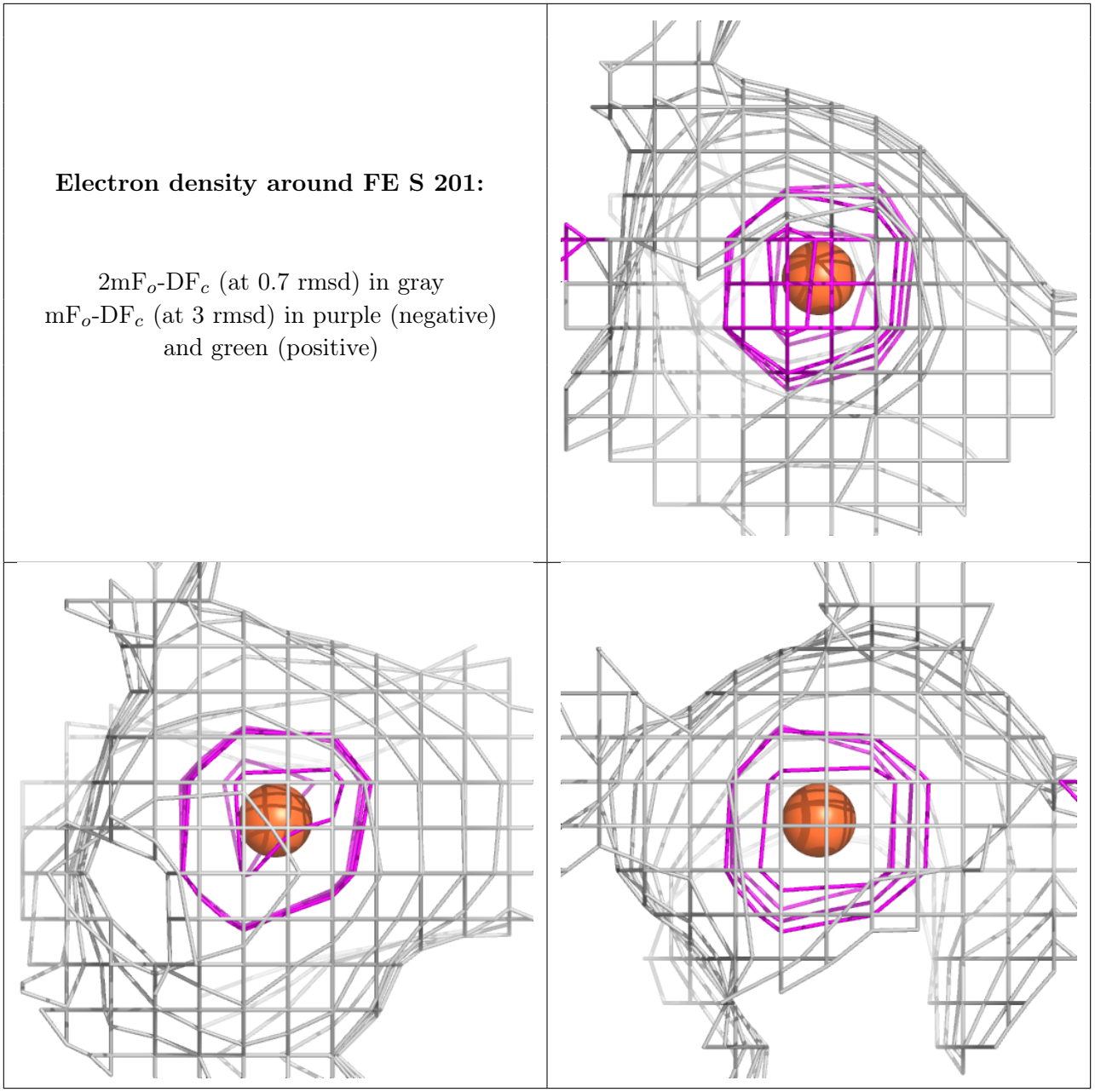
Electron density around FE E 201:

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



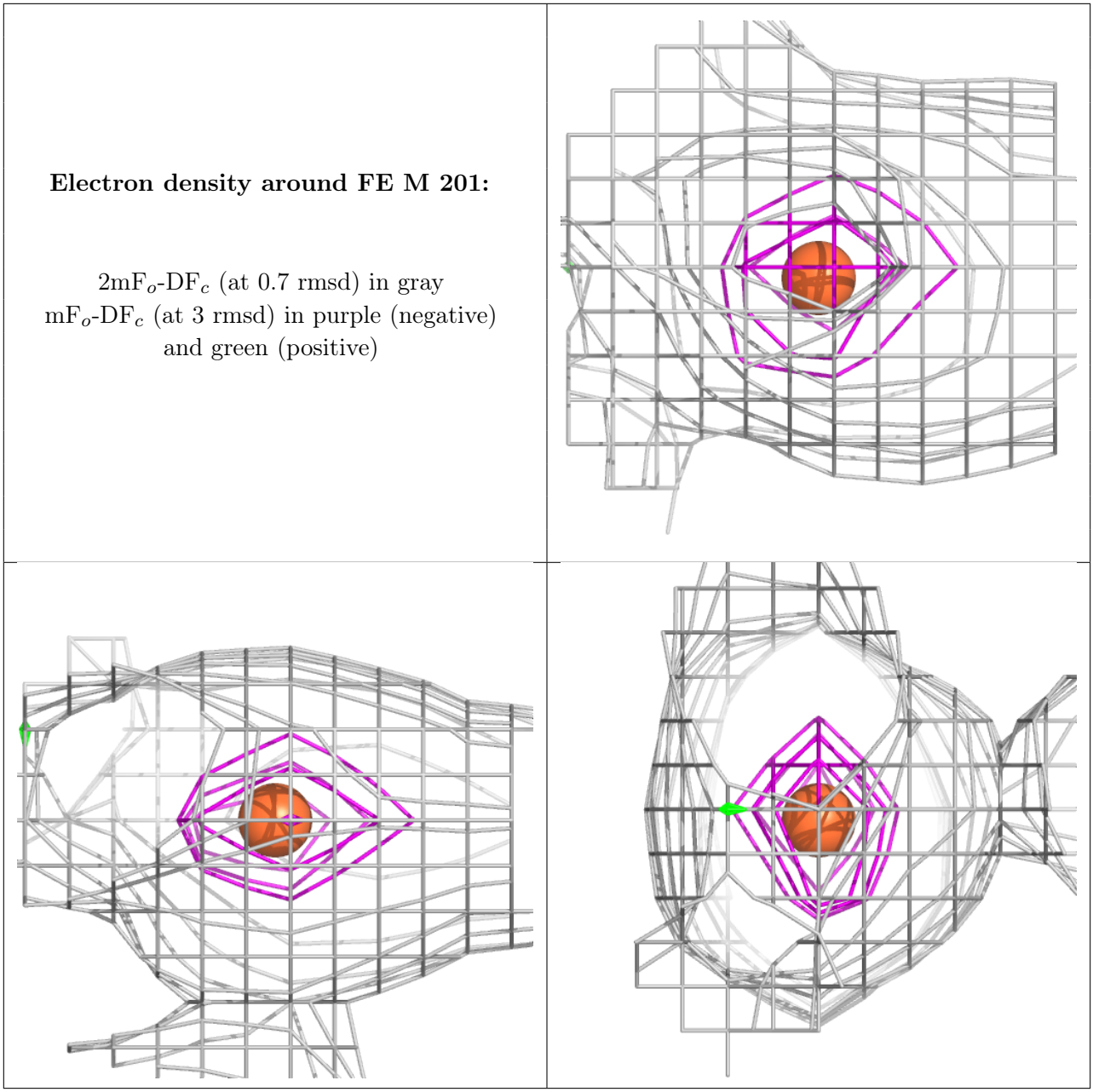
Electron density around FE S 201:

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



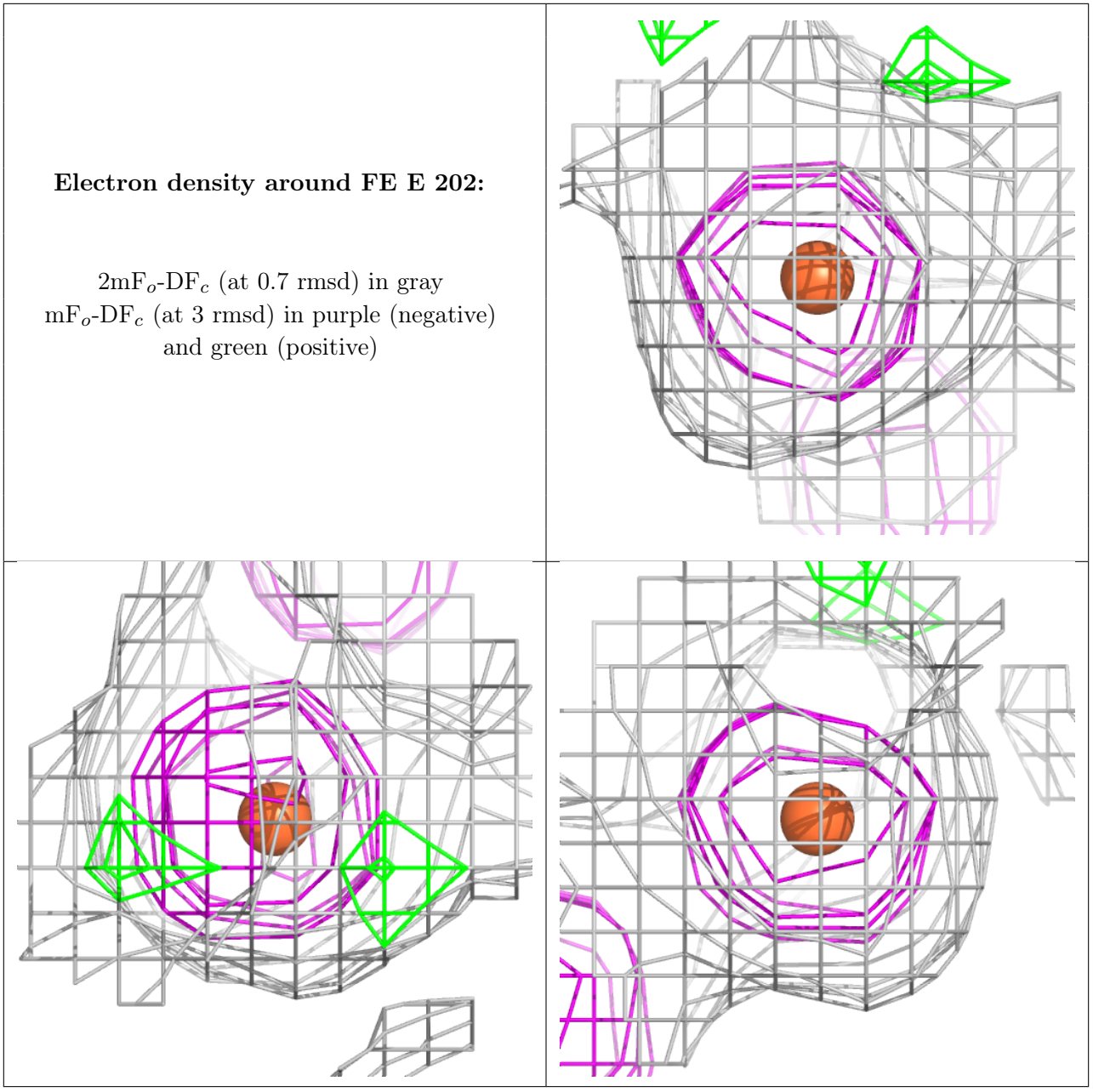
Electron density around FE M 201:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.