Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 12:05 AM JST

PDB ID	:	8JIB
Title	:	Crystal Structure of Prophenoloxidase PPO6 from Aedes aegypti
Authors	:	Zhu, X.; Zhang, L.; Yang, X.; Bao, P.; Ren, D.; Han, Q.
Deposited on	:	2023-05-26
Resolution	:	3.15 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 (i) 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 (i)) were used in the production of this report:

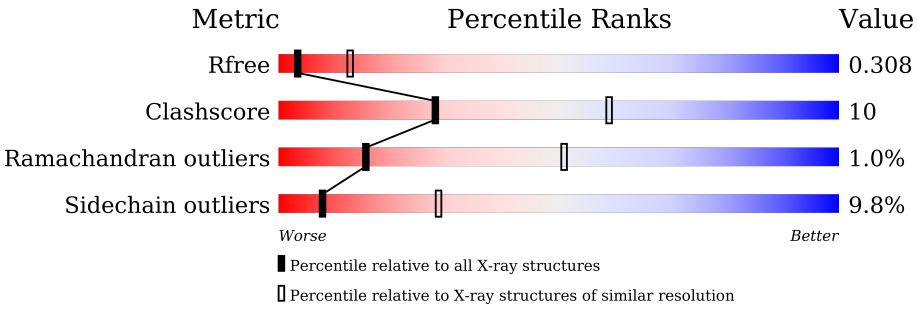
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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%

Mol	Chain	Length	Quality of chain
1	A	681	71% 20% 5% •
1	B	681	72% 19% • • 5%
1	C	681	71% 20% • • 5%
1	D	681	72% 20% • 5%
1	E	681	72% 21% • •
1	F	681	73% 18% • •
1	G	681	77% 17% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	681	75% 19%
1	I	681	75% 18%
1	J	681	74% 19%
1	K	681	77% 17%
1	L	681	75% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 65153 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 TK receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5377	3422	969	961	25			
1	B	645	Total	C	N	O	S	0	0	0
			5330	3395	960	952	23			
1	C	648	Total	C	N	O	S	0	0	0
			5358	3412	966	955	25			
1	D	650	Total	C	N	O	S	0	0	0
			5373	3420	968	960	25			
1	E	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	F	657	Total	C	N	O	S	0	0	0
			5421	3448	976	971	26			
1	G	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	H	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	I	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	J	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	K	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	L	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

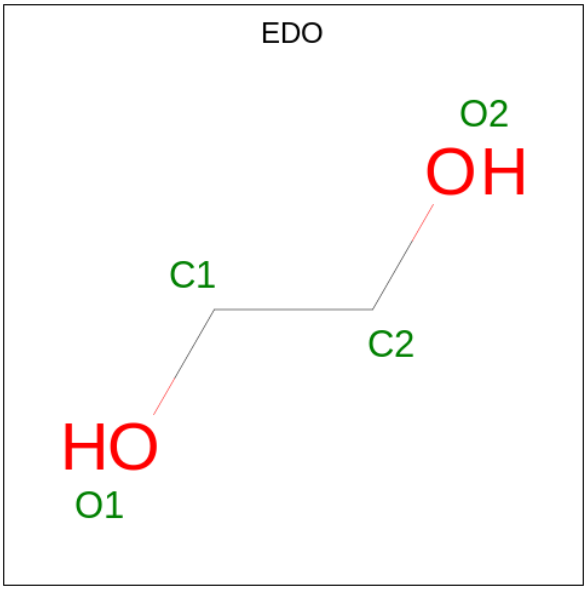
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0
2	G	2	Total Cu 2 2	0	0
2	H	2	Total Cu 2 2	0	0
2	I	2	Total Cu 2 2	0	0
2	J	2	Total Cu 2 2	0	0
2	K	2	Total Cu 2 2	0	0
2	L	2	Total Cu 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

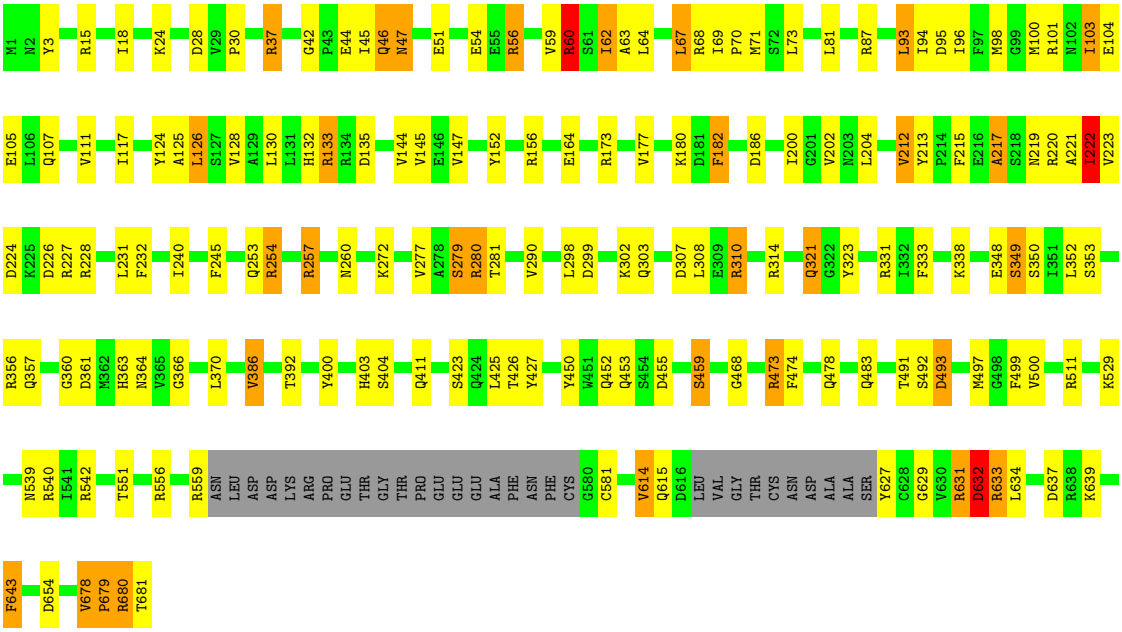
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	25	Total	O	0	0
			25	25		
4	C	23	Total	O	0	0
			23	23		
4	D	13	Total	O	0	0
			13	13		
4	E	14	Total	O	0	0
			14	14		
4	F	12	Total	O	0	0
			12	12		
4	G	8	Total	O	0	0
			8	8		
4	H	6	Total	O	0	0
			6	6		
4	I	8	Total	O	0	0
			8	8		
4	J	6	Total	O	0	0
			6	6		
4	K	1	Total	O	0	0
			1	1		
4	L	18	Total	O	0	0
			18	18		

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. 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. 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.

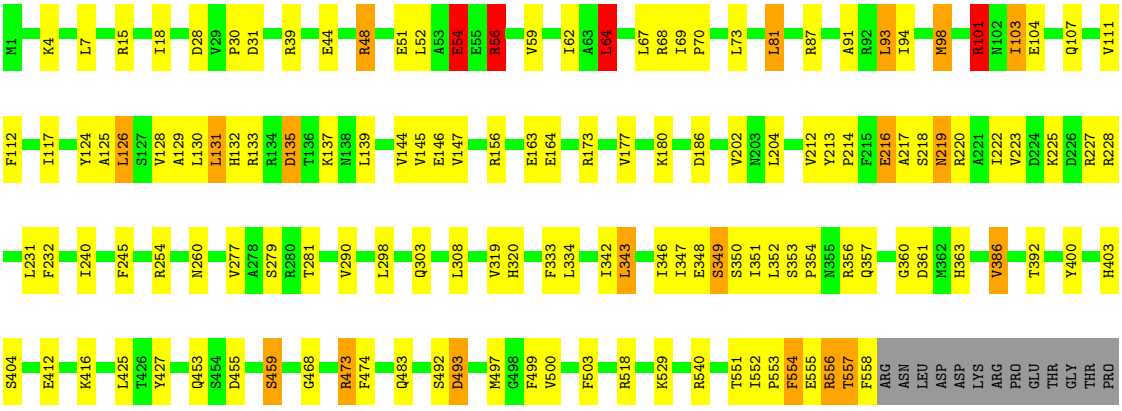
• Molecule 1: TK receptor

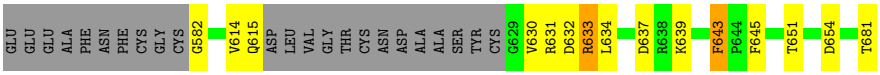
Chain A:



• Molecule 1: TK receptor

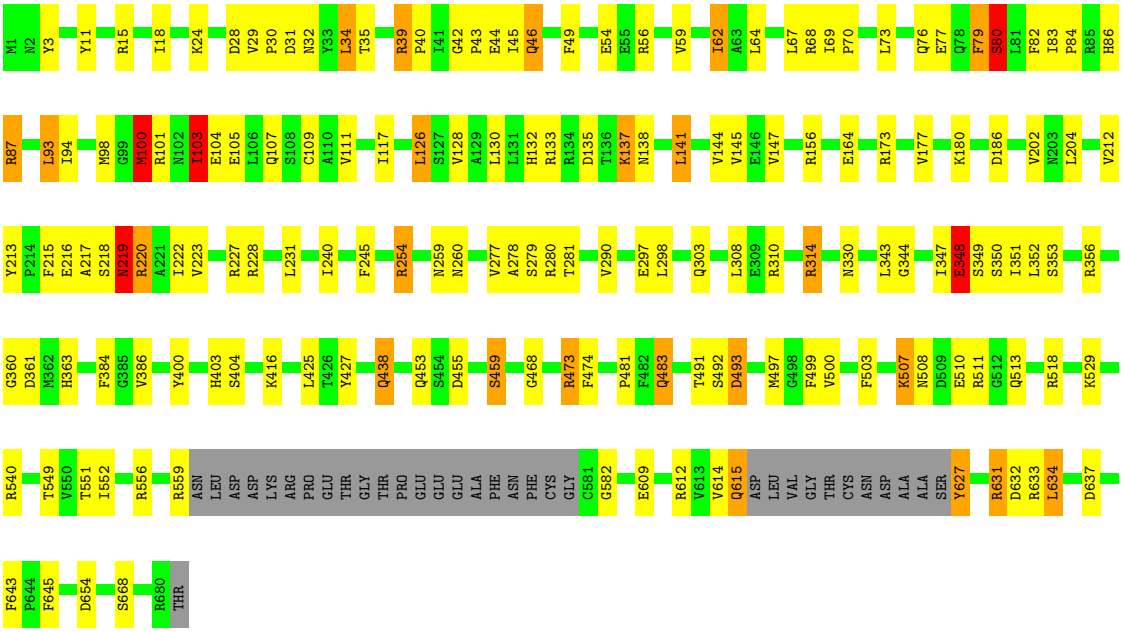
Chain B:





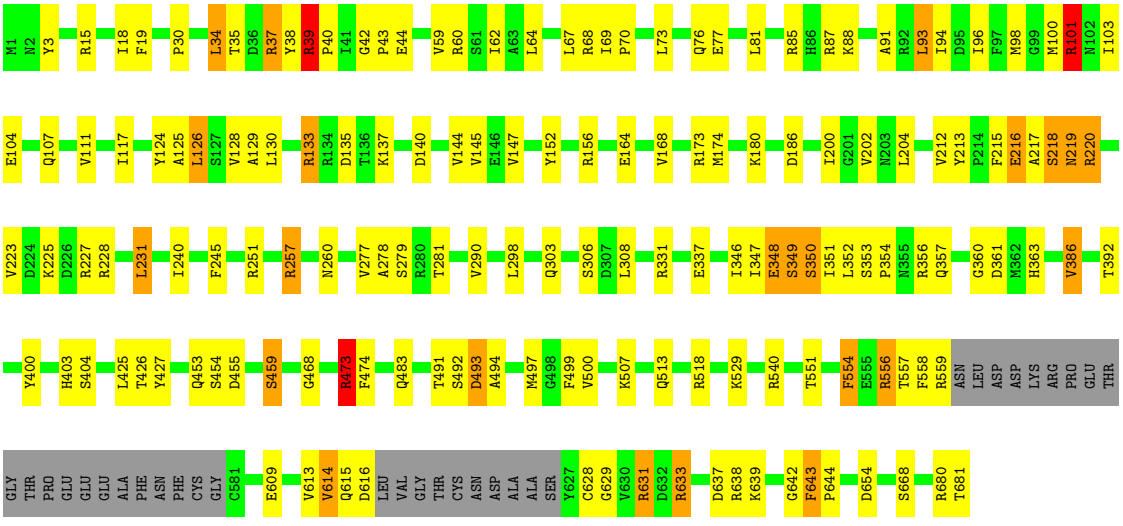
• Molecule 1: TK receptor

Chain C:



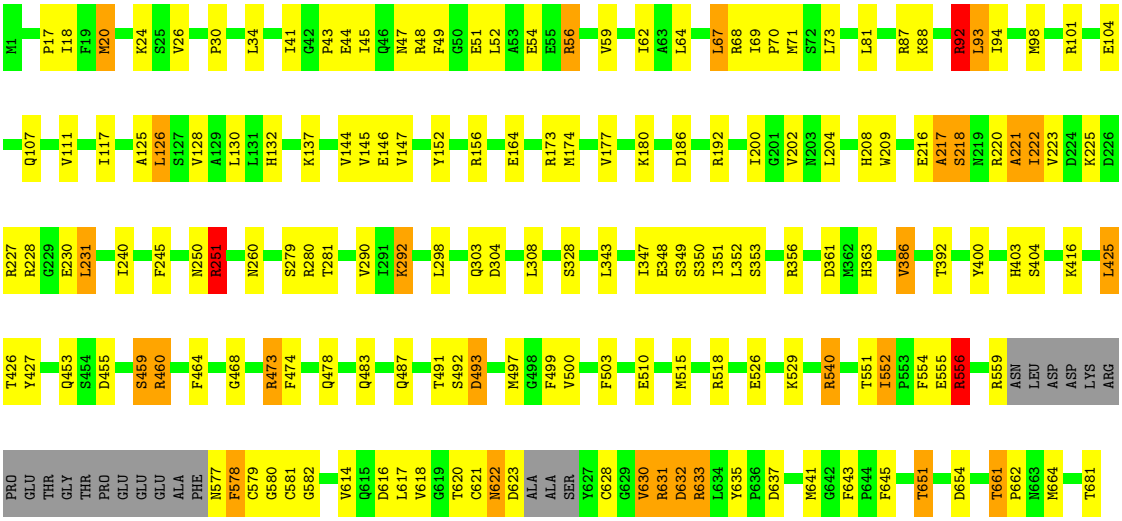
• Molecule 1: TK receptor

Chain D:



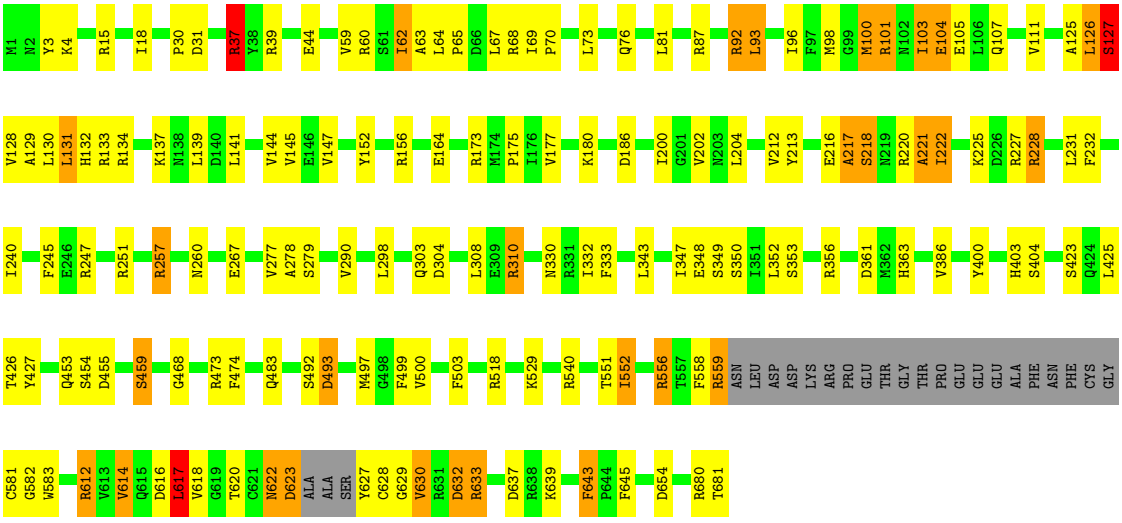
• Molecule 1: TK receptor

Chain E:



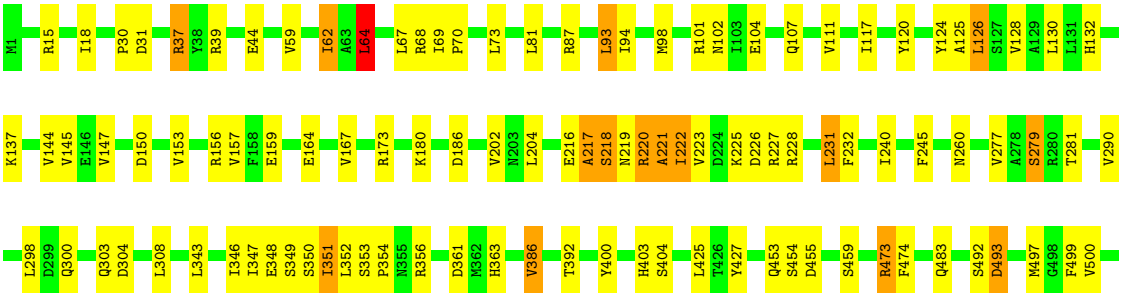
• Molecule 1: TK receptor

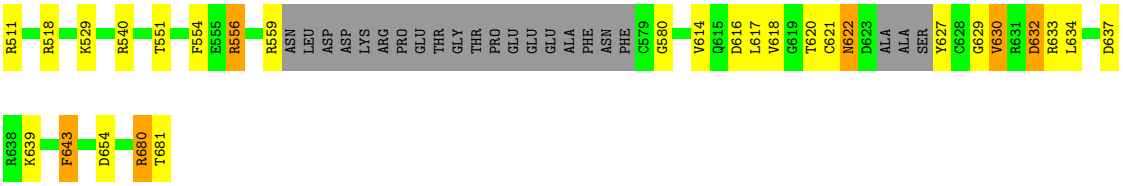
Chain F:



• Molecule 1: TK receptor

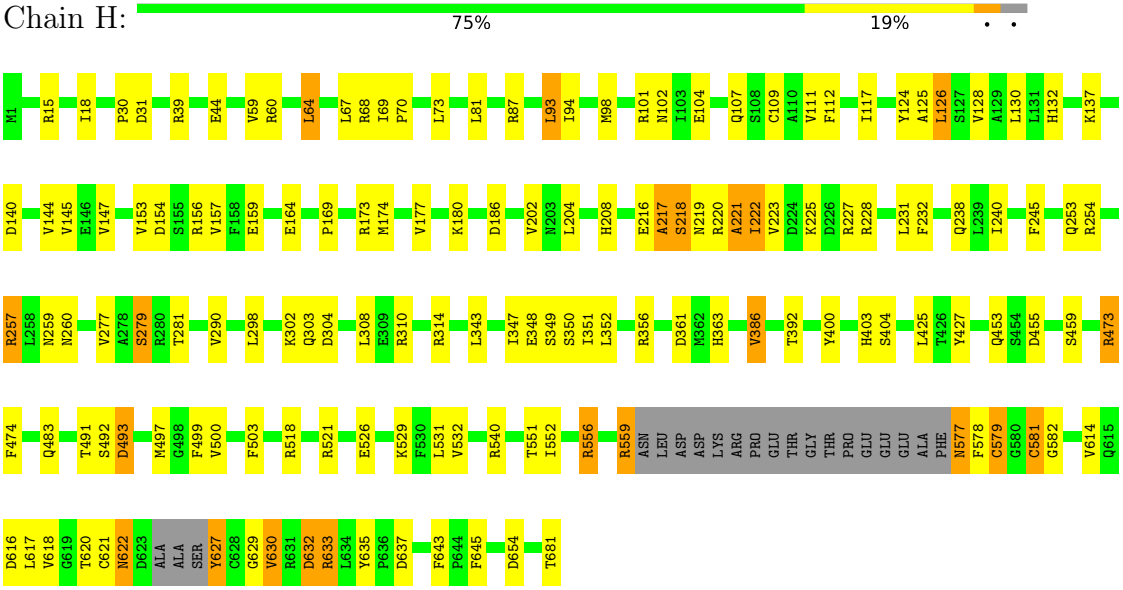
Chain G:





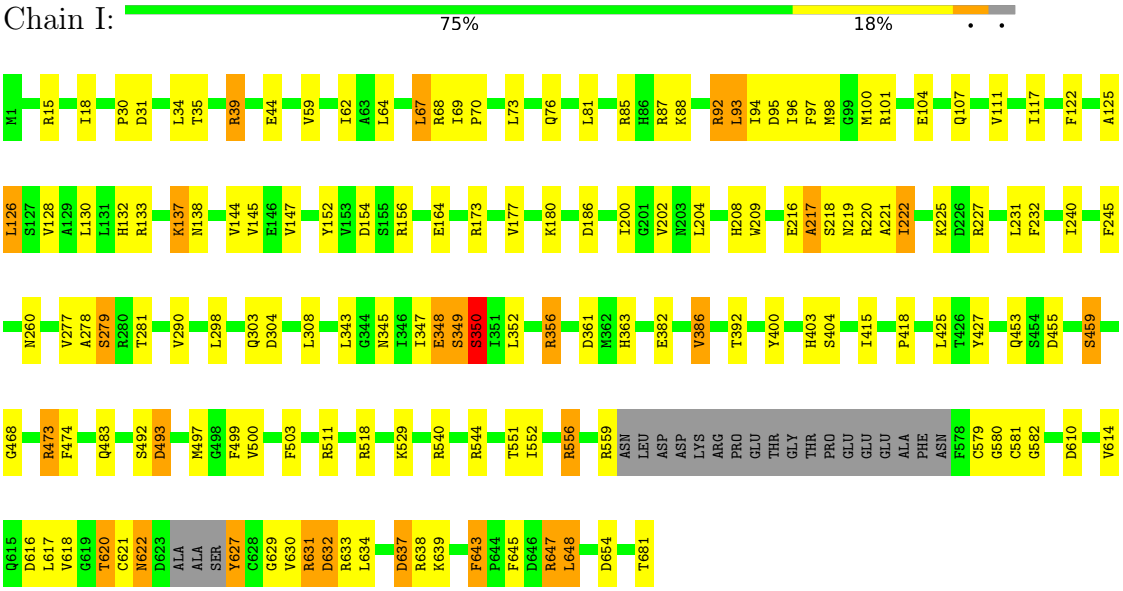
• Molecule 1: TK receptor

Chain H:



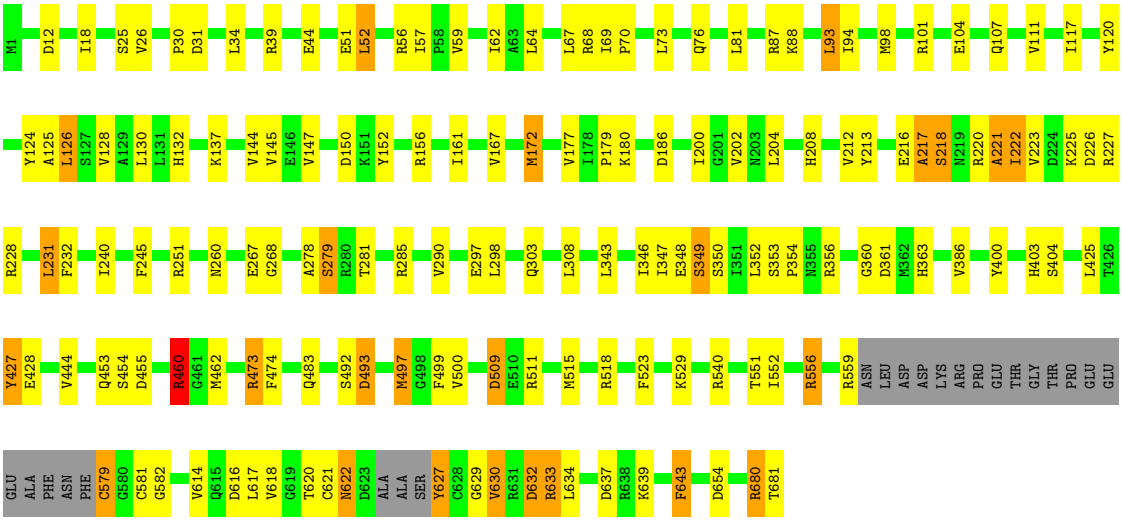
• Molecule 1: TK receptor

Chain I:



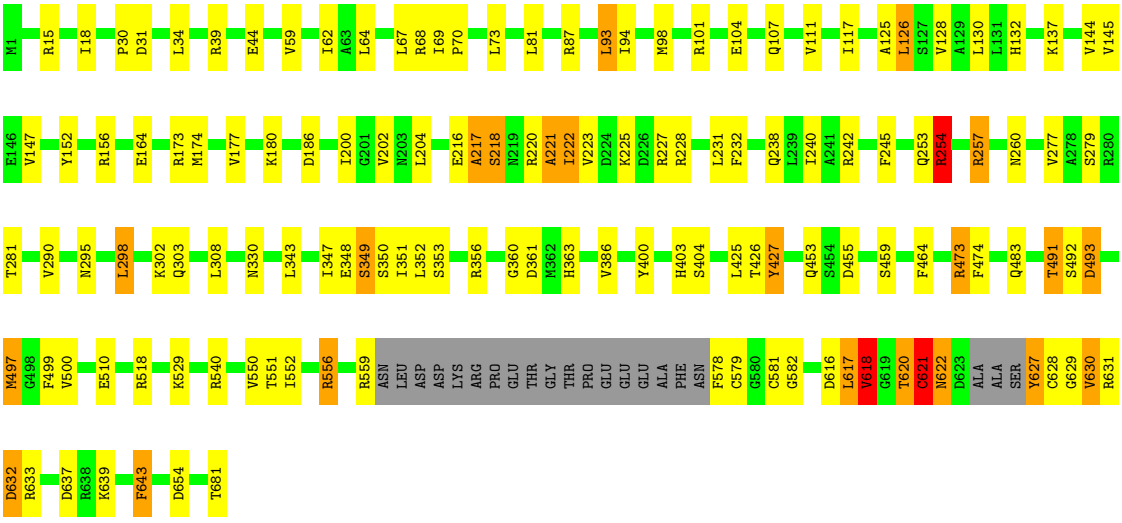
• Molecule 1: TK receptor

Chain J:



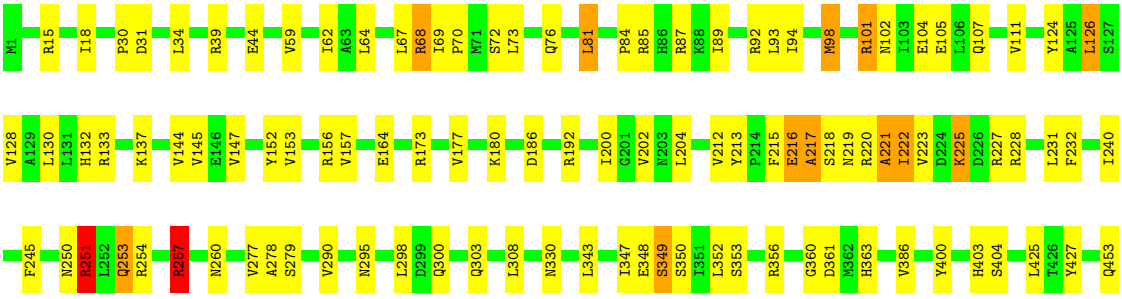
• Molecule 1: TK receptor

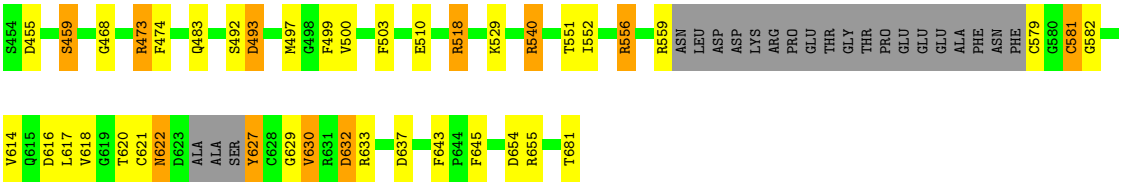
Chain K:



• Molecule 1: TK receptor

Chain L:




S454
D455
S459
G468
R473
F474
Q483
S492
D493
M497
G498
F499
V500
F503
E510
R518
K529
R540
T551
I552
R556
R559
ASN
LEU
ASP
ASP
LYS
ARG
PRO
GLU
THR
GLY
THR
PRO
GLU
GLU
GLU
ALA
PHE
ASN
PHE
C579
G580
C581
G582
V614
Q615
D616
L617
V618
G619
T620
C621
N622
D623
ALA
ALA
SER
Y627
C628
G629
V630
R631
D632
R633
D637
F643
P644
F645
D654
R655
T681

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.04Å 364.15Å 125.52Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	48.66 – 3.15 48.61 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.66-3.15) 98.1 (48.61-3.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.269 , 0.310 0.269 , 0.308	Depositor DCC
R_{free} test set	7921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.387 for h,-k,-h-l 0.047 for l,-k,h 0.047 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	65153	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% 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: EDO, CU

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	0.39	0/5513	0.80	12/7461 (0.2%)
1	B	0.37	0/5465	0.75	3/7397 (0.0%)
1	C	0.37	0/5494	0.78	8/7435 (0.1%)
1	D	0.39	0/5509	0.75	4/7456 (0.1%)
1	E	0.36	0/5587	0.74	7/7562 (0.1%)
1	F	0.36	0/5557	0.77	9/7522 (0.1%)
1	G	0.34	0/5567	0.67	0/7535
1	H	0.34	0/5587	0.68	1/7562 (0.0%)
1	I	0.35	0/5579	0.72	8/7551 (0.1%)
1	J	0.34	0/5567	0.70	4/7535 (0.1%)
1	K	0.33	0/5579	0.67	2/7551 (0.0%)
1	L	0.35	1/5567 (0.0%)	0.71	10/7535 (0.1%)
All	All	0.36	1/66571 (0.0%)	0.73	68/90102 (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	A	0	1
1	B	0	1
1	D	0	3
1	E	0	3
1	F	0	4
1	G	0	1
1	H	0	2
1	J	0	2
1	K	0	1
1	L	0	2
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	216	GLU	CD-OE2	-5.52	1.19	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	MET	CG-SD-CE	10.93	117.69	100.20
1	C	79	PHE	CB-CA-C	10.66	131.72	110.40
1	F	310	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	F	228	ARG	CG-CD-NE	-9.62	91.59	111.80
1	F	247	ARG	CG-CD-NE	-9.34	92.18	111.80
1	C	100	MET	CG-SD-CE	9.30	115.08	100.20
1	F	617	LEU	CB-CG-CD2	8.81	125.97	111.00
1	I	637	ASP	CB-CG-OD1	-8.20	110.92	118.30
1	I	348	GLU	CG-CD-OE2	7.76	133.83	118.30
1	J	509	ASP	CB-CG-OD2	7.63	125.17	118.30
1	L	655	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	L	216	GLU	CG-CD-OE1	7.54	133.39	118.30
1	I	350	SER	N-CA-CB	7.47	121.71	110.50
1	C	314	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	J	509	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	D	39	ARG	CG-CD-NE	7.05	126.60	111.80
1	A	257	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	L	257	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	L	655	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	E	20	MET	CG-SD-CE	6.57	110.71	100.20
1	E	515	MET	CG-SD-CE	6.51	110.62	100.20
1	A	310	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	F	612	ARG	CA-CB-CG	6.36	127.39	113.40
1	L	216	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	F	310	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	I	348	GLU	CG-CD-OE1	-6.22	105.86	118.30
1	H	302	LYS	CA-CB-CG	6.15	126.93	113.40
1	C	101	ARG	CG-CD-NE	-6.14	98.90	111.80
1	C	254	ARG	CG-CD-NE	6.10	124.60	111.80
1	F	559	ARG	N-CA-CB	6.04	121.47	110.60
1	B	56	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	D	101	ARG	CB-CA-C	-5.74	98.92	110.40
1	K	620	THR	CA-CB-OG1	-5.71	97.01	109.00
1	B	54	GLU	CG-CD-OE1	-5.60	107.09	118.30
1	A	182	PHE	CB-CG-CD2	5.60	124.72	120.80
1	E	92	ARG	CB-CG-CD	5.58	126.09	111.60
1	I	637	ASP	CB-CG-OD2	5.52	123.27	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ARG	CG-CD-NE	5.51	123.38	111.80
1	E	251	ARG	CA-CB-CG	5.50	125.50	113.40
1	I	348	GLU	N-CA-CB	5.48	120.47	110.60
1	E	623	ASP	CA-C-O	-5.46	108.64	120.10
1	A	60	ARG	CG-CD-NE	-5.42	100.41	111.80
1	C	254	ARG	CA-CB-CG	5.36	125.19	113.40
1	F	37	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	680	ARG	N-CA-CB	-5.35	100.97	110.60
1	D	642	GLY	C-N-CA	5.34	135.06	121.70
1	A	182	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	C	80	SER	N-CA-CB	5.32	118.49	110.50
1	E	651	THR	CA-CB-CG2	5.28	119.80	112.40
1	I	92	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	J	172	MET	CA-CB-CG	5.25	122.23	113.30
1	A	133	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	L	251	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	F	127	SER	CB-CA-C	5.20	119.98	110.10
1	I	137	LYS	CA-CB-CG	5.20	124.84	113.40
1	L	581	CYS	CB-CA-C	5.17	120.75	110.40
1	A	540	ARG	CA-CB-CG	-5.15	102.08	113.40
1	L	251	ARG	CG-CD-NE	5.13	122.58	111.80
1	D	337	GLU	CG-CD-OE1	-5.09	108.12	118.30
1	C	103	ILE	CA-CB-CG1	5.08	120.66	111.00
1	K	254	ARG	CA-CB-CG	5.08	124.59	113.40
1	L	85	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	310	ARG	CG-CD-NE	5.06	122.44	111.80
1	L	133	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	48	ARG	CA-CB-CG	5.05	124.50	113.40
1	A	60	ARG	CA-CB-CG	5.03	124.47	113.40
1	A	542	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	J	88	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
1	B	56	ARG	Sidechain
1	D	34	LEU	Mainchain
1	D	473	ARG	Sidechain
1	D	631	ARG	Sidechain
1	E	221	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	556	ARG	Sidechain
1	E	631	ARG	Sidechain
1	F	127	SER	Mainchain
1	F	221	ALA	Peptide
1	F	558	PHE	Peptide
1	F	92	ARG	Sidechain
1	G	221	ALA	Peptide
1	H	221	ALA	Peptide
1	H	257	ARG	Sidechain
1	J	221	ALA	Peptide
1	J	460	ARG	Sidechain
1	K	221	ALA	Peptide
1	L	221	ALA	Peptide
1	L	251	ARG	Sidechain

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	5377	0	5284	134	3
1	B	5330	0	5242	105	0
1	C	5358	0	5270	128	3
1	D	5373	0	5281	115	1
1	E	5450	0	5348	134	0
1	F	5421	0	5324	141	0
1	G	5431	0	5334	92	1
1	H	5450	0	5348	92	1
1	I	5442	0	5341	104	0
1	J	5431	0	5334	107	1
1	K	5442	0	5342	102	1
1	L	5431	0	5333	113	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	12	0	18	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
3	H	4	0	6	0	0
4	A	31	0	0	0	0
4	B	25	0	0	0	0
4	C	23	0	0	1	0
4	D	13	0	0	0	0
4	E	14	0	0	2	0
4	F	12	0	0	1	0
4	G	8	0	0	0	0
4	H	6	0	0	0	0
4	I	8	0	0	1	0
4	J	6	0	0	1	0
4	K	1	0	0	0	0
4	L	18	0	0	1	0
All	All	65153	0	63823	1273	6

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 10.

All (1273) 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:J:208:HIS:HB3	1:J:581:CYS:SG	1.38	1.60
1:A:132:HIS:CG	1:A:222:ILE:HD11	1.41	1.50
1:J:581:CYS:SG	1:J:622:ASN:HB3	1.55	1.46
1:B:28:ASP:OD1	1:B:56:ARG:NH1	1.60	1.33
1:B:493:ASP:O	1:D:101:ARG:HG2	1.34	1.27
1:B:101:ARG:HD2	1:D:493:ASP:O	1.36	1.26
1:H:349:SER:OG	1:H:361:ASP:OD1	1.54	1.25
1:F:349:SER:OG	1:F:361:ASP:OD1	1.53	1.24
1:A:132:HIS:CG	1:A:222:ILE:CD1	2.20	1.23
1:F:126:LEU:O	1:F:127:SER:O	1.57	1.23
1:I:208:HIS:CB	1:I:581:CYS:SG	2.27	1.23
1:B:319:VAL:CG1	1:B:412:GLU:O	1.87	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:HIS:CB	1:J:581:CYS:SG	2.26	1.22
1:F:100:MET:O	1:F:133:ARG:NH2	1.72	1.21
1:I:100:MET:O	1:I:133:ARG:NH2	1.75	1.19
1:D:124:TYR:O	1:D:128:VAL:HG23	1.40	1.17
1:B:101:ARG:HB3	1:D:494:ALA:HA	1.24	1.15
1:A:678:VAL:HG12	1:A:679:PRO:HD2	1.26	1.15
1:C:549:THR:O	1:C:627:TYR:CE2	2.01	1.14
1:B:28:ASP:CG	1:B:56:ARG:NH1	1.86	1.14
1:E:579:CYS:SG	1:E:635:TYR:HE2	1.71	1.13
1:J:581:CYS:SG	1:J:622:ASN:CB	2.36	1.12
1:I:208:HIS:HB2	1:I:581:CYS:SG	1.90	1.10
1:J:12:ASP:OD2	1:J:460:ARG:NH1	1.83	1.10
1:A:132:HIS:ND1	1:A:222:ILE:HD11	1.67	1.09
1:I:415:ILE:HG22	1:I:648:LEU:HD21	1.35	1.09
1:B:493:ASP:O	1:D:101:ARG:CG	2.00	1.08
1:A:366:GLY:O	1:A:370:LEU:HD13	1.52	1.08
1:D:39:ARG:HB3	1:D:40:PRO:HD3	1.19	1.06
1:A:678:VAL:HG12	1:A:679:PRO:CD	1.83	1.06
1:J:161:ILE:HG21	1:J:462:MET:HE2	1.07	1.05
1:I:209:TRP:N	1:I:581:CYS:SG	2.30	1.05
1:A:366:GLY:O	1:A:370:LEU:CD1	2.06	1.04
1:E:250:ASN:O	1:E:251:ARG:HD3	1.58	1.03
1:E:146:GLU:HB3	1:E:460:ARG:HD2	1.40	1.03
1:H:579:CYS:SG	1:H:630:VAL:HG21	1.97	1.03
1:K:620:THR:OG1	1:K:629:GLY:C	1.98	1.02
1:B:319:VAL:HG11	1:B:412:GLU:O	1.58	1.02
1:D:38:TYR:HE2	1:G:167:VAL:HG11	1.23	1.02
1:C:615:GLN:NE2	1:C:634:LEU:HB2	1.73	1.02
1:E:552:ILE:CG2	1:E:582:GLY:HA3	1.90	1.01
1:E:81:LEU:HD12	4:E:803:HOH:O	1.59	1.00
1:C:3:TYR:HB3	1:C:103:ILE:HD11	1.44	0.99
1:A:272:LYS:HE3	1:I:382:GLU:OE2	1.62	0.99
1:J:161:ILE:HG21	1:J:462:MET:CE	1.91	0.98
1:B:615:GLN:NE2	1:B:633:ARG:HB2	1.78	0.98
1:F:60:ARG:NE	1:F:104:GLU:OE2	1.96	0.98
1:L:253:GLN:HG2	1:L:510:GLU:OE2	1.64	0.97
1:D:38:TYR:CE2	1:G:167:VAL:HG11	1.98	0.97
1:A:132:HIS:CB	1:A:222:ILE:CD1	2.43	0.97
1:I:208:HIS:HB3	1:I:581:CYS:SG	2.04	0.96
1:A:67:LEU:CD1	1:A:96:ILE:HD13	1.96	0.95
1:J:161:ILE:CG2	1:J:462:MET:HE2	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:ARG:CZ	1:L:105:GLU:OE2	2.15	0.94
1:F:556:ARG:NE	1:F:623:ASP:OD2	1.99	0.94
1:H:257:ARG:NH2	1:I:304:ASP:OD1	2.00	0.94
1:F:60:ARG:CZ	1:F:104:GLU:OE2	2.16	0.93
1:I:579:CYS:SG	1:I:630:VAL:HG21	2.09	0.93
1:K:620:THR:CG2	1:K:629:GLY:HA3	1.98	0.92
1:C:549:THR:O	1:C:627:TYR:HE2	1.43	0.92
1:F:622:ASN:OD1	1:F:629:GLY:HA3	1.69	0.92
1:K:620:THR:HG23	1:K:629:GLY:HA3	1.52	0.92
1:I:345:ASN:O	1:I:349:SER:O	1.87	0.92
1:D:39:ARG:HB3	1:D:40:PRO:CD	2.01	0.91
1:G:349:SER:OG	1:G:356:ARG:NH1	2.02	0.91
1:H:579:CYS:SG	1:H:630:VAL:CG2	2.59	0.90
1:I:579:CYS:SG	1:I:630:VAL:CG2	2.60	0.90
1:F:98:MET:HE3	1:F:132:HIS:O	1.72	0.89
1:C:349:SER:HB3	1:C:356:ARG:HH11	1.35	0.88
1:I:208:HIS:C	1:I:581:CYS:SG	2.51	0.88
1:C:549:THR:O	1:C:627:TYR:CD2	2.27	0.88
1:C:615:GLN:HE21	1:C:634:LEU:HB2	1.33	0.88
1:C:615:GLN:HE21	1:C:634:LEU:CB	1.86	0.87
1:J:581:CYS:HG	1:J:622:ASN:HB3	0.93	0.86
1:F:131:LEU:HD21	1:F:141:LEU:HD21	1.57	0.86
1:F:70:PRO:HD3	1:F:92:ARG:HG2	1.58	0.85
1:J:25:SER:HB3	1:J:57:ILE:HD11	1.59	0.85
1:L:192:ARG:CZ	1:L:251:ARG:NH1	2.39	0.85
1:C:349:SER:OG	1:C:360:GLY:O	1.94	0.85
1:D:217:ALA:HA	1:D:351:ILE:HG21	1.59	0.85
1:B:28:ASP:HB2	1:B:56:ARG:CZ	2.06	0.84
1:D:124:TYR:O	1:D:128:VAL:CG2	2.24	0.84
1:D:140:ASP:OD1	1:D:556:ARG:NH2	2.11	0.84
1:J:454:SER:OG	1:J:680:ARG:HD3	1.78	0.83
1:L:192:ARG:NH2	1:L:251:ARG:HH11	1.76	0.83
1:E:552:ILE:HG21	1:E:582:GLY:HA3	1.61	0.82
1:D:628:CYS:SG	1:D:629:GLY:N	2.52	0.82
1:F:556:ARG:CG	1:F:623:ASP:OD2	2.28	0.82
1:L:579:CYS:SG	1:L:627:TYR:OH	2.35	0.82
1:A:132:HIS:CD2	1:A:222:ILE:HD11	2.12	0.81
1:C:3:TYR:CB	1:C:103:ILE:HD11	2.10	0.81
1:F:60:ARG:NH1	1:F:104:GLU:OE1	2.12	0.81
1:B:28:ASP:CB	1:B:56:ARG:CZ	2.40	0.81
1:C:348:GLU:HB2	1:C:363:HIS:HB3	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:SER:OG	1:L:89:ILE:CD1	2.29	0.81
1:L:540:ARG:O	1:L:540:ARG:HG3	1.81	0.81
1:A:349:SER:OG	1:A:360:GLY:O	1.99	0.81
1:H:581:CYS:SG	1:H:622:ASN:OD1	2.40	0.80
1:J:231:LEU:HD11	1:J:579:CYS:CB	2.11	0.80
1:A:333:PHE:CD1	1:F:333:PHE:CE1	2.68	0.80
1:G:454:SER:OG	1:G:680:ARG:HD2	1.82	0.80
1:B:615:GLN:HE22	1:B:633:ARG:HB2	1.46	0.80
1:L:349:SER:OG	1:L:360:GLY:O	2.00	0.80
1:C:215:PHE:CD1	1:C:216:GLU:HG3	2.16	0.80
1:C:348:GLU:HA	1:C:363:HIS:HB3	1.62	0.80
1:D:100:MET:SD	1:D:101:ARG:NH2	2.54	0.80
1:B:349:SER:OG	1:B:360:GLY:O	2.00	0.79
1:E:349:SER:HB3	1:E:361:ASP:HA	1.64	0.79
1:F:267:GLU:HG3	4:F:805:HOH:O	1.82	0.79
1:J:349:SER:OG	1:J:360:GLY:O	2.01	0.79
1:L:81:LEU:HD12	1:L:81:LEU:H	1.47	0.79
1:D:251:ARG:HE	1:L:251:ARG:HD2	1.47	0.79
1:D:349:SER:OG	1:D:360:GLY:O	1.98	0.79
1:I:117:ILE:HD11	1:I:122:PHE:HB2	1.65	0.78
1:K:349:SER:OG	1:K:360:GLY:O	2.01	0.78
1:F:60:ARG:NH1	1:F:104:GLU:CD	2.37	0.78
1:F:60:ARG:NH1	1:F:104:GLU:OE2	2.17	0.78
1:J:267:GLU:O	1:J:285:ARG:NH2	2.14	0.78
1:F:132:HIS:ND1	1:F:222:ILE:HD13	1.98	0.78
1:B:216:GLU:HB2	1:B:351:ILE:HG23	1.66	0.78
1:C:215:PHE:HD1	1:C:216:GLU:HG3	1.48	0.78
1:A:321:GLN:O	1:A:321:GLN:NE2	2.16	0.78
1:E:579:CYS:SG	1:E:635:TYR:CE2	2.59	0.77
1:F:232:PHE:CD1	1:F:348:GLU:OE1	2.37	0.77
1:I:208:HIS:CA	1:I:581:CYS:SG	2.72	0.77
1:A:67:LEU:HD11	1:A:96:ILE:HD13	1.66	0.77
1:D:164:GLU:OE2	1:G:37:ARG:NH1	2.18	0.77
1:K:618:VAL:HG23	1:K:632:ASP:OD1	1.84	0.77
1:F:349:SER:HB3	1:F:361:ASP:HA	1.67	0.77
1:J:231:LEU:HD11	1:J:579:CYS:HB3	1.67	0.77
1:F:556:ARG:CD	1:F:623:ASP:OD2	2.31	0.77
1:K:620:THR:HG23	1:K:628:CYS:O	1.85	0.77
1:I:621:CYS:C	1:I:631:ARG:NH1	2.38	0.76
1:K:620:THR:CG2	1:K:629:GLY:CA	2.63	0.76
1:A:132:HIS:HB3	1:A:222:ILE:HD12	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HG12	1:B:412:GLU:O	1.85	0.76
1:H:349:SER:HB3	1:H:361:ASP:HA	1.66	0.76
1:L:216:GLU:OE2	1:L:356:ARG:NH2	2.16	0.76
1:I:579:CYS:SG	1:I:579:CYS:O	2.42	0.76
1:K:618:VAL:CG2	1:K:632:ASP:OD1	2.34	0.76
1:F:60:ARG:HH11	1:F:104:GLU:CD	1.89	0.76
1:F:552:ILE:HD12	1:F:582:GLY:C	2.06	0.76
1:E:43:PRO:O	1:E:47:ASN:ND2	2.19	0.76
1:A:333:PHE:CE1	1:F:333:PHE:CE1	2.74	0.76
1:D:251:ARG:NE	1:L:251:ARG:HD2	2.01	0.76
1:E:67:LEU:HB3	1:E:71:MET:HE2	1.68	0.76
1:K:238:GLN:HB3	1:K:578:PHE:CZ	2.20	0.75
1:G:231:LEU:HD11	1:G:580:GLY:HA3	1.69	0.74
1:C:615:GLN:NE2	1:C:634:LEU:CB	2.46	0.74
1:A:28:ASP:OD1	1:A:56:ARG:NH2	2.21	0.74
1:D:94:ILE:HD13	1:D:128:VAL:HG11	1.69	0.74
1:H:257:ARG:HH22	1:I:304:ASP:CG	1.92	0.74
1:D:349:SER:HB2	1:D:361:ASP:HA	1.70	0.73
1:E:17:PRO:HD2	1:E:20:MET:CE	2.18	0.73
1:E:208:HIS:HB3	1:E:581:CYS:HB2	1.70	0.73
1:L:72:SER:OG	1:L:89:ILE:HD13	1.87	0.73
1:C:220:ARG:O	1:C:220:ARG:HG2	1.88	0.73
1:D:37:ARG:NH1	1:G:164:GLU:OE2	2.19	0.73
1:K:620:THR:OG1	1:K:629:GLY:CA	2.36	0.73
1:C:330:ASN:ND2	1:F:332:ILE:HD13	2.02	0.73
1:I:621:CYS:O	1:I:631:ARG:NH1	2.22	0.73
1:J:515:MET:HE1	1:J:523:PHE:CD2	2.24	0.73
1:D:212:VAL:HG22	1:D:213:TYR:CD1	2.23	0.73
1:F:132:HIS:CD2	1:F:222:ILE:HG12	2.24	0.73
1:F:131:LEU:HD21	1:F:141:LEU:CD2	2.19	0.72
1:I:415:ILE:HG22	1:I:648:LEU:CD2	2.16	0.72
1:C:82:PHE:O	1:C:87:ARG:NH2	2.23	0.72
1:K:620:THR:CB	1:K:629:GLY:HA3	2.18	0.72
1:A:132:HIS:HB3	1:A:222:ILE:CD1	2.17	0.72
1:F:132:HIS:ND1	1:F:222:ILE:CD1	2.53	0.72
1:C:217:ALA:HB3	1:C:223:VAL:HG23	1.71	0.72
1:F:552:ILE:HD13	1:F:552:ILE:H	1.55	0.72
1:D:39:ARG:CB	1:D:40:PRO:HD3	2.07	0.72
1:A:67:LEU:CD1	1:A:96:ILE:CD1	2.68	0.72
1:A:272:LYS:CE	1:I:382:GLU:OE2	2.37	0.72
1:C:28:ASP:OD1	1:C:56:ARG:NH2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:TYR:CD1	1:A:678:VAL:CG2	2.74	0.71
1:F:4:LYS:HE2	1:F:139:LEU:HD13	1.73	0.71
1:A:581:CYS:SG	1:A:581:CYS:O	2.49	0.71
1:C:310:ARG:O	1:C:314:ARG:HG3	1.89	0.71
1:J:161:ILE:CG2	1:J:462:MET:CE	2.63	0.71
1:K:242:ARG:HD2	1:K:578:PHE:CZ	2.25	0.71
1:C:349:SER:HB3	1:C:356:ARG:NH1	2.05	0.70
1:E:70:PRO:HD3	1:E:92:ARG:HD2	1.72	0.70
1:H:310:ARG:O	1:H:314:ARG:HG3	1.91	0.70
1:L:579:CYS:SG	1:L:630:VAL:HG21	2.30	0.70
1:A:254:ARG:CB	1:A:254:ARG:HH11	2.04	0.70
1:A:366:GLY:O	1:A:370:LEU:HD12	1.88	0.70
1:B:554:PHE:HD1	1:B:554:PHE:H	1.36	0.70
1:L:68:ARG:HD2	1:L:68:ARG:C	2.10	0.70
1:A:331:ARG:CZ	1:F:330:ASN:HB3	2.22	0.70
1:C:132:HIS:CG	1:C:222:ILE:HD11	2.26	0.70
1:E:579:CYS:HA	1:E:630:VAL:HG21	1.74	0.70
1:L:192:ARG:CZ	1:L:251:ARG:HH11	2.04	0.69
1:C:348:GLU:CB	1:C:363:HIS:HB3	2.21	0.69
1:A:310:ARG:O	1:A:314:ARG:HG3	1.91	0.69
1:E:620:THR:N	1:E:628:CYS:HB3	2.08	0.69
1:C:347:ILE:O	1:C:348:GLU:HB3	1.93	0.68
1:C:348:GLU:CA	1:C:363:HIS:HB3	2.23	0.68
1:D:60:ARG:NH1	1:D:104:GLU:OE1	2.26	0.68
1:C:132:HIS:CG	1:C:222:ILE:CD1	2.75	0.68
1:E:17:PRO:HD2	1:E:20:MET:HE3	1.74	0.68
1:F:126:LEU:C	1:F:127:SER:O	2.30	0.68
1:I:621:CYS:C	1:I:631:ARG:HH12	1.95	0.68
1:C:3:TYR:HB3	1:C:103:ILE:CD1	2.21	0.68
1:E:24:LYS:HD3	1:E:54:GLU:OE2	1.92	0.68
1:E:578:PHE:HB3	1:E:579:CYS:SG	2.34	0.68
1:L:132:HIS:ND1	1:L:222:ILE:HD13	2.09	0.68
1:D:231:LEU:HD11	1:D:629:GLY:HA2	1.73	0.68
1:F:132:HIS:CG	1:F:222:ILE:HG12	2.29	0.67
1:K:242:ARG:CD	1:K:578:PHE:CZ	2.77	0.67
1:K:620:THR:OG1	1:K:629:GLY:HA3	1.94	0.67
1:E:146:GLU:HB3	1:E:460:ARG:CD	2.21	0.67
1:E:487:GLN:OE1	1:E:540:ARG:NH1	2.28	0.67
1:A:450:TYR:CD1	1:A:678:VAL:HG23	2.29	0.67
1:B:555:GLU:O	1:B:558:PHE:HD2	1.77	0.67
1:A:678:VAL:CG1	1:A:679:PRO:CD	2.68	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:OE1	1:A:46:GLN:O	2.12	0.66
1:B:554:PHE:CD1	1:B:554:PHE:N	2.64	0.66
1:I:97:PHE:O	1:I:133:ARG:NH1	2.27	0.66
1:A:221:ALA:O	1:A:222:ILE:HG22	1.96	0.66
1:B:552:ILE:HG23	1:B:582:GLY:HA3	1.77	0.66
1:G:629:GLY:O	1:G:630:VAL:HG22	1.96	0.66
1:L:192:ARG:NH2	1:L:251:ARG:NH1	2.44	0.66
1:L:68:ARG:HD2	1:L:68:ARG:O	1.94	0.66
1:L:629:GLY:O	1:L:630:VAL:HG22	1.95	0.66
1:G:349:SER:HB3	1:G:361:ASP:OD1	1.95	0.66
1:E:552:ILE:HG23	1:E:582:GLY:HA3	1.77	0.65
1:F:104:GLU:OE1	1:F:105:GLU:HG3	1.96	0.65
1:F:629:GLY:O	1:F:630:VAL:HG22	1.96	0.65
1:H:577:ASN:N	1:H:627:TYR:HH	1.94	0.65
1:D:613:VAL:O	1:D:614:VAL:C	2.34	0.65
1:H:629:GLY:O	1:H:630:VAL:HG22	1.97	0.65
1:K:629:GLY:O	1:K:630:VAL:HG22	1.97	0.65
1:E:581:CYS:HA	1:E:622:ASN:HB2	1.78	0.65
1:H:257:ARG:NH2	1:I:304:ASP:CG	2.50	0.65
1:J:268:GLY:HA2	1:J:285:ARG:NH1	2.11	0.65
1:D:168:VAL:HG21	1:G:37:ARG:NH1	2.11	0.65
1:F:93:LEU:HD13	1:F:125:ALA:CB	2.26	0.65
1:C:349:SER:HB2	1:C:361:ASP:OD1	1.97	0.65
1:F:581:CYS:SG	1:F:623:ASP:C	2.75	0.65
1:J:629:GLY:O	1:J:630:VAL:HG22	1.96	0.64
1:L:579:CYS:HG	1:L:627:TYR:HH	1.44	0.64
1:F:556:ARG:HG2	1:F:623:ASP:OD2	1.96	0.64
1:G:680:ARG:HG2	1:G:680:ARG:HH21	1.60	0.64
1:L:101:ARG:NH2	1:L:105:GLU:OE2	2.29	0.64
1:L:232:PHE:CE1	1:L:348:GLU:OE2	2.50	0.64
1:B:219:ASN:HD21	1:D:609:GLU:HG2	1.63	0.64
1:J:25:SER:HB3	1:J:57:ILE:CD1	2.27	0.64
1:H:132:HIS:ND1	1:H:222:ILE:HD13	2.13	0.64
1:F:132:HIS:CG	1:F:222:ILE:CD1	2.81	0.63
1:I:349:SER:OG	1:I:356:ARG:HD2	1.99	0.63
1:F:37:ARG:CD	1:F:37:ARG:O	2.45	0.63
1:F:37:ARG:O	1:F:37:ARG:HD3	1.97	0.63
1:E:349:SER:CB	1:E:361:ASP:HA	2.28	0.63
1:G:37:ARG:HD2	1:G:37:ARG:C	2.18	0.63
1:D:349:SER:CB	1:D:361:ASP:HA	2.27	0.63
1:G:37:ARG:C	1:G:37:ARG:CD	2.67	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:550:VAL:HG13	1:K:578:PHE:HB2	1.80	0.63
1:K:132:HIS:ND1	1:K:222:ILE:HD13	2.13	0.63
1:E:132:HIS:ND1	1:E:222:ILE:HD13	2.14	0.63
1:I:579:CYS:SG	1:I:630:VAL:HG23	2.38	0.63
1:I:629:GLY:O	1:I:630:VAL:HG22	1.99	0.63
1:A:37:ARG:HD2	1:A:37:ARG:O	1.99	0.62
1:A:62:ILE:HD13	1:A:63:ALA:H	1.64	0.62
1:A:450:TYR:CD1	1:A:678:VAL:HG21	2.35	0.62
1:C:11:TYR:OH	1:C:141:LEU:HD21	1.99	0.62
1:G:37:ARG:CD	1:G:37:ARG:O	2.47	0.62
1:F:37:ARG:CD	1:F:37:ARG:C	2.67	0.62
1:A:615:GLN:O	1:E:220:ARG:NH2	2.28	0.62
1:A:678:VAL:HG12	1:A:679:PRO:HD3	1.75	0.62
1:D:19:PHE:HZ	1:D:38:TYR:CD2	2.18	0.62
1:F:62:ILE:HD12	1:F:105:GLU:HG2	1.80	0.62
1:J:349:SER:CB	1:J:361:ASP:HA	2.30	0.62
1:L:400:TYR:O	1:L:404:SER:HB2	2.00	0.62
1:B:146:GLU:OE2	1:B:558:PHE:HE1	1.83	0.62
1:G:132:HIS:ND1	1:G:222:ILE:HD13	2.14	0.62
1:J:132:HIS:ND1	1:J:222:ILE:HD13	2.13	0.62
1:C:400:TYR:O	1:C:404:SER:HB2	2.00	0.62
1:D:613:VAL:O	1:D:614:VAL:O	2.16	0.62
1:E:208:HIS:CB	1:E:581:CYS:HB2	2.30	0.62
1:J:179:PRO:HB3	4:J:805:HOH:O	1.97	0.62
1:L:349:SER:CB	1:L:361:ASP:HA	2.30	0.62
1:B:400:TYR:O	1:B:404:SER:HB2	2.00	0.62
1:C:216:GLU:OE2	1:C:356:ARG:NH2	2.26	0.62
1:G:349:SER:HB2	1:G:361:ASP:HA	1.81	0.62
1:K:349:SER:HB3	1:K:356:ARG:HH11	1.63	0.62
1:L:232:PHE:CD1	1:L:348:GLU:OE2	2.53	0.62
1:B:493:ASP:O	1:D:101:ARG:HG3	1.96	0.62
1:D:15:ARG:NH1	1:G:159:GLU:OE2	2.33	0.62
1:G:400:TYR:O	1:G:404:SER:HB2	2.00	0.62
1:C:77:GLU:OE1	1:H:156:ARG:NH2	2.32	0.61
1:C:280:ARG:HH21	1:H:154:ASP:CG	2.03	0.61
1:F:349:SER:CB	1:F:361:ASP:HA	2.30	0.61
1:K:400:TYR:O	1:K:404:SER:HB2	2.00	0.61
1:K:579:CYS:HA	1:K:627:TYR:CE2	2.35	0.61
1:B:349:SER:HB3	1:B:356:ARG:HH11	1.65	0.61
1:D:557:THR:HG22	1:D:557:THR:O	2.01	0.61
1:F:400:TYR:O	1:F:404:SER:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:400:TYR:O	1:H:404:SER:HB2	2.00	0.61
1:A:3:TYR:HB3	1:A:103:ILE:CG2	2.30	0.61
1:A:631:ARG:O	1:A:632:ASP:HB2	1.99	0.61
1:B:219:ASN:ND2	1:D:609:GLU:HG2	2.16	0.61
1:I:639:LYS:HE3	1:I:643:PHE:CZ	2.36	0.61
1:J:400:TYR:O	1:J:404:SER:HB2	2.00	0.61
1:A:254:ARG:HH11	1:A:254:ARG:HB3	1.65	0.61
1:J:349:SER:HB3	1:J:356:ARG:HH11	1.65	0.61
1:D:400:TYR:O	1:D:404:SER:HB2	2.00	0.61
1:F:240:ILE:HD11	1:F:403:HIS:HB3	1.83	0.61
1:I:117:ILE:HD11	1:I:122:PHE:CB	2.30	0.61
1:C:94:ILE:HD13	1:C:128:VAL:HB	1.81	0.61
1:J:349:SER:HB2	1:J:361:ASP:HA	1.82	0.61
1:A:400:TYR:O	1:A:404:SER:HB2	2.00	0.61
1:C:11:TYR:OH	1:C:141:LEU:CD2	2.49	0.61
1:D:227:ARG:NH2	1:D:637:ASP:O	2.34	0.61
1:F:37:ARG:C	1:F:37:ARG:HD2	2.21	0.61
1:I:227:ARG:NH2	1:I:637:ASP:O	2.34	0.61
1:C:227:ARG:NH2	1:C:637:ASP:O	2.34	0.61
1:H:349:SER:CB	1:H:361:ASP:HA	2.31	0.61
1:I:400:TYR:O	1:I:404:SER:HB2	2.00	0.61
1:C:137:LYS:HD3	1:C:137:LYS:C	2.21	0.61
1:D:164:GLU:CD	1:G:37:ARG:HH11	2.04	0.61
1:H:208:HIS:CB	1:H:581:CYS:HB2	2.31	0.61
1:J:208:HIS:CG	1:J:581:CYS:SG	2.93	0.61
1:C:103:ILE:HG22	1:C:135:ASP:OD2	2.00	0.61
1:E:240:ILE:HD11	1:E:403:HIS:HB3	1.83	0.61
1:F:65:PRO:HB2	1:F:96:ILE:CD1	2.30	0.61
1:I:240:ILE:HD11	1:I:403:HIS:HB3	1.82	0.61
1:A:240:ILE:HD11	1:A:403:HIS:HB3	1.83	0.60
1:E:230:GLU:C	1:E:641:MET:HE3	2.21	0.60
1:L:240:ILE:HD11	1:L:403:HIS:HB3	1.83	0.60
1:A:227:ARG:NH2	1:A:637:ASP:O	2.34	0.60
1:A:349:SER:HB2	1:A:361:ASP:HA	1.83	0.60
1:B:240:ILE:HD11	1:B:403:HIS:HB3	1.83	0.60
1:B:349:SER:CB	1:B:361:ASP:HA	2.30	0.60
1:E:400:TYR:O	1:E:404:SER:HB2	2.01	0.60
1:G:227:ARG:NH2	1:G:637:ASP:O	2.34	0.60
1:H:227:ARG:NH2	1:H:637:ASP:O	2.34	0.60
1:J:227:ARG:NH2	1:J:637:ASP:O	2.34	0.60
1:K:227:ARG:NH2	1:K:637:ASP:O	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:ARG:NH1	1:L:251:ARG:HE	1.99	0.60
1:L:227:ARG:NH2	1:L:637:ASP:O	2.35	0.60
1:E:227:ARG:NH2	1:E:637:ASP:O	2.34	0.60
1:D:37:ARG:HD3	1:D:37:ARG:C	2.22	0.60
1:G:304:ASP:OD2	1:L:257:ARG:NH1	2.34	0.60
1:J:240:ILE:HD11	1:J:403:HIS:HB3	1.83	0.60
1:L:349:SER:HB2	1:L:361:ASP:HA	1.83	0.60
1:A:30:PRO:HD3	1:A:59:VAL:HG13	1.81	0.60
1:A:349:SER:CB	1:A:361:ASP:HA	2.31	0.60
1:D:240:ILE:HD11	1:D:403:HIS:HB3	1.83	0.60
1:K:349:SER:CB	1:K:361:ASP:HA	2.32	0.60
1:A:452:GLN:OE1	1:A:478:GLN:HG2	2.02	0.60
1:F:98:MET:CE	1:F:132:HIS:O	2.48	0.60
1:C:11:TYR:CZ	1:C:141:LEU:HD23	2.37	0.60
1:G:349:SER:CB	1:G:361:ASP:HA	2.31	0.60
1:H:240:ILE:HD11	1:H:403:HIS:HB3	1.83	0.60
1:B:227:ARG:NH2	1:B:637:ASP:O	2.34	0.60
1:A:307:ASP:OD1	1:A:310:ARG:NH1	2.29	0.59
1:B:349:SER:HB2	1:B:361:ASP:HA	1.83	0.59
1:C:330:ASN:ND2	1:F:332:ILE:CD1	2.65	0.59
1:G:37:ARG:O	1:G:37:ARG:HD3	2.02	0.59
1:H:208:HIS:HB3	1:H:581:CYS:HB2	1.84	0.59
1:K:349:SER:HB2	1:K:361:ASP:HA	1.83	0.59
1:I:117:ILE:HD11	1:I:122:PHE:CA	2.33	0.59
1:K:240:ILE:HD11	1:K:403:HIS:HB3	1.83	0.59
1:F:227:ARG:NH2	1:F:637:ASP:O	2.35	0.59
1:F:552:ILE:HG23	1:F:582:GLY:HA3	1.84	0.59
1:A:81:LEU:O	1:A:87:ARG:HD2	2.03	0.59
1:C:348:GLU:HB2	1:C:363:HIS:CB	2.30	0.59
1:C:348:GLU:HG3	1:C:363:HIS:HD1	1.66	0.59
1:L:349:SER:HB3	1:L:356:ARG:HH11	1.67	0.59
1:C:132:HIS:CE1	1:C:222:ILE:HD11	2.37	0.59
1:G:240:ILE:HD11	1:G:403:HIS:HB3	1.83	0.59
1:C:330:ASN:HD21	1:F:332:ILE:HD13	1.66	0.59
1:G:304:ASP:CG	1:L:257:ARG:HH12	2.06	0.59
1:C:349:SER:HG	1:C:361:ASP:HA	1.66	0.59
1:L:132:HIS:CG	1:L:222:ILE:CD1	2.85	0.59
1:F:30:PRO:HD3	1:F:59:VAL:HG13	1.85	0.58
1:I:579:CYS:HA	1:I:627:TYR:CE2	2.38	0.58
1:A:349:SER:HB3	1:A:356:ARG:HH11	1.67	0.58
1:D:30:PRO:HD3	1:D:59:VAL:HG13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ASN:C	1:E:251:ARG:HD3	2.22	0.58
1:K:620:THR:HG23	1:K:629:GLY:CA	2.25	0.58
1:D:81:LEU:O	1:D:87:ARG:HD2	2.03	0.58
1:J:515:MET:CE	1:J:523:PHE:CD2	2.86	0.58
1:C:44:GLU:HG2	1:H:169:PRO:HG2	1.85	0.58
1:D:349:SER:O	1:D:356:ARG:NH1	2.37	0.58
1:F:455:ASP:OD1	1:F:473:ARG:HG3	2.02	0.58
1:B:333:PHE:CZ	1:D:331:ARG:HB2	2.38	0.58
1:D:348:GLU:HA	1:D:363:HIS:HB3	1.84	0.58
1:G:62:ILE:CG2	1:G:64:LEU:HD13	2.34	0.58
1:J:30:PRO:HD3	1:J:59:VAL:HG13	1.86	0.58
1:K:30:PRO:HD3	1:K:59:VAL:HG13	1.86	0.58
1:F:101:ARG:H	1:F:101:ARG:HD2	1.69	0.58
1:H:552:ILE:HG23	1:H:582:GLY:HA3	1.84	0.58
1:L:30:PRO:HD3	1:L:59:VAL:HG13	1.86	0.58
1:C:240:ILE:HD11	1:C:403:HIS:HB3	1.85	0.58
1:E:81:LEU:O	1:E:87:ARG:HD2	2.04	0.58
1:E:581:CYS:SG	1:E:622:ASN:ND2	2.76	0.58
1:A:46:GLN:OE1	1:A:46:GLN:C	2.42	0.58
1:J:81:LEU:O	1:J:87:ARG:HD2	2.04	0.58
1:J:552:ILE:HG23	1:J:582:GLY:HA3	1.86	0.58
1:B:615:GLN:HE22	1:B:634:LEU:H	1.51	0.57
1:D:631:ARG:HG3	1:D:633:ARG:HG3	1.85	0.57
1:F:81:LEU:O	1:F:87:ARG:HD2	2.04	0.57
1:H:81:LEU:O	1:H:87:ARG:HD2	2.04	0.57
1:A:132:HIS:CD2	1:A:222:ILE:CD1	2.79	0.57
1:B:615:GLN:HE21	1:B:633:ARG:HB2	1.68	0.57
1:H:30:PRO:HD3	1:H:59:VAL:HG13	1.85	0.57
1:G:81:LEU:O	1:G:87:ARG:HD2	2.04	0.57
1:D:615:GLN:HE22	1:D:633:ARG:HB2	1.69	0.57
1:G:30:PRO:HD3	1:G:59:VAL:HG13	1.85	0.57
1:I:30:PRO:HD3	1:I:59:VAL:HG13	1.86	0.57
1:I:132:HIS:NE2	1:I:222:ILE:HG21	2.19	0.57
1:L:69:ILE:HB	1:L:70:PRO:HD3	1.86	0.57
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.19	0.57
1:B:91:ALA:HB1	1:B:217:ALA:O	2.04	0.57
1:E:231:LEU:HD21	1:E:579:CYS:HB2	1.87	0.57
1:I:349:SER:HB2	1:I:361:ASP:HA	1.87	0.57
1:L:253:GLN:CG	1:L:510:GLU:OE2	2.47	0.57
1:B:30:PRO:HD3	1:B:59:VAL:HG13	1.86	0.57
1:E:579:CYS:HB3	1:E:630:VAL:HG11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:LEU:HD12	1:L:81:LEU:N	2.17	0.57
1:B:81:LEU:O	1:B:87:ARG:HD2	2.05	0.57
1:C:552:ILE:HG23	1:C:582:GLY:HA3	1.87	0.57
1:D:357:GLN:HG2	1:E:416:LYS:NZ	2.19	0.57
1:E:69:ILE:HB	1:E:70:PRO:HD3	1.85	0.57
1:K:552:ILE:HG23	1:K:582:GLY:HA3	1.86	0.57
1:E:526:GLU:OE2	1:E:578:PHE:CE2	2.58	0.57
1:E:552:ILE:HD12	1:E:556:ARG:HG2	1.87	0.57
1:G:218:SER:OG	1:G:220:ARG:HG3	2.05	0.57
1:C:481:PRO:HD2	4:C:817:HOH:O	2.05	0.57
1:E:556:ARG:NH2	1:E:621:CYS:SG	2.78	0.57
1:F:132:HIS:CE1	1:F:222:ILE:HD13	2.40	0.57
1:D:69:ILE:HB	1:D:70:PRO:HD3	1.86	0.56
1:F:617:LEU:HD13	1:F:617:LEU:N	2.21	0.56
1:B:492:SER:O	1:B:493:ASP:HB2	2.06	0.56
1:C:349:SER:CB	1:C:361:ASP:HA	2.36	0.56
1:K:81:LEU:O	1:K:87:ARG:HD2	2.05	0.56
1:L:81:LEU:H	1:L:81:LEU:CD1	2.15	0.56
1:D:91:ALA:HB2	1:D:216:GLU:OE2	2.05	0.56
1:C:492:SER:O	1:C:493:ASP:HB2	2.06	0.56
1:C:507:LYS:HE2	1:C:668:SER:OG	2.06	0.56
1:F:62:ILE:CD1	1:F:105:GLU:HG2	2.35	0.56
1:I:348:GLU:HA	1:I:363:HIS:HB3	1.85	0.56
1:L:552:ILE:HG23	1:L:582:GLY:HA3	1.87	0.56
1:B:4:LYS:HE2	1:B:139:LEU:HD13	1.86	0.56
1:C:612:ARG:NH2	1:F:101:ARG:HB3	2.21	0.56
1:E:552:ILE:HD11	1:E:556:ARG:HB3	1.87	0.56
1:F:492:SER:O	1:F:493:ASP:HB2	2.05	0.56
1:I:81:LEU:O	1:I:87:ARG:HD2	2.05	0.56
1:J:492:SER:O	1:J:493:ASP:HB2	2.06	0.56
1:C:349:SER:OG	1:C:361:ASP:HA	2.05	0.56
1:K:620:THR:HB	1:K:631:ARG:H	1.70	0.56
1:E:146:GLU:CB	1:E:460:ARG:HD2	2.24	0.56
1:I:492:SER:O	1:I:493:ASP:HB2	2.06	0.56
1:K:492:SER:O	1:K:493:ASP:HB2	2.06	0.56
1:K:620:THR:HG21	1:K:630:VAL:H	1.71	0.56
1:B:216:GLU:HB2	1:B:351:ILE:CG2	2.35	0.56
1:B:348:GLU:HA	1:B:363:HIS:HB3	1.88	0.56
1:E:30:PRO:HD3	1:E:59:VAL:HG13	1.87	0.56
1:E:132:HIS:CG	1:E:222:ILE:CD1	2.89	0.56
1:E:492:SER:O	1:E:493:ASP:HB2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:ARG:NH1	1:F:310:ARG:HG3	2.20	0.56
1:A:103:ILE:HG13	1:A:135:ASP:OD2	2.05	0.55
1:C:132:HIS:ND1	1:C:222:ILE:HD11	2.21	0.55
1:H:492:SER:O	1:H:493:ASP:HB2	2.06	0.55
1:K:242:ARG:NE	1:K:578:PHE:CZ	2.75	0.55
1:K:579:CYS:HA	1:K:627:TYR:HE2	1.69	0.55
1:A:492:SER:O	1:A:493:ASP:HB2	2.06	0.55
1:B:633:ARG:HH21	1:D:616:ASP:HB3	1.70	0.55
1:J:132:HIS:CG	1:J:222:ILE:CD1	2.89	0.55
1:K:132:HIS:CG	1:K:222:ILE:CD1	2.89	0.55
1:I:620:THR:O	1:I:631:ARG:HG2	2.06	0.55
1:C:100:MET:SD	1:C:109:CYS:HB2	2.46	0.55
1:A:69:ILE:HB	1:A:70:PRO:HD3	1.87	0.55
1:A:132:HIS:CG	1:A:222:ILE:HD12	2.31	0.55
1:E:132:HIS:CD2	1:E:222:ILE:HG12	2.41	0.55
1:G:132:HIS:CD2	1:G:222:ILE:HG12	2.42	0.55
1:G:132:HIS:CG	1:G:222:ILE:CD1	2.89	0.55
1:H:577:ASN:ND2	1:H:635:TYR:OH	2.39	0.55
1:H:132:HIS:CG	1:H:222:ILE:CD1	2.89	0.55
1:L:72:SER:OG	1:L:89:ILE:HD11	2.02	0.55
1:A:94:ILE:O	1:A:98:MET:HB2	2.07	0.55
1:C:348:GLU:O	1:C:348:GLU:HG2	2.06	0.55
1:H:531:LEU:HD12	1:H:532:VAL:N	2.22	0.55
1:J:132:HIS:CD2	1:J:222:ILE:HG12	2.42	0.55
1:K:550:VAL:HG13	1:K:578:PHE:CB	2.37	0.55
1:L:81:LEU:O	1:L:87:ARG:HD2	2.06	0.55
1:L:492:SER:O	1:L:493:ASP:HB2	2.06	0.55
1:A:156:ARG:HA	1:I:279:SER:HB3	1.87	0.55
1:B:64:LEU:HD13	1:B:112:PHE:CD2	2.42	0.55
1:B:319:VAL:HG13	1:B:412:GLU:O	1.98	0.55
1:D:94:ILE:O	1:D:98:MET:HB2	2.07	0.55
1:D:42:GLY:N	1:D:43:PRO:HD2	2.20	0.55
1:L:72:SER:HG	1:L:89:ILE:CD1	2.19	0.55
1:L:348:GLU:HA	1:L:363:HIS:HB3	1.89	0.55
1:A:226:ASP:CG	1:A:634:LEU:CD1	2.75	0.54
1:C:219:ASN:OD1	1:F:614:VAL:CG2	2.55	0.54
1:D:492:SER:O	1:D:493:ASP:HB2	2.06	0.54
1:F:616:ASP:O	1:F:632:ASP:OD2	2.25	0.54
1:G:492:SER:O	1:G:493:ASP:HB2	2.06	0.54
1:I:621:CYS:HA	1:I:631:ARG:CZ	2.37	0.54
1:C:609:GLU:HG2	1:F:101:ARG:HG2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HB	1:G:70:PRO:HD3	1.90	0.54
1:E:661:THR:OG1	1:E:662:PRO:HD2	2.08	0.54
1:D:615:GLN:NE2	1:D:633:ARG:HB2	2.23	0.54
1:F:98:MET:HE3	1:F:132:HIS:C	2.27	0.54
1:H:132:HIS:CD2	1:H:222:ILE:HG12	2.42	0.54
1:K:132:HIS:CD2	1:K:222:ILE:HG12	2.43	0.54
1:A:132:HIS:CB	1:A:222:ILE:HD12	2.26	0.54
1:E:503:PHE:CD1	1:E:645:PHE:HE1	2.26	0.54
1:I:69:ILE:HB	1:I:70:PRO:HD3	1.90	0.54
1:J:268:GLY:HA2	1:J:285:ARG:HH12	1.73	0.54
1:A:132:HIS:CE1	1:A:222:ILE:HD11	2.40	0.54
1:B:633:ARG:NH2	1:D:616:ASP:HB3	2.22	0.54
1:C:69:ILE:HB	1:C:70:PRO:HD3	1.90	0.53
1:E:425:LEU:O	1:E:661:THR:HG21	2.08	0.53
1:C:62:ILE:CD1	1:C:105:GLU:HG2	2.38	0.53
1:E:156:ARG:HA	1:J:279:SER:HB3	1.90	0.53
1:L:132:HIS:ND1	1:L:222:ILE:CD1	2.71	0.53
1:L:215:PHE:HB3	1:L:348:GLU:OE1	2.08	0.53
1:I:556:ARG:HD2	1:I:622:ASN:HD21	1.72	0.53
1:J:120:TYR:OH	1:J:150:ASP:OD2	2.24	0.53
1:D:3:TYR:HB3	1:D:103:ILE:HG12	1.90	0.53
1:E:20:MET:HE2	1:J:167:VAL:HG22	1.91	0.53
1:F:103:ILE:HG23	1:F:103:ILE:O	2.08	0.53
1:G:120:TYR:OH	1:G:150:ASP:OD2	2.24	0.53
1:L:216:GLU:O	1:L:217:ALA:HB2	2.09	0.53
1:C:30:PRO:HD3	1:C:59:VAL:HG13	1.88	0.53
1:A:215:PHE:CE2	1:A:364:ASN:ND2	2.77	0.53
1:K:242:ARG:NE	1:K:578:PHE:CE2	2.71	0.53
1:K:621:CYS:SG	1:K:622:ASN:ND2	2.81	0.53
1:A:349:SER:O	1:A:356:ARG:NH1	2.42	0.53
1:C:132:HIS:CD2	1:C:222:ILE:HD11	2.44	0.53
1:B:101:ARG:CB	1:D:494:ALA:HA	2.17	0.53
1:C:83:ILE:O	1:C:87:ARG:HG2	2.09	0.53
1:E:231:LEU:HD21	1:E:579:CYS:CB	2.39	0.53
1:E:581:CYS:SG	1:E:622:ASN:CG	2.87	0.53
1:L:503:PHE:CD1	1:L:645:PHE:HE2	2.27	0.53
1:E:218:SER:OG	1:E:220:ARG:HG3	2.09	0.53
1:E:552:ILE:CD1	1:E:556:ARG:HB3	2.39	0.53
1:H:145:VAL:HG23	1:H:204:LEU:HD21	1.91	0.53
1:I:552:ILE:HG23	1:I:582:GLY:HA3	1.90	0.53
1:K:348:GLU:HA	1:K:363:HIS:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:579:CYS:SG	1:L:627:TYR:CZ	2.99	0.53
1:H:348:GLU:HA	1:H:363:HIS:HB3	1.91	0.52
1:E:49:PHE:HZ	1:J:167:VAL:HA	1.74	0.52
1:C:216:GLU:CD	1:C:356:ARG:HH22	2.12	0.52
1:C:349:SER:HB2	1:C:361:ASP:HA	1.90	0.52
1:H:69:ILE:HB	1:H:70:PRO:HD3	1.92	0.52
1:I:145:VAL:HG23	1:I:204:LEU:HD21	1.92	0.52
1:L:132:HIS:CD2	1:L:222:ILE:HG12	2.45	0.52
1:C:348:GLU:HG3	1:C:363:HIS:ND1	2.24	0.52
1:D:279:SER:HB3	1:G:156:ARG:HA	1.92	0.52
1:J:145:VAL:HG23	1:J:204:LEU:HD21	1.91	0.52
1:K:145:VAL:HG23	1:K:204:LEU:HD21	1.92	0.52
1:K:69:ILE:HB	1:K:70:PRO:HD3	1.91	0.52
1:L:295:ASN:HB2	4:L:805:HOH:O	2.08	0.52
1:A:226:ASP:CG	1:A:634:LEU:HD13	2.30	0.52
1:D:60:ARG:CZ	1:D:104:GLU:OE1	2.58	0.52
1:E:304:ASP:CG	1:F:257:ARG:HH12	2.12	0.52
1:F:348:GLU:HA	1:F:363:HIS:HB3	1.91	0.52
1:H:531:LEU:HD12	1:H:532:VAL:H	1.75	0.52
1:J:231:LEU:HD11	1:J:579:CYS:HB2	1.92	0.52
1:A:423:SER:HB2	1:F:423:SER:OG	2.08	0.52
1:C:145:VAL:HG23	1:C:204:LEU:HD21	1.92	0.52
1:D:349:SER:HB3	1:D:356:ARG:HH11	1.74	0.52
1:E:67:LEU:HB3	1:E:71:MET:CE	2.36	0.52
1:E:304:ASP:OD2	1:F:257:ARG:NH1	2.42	0.52
1:F:92:ARG:NH2	1:F:96:ILE:HD11	2.25	0.52
1:J:218:SER:OG	1:J:220:ARG:HG3	2.10	0.52
1:K:216:GLU:O	1:K:217:ALA:HB2	2.09	0.52
1:C:94:ILE:HD13	1:C:128:VAL:CB	2.40	0.52
1:G:37:ARG:HD2	1:G:37:ARG:O	2.10	0.52
1:D:281:THR:HG23	1:G:281:THR:HG23	1.91	0.52
1:E:216:GLU:O	1:E:217:ALA:HB2	2.10	0.52
1:E:552:ILE:CD1	1:E:556:ARG:HG2	2.40	0.52
1:J:579:CYS:N	1:J:627:TYR:CE2	2.78	0.52
1:C:279:SER:HB3	1:H:156:ARG:HA	1.92	0.52
1:D:85:ARG:O	1:D:88:LYS:HG2	2.10	0.51
1:F:145:VAL:HG23	1:F:204:LEU:HD21	1.91	0.51
1:H:132:HIS:CG	1:H:222:ILE:HG12	2.45	0.51
1:C:609:GLU:OE1	1:F:101:ARG:HD3	2.09	0.51
1:E:145:VAL:HG23	1:E:204:LEU:HD21	1.91	0.51
1:E:192:ARG:NH1	1:E:251:ARG:NE	2.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:GLU:O	1:J:217:ALA:HB2	2.10	0.51
1:A:333:PHE:CE1	1:F:333:PHE:CD1	2.98	0.51
1:G:556:ARG:HD2	1:G:622:ASN:HD21	1.76	0.51
1:K:620:THR:O	1:K:621:CYS:HB3	2.10	0.51
1:F:3:TYR:HB3	1:F:103:ILE:HG23	1.93	0.51
1:F:216:GLU:O	1:F:217:ALA:HB2	2.10	0.51
1:J:500:VAL:O	1:J:529:LYS:HA	2.11	0.51
1:L:540:ARG:O	1:L:540:ARG:CG	2.54	0.51
1:A:42:GLY:O	1:A:45:ILE:HB	2.09	0.51
1:D:145:VAL:HG23	1:D:204:LEU:HD21	1.91	0.51
1:G:145:VAL:HG23	1:G:204:LEU:HD21	1.92	0.51
1:A:223:VAL:O	1:A:228:ARG:HD2	2.11	0.51
1:C:79:PHE:O	1:C:86:HIS:CD2	2.63	0.51
1:D:218:SER:OG	1:D:219:ASN:N	2.44	0.51
1:E:478:GLN:NE2	1:E:554:PHE:HZ	2.09	0.51
1:G:216:GLU:O	1:G:217:ALA:HB2	2.11	0.51
1:H:556:ARG:HD2	1:H:622:ASN:HD21	1.74	0.51
1:J:132:HIS:CG	1:J:222:ILE:HG12	2.46	0.51
1:K:500:VAL:O	1:K:529:LYS:HA	2.11	0.51
1:B:146:GLU:OE2	1:B:558:PHE:CE1	2.63	0.51
1:B:500:VAL:O	1:B:529:LYS:HA	2.11	0.51
1:F:3:TYR:HB3	1:F:103:ILE:CG2	2.41	0.51
1:F:500:VAL:O	1:F:529:LYS:HA	2.11	0.51
1:H:500:VAL:O	1:H:529:LYS:HA	2.11	0.51
1:I:209:TRP:HD1	1:I:580:GLY:HA3	1.76	0.51
1:I:500:VAL:O	1:I:529:LYS:HA	2.11	0.51
1:K:556:ARG:HD2	1:K:622:ASN:HD21	1.76	0.51
1:A:321:GLN:HG3	1:A:323:TYR:CZ	2.45	0.51
1:I:453:GLN:HA	1:I:474:PHE:O	2.11	0.51
1:J:515:MET:HE1	1:J:523:PHE:CE2	2.44	0.51
1:D:39:ARG:HG2	1:D:39:ARG:HH21	1.75	0.51
1:D:500:VAL:O	1:D:529:LYS:HA	2.11	0.51
1:I:31:ASP:O	1:I:39:ARG:HD3	2.09	0.51
1:L:145:VAL:HG23	1:L:204:LEU:HD21	1.91	0.51
1:L:579:CYS:HA	1:L:627:TYR:CE2	2.46	0.51
1:C:31:ASP:O	1:C:39:ARG:HD3	2.11	0.51
1:D:77:GLU:OE1	1:G:156:ARG:NH2	2.36	0.51
1:D:613:VAL:O	1:D:615:GLN:HB2	2.11	0.51
1:E:500:VAL:O	1:E:529:LYS:HA	2.11	0.51
1:J:69:ILE:HB	1:J:70:PRO:HD3	1.93	0.51
1:L:453:GLN:HA	1:L:474:PHE:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:O	1:B:228:ARG:HD2	2.11	0.50
1:D:453:GLN:HA	1:D:474:PHE:O	2.11	0.50
1:E:20:MET:CE	1:J:167:VAL:HG22	2.40	0.50
1:E:132:HIS:CG	1:E:222:ILE:HG12	2.45	0.50
1:E:453:GLN:HA	1:E:474:PHE:O	2.11	0.50
1:F:93:LEU:HD13	1:F:125:ALA:HB1	1.93	0.50
1:A:145:VAL:HG23	1:A:204:LEU:HD21	1.92	0.50
1:A:217:ALA:HB3	1:A:223:VAL:HG23	1.92	0.50
1:B:156:ARG:HA	1:K:279:SER:HB3	1.93	0.50
1:D:507:LYS:HE3	1:D:668:SER:OG	2.12	0.50
1:G:348:GLU:HA	1:G:363:HIS:HB3	1.92	0.50
1:H:140:ASP:OD2	1:H:559:ARG:CZ	2.60	0.50
1:I:85:ARG:O	1:I:88:LYS:HG2	2.11	0.50
1:L:192:ARG:NH1	1:L:251:ARG:NE	2.59	0.50
1:C:330:ASN:HD22	1:F:332:ILE:CD1	2.25	0.50
1:C:500:VAL:O	1:C:529:LYS:HA	2.11	0.50
1:F:251:ARG:HE	1:J:251:ARG:NE	2.08	0.50
1:J:52:LEU:O	1:J:52:LEU:HD23	2.11	0.50
1:J:453:GLN:HA	1:J:474:PHE:O	2.11	0.50
1:E:348:GLU:HA	1:E:363:HIS:HB3	1.93	0.50
1:F:453:GLN:HA	1:F:474:PHE:O	2.11	0.50
1:J:348:GLU:HA	1:J:363:HIS:HB3	1.93	0.50
1:E:581:CYS:SG	1:E:622:ASN:HB2	2.52	0.50
1:F:132:HIS:CG	1:F:222:ILE:CG1	2.95	0.50
1:F:552:ILE:HD13	1:F:583:TRP:O	2.12	0.50
1:G:62:ILE:HG22	1:G:64:LEU:CD1	2.42	0.50
1:G:62:ILE:HG23	1:G:64:LEU:HD13	1.94	0.50
1:B:353:SER:HB3	1:B:356:ARG:HG2	1.94	0.50
1:E:349:SER:O	1:E:356:ARG:NH1	2.45	0.50
1:E:353:SER:HB3	1:E:356:ARG:HG2	1.93	0.50
1:E:478:GLN:NE2	1:E:554:PHE:CZ	2.80	0.50
1:G:453:GLN:HA	1:G:474:PHE:O	2.11	0.50
1:J:556:ARG:HD2	1:J:622:ASN:HD21	1.77	0.50
1:E:132:HIS:ND1	1:E:222:ILE:CD1	2.74	0.50
1:H:216:GLU:O	1:H:217:ALA:HB2	2.11	0.50
1:K:132:HIS:CG	1:K:222:ILE:HG12	2.47	0.50
1:K:620:THR:OG1	1:K:630:VAL:N	2.45	0.50
1:A:321:GLN:NE2	1:A:323:TYR:CE2	2.79	0.50
1:B:145:VAL:HG23	1:B:204:LEU:HD21	1.92	0.50
1:C:156:ARG:HA	1:H:279:SER:HB3	1.94	0.50
1:G:500:VAL:O	1:G:529:LYS:HA	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:HIS:CD2	1:I:222:ILE:HG21	2.47	0.50
1:B:453:GLN:HA	1:B:474:PHE:O	2.11	0.50
1:H:526:GLU:OE2	1:H:577:ASN:HB2	2.11	0.50
1:L:500:VAL:O	1:L:529:LYS:HA	2.11	0.50
1:A:103:ILE:CG2	1:A:103:ILE:O	2.60	0.49
1:C:609:GLU:OE1	1:F:101:ARG:NH1	2.42	0.49
1:F:69:ILE:HB	1:F:70:PRO:HD3	1.94	0.49
1:F:622:ASN:OD1	1:F:629:GLY:CA	2.54	0.49
1:G:621:CYS:SG	1:G:622:ASN:N	2.85	0.49
1:K:238:GLN:HB3	1:K:578:PHE:CE2	2.47	0.49
1:K:453:GLN:HA	1:K:474:PHE:O	2.11	0.49
1:L:556:ARG:HD2	1:L:622:ASN:HD21	1.76	0.49
1:A:453:GLN:HA	1:A:474:PHE:O	2.12	0.49
1:C:223:VAL:O	1:C:228:ARG:HD2	2.12	0.49
1:C:453:GLN:HA	1:C:474:PHE:O	2.11	0.49
1:F:132:HIS:CG	1:F:222:ILE:HD11	2.46	0.49
1:H:132:HIS:ND1	1:H:222:ILE:CD1	2.75	0.49
1:K:132:HIS:ND1	1:K:222:ILE:CD1	2.74	0.49
1:F:37:ARG:NH2	1:L:164:GLU:OE2	2.46	0.49
1:H:453:GLN:HA	1:H:474:PHE:O	2.11	0.49
1:I:216:GLU:O	1:I:217:ALA:HB2	2.10	0.49
1:J:581:CYS:SG	1:J:622:ASN:OD1	2.70	0.49
1:K:223:VAL:O	1:K:228:ARG:HD2	2.12	0.49
1:A:24:LYS:HB3	1:A:54:GLU:HG3	1.95	0.49
1:A:220:ARG:HB3	1:A:224:ASP:HB2	1.93	0.49
1:B:503:PHE:CD1	1:B:645:PHE:HE1	2.30	0.49
1:D:19:PHE:CZ	1:D:38:TYR:CD2	3.00	0.49
1:F:37:ARG:O	1:F:37:ARG:HD2	2.11	0.49
1:F:353:SER:HB3	1:F:356:ARG:HG2	1.94	0.49
1:D:93:LEU:HD11	1:D:117:ILE:CD1	2.42	0.49
1:J:132:HIS:ND1	1:J:222:ILE:CD1	2.75	0.49
1:J:621:CYS:SG	1:J:622:ASN:N	2.85	0.49
1:A:423:SER:CB	1:F:423:SER:OG	2.60	0.49
1:A:500:VAL:O	1:A:529:LYS:HA	2.11	0.49
1:E:94:ILE:O	1:E:98:MET:HB2	2.13	0.49
1:C:42:GLY:N	1:C:43:PRO:HD2	2.26	0.49
1:C:627:TYR:HE1	1:C:631:ARG:HH12	1.59	0.49
1:D:353:SER:HB3	1:D:356:ARG:HG2	1.94	0.49
1:G:353:SER:HB3	1:G:356:ARG:HG2	1.94	0.49
1:H:503:PHE:CD1	1:H:645:PHE:HE1	2.30	0.49
1:J:26:VAL:CG1	1:J:56:ARG:HG3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:SER:OG	1:K:220:ARG:HG3	2.13	0.49
1:A:67:LEU:HD12	1:A:96:ILE:CD1	2.42	0.49
1:C:84:PRO:HA	1:C:87:ARG:HG3	1.95	0.49
1:J:223:VAL:O	1:J:228:ARG:HD2	2.13	0.49
1:A:338:LYS:HZ3	1:E:328:SER:CB	2.25	0.49
1:E:581:CYS:SG	1:E:622:ASN:CB	3.01	0.49
1:L:223:VAL:O	1:L:228:ARG:HD2	2.13	0.49
1:L:349:SER:HG	1:L:361:ASP:HA	1.77	0.49
1:D:212:VAL:HG22	1:D:213:TYR:CE1	2.49	0.48
1:L:621:CYS:SG	1:L:622:ASN:N	2.86	0.48
1:A:450:TYR:CE1	1:A:678:VAL:HG21	2.47	0.48
1:B:69:ILE:HB	1:B:70:PRO:HD3	1.94	0.48
1:C:281:THR:HG23	1:H:281:THR:HG23	1.95	0.48
1:L:132:HIS:CE1	1:L:222:ILE:HD13	2.48	0.48
1:I:232:PHE:CZ	1:I:348:GLU:HB3	2.47	0.48
1:I:349:SER:CB	1:I:361:ASP:OD1	2.61	0.48
1:I:621:CYS:SG	1:I:622:ASN:N	2.85	0.48
1:L:44:GLU:N	1:L:44:GLU:OE1	2.46	0.48
1:B:128:VAL:HA	1:B:131:LEU:CD1	2.43	0.48
1:C:615:GLN:HE21	1:C:634:LEU:CG	2.24	0.48
1:E:459:SER:OG	1:E:468:GLY:O	2.30	0.48
1:G:132:HIS:CG	1:G:222:ILE:HG12	2.47	0.48
1:I:349:SER:HB3	1:I:361:ASP:OD1	2.12	0.48
1:A:126:LEU:HD22	1:A:130:LEU:HG	1.96	0.48
1:C:94:ILE:HD13	1:C:128:VAL:CG1	2.43	0.48
1:A:348:GLU:HA	1:A:363:HIS:HB3	1.94	0.48
1:C:219:ASN:OD1	1:F:614:VAL:HG23	2.12	0.48
1:E:192:ARG:CZ	1:E:251:ARG:CZ	2.91	0.48
1:F:31:ASP:O	1:F:39:ARG:HD3	2.14	0.48
1:G:44:GLU:N	1:G:44:GLU:OE1	2.46	0.48
1:H:621:CYS:SG	1:H:622:ASN:N	2.85	0.48
1:A:44:GLU:OE1	1:A:44:GLU:N	2.45	0.48
1:D:219:ASN:OD1	1:D:220:ARG:N	2.47	0.48
1:L:353:SER:HB3	1:L:356:ARG:HG2	1.95	0.48
1:A:353:SER:HB3	1:A:356:ARG:HG2	1.96	0.48
1:E:192:ARG:HH11	1:E:251:ARG:HD3	1.79	0.48
1:E:223:VAL:O	1:E:228:ARG:HD2	2.13	0.48
1:I:44:GLU:N	1:I:44:GLU:OE1	2.46	0.48
1:I:94:ILE:HD13	1:I:128:VAL:HG11	1.94	0.48
1:K:44:GLU:N	1:K:44:GLU:OE1	2.46	0.48
1:L:215:PHE:CD1	1:L:216:GLU:HG3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:NH1	1:H:159:GLU:OE2	2.43	0.48
1:D:44:GLU:N	1:D:44:GLU:OE1	2.47	0.48
1:G:132:HIS:ND1	1:G:222:ILE:CD1	2.76	0.48
1:G:223:VAL:O	1:G:228:ARG:HD2	2.14	0.48
1:H:223:VAL:O	1:H:228:ARG:HD2	2.14	0.48
1:J:349:SER:OG	1:J:361:ASP:HA	2.14	0.48
1:J:581:CYS:SG	1:J:622:ASN:CG	2.92	0.48
1:L:221:ALA:C	1:L:222:ILE:HG13	2.34	0.48
1:E:231:LEU:HD22	1:E:641:MET:HE1	1.95	0.48
1:F:132:HIS:NE2	1:F:222:ILE:HG21	2.29	0.48
1:H:581:CYS:CB	1:H:622:ASN:OD1	2.63	0.47
1:J:44:GLU:OE1	1:J:44:GLU:N	2.46	0.47
1:K:621:CYS:SG	1:K:622:ASN:N	2.87	0.47
1:L:349:SER:OG	1:L:361:ASP:HA	2.14	0.47
1:D:223:VAL:O	1:D:228:ARG:HD2	2.14	0.47
1:E:44:GLU:OE1	1:E:44:GLU:N	2.46	0.47
1:F:221:ALA:C	1:F:222:ILE:HG13	2.34	0.47
1:J:12:ASP:OD2	1:J:460:ARG:CZ	2.58	0.47
1:A:254:ARG:CB	1:A:254:ARG:NH1	2.76	0.47
1:H:218:SER:OG	1:H:220:ARG:HG3	2.14	0.47
1:I:622:ASN:HA	1:I:631:ARG:HH12	1.79	0.47
1:L:94:ILE:O	1:L:98:MET:HB2	2.13	0.47
1:B:81:LEU:HD12	1:B:81:LEU:H	1.80	0.47
1:B:553:PRO:HD2	1:B:556:ARG:HG3	1.96	0.47
1:F:3:TYR:CB	1:F:103:ILE:CG2	2.92	0.47
1:I:209:TRP:CD1	1:I:580:GLY:HA3	2.49	0.47
1:A:182:PHE:HE1	1:A:272:LYS:HB2	1.78	0.47
1:F:44:GLU:N	1:F:44:GLU:OE1	2.46	0.47
1:F:70:PRO:HD3	1:F:92:ARG:CG	2.38	0.47
1:I:511:ARG:HH12	1:K:298:LEU:HD23	1.79	0.47
1:A:349:SER:HG	1:A:361:ASP:HA	1.80	0.47
1:F:218:SER:OG	1:F:220:ARG:HG3	2.14	0.47
1:J:221:ALA:C	1:J:222:ILE:HG13	2.35	0.47
1:A:633:ARG:HD2	1:A:633:ARG:HA	1.51	0.47
1:A:678:VAL:CG1	1:A:679:PRO:HD2	2.20	0.47
1:B:349:SER:OG	1:B:361:ASP:HA	2.14	0.47
1:C:353:SER:HB3	1:C:356:ARG:HG2	1.96	0.47
1:E:92:ARG:HG2	1:E:92:ARG:NH2	2.29	0.47
1:E:192:ARG:NH1	1:E:251:ARG:HD3	2.29	0.47
1:E:221:ALA:C	1:E:222:ILE:HG13	2.34	0.47
1:E:620:THR:OG1	1:E:631:ARG:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:GLN:OE1	1:K:510:GLU:OE2	2.33	0.47
1:K:620:THR:CB	1:K:629:GLY:CA	2.88	0.47
1:H:44:GLU:OE1	1:H:44:GLU:N	2.46	0.47
1:H:304:ASP:OD2	1:K:257:ARG:NH1	2.48	0.47
1:J:353:SER:HB3	1:J:356:ARG:HG2	1.95	0.47
1:A:182:PHE:CE1	1:A:272:LYS:HB2	2.50	0.47
1:A:455:ASP:OD1	1:A:473:ARG:HG2	2.15	0.47
1:F:279:SER:HB3	1:L:156:ARG:HA	1.97	0.47
1:L:132:HIS:CG	1:L:222:ILE:HG12	2.50	0.47
1:C:344:GLY:O	1:C:347:ILE:O	2.33	0.47
1:E:70:PRO:CD	1:E:92:ARG:HD2	2.41	0.47
1:G:346:ILE:HG12	1:G:354:PRO:HD2	1.97	0.47
1:H:221:ALA:C	1:H:222:ILE:HG13	2.34	0.47
1:A:67:LEU:HD12	1:A:70:PRO:HG2	1.97	0.46
1:A:459:SER:OG	1:A:468:GLY:O	2.30	0.46
1:B:31:ASP:O	1:B:39:ARG:HD3	2.16	0.46
1:K:31:ASP:O	1:K:39:ARG:HD3	2.16	0.46
1:B:279:SER:HB3	1:K:156:ARG:HA	1.97	0.46
1:D:455:ASP:OD1	1:D:473:ARG:HG2	2.15	0.46
1:E:455:ASP:OD1	1:E:473:ARG:HG2	2.16	0.46
1:J:454:SER:CB	1:J:680:ARG:HD3	2.45	0.46
1:K:353:SER:HB3	1:K:356:ARG:HG2	1.97	0.46
1:K:455:ASP:OD1	1:K:473:ARG:HG2	2.16	0.46
1:L:579:CYS:SG	1:L:579:CYS:O	2.73	0.46
1:C:44:GLU:O	1:C:44:GLU:HG3	2.15	0.46
1:E:24:LYS:CD	1:E:54:GLU:OE2	2.63	0.46
1:H:94:ILE:O	1:H:98:MET:HB2	2.16	0.46
1:A:144:VAL:HA	1:A:147:VAL:HG22	1.98	0.46
1:F:100:MET:O	1:F:133:ARG:CZ	2.55	0.46
1:F:100:MET:HA	1:F:100:MET:CE	2.45	0.46
1:I:94:ILE:O	1:I:98:MET:HB2	2.15	0.46
1:I:217:ALA:O	1:I:218:SER:OG	2.26	0.46
1:J:509:ASP:OD1	1:J:511:ARG:N	2.38	0.46
1:L:192:ARG:CZ	1:L:251:ARG:CZ	2.94	0.46
1:C:503:PHE:CD1	1:C:645:PHE:HE1	2.34	0.46
1:F:126:LEU:HD22	1:F:130:LEU:HG	1.96	0.46
1:G:621:CYS:SG	1:G:622:ASN:ND2	2.89	0.46
1:K:349:SER:HG	1:K:361:ASP:HA	1.81	0.46
1:A:103:ILE:O	1:A:103:ILE:HG23	2.15	0.46
1:B:44:GLU:N	1:B:44:GLU:OE1	2.46	0.46
1:D:643:PHE:HB3	1:D:644:PRO:HD3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:ALA:C	1:K:222:ILE:HG13	2.35	0.46
1:C:459:SER:OG	1:C:468:GLY:O	2.30	0.46
1:D:19:PHE:HZ	1:D:38:TYR:HD2	1.61	0.46
1:H:31:ASP:O	1:H:39:ARG:HD3	2.16	0.46
1:I:579:CYS:H	1:I:627:TYR:HE2	1.62	0.46
1:A:67:LEU:HD13	1:A:96:ILE:HD13	1.94	0.46
1:A:615:GLN:NE2	1:A:633:ARG:HB3	2.31	0.46
1:D:156:ARG:HA	1:G:279:SER:HB3	1.97	0.46
1:I:132:HIS:CG	1:I:222:ILE:HG13	2.50	0.46
1:I:579:CYS:HB2	1:I:627:TYR:OH	2.15	0.46
1:K:94:ILE:O	1:K:98:MET:HB2	2.15	0.46
1:L:31:ASP:O	1:L:39:ARG:HD3	2.15	0.46
1:B:349:SER:HB2	1:B:361:ASP:OD1	2.16	0.46
1:E:661:THR:OG1	1:E:662:PRO:CD	2.64	0.46
1:I:503:PHE:CD1	1:I:645:PHE:HE1	2.34	0.46
1:I:621:CYS:SG	1:I:622:ASN:ND2	2.89	0.46
1:K:620:THR:CB	1:K:631:ARG:H	2.29	0.46
1:E:292:LYS:HA	1:E:292:LYS:HE2	1.98	0.46
1:G:221:ALA:C	1:G:222:ILE:HG13	2.35	0.46
1:H:621:CYS:SG	1:H:622:ASN:ND2	2.89	0.46
1:E:126:LEU:HD22	1:E:130:LEU:HG	1.98	0.45
1:G:511:ARG:NH2	1:J:297:GLU:OE1	2.49	0.45
1:H:94:ILE:HD13	1:H:128:VAL:HG11	1.98	0.45
1:I:221:ALA:C	1:I:222:ILE:HG12	2.37	0.45
1:C:11:TYR:CZ	1:C:141:LEU:CD2	2.99	0.45
1:C:100:MET:O	1:C:133:ARG:NH2	2.49	0.45
1:D:459:SER:OG	1:D:468:GLY:O	2.30	0.45
1:E:93:LEU:HD11	1:E:117:ILE:CD1	2.45	0.45
1:E:231:LEU:N	1:E:641:MET:HE3	2.32	0.45
1:I:93:LEU:HD13	1:I:125:ALA:CB	2.46	0.45
1:J:94:ILE:O	1:J:98:MET:HB2	2.15	0.45
1:J:579:CYS:N	1:J:627:TYR:HE2	2.14	0.45
1:D:454:SER:CB	1:D:554:PHE:HZ	2.29	0.45
1:G:680:ARG:HG2	1:G:680:ARG:NH2	2.30	0.45
1:A:614:VAL:HG23	1:E:220:ARG:HD2	1.99	0.45
1:G:94:ILE:O	1:G:98:MET:HB2	2.16	0.45
1:G:639:LYS:HD2	1:G:643:PHE:CE1	2.52	0.45
1:J:346:ILE:HG12	1:J:354:PRO:HD2	1.98	0.45
1:J:639:LYS:HD2	1:J:643:PHE:CE1	2.51	0.45
1:L:222:ILE:HA	1:L:225:LYS:NZ	2.32	0.45
1:L:621:CYS:SG	1:L:622:ASN:ND2	2.89	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:SER:HB3	1:I:156:ARG:HA	1.99	0.45
1:B:552:ILE:CG2	1:B:582:GLY:HA3	2.44	0.45
1:C:631:ARG:HA	1:C:631:ARG:HD3	1.53	0.45
1:E:17:PRO:HD2	1:E:20:MET:HE2	1.93	0.45
1:E:661:THR:CG2	1:E:664:MET:CE	2.95	0.45
1:G:31:ASP:O	1:G:39:ARG:HD3	2.16	0.45
1:H:556:ARG:O	1:H:559:ARG:HG2	2.17	0.45
1:A:200:ILE:HG12	1:A:474:PHE:CE1	2.52	0.45
1:C:107:GLN:O	1:C:111:VAL:HG23	2.17	0.45
1:K:620:THR:CB	1:K:630:VAL:N	2.80	0.45
1:D:212:VAL:CG2	1:D:213:TYR:CE1	3.00	0.45
1:J:93:LEU:HD13	1:J:125:ALA:CB	2.47	0.45
1:J:349:SER:HG	1:J:361:ASP:HA	1.82	0.45
1:J:621:CYS:SG	1:J:622:ASN:ND2	2.89	0.45
1:A:164:GLU:HG3	1:A:173:ARG:HG3	1.98	0.45
1:B:135:ASP:N	1:B:135:ASP:OD1	2.50	0.45
1:F:139:LEU:HD12	1:F:139:LEU:HA	1.84	0.45
1:I:343:LEU:O	1:I:347:ILE:HG13	2.17	0.45
1:K:94:ILE:HD13	1:K:128:VAL:HG11	1.99	0.45
1:A:3:TYR:CB	1:A:103:ILE:CG2	2.95	0.45
1:B:98:MET:HE2	1:B:132:HIS:HB2	1.99	0.45
1:B:349:SER:HG	1:B:361:ASP:HA	1.81	0.45
1:D:93:LEU:HD13	1:D:125:ALA:CB	2.46	0.45
1:E:250:ASN:O	1:E:251:ARG:CD	2.47	0.45
1:K:126:LEU:HD22	1:K:130:LEU:HG	1.99	0.45
1:D:19:PHE:CZ	1:D:38:TYR:HD2	2.35	0.44
1:J:126:LEU:HD22	1:J:130:LEU:HG	1.99	0.44
1:K:144:VAL:HA	1:K:147:VAL:HG22	1.99	0.44
1:L:144:VAL:HA	1:L:147:VAL:HG22	2.00	0.44
1:A:349:SER:OG	1:A:361:ASP:HA	2.16	0.44
1:B:357:GLN:HG2	1:C:416:LYS:NZ	2.32	0.44
1:H:64:LEU:HD22	1:H:109:CYS:HA	1.98	0.44
1:I:117:ILE:CD1	1:I:122:PHE:HB2	2.42	0.44
1:I:418:PRO:O	1:I:647:ARG:HD3	2.17	0.44
1:J:31:ASP:O	1:J:39:ARG:HD3	2.16	0.44
1:L:349:SER:HB3	1:L:356:ARG:NH1	2.31	0.44
1:L:455:ASP:OD1	1:L:473:ARG:HG2	2.17	0.44
1:C:144:VAL:HA	1:C:147:VAL:HG22	2.00	0.44
1:D:231:LEU:HD11	1:D:629:GLY:CA	2.46	0.44
1:F:459:SER:OG	1:F:468:GLY:O	2.29	0.44
1:K:620:THR:HG23	1:K:628:CYS:C	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:126:LEU:HD22	1:L:130:LEU:HG	2.00	0.44
1:B:349:SER:HB3	1:B:356:ARG:NH1	2.32	0.44
1:F:131:LEU:N	1:F:131:LEU:HD23	2.32	0.44
1:F:556:ARG:HA	1:F:556:ARG:HD3	1.68	0.44
1:H:93:LEU:HD13	1:H:125:ALA:CB	2.47	0.44
1:H:126:LEU:HD22	1:H:130:LEU:HG	1.99	0.44
1:J:455:ASP:OD1	1:J:473:ARG:HG2	2.17	0.44
1:E:93:LEU:HD13	1:E:125:ALA:CB	2.47	0.44
1:G:62:ILE:HG22	1:G:64:LEU:HD13	2.00	0.44
1:G:93:LEU:HD13	1:G:125:ALA:CB	2.48	0.44
1:A:212:VAL:HG22	1:A:213:TYR:CD1	2.52	0.44
1:I:610:ASP:O	1:I:638:ARG:HD3	2.18	0.44
1:J:144:VAL:HA	1:J:147:VAL:HG22	1.99	0.44
1:K:93:LEU:HD13	1:K:125:ALA:CB	2.48	0.44
1:D:129:ALA:O	1:D:133:ARG:HB2	2.18	0.44
1:F:552:ILE:HD13	1:F:552:ILE:N	2.25	0.44
1:K:349:SER:OG	1:K:361:ASP:HA	2.17	0.44
1:B:334:LEU:HD13	1:B:343:LEU:HD11	2.00	0.44
1:E:280:ARG:HB2	4:E:809:HOH:O	2.16	0.44
1:H:552:ILE:CG2	1:H:582:GLY:HA3	2.48	0.44
1:A:124:TYR:O	1:A:128:VAL:HG23	2.17	0.44
1:C:280:ARG:NH2	1:H:154:ASP:OD2	2.51	0.44
1:E:164:GLU:HG3	1:E:173:ARG:HG3	2.00	0.44
1:I:350:SER:C	1:I:352:LEU:N	2.71	0.44
1:L:232:PHE:CZ	1:L:348:GLU:HB2	2.53	0.44
1:F:127:SER:O	1:F:129:ALA:N	2.51	0.43
1:G:350:SER:C	1:G:352:LEU:N	2.71	0.43
1:I:144:VAL:HA	1:I:147:VAL:HG22	1.99	0.43
1:L:350:SER:C	1:L:352:LEU:N	2.71	0.43
1:A:357:GLN:HG2	1:B:416:LYS:NZ	2.33	0.43
1:B:163:GLU:HG3	1:K:464:PHE:CZ	2.53	0.43
1:C:24:LYS:HD3	1:C:54:GLU:OE1	2.17	0.43
1:C:455:ASP:OD1	1:C:473:ARG:HG2	2.17	0.43
1:D:37:ARG:C	1:D:37:ARG:CD	2.86	0.43
1:D:43:PRO:HG2	1:D:44:GLU:OE1	2.18	0.43
1:E:144:VAL:HA	1:E:147:VAL:HG22	2.00	0.43
1:G:94:ILE:HD13	1:G:128:VAL:HG11	2.00	0.43
1:H:257:ARG:NH2	1:H:259:ASN:HD22	2.15	0.43
1:I:544:ARG:HG2	4:I:802:HOH:O	2.18	0.43
1:J:343:LEU:O	1:J:347:ILE:HG13	2.18	0.43
1:B:7:LEU:HD11	1:B:103:ILE:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:HD22	1:D:130:LEU:HG	2.00	0.43
1:F:107:GLN:O	1:F:111:VAL:HG23	2.18	0.43
1:F:454:SER:HA	1:F:680:ARG:HD3	1.99	0.43
1:G:107:GLN:O	1:G:111:VAL:HG23	2.18	0.43
1:H:107:GLN:O	1:H:111:VAL:HG23	2.18	0.43
1:H:144:VAL:HA	1:H:147:VAL:HG22	2.00	0.43
1:K:343:LEU:O	1:K:347:ILE:HG13	2.19	0.43
1:K:620:THR:CB	1:K:629:GLY:C	2.83	0.43
1:L:349:SER:HB2	1:L:361:ASP:OD1	2.18	0.43
1:A:93:LEU:HD11	1:A:117:ILE:CD1	2.49	0.43
1:B:343:LEU:O	1:B:347:ILE:HG13	2.18	0.43
1:C:93:LEU:HD11	1:C:117:ILE:CD1	2.49	0.43
1:D:346:ILE:HG12	1:D:354:PRO:HD2	1.99	0.43
1:F:232:PHE:CZ	1:F:348:GLU:HB2	2.54	0.43
1:F:350:SER:C	1:F:352:LEU:N	2.71	0.43
1:I:126:LEU:HD22	1:I:130:LEU:HG	2.00	0.43
1:A:678:VAL:CG1	1:A:679:PRO:HD3	2.43	0.43
1:B:107:GLN:O	1:B:111:VAL:HG23	2.18	0.43
1:B:459:SER:OG	1:B:468:GLY:O	2.30	0.43
1:E:92:ARG:HD3	1:E:92:ARG:C	2.38	0.43
1:F:156:ARG:HA	1:L:279:SER:HB3	1.99	0.43
1:F:221:ALA:C	1:F:222:ILE:CG1	2.87	0.43
1:H:350:SER:C	1:H:352:LEU:N	2.71	0.43
1:J:94:ILE:HD13	1:J:128:VAL:HG11	1.99	0.43
1:C:87:ARG:HG2	1:C:87:ARG:H	1.66	0.43
1:C:132:HIS:CD2	1:C:222:ILE:CD1	3.01	0.43
1:D:107:GLN:O	1:D:111:VAL:HG23	2.18	0.43
1:H:350:SER:O	1:H:352:LEU:N	2.52	0.43
1:K:295:ASN:HD22	1:K:302:LYS:HD3	1.83	0.43
1:C:350:SER:C	1:C:352:LEU:N	2.71	0.43
1:E:209:TRP:CD1	1:E:580:GLY:HA3	2.54	0.43
1:E:250:ASN:C	1:E:251:ARG:CD	2.85	0.43
1:J:350:SER:C	1:J:352:LEU:N	2.72	0.43
1:K:350:SER:C	1:K:352:LEU:N	2.71	0.43
1:L:107:GLN:O	1:L:111:VAL:HG23	2.19	0.43
1:D:350:SER:C	1:D:352:LEU:N	2.72	0.43
1:F:350:SER:O	1:F:352:LEU:N	2.52	0.43
1:H:579:CYS:H	1:H:627:TYR:HE2	1.65	0.43
1:I:455:ASP:OD1	1:I:473:ARG:HG2	2.19	0.43
1:L:94:ILE:HD13	1:L:128:VAL:HG11	2.00	0.43
1:L:459:SER:OG	1:L:468:GLY:O	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HH11	1:A:254:ARG:HB2	1.79	0.43
1:A:639:LYS:HD2	1:A:643:PHE:CE1	2.54	0.43
1:B:94:ILE:HD13	1:B:128:VAL:HG11	2.00	0.43
1:D:639:LYS:HD2	1:D:643:PHE:CE1	2.53	0.43
1:E:223:VAL:HG11	1:E:351:ILE:HG12	2.00	0.43
1:E:552:ILE:HD12	1:E:556:ARG:CG	2.47	0.43
1:F:62:ILE:HG22	1:F:63:ALA:N	2.33	0.43
1:F:343:LEU:O	1:F:347:ILE:HG13	2.19	0.43
1:G:164:GLU:HG3	1:G:173:ARG:HG3	2.00	0.43
1:H:238:GLN:HB3	1:H:578:PHE:CZ	2.54	0.43
1:I:67:LEU:HD12	1:I:96:ILE:HD13	2.01	0.43
1:J:349:SER:HB2	1:J:361:ASP:OD1	2.19	0.43
1:B:129:ALA:O	1:B:133:ARG:HB2	2.19	0.43
1:B:455:ASP:OD1	1:B:473:ARG:HG2	2.18	0.43
1:B:557:THR:O	1:B:558:PHE:C	2.56	0.43
1:C:15:ARG:HD3	1:C:277:VAL:HA	2.01	0.43
1:E:26:VAL:CG1	1:E:56:ARG:HD2	2.48	0.43
1:F:144:VAL:HA	1:F:147:VAL:HG22	2.01	0.43
1:H:455:ASP:OD1	1:H:473:ARG:HG2	2.19	0.43
1:H:577:ASN:CA	1:H:627:TYR:HH	2.31	0.43
1:I:222:ILE:HG22	1:I:222:ILE:O	2.18	0.43
1:J:107:GLN:O	1:J:111:VAL:HG23	2.19	0.43
1:J:349:SER:HB3	1:J:356:ARG:NH1	2.34	0.43
1:A:331:ARG:NH1	1:F:330:ASN:HB3	2.34	0.42
1:D:144:VAL:HA	1:D:147:VAL:HG22	2.01	0.42
1:E:281:THR:HG23	1:J:281:THR:HG23	2.01	0.42
1:E:661:THR:OG1	1:E:662:PRO:N	2.51	0.42
1:G:64:LEU:HD13	1:G:64:LEU:N	2.34	0.42
1:H:491:THR:O	1:H:491:THR:OG1	2.37	0.42
1:K:350:SER:O	1:K:352:LEU:N	2.52	0.42
1:A:18:ILE:HD13	1:A:111:VAL:HG13	2.00	0.42
1:D:257:ARG:NH1	1:F:304:ASP:OD2	2.52	0.42
1:E:491:THR:O	1:E:491:THR:OG1	2.37	0.42
1:F:212:VAL:HG22	1:F:213:TYR:CD2	2.54	0.42
1:H:629:GLY:O	1:H:630:VAL:CG2	2.66	0.42
1:I:164:GLU:HG3	1:I:173:ARG:HG3	2.01	0.42
1:I:632:ASP:O	1:I:633:ARG:C	2.58	0.42
1:K:427:TYR:OH	1:K:497:MET:O	2.30	0.42
1:B:552:ILE:HD11	1:B:557:THR:HG23	2.01	0.42
1:E:107:GLN:O	1:E:111:VAL:HG23	2.18	0.42
1:E:221:ALA:C	1:E:222:ILE:CG1	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:N	1:F:131:LEU:CD2	2.82	0.42
1:G:93:LEU:HD11	1:G:117:ILE:CD1	2.49	0.42
1:G:126:LEU:HD22	1:G:130:LEU:HG	2.01	0.42
1:G:144:VAL:HA	1:G:147:VAL:HG22	2.00	0.42
1:G:349:SER:HG	1:G:356:ARG:NH1	2.14	0.42
1:I:459:SER:OG	1:I:468:GLY:O	2.30	0.42
1:K:132:HIS:CE1	1:K:222:ILE:HD13	2.55	0.42
1:E:343:LEU:O	1:E:347:ILE:HG13	2.19	0.42
1:G:300:GLN:HG2	1:L:518:ARG:NH1	2.34	0.42
1:K:107:GLN:O	1:K:111:VAL:HG23	2.19	0.42
1:L:132:HIS:CG	1:L:222:ILE:HD11	2.53	0.42
1:B:232:PHE:CZ	1:B:348:GLU:HB2	2.54	0.42
1:B:492:SER:O	1:B:493:ASP:CB	2.68	0.42
1:C:32:ASN:OD1	1:C:32:ASN:N	2.44	0.42
1:C:62:ILE:HD13	1:C:105:GLU:HG2	2.01	0.42
1:C:164:GLU:HG3	1:C:173:ARG:HG3	2.01	0.42
1:D:140:ASP:CG	1:D:556:ARG:HH22	2.16	0.42
1:D:454:SER:HG	1:D:554:PHE:HE2	1.59	0.42
1:G:221:ALA:C	1:G:222:ILE:CG1	2.88	0.42
1:I:629:GLY:O	1:I:630:VAL:CG2	2.67	0.42
1:J:222:ILE:O	1:J:222:ILE:HG22	2.19	0.42
1:J:552:ILE:CG2	1:J:582:GLY:HA3	2.49	0.42
1:L:164:GLU:HG3	1:L:173:ARG:HG3	2.02	0.42
1:A:357:GLN:HG2	1:B:416:LYS:HZ3	1.84	0.42
1:B:386:VAL:HG22	1:B:392:THR:HB	2.02	0.42
1:C:94:ILE:HD13	1:C:128:VAL:HG11	2.02	0.42
1:C:552:ILE:CG2	1:C:582:GLY:HA3	2.49	0.42
1:D:357:GLN:HG2	1:E:416:LYS:HZ2	1.84	0.42
1:D:492:SER:O	1:D:493:ASP:CB	2.68	0.42
1:G:18:ILE:HD13	1:G:111:VAL:HG13	2.01	0.42
1:G:455:ASP:OD1	1:G:473:ARG:HG2	2.20	0.42
1:H:18:ILE:HD13	1:H:111:VAL:HG13	2.00	0.42
1:H:232:PHE:CZ	1:H:348:GLU:HB2	2.54	0.42
1:H:343:LEU:O	1:H:347:ILE:HG13	2.18	0.42
1:I:132:HIS:CE1	1:I:222:ILE:HG21	2.54	0.42
1:J:18:ILE:HD13	1:J:111:VAL:HG13	2.02	0.42
1:K:254:ARG:HH11	1:K:254:ARG:CG	2.33	0.42
1:L:250:ASN:C	1:L:251:ARG:HG3	2.39	0.42
1:L:492:SER:O	1:L:493:ASP:CB	2.68	0.42
1:A:281:THR:HG23	1:I:281:THR:HG23	2.01	0.42
1:A:350:SER:C	1:A:352:LEU:N	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HA	1:B:147:VAL:HG22	2.01	0.42
1:C:79:PHE:O	1:C:86:HIS:HD2	2.03	0.42
1:C:223:VAL:HG11	1:C:351:ILE:HG12	2.00	0.42
1:D:152:TYR:HB3	1:D:200:ILE:CD1	2.50	0.42
1:D:164:GLU:HG3	1:D:173:ARG:HG3	2.01	0.42
1:E:18:ILE:HD13	1:E:111:VAL:HG13	2.01	0.42
1:E:132:HIS:CE1	1:E:222:ILE:HD13	2.54	0.42
1:E:279:SER:HB3	1:J:156:ARG:HA	2.00	0.42
1:H:64:LEU:HD13	1:H:112:PHE:CD2	2.54	0.42
1:H:221:ALA:C	1:H:222:ILE:CG1	2.88	0.42
1:L:18:ILE:HD13	1:L:111:VAL:HG13	2.02	0.42
1:L:253:GLN:NE2	1:L:254:ARG:O	2.52	0.42
1:A:386:VAL:HG22	1:A:392:THR:HB	2.02	0.42
1:E:350:SER:C	1:E:352:LEU:N	2.72	0.42
1:F:222:ILE:HG22	1:F:222:ILE:O	2.19	0.42
1:G:222:ILE:HG22	1:G:222:ILE:O	2.20	0.42
1:J:492:SER:O	1:J:493:ASP:CB	2.68	0.42
1:K:18:ILE:HD13	1:K:111:VAL:HG13	2.02	0.42
1:K:492:SER:O	1:K:493:ASP:CB	2.68	0.42
1:L:222:ILE:O	1:L:222:ILE:HG22	2.20	0.42
1:A:100:MET:O	1:A:133:ARG:NH1	2.46	0.42
1:B:281:THR:HG23	1:K:281:THR:HG23	2.02	0.42
1:C:18:ILE:HD13	1:C:111:VAL:HG13	2.02	0.42
1:C:34:LEU:CD2	1:C:46:GLN:HE22	2.32	0.42
1:C:348:GLU:CG	1:C:363:HIS:HD1	2.31	0.42
1:D:212:VAL:CG2	1:D:213:TYR:CD1	2.98	0.42
1:E:94:ILE:HD13	1:E:128:VAL:HG11	2.00	0.42
1:G:350:SER:O	1:G:352:LEU:N	2.51	0.42
1:G:554:PHE:CD2	1:G:680:ARG:NH2	2.88	0.42
1:H:577:ASN:N	1:H:627:TYR:OH	2.53	0.42
1:I:222:ILE:HD13	1:I:222:ILE:N	2.35	0.42
1:I:492:SER:O	1:I:493:ASP:CB	2.68	0.42
1:J:232:PHE:CZ	1:J:348:GLU:HB2	2.55	0.42
1:K:232:PHE:CZ	1:K:348:GLU:HB2	2.55	0.42
1:L:84:PRO:HG2	1:L:300:GLN:O	2.20	0.42
1:B:214:PRO:O	1:B:223:VAL:HG13	2.19	0.42
1:B:350:SER:C	1:B:352:LEU:N	2.73	0.42
1:D:350:SER:O	1:D:352:LEU:N	2.52	0.42
1:F:15:ARG:HD3	1:F:277:VAL:HA	2.01	0.42
1:F:18:ILE:HD13	1:F:111:VAL:HG13	2.01	0.42
1:H:222:ILE:HG22	1:H:222:ILE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:SER:O	1:L:352:LEU:N	2.53	0.42
1:L:629:GLY:O	1:L:630:VAL:CG2	2.66	0.42
1:A:357:GLN:HE21	1:B:320:HIS:HD2	1.68	0.41
1:B:346:ILE:HG12	1:B:354:PRO:HD2	2.02	0.41
1:C:103:ILE:HD12	1:C:103:ILE:O	2.20	0.41
1:C:126:LEU:HD22	1:C:130:LEU:HG	2.01	0.41
1:D:37:ARG:HB3	1:D:38:TYR:HD1	1.85	0.41
1:E:492:SER:O	1:E:493:ASP:CB	2.67	0.41
1:F:175:PRO:HG2	1:F:473:ARG:CZ	2.50	0.41
1:A:492:SER:O	1:A:493:ASP:CB	2.67	0.41
1:C:80:SER:HB2	1:C:384:PHE:CZ	2.55	0.41
1:C:634:LEU:HD22	1:C:634:LEU:HA	1.79	0.41
1:D:67:LEU:HD12	1:D:96:ILE:HD13	2.01	0.41
1:E:192:ARG:NH1	1:E:251:ARG:CD	2.84	0.41
1:F:69:ILE:HB	1:F:92:ARG:HG2	2.02	0.41
1:G:15:ARG:HD3	1:G:277:VAL:HA	2.02	0.41
1:J:93:LEU:HD11	1:J:117:ILE:CD1	2.50	0.41
1:J:632:ASP:O	1:J:633:ARG:C	2.59	0.41
1:L:15:ARG:HD3	1:L:277:VAL:HA	2.02	0.41
1:B:93:LEU:HD13	1:B:125:ALA:CB	2.50	0.41
1:B:126:LEU:HD22	1:B:130:LEU:HG	2.02	0.41
1:E:209:TRP:HD1	1:E:580:GLY:HA3	1.84	0.41
1:G:153:VAL:HG11	1:G:157:VAL:HG21	2.02	0.41
1:G:343:LEU:O	1:G:347:ILE:HG13	2.20	0.41
1:H:164:GLU:HG3	1:H:173:ARG:HG3	2.02	0.41
1:A:220:ARG:O	1:A:224:ASP:N	2.49	0.41
1:B:615:GLN:NE2	1:B:633:ARG:CB	2.66	0.41
1:D:37:ARG:HD3	1:D:38:TYR:CD1	2.55	0.41
1:F:492:SER:O	1:F:493:ASP:CB	2.67	0.41
1:G:632:ASP:O	1:G:633:ARG:C	2.59	0.41
1:L:343:LEU:O	1:L:347:ILE:HG13	2.19	0.41
1:A:107:GLN:O	1:A:111:VAL:HG23	2.20	0.41
1:A:349:SER:HB2	1:A:361:ASP:OD1	2.20	0.41
1:E:216:GLU:O	1:E:217:ALA:CB	2.69	0.41
1:G:232:PHE:CZ	1:G:348:GLU:HB2	2.56	0.41
1:H:526:GLU:OE1	1:H:577:ASN:HB3	2.21	0.41
1:H:632:ASP:O	1:H:633:ARG:C	2.59	0.41
1:I:107:GLN:O	1:I:111:VAL:HG23	2.19	0.41
1:I:221:ALA:C	1:I:222:ILE:CG1	2.89	0.41
1:J:152:TYR:HB3	1:J:200:ILE:HD12	2.02	0.41
1:K:15:ARG:HD3	1:K:277:VAL:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:491:THR:O	1:K:491:THR:OG1	2.37	0.41
1:A:215:PHE:HB2	1:A:350:SER:HA	2.02	0.41
1:A:219:ASN:N	1:A:219:ASN:ND2	2.69	0.41
1:A:280:ARG:NH1	1:I:154:ASP:OD1	2.53	0.41
1:A:634:LEU:HD13	1:A:634:LEU:HA	1.95	0.41
1:B:220:ARG:HH12	1:D:638:ARG:HH12	1.68	0.41
1:C:350:SER:O	1:C:352:LEU:N	2.53	0.41
1:E:20:MET:HE3	1:E:464:PHE:HE1	1.86	0.41
1:G:132:HIS:CE1	1:G:222:ILE:HD13	2.55	0.41
1:G:492:SER:O	1:G:493:ASP:CB	2.68	0.41
1:H:132:HIS:CE1	1:H:222:ILE:HD13	2.55	0.41
1:J:350:SER:O	1:J:352:LEU:N	2.54	0.41
1:L:132:HIS:CB	1:L:222:ILE:HD11	2.51	0.41
1:L:221:ALA:C	1:L:222:ILE:CG1	2.88	0.41
1:A:152:TYR:HB3	1:A:200:ILE:CD1	2.51	0.41
1:B:18:ILE:HD13	1:B:111:VAL:HG13	2.02	0.41
1:B:164:GLU:HG3	1:B:173:ARG:HG3	2.02	0.41
1:B:350:SER:O	1:B:352:LEU:N	2.54	0.41
1:D:386:VAL:HG22	1:D:392:THR:HB	2.03	0.41
1:F:164:GLU:HG3	1:F:173:ARG:HG3	2.02	0.41
1:F:216:GLU:O	1:F:217:ALA:CB	2.69	0.41
1:G:62:ILE:CG2	1:G:64:LEU:CD1	2.98	0.41
1:H:124:TYR:O	1:H:128:VAL:HG23	2.21	0.41
1:H:153:VAL:HG11	1:H:157:VAL:HG21	2.02	0.41
1:I:348:GLU:O	1:I:348:GLU:HG3	2.21	0.41
1:J:221:ALA:C	1:J:222:ILE:CG1	2.88	0.41
1:K:221:ALA:C	1:K:222:ILE:CG1	2.88	0.41
1:L:124:TYR:O	1:L:128:VAL:HG23	2.21	0.41
1:A:15:ARG:HD3	1:A:277:VAL:HA	2.02	0.41
1:C:212:VAL:HG22	1:C:213:TYR:CD2	2.56	0.41
1:F:251:ARG:HE	1:J:251:ARG:HE	1.69	0.41
1:F:503:PHE:CD1	1:F:645:PHE:HE1	2.38	0.41
1:L:101:ARG:HD2	1:L:102:ASN:H	1.86	0.41
1:L:152:TYR:HB3	1:L:200:ILE:HD12	2.03	0.41
1:L:152:TYR:HB3	1:L:200:ILE:CD1	2.51	0.41
1:B:54:GLU:H	1:B:54:GLU:HG2	1.52	0.41
1:B:212:VAL:HG22	1:B:213:TYR:CD2	2.56	0.41
1:B:639:LYS:HD2	1:B:643:PHE:CE1	2.56	0.41
1:C:343:LEU:O	1:C:347:ILE:HG13	2.20	0.41
1:D:18:ILE:HD13	1:D:111:VAL:HG13	2.03	0.41
1:D:215:PHE:HB2	1:D:350:SER:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:552:ILE:N	1:F:552:ILE:CD1	2.84	0.41
1:G:216:GLU:O	1:G:217:ALA:CB	2.69	0.41
1:G:223:VAL:HG11	1:G:351:ILE:HG12	2.02	0.41
1:H:15:ARG:HD3	1:H:277:VAL:HA	2.03	0.41
1:H:93:LEU:HD11	1:H:117:ILE:CD1	2.50	0.41
1:I:15:ARG:HD3	1:I:277:VAL:HA	2.02	0.41
1:I:76:GLN:O	1:I:278:ALA:HA	2.21	0.41
1:I:152:TYR:HB3	1:I:200:ILE:CD1	2.51	0.41
1:J:427:TYR:OH	1:J:497:MET:O	2.29	0.41
1:K:93:LEU:HD11	1:K:117:ILE:CD1	2.51	0.41
1:K:152:TYR:HB3	1:K:200:ILE:CD1	2.51	0.41
1:K:164:GLU:HG3	1:K:173:ARG:HG3	2.02	0.41
1:K:216:GLU:O	1:K:217:ALA:CB	2.69	0.41
1:K:349:SER:HB2	1:K:361:ASP:OD1	2.20	0.41
1:K:350:SER:C	1:K:352:LEU:H	2.25	0.41
1:K:552:ILE:CG2	1:K:582:GLY:HA3	2.49	0.41
1:K:617:LEU:H	1:K:617:LEU:CD1	2.34	0.41
1:K:632:ASP:O	1:K:633:ARG:C	2.59	0.41
1:L:212:VAL:HG22	1:L:213:TYR:CD2	2.56	0.41
1:L:552:ILE:CG2	1:L:582:GLY:HA3	2.49	0.41
1:B:93:LEU:HD11	1:B:117:ILE:CD1	2.51	0.41
1:B:124:TYR:O	1:B:128:VAL:HG23	2.21	0.41
1:C:492:SER:O	1:C:493:ASP:CB	2.68	0.41
1:E:386:VAL:HG22	1:E:392:THR:HB	2.02	0.41
1:L:76:GLN:O	1:L:278:ALA:HA	2.21	0.41
1:B:15:ARG:HD3	1:B:277:VAL:HA	2.03	0.40
1:C:491:THR:O	1:C:491:THR:OG1	2.38	0.40
1:E:350:SER:O	1:E:352:LEU:N	2.54	0.40
1:F:152:TYR:HB3	1:F:200:ILE:CD1	2.51	0.40
1:G:386:VAL:HG22	1:G:392:THR:HB	2.04	0.40
1:I:386:VAL:HG22	1:I:392:THR:HB	2.02	0.40
1:J:124:TYR:O	1:J:128:VAL:HG23	2.21	0.40
1:B:334:LEU:HD13	1:B:343:LEU:CD1	2.51	0.40
1:C:76:GLN:O	1:C:278:ALA:HA	2.22	0.40
1:F:76:GLN:O	1:F:278:ALA:HA	2.21	0.40
1:F:632:ASP:O	1:F:633:ARG:C	2.59	0.40
1:G:226:ASP:CG	1:G:634:LEU:HD13	2.41	0.40
1:H:492:SER:O	1:H:493:ASP:CB	2.68	0.40
1:I:18:ILE:HD13	1:I:111:VAL:HG13	2.02	0.40
1:I:209:TRP:H	1:I:581:CYS:HG	1.69	0.40
1:I:350:SER:C	1:I:352:LEU:H	2.25	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:552:ILE:CG2	1:I:582:GLY:HA3	2.49	0.40
1:J:226:ASP:CG	1:J:634:LEU:HD13	2.42	0.40
1:L:222:ILE:HA	1:L:225:LYS:HZ2	1.85	0.40
1:A:93:LEU:HD13	1:A:125:ALA:CB	2.52	0.40
1:A:350:SER:O	1:A:352:LEU:N	2.54	0.40
1:B:48:ARG:HG2	1:B:48:ARG:HH11	1.86	0.40
1:B:219:ASN:HB3	1:B:222:ILE:HD12	2.03	0.40
1:E:556:ARG:CZ	1:E:621:CYS:SG	3.10	0.40
1:H:386:VAL:HG22	1:H:392:THR:HB	2.03	0.40
1:H:521:ARG:HB2	1:H:645:PHE:HB3	2.04	0.40
1:J:76:GLN:O	1:J:278:ALA:HA	2.21	0.40
1:J:132:HIS:CE1	1:J:222:ILE:HD13	2.55	0.40
1:J:212:VAL:HG22	1:J:213:TYR:CD2	2.56	0.40
1:K:620:THR:OG1	1:K:621:CYS:N	2.54	0.40
1:L:153:VAL:HG11	1:L:157:VAL:HG21	2.04	0.40
1:A:232:PHE:CZ	1:A:348:GLU:HB2	2.56	0.40
1:A:338:LYS:NZ	1:E:328:SER:HB3	2.36	0.40
1:A:615:GLN:C	1:E:220:ARG:HH21	2.18	0.40
1:C:39:ARG:N	1:C:40:PRO:CD	2.85	0.40
1:D:15:ARG:HD3	1:D:277:VAL:HA	2.04	0.40
1:I:152:TYR:HB3	1:I:200:ILE:HD12	2.03	0.40
1:D:76:GLN:O	1:D:278:ALA:HA	2.22	0.40
1:E:152:TYR:HB3	1:E:200:ILE:CD1	2.51	0.40
1:E:222:ILE:O	1:E:222:ILE:HG22	2.21	0.40
1:E:632:ASP:O	1:E:633:ARG:C	2.59	0.40
1:F:552:ILE:HD12	1:F:582:GLY:CA	2.50	0.40
1:F:639:LYS:HD2	1:F:643:PHE:CE1	2.57	0.40
1:G:124:TYR:O	1:G:128:VAL:HG23	2.21	0.40
1:J:152:TYR:HB3	1:J:200:ILE:CD1	2.51	0.40
1:K:639:LYS:HD2	1:K:643:PHE:CE1	2.57	0.40
1:L:632:ASP:O	1:L:633:ARG:C	2.59	0.40

All (6) 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:D:44:GLU:OE2	1:J:444:VAL:CG1[1_655]	1.59	0.61
1:A:47:ASN:OD1	1:C:438:GLN:NE2[1_656]	1.60	0.60
1:G:102:ASN:OD1	1:K:330:ASN:ND2[2_645]	1.95	0.25
1:A:47:ASN:OD1	1:C:438:GLN:CD[1_656]	1.96	0.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:ASN:OD1	1:L:330:ASN:ND2[2_555]	2.03	0.17
1:A:47:ASN:ND2	1:C:483:GLN:OE1[1_656]	2.18	0.02

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	645/681 (95%)	608 (94%)	30 (5%)	7 (1%)	14	48
1	B	639/681 (94%)	602 (94%)	32 (5%)	5 (1%)	19	55
1	C	642/681 (94%)	609 (95%)	27 (4%)	6 (1%)	17	53
1	D	644/681 (95%)	610 (95%)	29 (4%)	5 (1%)	19	55
1	E	655/681 (96%)	620 (95%)	30 (5%)	5 (1%)	19	55
1	F	651/681 (96%)	614 (94%)	29 (4%)	8 (1%)	13	46
1	G	653/681 (96%)	615 (94%)	32 (5%)	6 (1%)	17	53
1	H	655/681 (96%)	616 (94%)	32 (5%)	7 (1%)	14	48
1	I	654/681 (96%)	618 (94%)	30 (5%)	6 (1%)	17	53
1	J	653/681 (96%)	614 (94%)	33 (5%)	6 (1%)	17	53
1	K	654/681 (96%)	617 (94%)	29 (4%)	8 (1%)	13	46
1	L	653/681 (96%)	616 (94%)	31 (5%)	6 (1%)	17	53
All	All	7798/8172 (95%)	7359 (94%)	364 (5%)	75 (1%)	15	51

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	SER
1	B	630	VAL
1	D	614	VAL
1	D	643	PHE
1	E	217	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	222	ILE
1	F	127	SER
1	F	217	ALA
1	F	222	ILE
1	G	217	ALA
1	G	222	ILE
1	H	217	ALA
1	H	222	ILE
1	I	217	ALA
1	I	222	ILE
1	J	217	ALA
1	J	222	ILE
1	K	217	ALA
1	K	222	ILE
1	K	621	CYS
1	L	217	ALA
1	L	222	ILE
1	A	222	ILE
1	A	493	ASP
1	A	632	ASP
1	B	493	ASP
1	C	493	ASP
1	C	632	ASP
1	D	493	ASP
1	E	493	ASP
1	E	633	ARG
1	F	128	VAL
1	F	493	ASP
1	G	493	ASP
1	H	493	ASP
1	I	493	ASP
1	J	493	ASP
1	K	493	ASP
1	L	493	ASP
1	L	581	CYS
1	A	217	ALA
1	I	350	SER
1	A	64	LEU
1	B	64	LEU
1	C	64	LEU
1	C	348	GLU
1	D	64	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	218	SER
1	E	64	LEU
1	F	64	LEU
1	G	64	LEU
1	H	64	LEU
1	I	64	LEU
1	I	349	SER
1	J	64	LEU
1	K	64	LEU
1	L	64	LEU
1	B	219	ASN
1	C	80	SER
1	C	219	ASN
1	H	633	ARG
1	J	633	ARG
1	F	633	ARG
1	A	629	GLY
1	K	618	VAL
1	A	679	PRO
1	F	630	VAL
1	G	351	ILE
1	G	630	VAL
1	H	351	ILE
1	J	630	VAL
1	K	351	ILE
1	K	630	VAL
1	L	630	VAL
1	H	630	VAL

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	585/610 (96%)	520 (89%)	65 (11%)	6 24
1	B	580/610 (95%)	521 (90%)	59 (10%)	7 27
1	C	583/610 (96%)	517 (89%)	66 (11%)	6 23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	585/610 (96%)	529 (90%)	56 (10%)	8 29
1	E	594/610 (97%)	529 (89%)	65 (11%)	6 24
1	F	591/610 (97%)	535 (90%)	56 (10%)	8 30
1	G	592/610 (97%)	541 (91%)	51 (9%)	10 35
1	H	594/610 (97%)	539 (91%)	55 (9%)	9 31
1	I	593/610 (97%)	534 (90%)	59 (10%)	8 28
1	J	592/610 (97%)	537 (91%)	55 (9%)	9 31
1	K	593/610 (97%)	540 (91%)	53 (9%)	9 33
1	L	592/610 (97%)	536 (90%)	56 (10%)	8 30
All	All	7074/7320 (97%)	6378 (90%)	696 (10%)	8 28

All (696) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	46	GLN
1	A	47	ASN
1	A	51	GLU
1	A	56	ARG
1	A	60	ARG
1	A	62	ILE
1	A	67	LEU
1	A	68	ARG
1	A	73	LEU
1	A	93	LEU
1	A	95	ASP
1	A	101	ARG
1	A	103	ILE
1	A	104	GLU
1	A	105	GLU
1	A	126	LEU
1	A	177	VAL
1	A	180	LYS
1	A	186	ASP
1	A	202	VAL
1	A	212	VAL
1	A	222	ILE
1	A	231	LEU
1	A	245	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	GLN
1	A	254	ARG
1	A	257	ARG
1	A	260	ASN
1	A	279	SER
1	A	280	ARG
1	A	290	VAL
1	A	298	LEU
1	A	299	ASP
1	A	302	LYS
1	A	303	GLN
1	A	308	LEU
1	A	321	GLN
1	A	349	SER
1	A	386	VAL
1	A	411	GLN
1	A	425	LEU
1	A	426	THR
1	A	427	TYR
1	A	459	SER
1	A	473	ARG
1	A	483	GLN
1	A	491	THR
1	A	497	MET
1	A	499	PHE
1	A	511	ARG
1	A	539	ASN
1	A	551	THR
1	A	556	ARG
1	A	559	ARG
1	A	614	VAL
1	A	627	TYR
1	A	631	ARG
1	A	632	ASP
1	A	633	ARG
1	A	643	PHE
1	A	654	ASP
1	A	678	VAL
1	A	680	ARG
1	A	681	THR
1	B	48	ARG
1	B	51	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	52	LEU
1	B	54	GLU
1	B	56	ARG
1	B	62	ILE
1	B	64	LEU
1	B	67	LEU
1	B	68	ARG
1	B	73	LEU
1	B	81	LEU
1	B	93	LEU
1	B	98	MET
1	B	101	ARG
1	B	103	ILE
1	B	104	GLU
1	B	126	LEU
1	B	131	LEU
1	B	135	ASP
1	B	137	LYS
1	B	177	VAL
1	B	180	LYS
1	B	186	ASP
1	B	202	VAL
1	B	216	GLU
1	B	225	LYS
1	B	231	LEU
1	B	245	PHE
1	B	254	ARG
1	B	260	ASN
1	B	290	VAL
1	B	298	LEU
1	B	303	GLN
1	B	308	LEU
1	B	342	ILE
1	B	343	LEU
1	B	349	SER
1	B	386	VAL
1	B	425	LEU
1	B	427	TYR
1	B	459	SER
1	B	473	ARG
1	B	483	GLN
1	B	497	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	499	PHE
1	B	518	ARG
1	B	540	ARG
1	B	551	THR
1	B	554	PHE
1	B	556	ARG
1	B	557	THR
1	B	614	VAL
1	B	631	ARG
1	B	632	ASP
1	B	633	ARG
1	B	643	PHE
1	B	651	THR
1	B	654	ASP
1	B	681	THR
1	C	29	VAL
1	C	34	LEU
1	C	35	THR
1	C	39	ARG
1	C	45	ILE
1	C	46	GLN
1	C	49	PHE
1	C	62	ILE
1	C	67	LEU
1	C	68	ARG
1	C	73	LEU
1	C	87	ARG
1	C	93	LEU
1	C	98	MET
1	C	100	MET
1	C	103	ILE
1	C	104	GLU
1	C	126	LEU
1	C	137	LYS
1	C	138	ASN
1	C	141	LEU
1	C	177	VAL
1	C	180	LYS
1	C	186	ASP
1	C	202	VAL
1	C	218	SER
1	C	219	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	220	ARG
1	C	231	LEU
1	C	245	PHE
1	C	254	ARG
1	C	259	ASN
1	C	260	ASN
1	C	290	VAL
1	C	297	GLU
1	C	298	LEU
1	C	303	GLN
1	C	308	LEU
1	C	348	GLU
1	C	386	VAL
1	C	425	LEU
1	C	427	TYR
1	C	438	GLN
1	C	459	SER
1	C	473	ARG
1	C	483	GLN
1	C	497	MET
1	C	499	PHE
1	C	507	LYS
1	C	508	ASN
1	C	510	GLU
1	C	511	ARG
1	C	513	GLN
1	C	518	ARG
1	C	540	ARG
1	C	551	THR
1	C	556	ARG
1	C	559	ARG
1	C	614	VAL
1	C	615	GLN
1	C	627	TYR
1	C	631	ARG
1	C	633	ARG
1	C	634	LEU
1	C	643	PHE
1	C	654	ASP
1	D	34	LEU
1	D	35	THR
1	D	37	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	39	ARG
1	D	62	ILE
1	D	68	ARG
1	D	73	LEU
1	D	93	LEU
1	D	101	ARG
1	D	126	LEU
1	D	133	ARG
1	D	135	ASP
1	D	137	LYS
1	D	174	MET
1	D	180	LYS
1	D	186	ASP
1	D	202	VAL
1	D	216	GLU
1	D	219	ASN
1	D	220	ARG
1	D	225	LYS
1	D	231	LEU
1	D	245	PHE
1	D	257	ARG
1	D	260	ASN
1	D	290	VAL
1	D	298	LEU
1	D	303	GLN
1	D	306	SER
1	D	308	LEU
1	D	347	ILE
1	D	348	GLU
1	D	349	SER
1	D	350	SER
1	D	386	VAL
1	D	425	LEU
1	D	426	THR
1	D	427	TYR
1	D	459	SER
1	D	473	ARG
1	D	483	GLN
1	D	491	THR
1	D	497	MET
1	D	499	PHE
1	D	513	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	518	ARG
1	D	540	ARG
1	D	551	THR
1	D	554	PHE
1	D	556	ARG
1	D	558	PHE
1	D	559	ARG
1	D	633	ARG
1	D	654	ASP
1	D	680	ARG
1	D	681	THR
1	E	34	LEU
1	E	41	ILE
1	E	45	ILE
1	E	51	GLU
1	E	52	LEU
1	E	56	ARG
1	E	62	ILE
1	E	67	LEU
1	E	68	ARG
1	E	73	LEU
1	E	88	LYS
1	E	92	ARG
1	E	93	LEU
1	E	101	ARG
1	E	104	GLU
1	E	126	LEU
1	E	137	LYS
1	E	174	MET
1	E	177	VAL
1	E	180	LYS
1	E	186	ASP
1	E	202	VAL
1	E	218	SER
1	E	225	LYS
1	E	231	LEU
1	E	245	PHE
1	E	251	ARG
1	E	260	ASN
1	E	290	VAL
1	E	292	LYS
1	E	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	303	GLN
1	E	308	LEU
1	E	386	VAL
1	E	425	LEU
1	E	426	THR
1	E	427	TYR
1	E	459	SER
1	E	460	ARG
1	E	473	ARG
1	E	483	GLN
1	E	497	MET
1	E	499	PHE
1	E	510	GLU
1	E	518	ARG
1	E	540	ARG
1	E	551	THR
1	E	552	ILE
1	E	555	GLU
1	E	556	ARG
1	E	559	ARG
1	E	577	ASN
1	E	578	PHE
1	E	614	VAL
1	E	616	ASP
1	E	617	LEU
1	E	618	VAL
1	E	622	ASN
1	E	630	VAL
1	E	632	ASP
1	E	643	PHE
1	E	651	THR
1	E	654	ASP
1	E	661	THR
1	E	681	THR
1	F	37	ARG
1	F	62	ILE
1	F	67	LEU
1	F	68	ARG
1	F	73	LEU
1	F	93	LEU
1	F	100	MET
1	F	101	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	103	ILE
1	F	104	GLU
1	F	126	LEU
1	F	131	LEU
1	F	134	ARG
1	F	137	LYS
1	F	177	VAL
1	F	180	LYS
1	F	186	ASP
1	F	202	VAL
1	F	218	SER
1	F	225	LYS
1	F	228	ARG
1	F	231	LEU
1	F	245	PHE
1	F	257	ARG
1	F	260	ASN
1	F	290	VAL
1	F	298	LEU
1	F	303	GLN
1	F	308	LEU
1	F	386	VAL
1	F	425	LEU
1	F	426	THR
1	F	427	TYR
1	F	459	SER
1	F	483	GLN
1	F	497	MET
1	F	499	PHE
1	F	518	ARG
1	F	540	ARG
1	F	551	THR
1	F	552	ILE
1	F	556	ARG
1	F	559	ARG
1	F	612	ARG
1	F	614	VAL
1	F	617	LEU
1	F	618	VAL
1	F	620	THR
1	F	622	ASN
1	F	623	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	627	TYR
1	F	628	CYS
1	F	632	ASP
1	F	643	PHE
1	F	654	ASP
1	F	681	THR
1	G	37	ARG
1	G	62	ILE
1	G	64	LEU
1	G	67	LEU
1	G	68	ARG
1	G	73	LEU
1	G	93	LEU
1	G	101	ARG
1	G	104	GLU
1	G	126	LEU
1	G	137	LYS
1	G	180	LYS
1	G	186	ASP
1	G	202	VAL
1	G	218	SER
1	G	219	ASN
1	G	220	ARG
1	G	225	LYS
1	G	231	LEU
1	G	245	PHE
1	G	260	ASN
1	G	279	SER
1	G	290	VAL
1	G	298	LEU
1	G	303	GLN
1	G	308	LEU
1	G	386	VAL
1	G	425	LEU
1	G	427	TYR
1	G	459	SER
1	G	473	ARG
1	G	483	GLN
1	G	497	MET
1	G	499	PHE
1	G	518	ARG
1	G	540	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	551	THR
1	G	556	ARG
1	G	559	ARG
1	G	614	VAL
1	G	616	ASP
1	G	617	LEU
1	G	618	VAL
1	G	620	THR
1	G	622	ASN
1	G	627	TYR
1	G	632	ASP
1	G	643	PHE
1	G	654	ASP
1	G	680	ARG
1	G	681	THR
1	H	60	ARG
1	H	67	LEU
1	H	68	ARG
1	H	73	LEU
1	H	93	LEU
1	H	101	ARG
1	H	104	GLU
1	H	126	LEU
1	H	137	LYS
1	H	174	MET
1	H	177	VAL
1	H	180	LYS
1	H	186	ASP
1	H	202	VAL
1	H	218	SER
1	H	219	ASN
1	H	225	LYS
1	H	231	LEU
1	H	245	PHE
1	H	253	GLN
1	H	254	ARG
1	H	260	ASN
1	H	279	SER
1	H	290	VAL
1	H	298	LEU
1	H	303	GLN
1	H	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	356	ARG
1	H	386	VAL
1	H	425	LEU
1	H	427	TYR
1	H	459	SER
1	H	473	ARG
1	H	483	GLN
1	H	497	MET
1	H	499	PHE
1	H	518	ARG
1	H	540	ARG
1	H	551	THR
1	H	556	ARG
1	H	559	ARG
1	H	577	ASN
1	H	579	CYS
1	H	581	CYS
1	H	614	VAL
1	H	616	ASP
1	H	617	LEU
1	H	618	VAL
1	H	620	THR
1	H	622	ASN
1	H	627	TYR
1	H	632	ASP
1	H	643	PHE
1	H	654	ASP
1	H	681	THR
1	I	34	LEU
1	I	35	THR
1	I	39	ARG
1	I	62	ILE
1	I	67	LEU
1	I	68	ARG
1	I	73	LEU
1	I	92	ARG
1	I	93	LEU
1	I	95	ASP
1	I	101	ARG
1	I	104	GLU
1	I	126	LEU
1	I	137	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	138	ASN
1	I	177	VAL
1	I	180	LYS
1	I	186	ASP
1	I	202	VAL
1	I	219	ASN
1	I	220	ARG
1	I	225	LYS
1	I	231	LEU
1	I	245	PHE
1	I	260	ASN
1	I	279	SER
1	I	290	VAL
1	I	298	LEU
1	I	303	GLN
1	I	308	LEU
1	I	356	ARG
1	I	386	VAL
1	I	425	LEU
1	I	427	TYR
1	I	459	SER
1	I	473	ARG
1	I	483	GLN
1	I	497	MET
1	I	499	PHE
1	I	518	ARG
1	I	540	ARG
1	I	551	THR
1	I	556	ARG
1	I	559	ARG
1	I	614	VAL
1	I	616	ASP
1	I	617	LEU
1	I	618	VAL
1	I	620	THR
1	I	622	ASN
1	I	627	TYR
1	I	631	ARG
1	I	632	ASP
1	I	634	LEU
1	I	643	PHE
1	I	647	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	648	LEU
1	I	654	ASP
1	I	681	THR
1	J	34	LEU
1	J	51	GLU
1	J	52	LEU
1	J	62	ILE
1	J	67	LEU
1	J	68	ARG
1	J	73	LEU
1	J	93	LEU
1	J	101	ARG
1	J	104	GLU
1	J	126	LEU
1	J	137	LYS
1	J	172	MET
1	J	177	VAL
1	J	180	LYS
1	J	186	ASP
1	J	202	VAL
1	J	218	SER
1	J	225	LYS
1	J	231	LEU
1	J	245	PHE
1	J	260	ASN
1	J	279	SER
1	J	290	VAL
1	J	298	LEU
1	J	303	GLN
1	J	308	LEU
1	J	349	SER
1	J	386	VAL
1	J	425	LEU
1	J	427	TYR
1	J	428	GLU
1	J	460	ARG
1	J	473	ARG
1	J	483	GLN
1	J	497	MET
1	J	499	PHE
1	J	518	ARG
1	J	540	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	551	THR
1	J	556	ARG
1	J	559	ARG
1	J	579	CYS
1	J	614	VAL
1	J	616	ASP
1	J	617	LEU
1	J	618	VAL
1	J	620	THR
1	J	622	ASN
1	J	627	TYR
1	J	632	ASP
1	J	643	PHE
1	J	654	ASP
1	J	680	ARG
1	J	681	THR
1	K	34	LEU
1	K	62	ILE
1	K	67	LEU
1	K	68	ARG
1	K	73	LEU
1	K	93	LEU
1	K	101	ARG
1	K	104	GLU
1	K	126	LEU
1	K	137	LYS
1	K	174	MET
1	K	177	VAL
1	K	180	LYS
1	K	186	ASP
1	K	202	VAL
1	K	218	SER
1	K	225	LYS
1	K	231	LEU
1	K	245	PHE
1	K	254	ARG
1	K	257	ARG
1	K	260	ASN
1	K	290	VAL
1	K	298	LEU
1	K	303	GLN
1	K	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	349	SER
1	K	386	VAL
1	K	425	LEU
1	K	426	THR
1	K	427	TYR
1	K	459	SER
1	K	473	ARG
1	K	483	GLN
1	K	491	THR
1	K	497	MET
1	K	499	PHE
1	K	518	ARG
1	K	540	ARG
1	K	551	THR
1	K	556	ARG
1	K	559	ARG
1	K	581	CYS
1	K	616	ASP
1	K	617	LEU
1	K	618	VAL
1	K	621	CYS
1	K	622	ASN
1	K	627	TYR
1	K	632	ASP
1	K	643	PHE
1	K	654	ASP
1	K	681	THR
1	L	34	LEU
1	L	62	ILE
1	L	67	LEU
1	L	68	ARG
1	L	73	LEU
1	L	81	LEU
1	L	92	ARG
1	L	93	LEU
1	L	98	MET
1	L	101	ARG
1	L	104	GLU
1	L	126	LEU
1	L	137	LYS
1	L	177	VAL
1	L	180	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	186	ASP
1	L	202	VAL
1	L	218	SER
1	L	219	ASN
1	L	220	ARG
1	L	225	LYS
1	L	231	LEU
1	L	245	PHE
1	L	251	ARG
1	L	253	GLN
1	L	257	ARG
1	L	260	ASN
1	L	290	VAL
1	L	298	LEU
1	L	303	GLN
1	L	308	LEU
1	L	349	SER
1	L	386	VAL
1	L	425	LEU
1	L	427	TYR
1	L	459	SER
1	L	473	ARG
1	L	483	GLN
1	L	497	MET
1	L	499	PHE
1	L	518	ARG
1	L	540	ARG
1	L	551	THR
1	L	556	ARG
1	L	559	ARG
1	L	614	VAL
1	L	616	ASP
1	L	617	LEU
1	L	618	VAL
1	L	620	THR
1	L	622	ASN
1	L	627	TYR
1	L	632	ASP
1	L	643	PHE
1	L	654	ASP
1	L	681	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	219	ASN
1	A	259	ASN
1	A	438	GLN
1	A	483	GLN
1	A	539	ASN
1	A	615	GLN
1	A	673	HIS
1	B	86	HIS
1	B	219	ASN
1	B	320	HIS
1	B	438	GLN
1	B	483	GLN
1	B	615	GLN
1	B	673	HIS
1	C	46	GLN
1	C	86	HIS
1	C	205	HIS
1	C	253	GLN
1	C	330	ASN
1	C	483	GLN
1	C	615	GLN
1	C	673	HIS
1	D	86	HIS
1	D	138	ASN
1	D	253	GLN
1	D	259	ASN
1	D	483	GLN
1	D	615	GLN
1	D	673	HIS
1	E	47	ASN
1	E	208	HIS
1	E	259	ASN
1	E	330	ASN
1	E	615	GLN
1	E	622	ASN
1	E	673	HIS
1	F	438	GLN
1	F	483	GLN
1	F	673	HIS
1	G	86	HIS
1	G	259	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	438	GLN
1	G	483	GLN
1	G	615	GLN
1	G	622	ASN
1	G	673	HIS
1	H	259	ASN
1	H	260	ASN
1	H	438	GLN
1	H	483	GLN
1	H	577	ASN
1	H	615	GLN
1	H	622	ASN
1	H	673	HIS
1	I	253	GLN
1	I	259	ASN
1	I	438	GLN
1	I	483	GLN
1	I	622	ASN
1	I	673	HIS
1	J	253	GLN
1	J	259	ASN
1	J	438	GLN
1	J	483	GLN
1	J	615	GLN
1	J	622	ASN
1	J	673	HIS
1	K	253	GLN
1	K	259	ASN
1	K	295	ASN
1	K	438	GLN
1	K	483	GLN
1	K	622	ASN
1	K	673	HIS
1	L	86	HIS
1	L	205	HIS
1	L	259	ASN
1	L	295	ASN
1	L	438	GLN
1	L	483	GLN
1	L	615	GLN
1	L	622	ASN
1	L	673	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 24 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	705	-	3,3,3	0.21	0	2,2,2	0.42	0
3	EDO	H	703	-	3,3,3	0.18	0	2,2,2	0.33	0
3	EDO	A	703	-	3,3,3	0.25	0	2,2,2	0.42	0
3	EDO	D	703	-	3,3,3	0.60	0	2,2,2	0.60	0
3	EDO	A	704	-	3,3,3	0.36	0	2,2,2	0.55	0
3	EDO	F	703	-	3,3,3	0.08	0	2,2,2	0.16	0
3	EDO	D	704	-	3,3,3	0.25	0	2,2,2	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	H	703	-	-	1/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	703	-	-	1/1/1/1	-
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	F	703	-	-	1/1/1/1	-
3	EDO	D	704	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	EDO	O1-C1-C2-O2
3	H	703	EDO	O1-C1-C2-O2
3	D	703	EDO	O1-C1-C2-O2
3	F	703	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

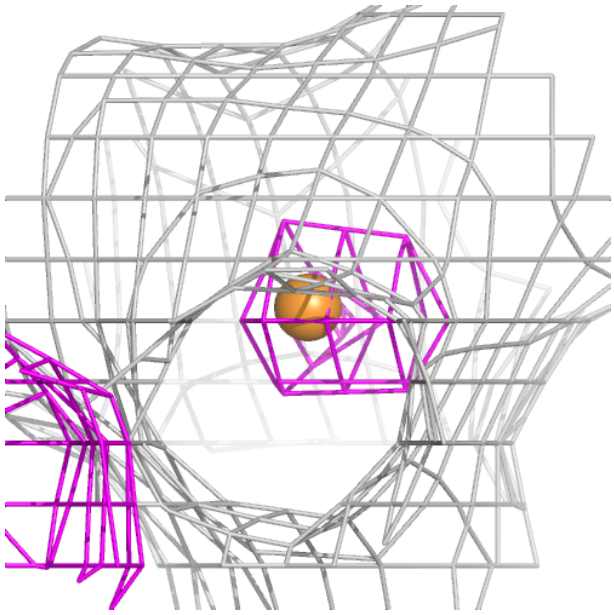
6.4 Ligands

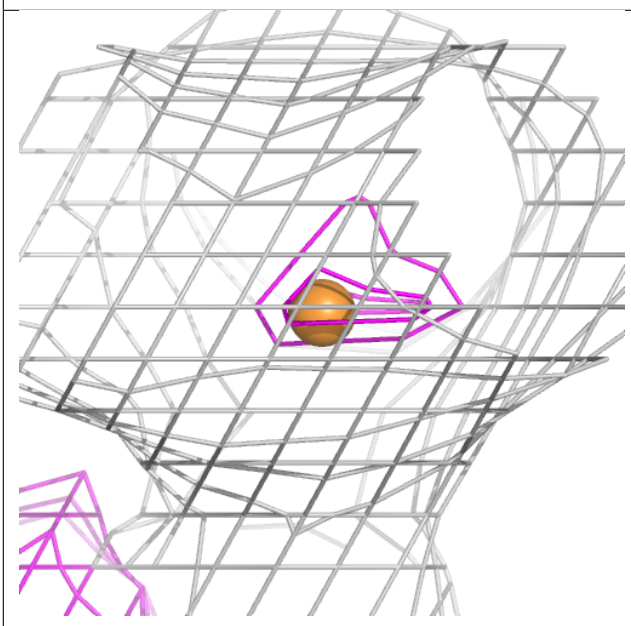
Unable to reproduce the depositors R factor - this section is therefore empty.

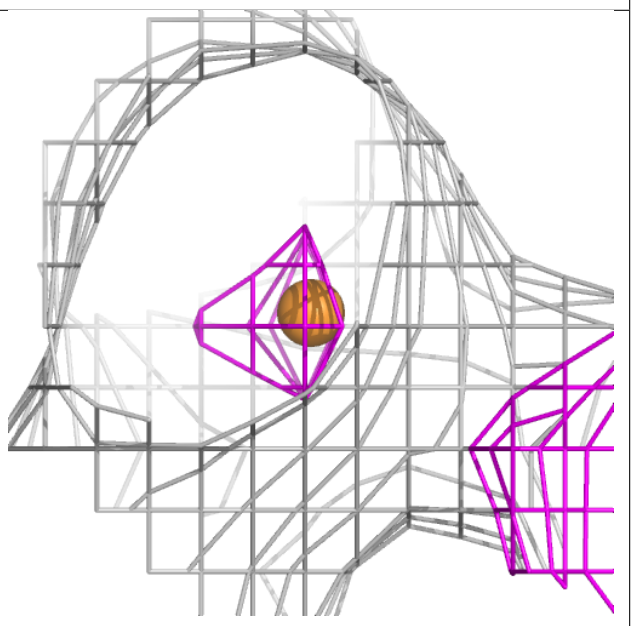
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CU A 701:

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

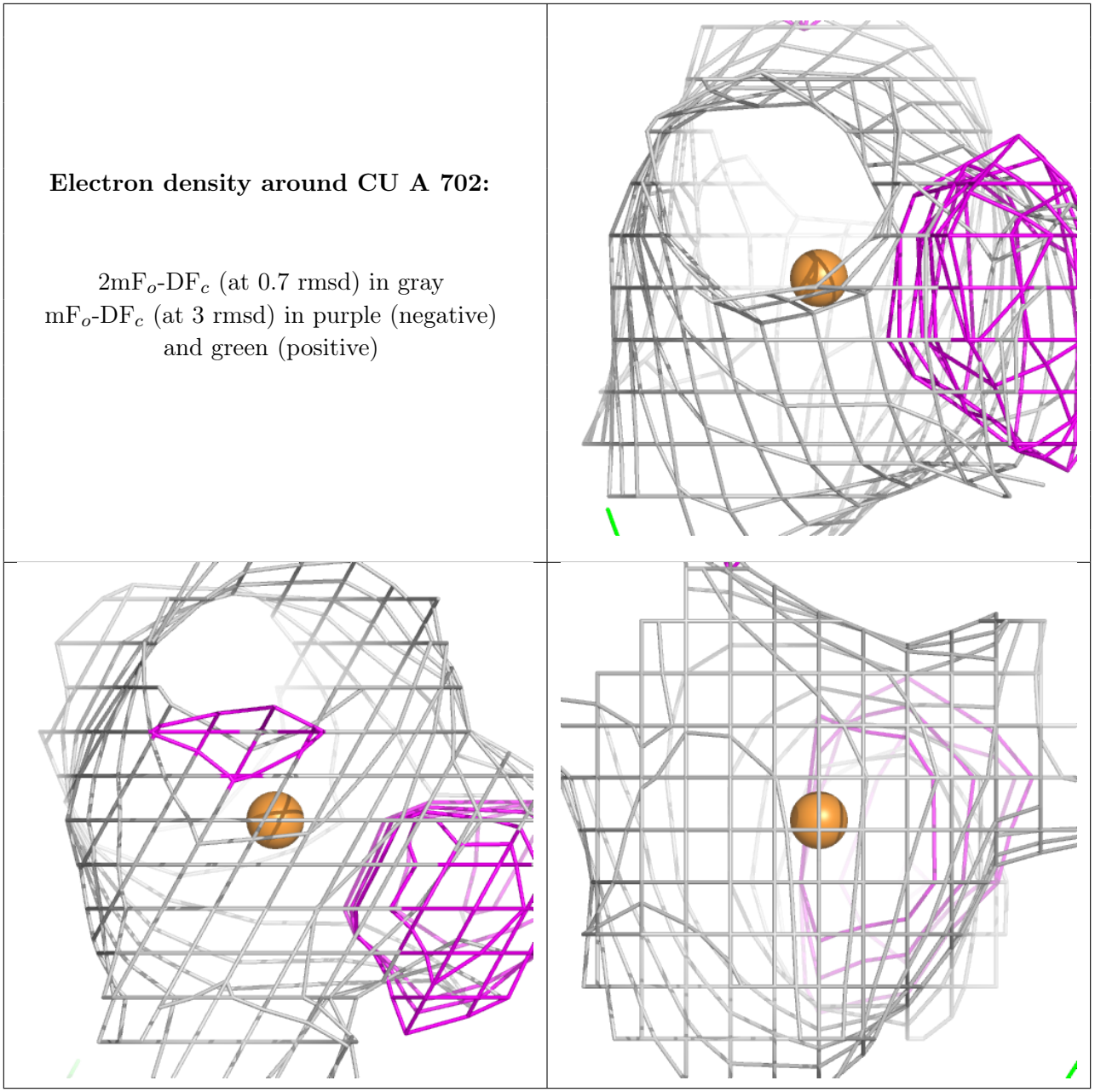






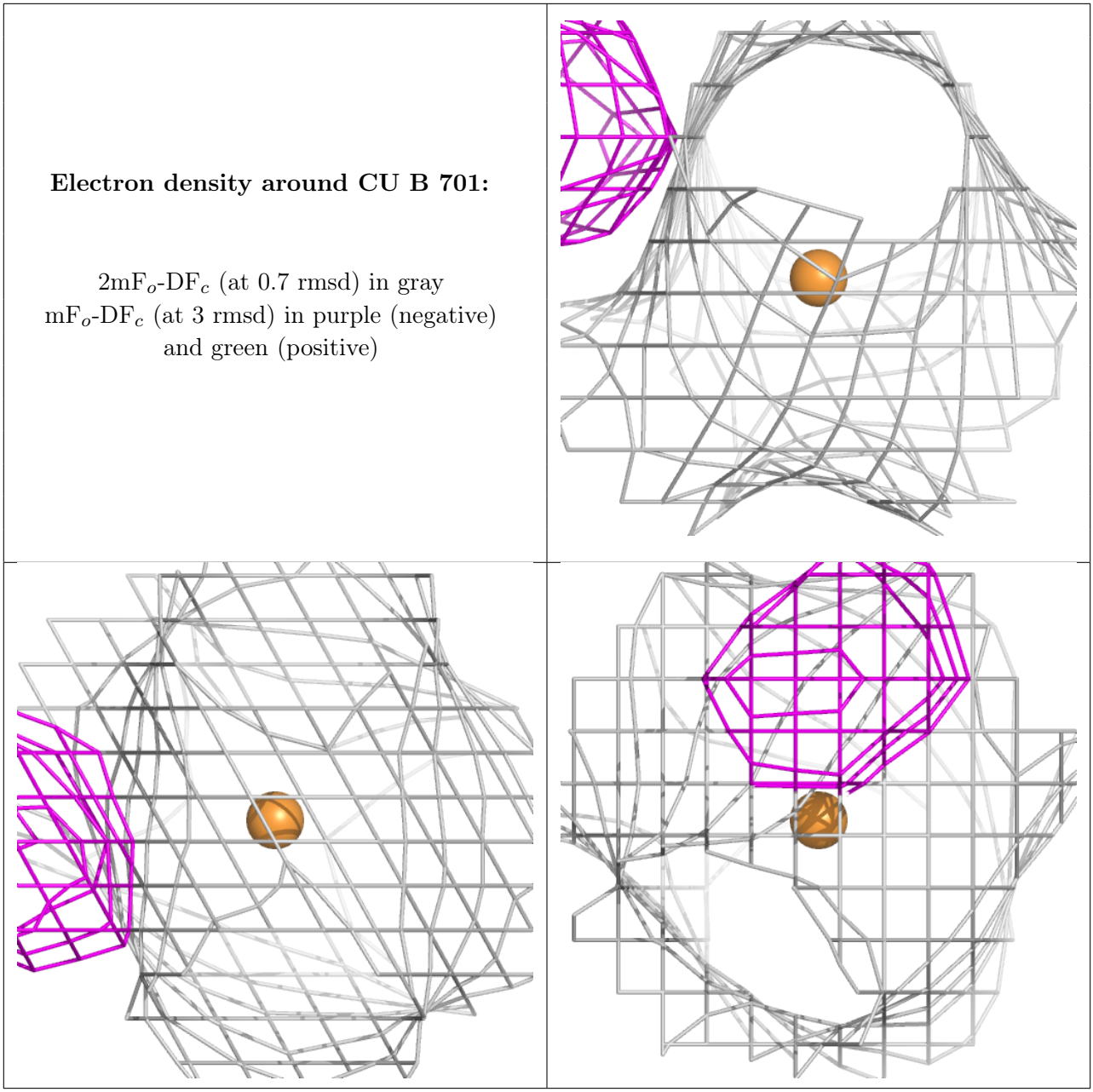
Electron density around CU A 702:

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



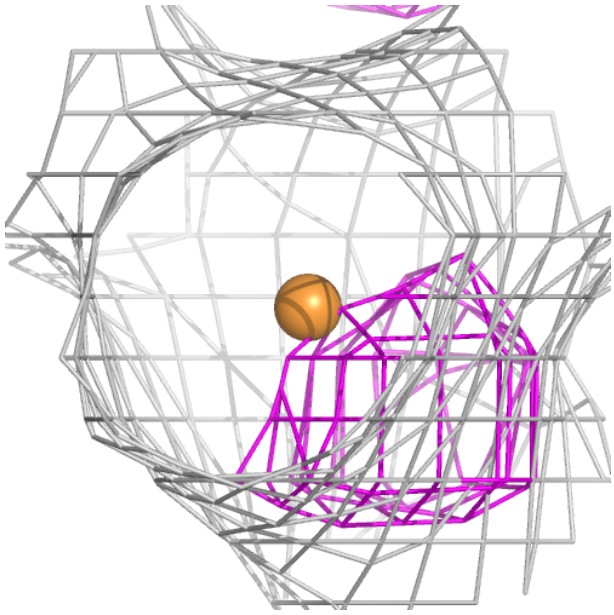
Electron density around CU B 701:

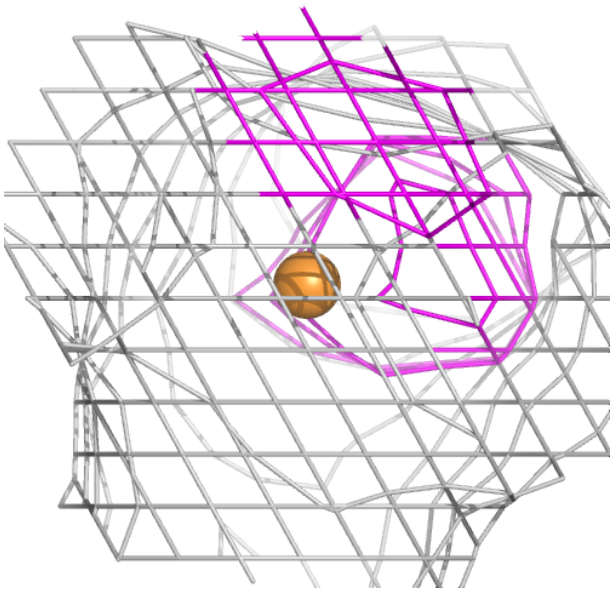
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

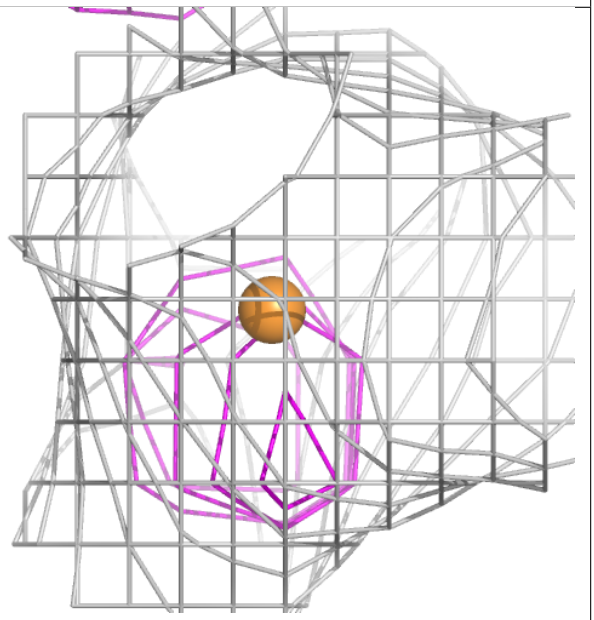


Electron density around CU B 702:

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

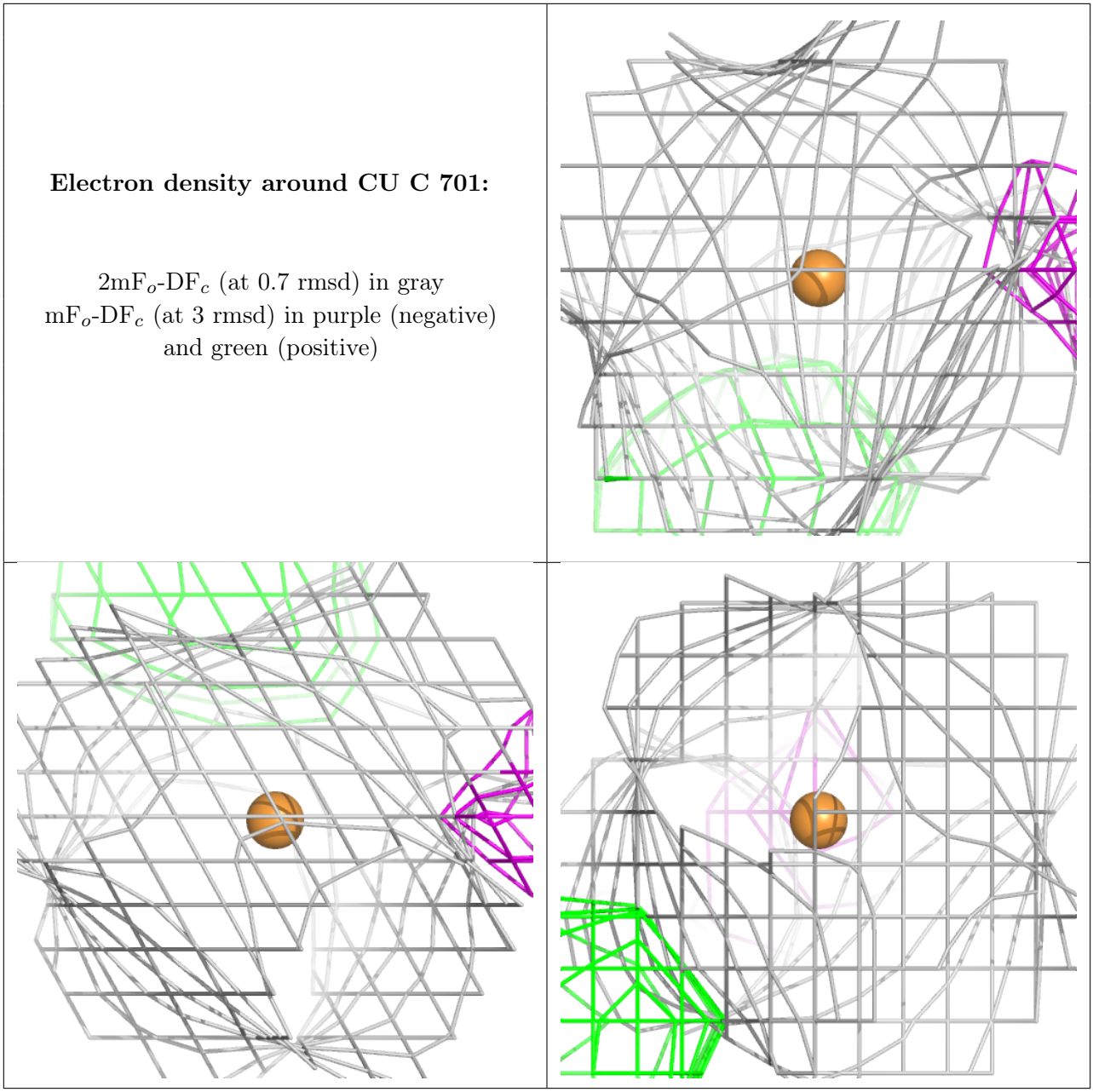






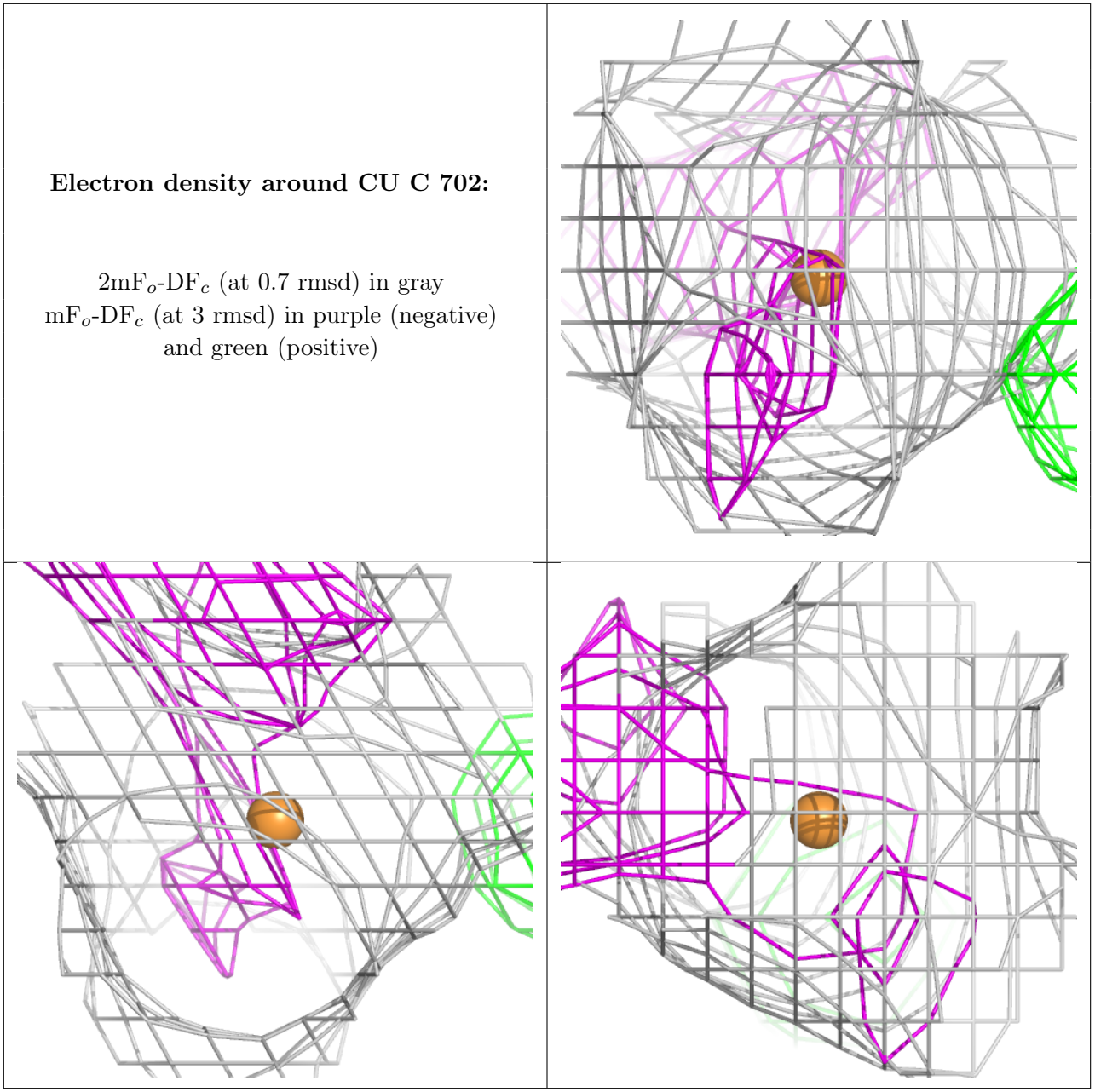
Electron density around CU C 701:

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



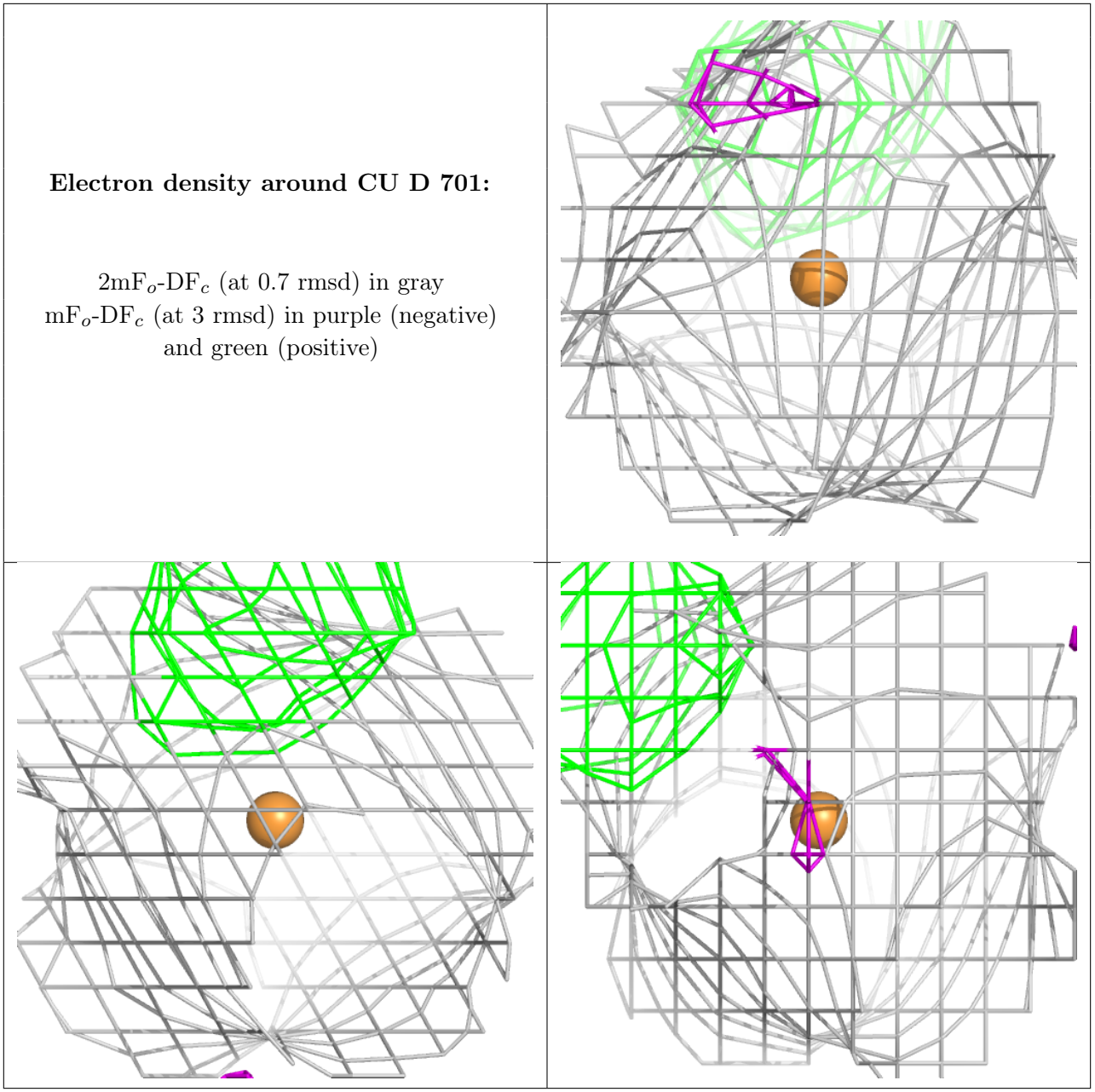
Electron density around CU C 702:

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



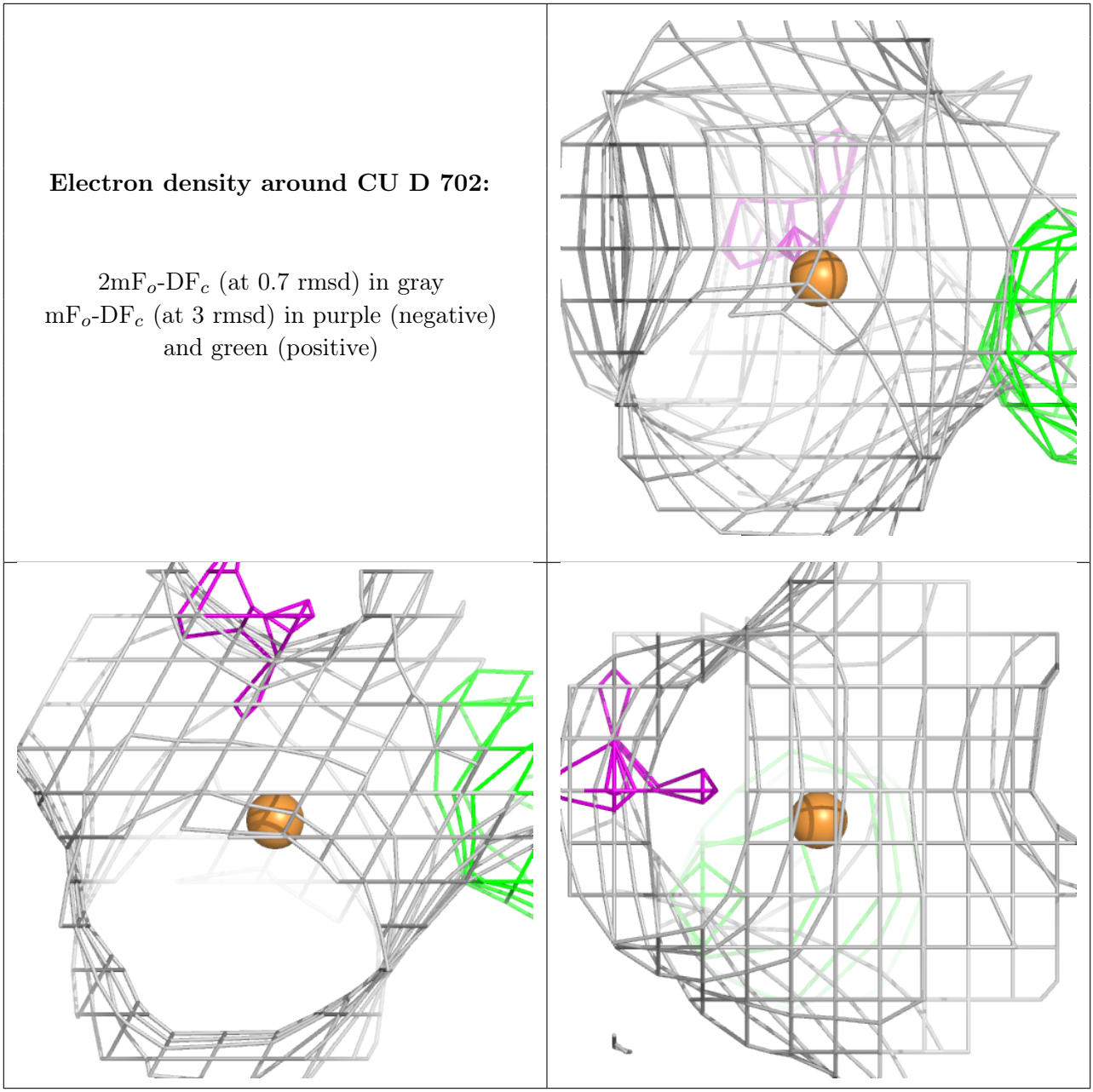
Electron density around CU D 701:

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



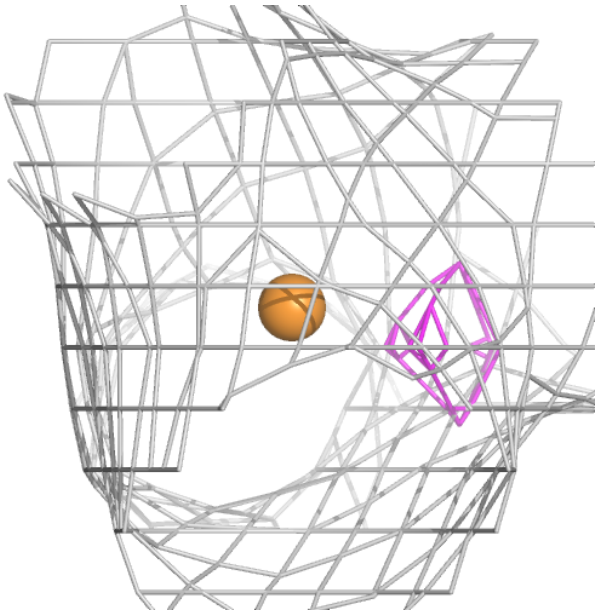
Electron density around CU D 702:

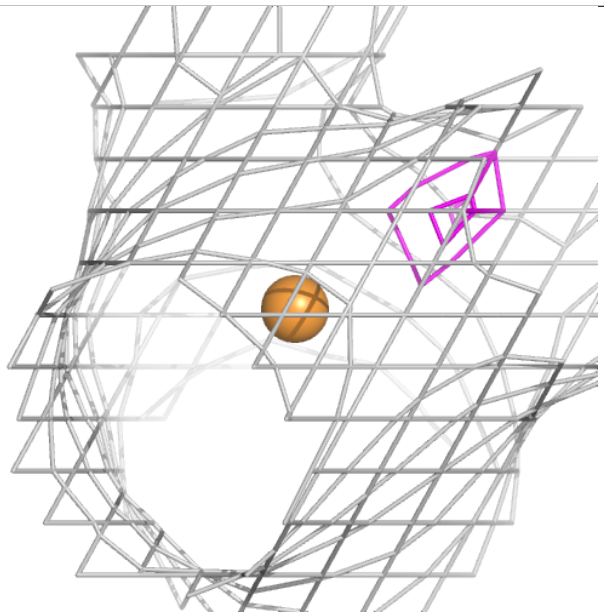
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

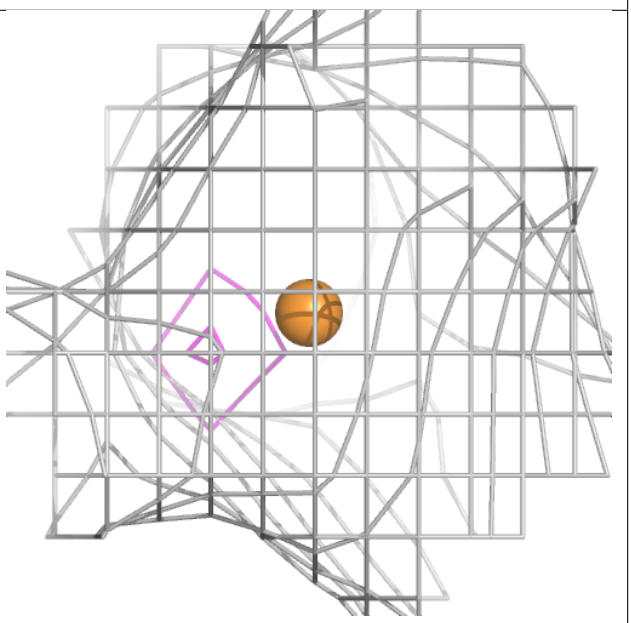


Electron density around CU E 701:

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

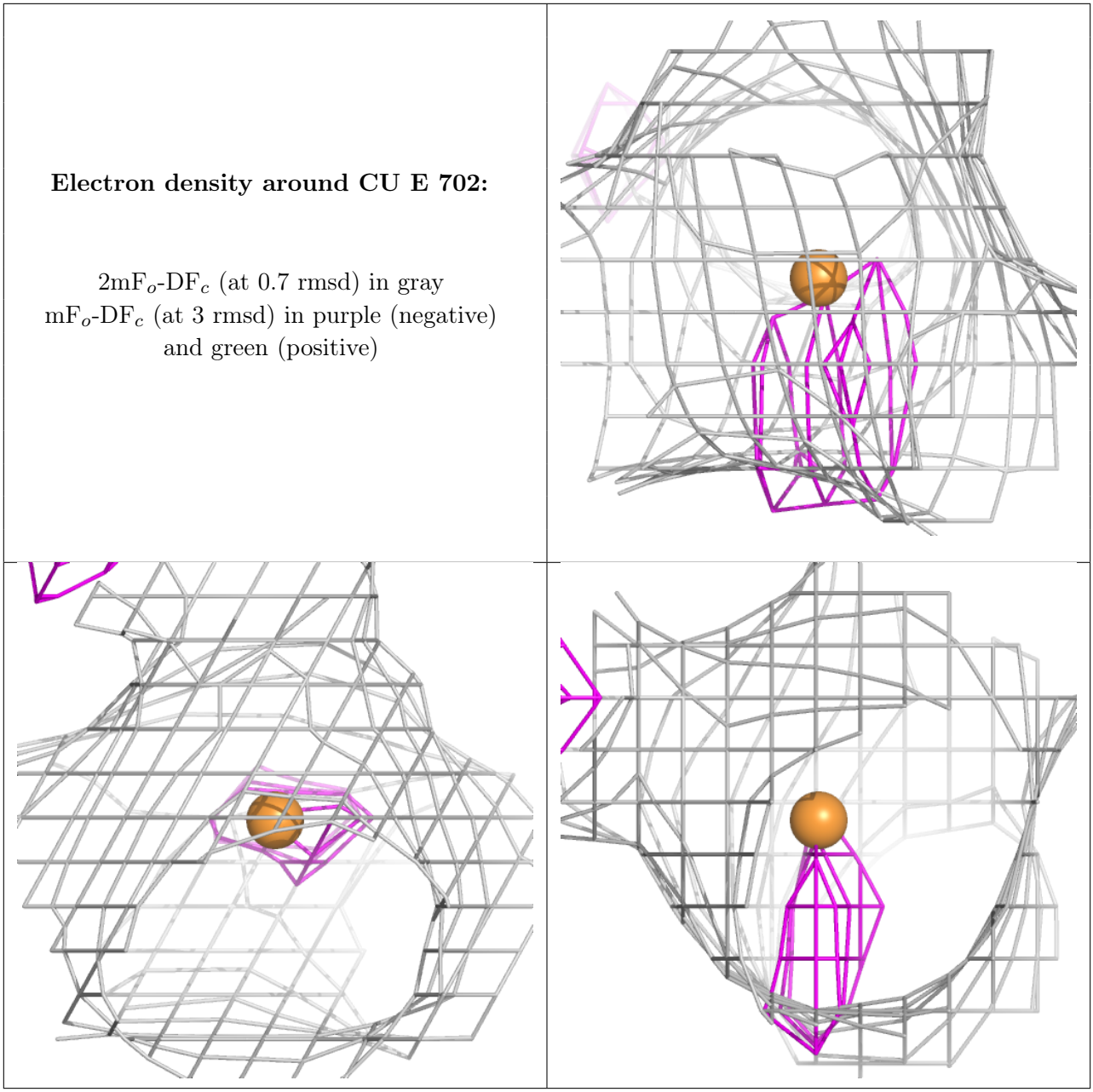






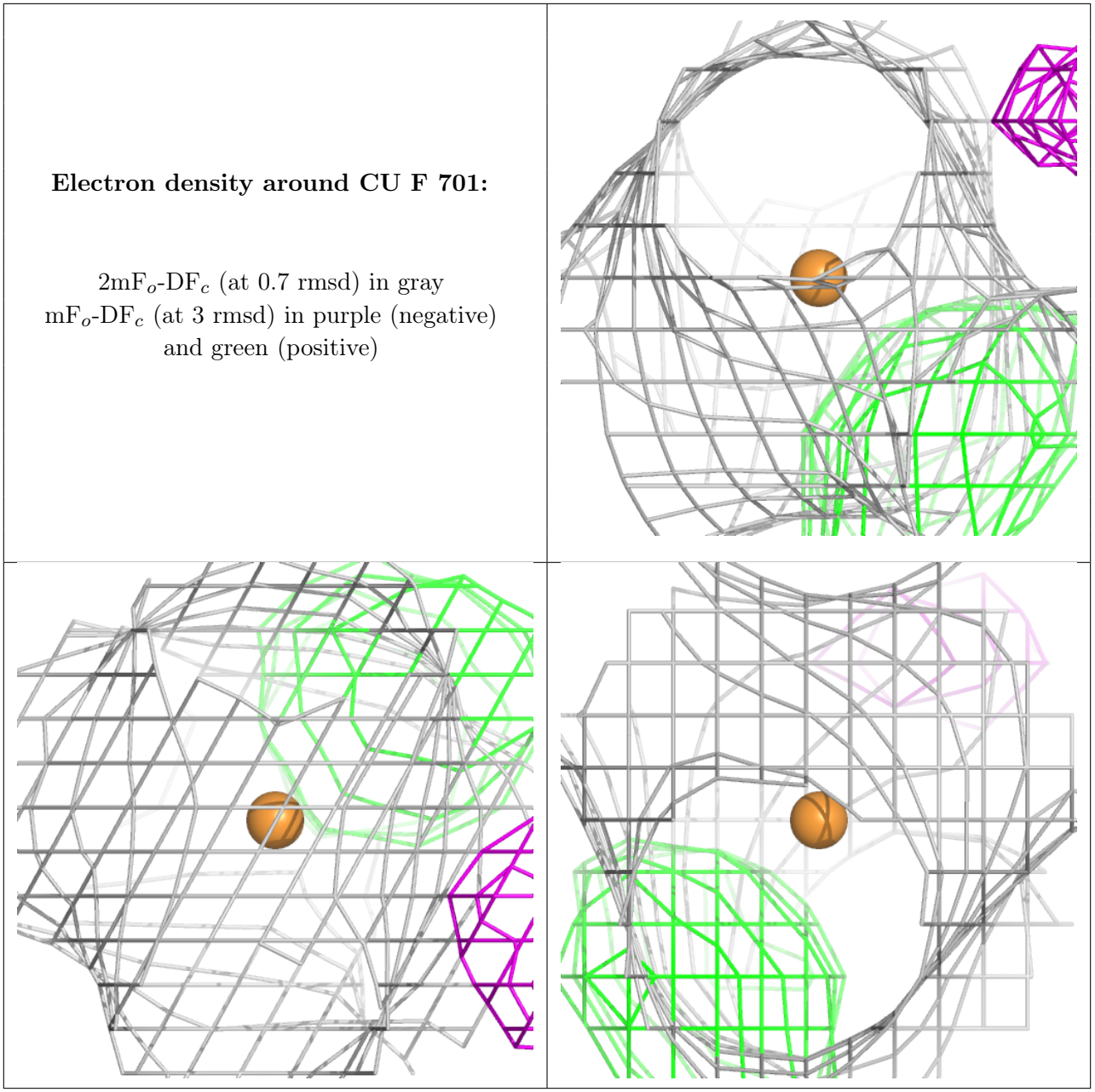
Electron density around CU E 702:

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



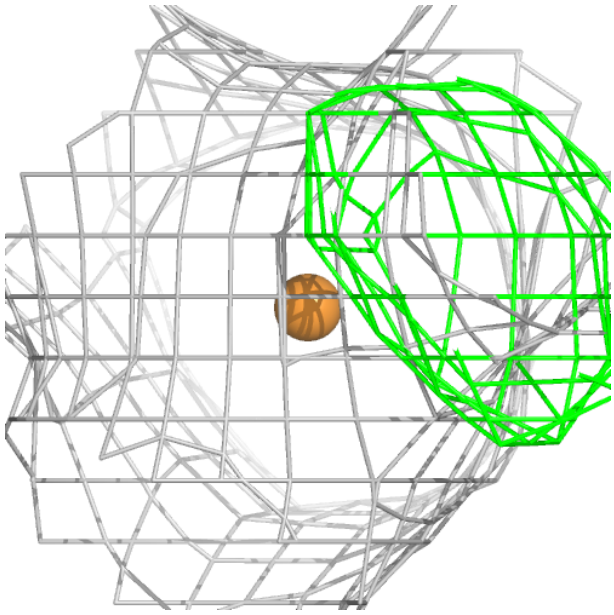
Electron density around CU F 701:

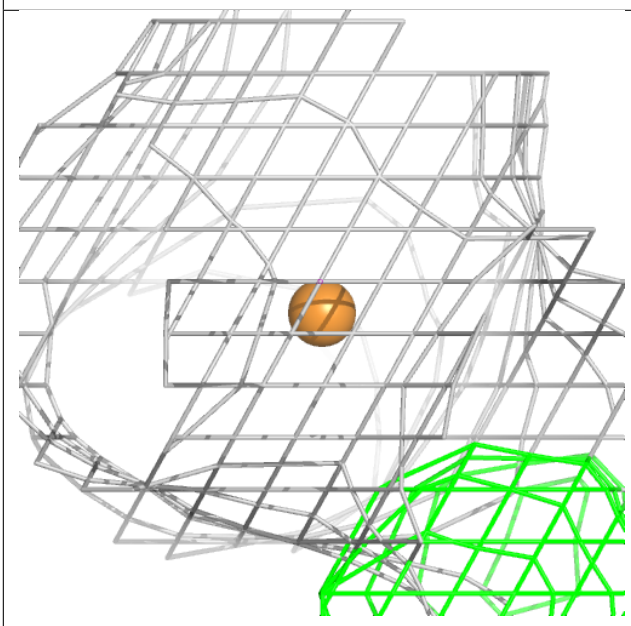
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

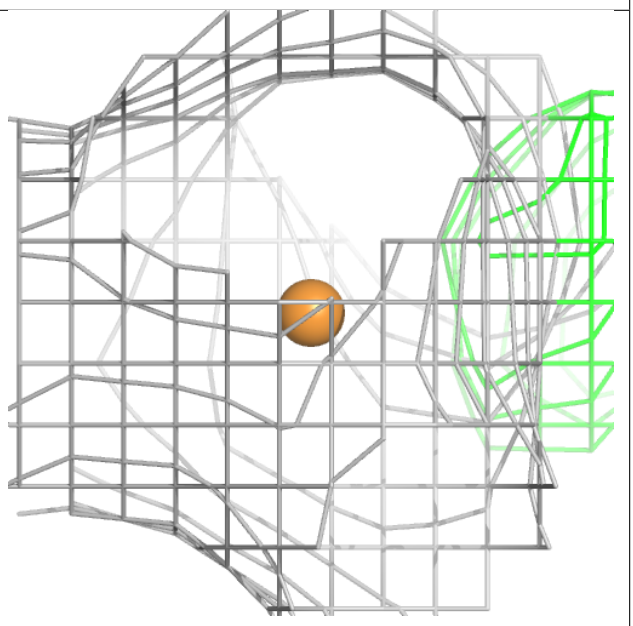


Electron density around CU F 702:

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

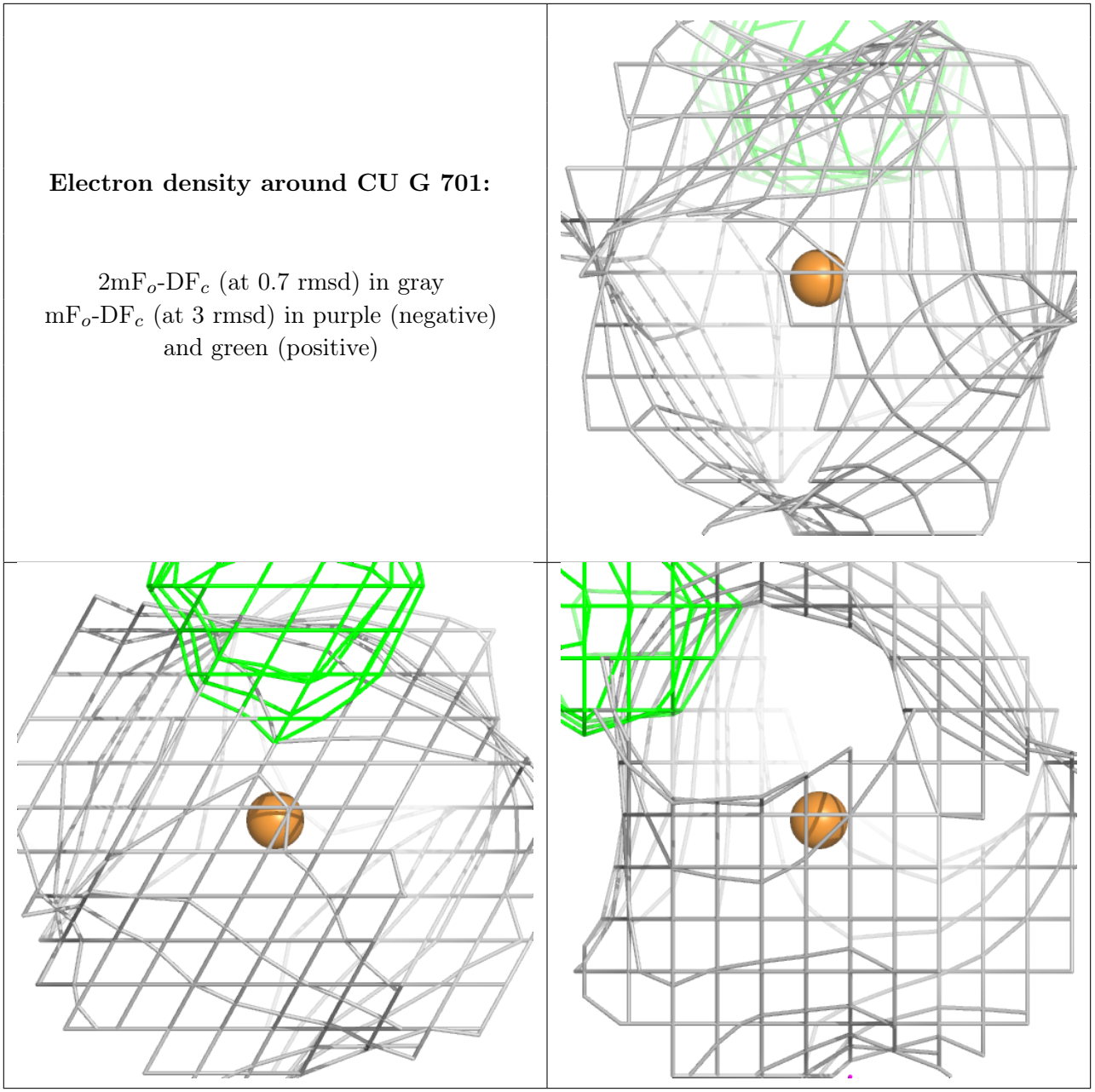






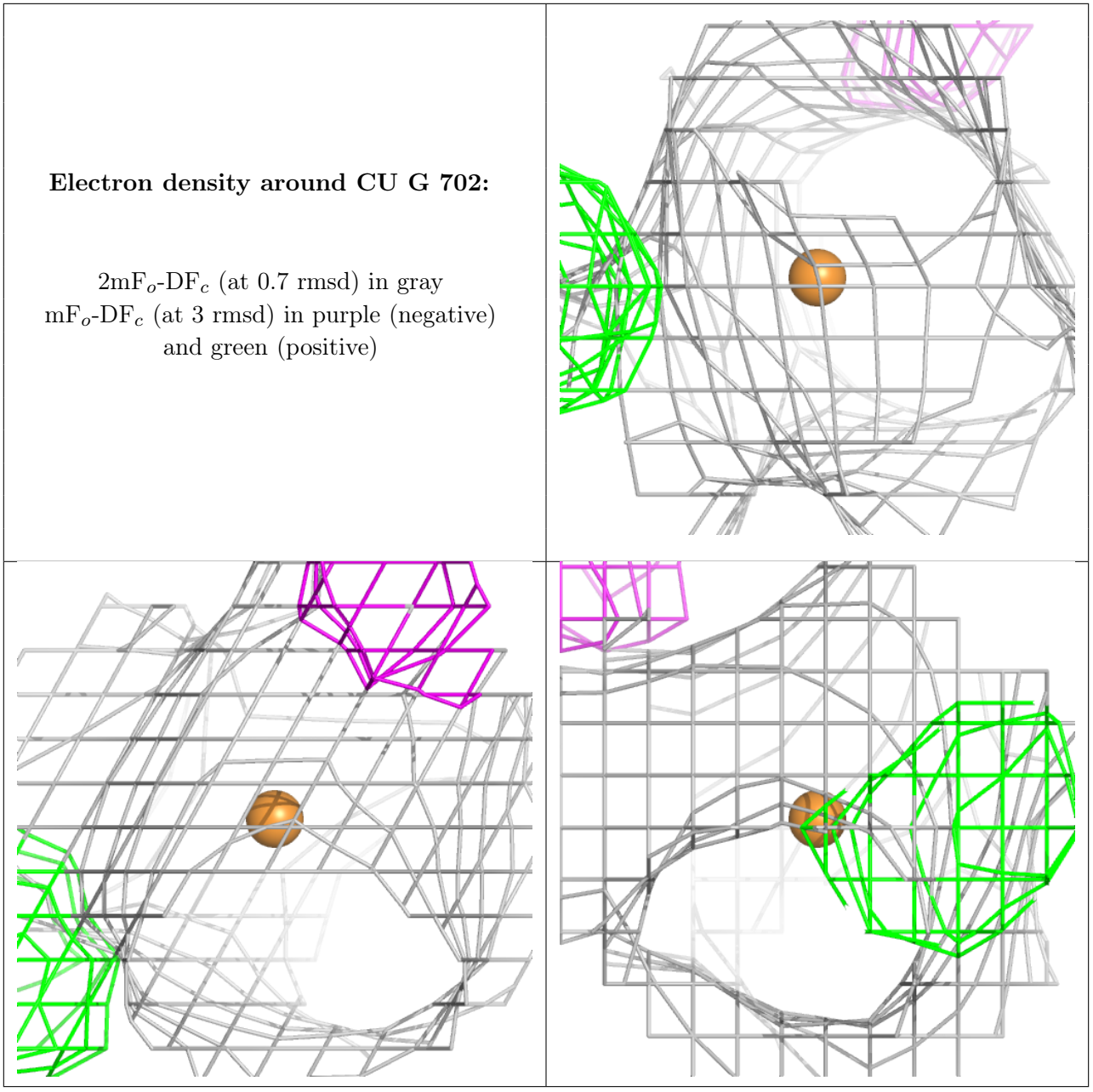
Electron density around CU G 701:

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



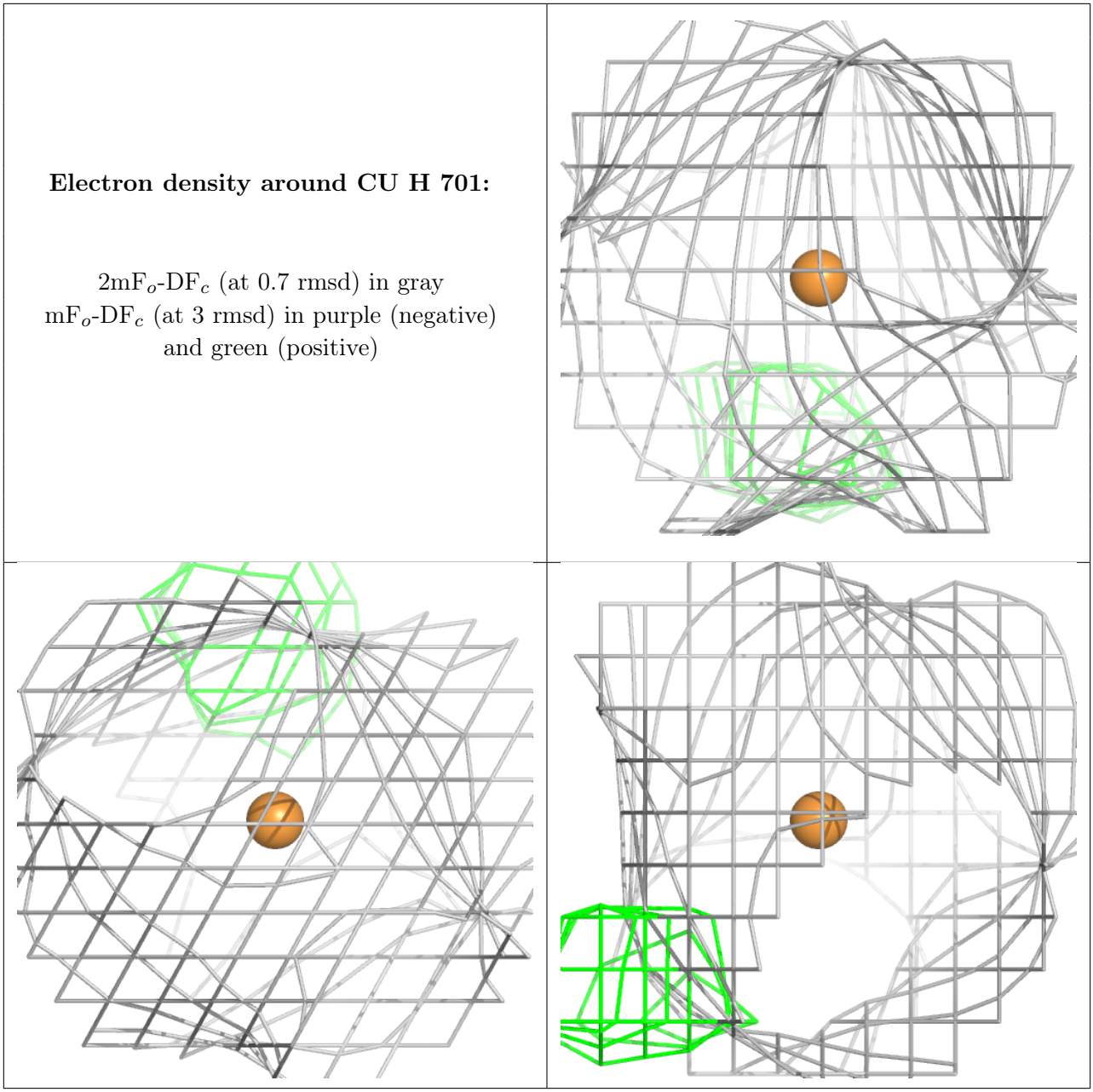
Electron density around CU G 702:

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



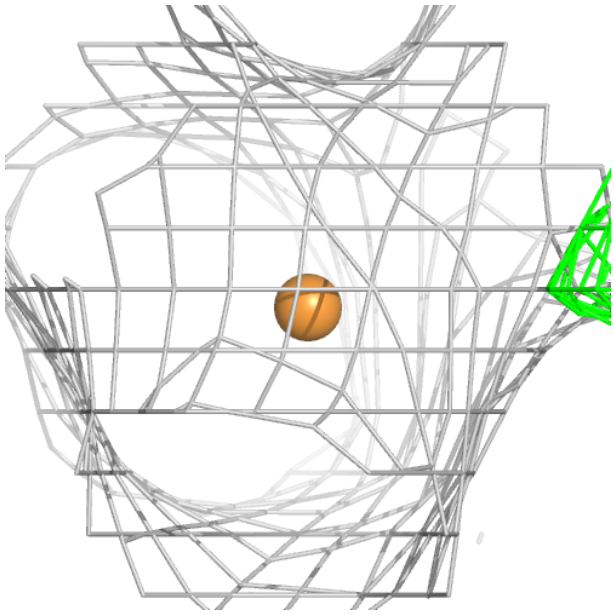
Electron density around CU H 701:

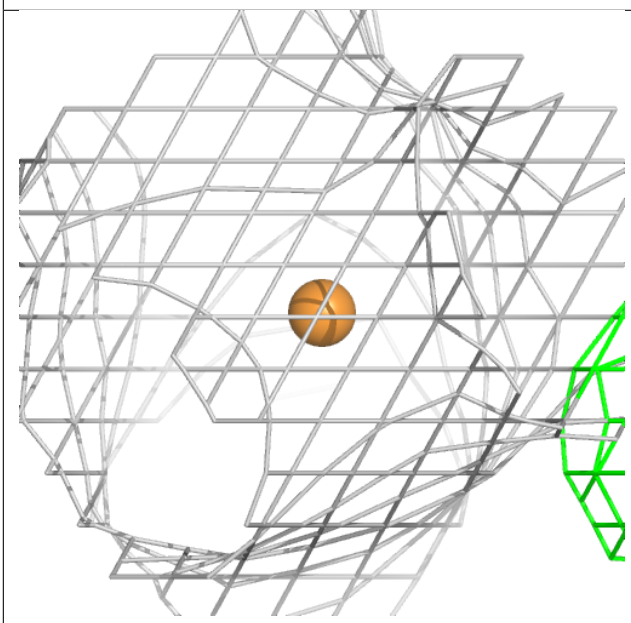
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

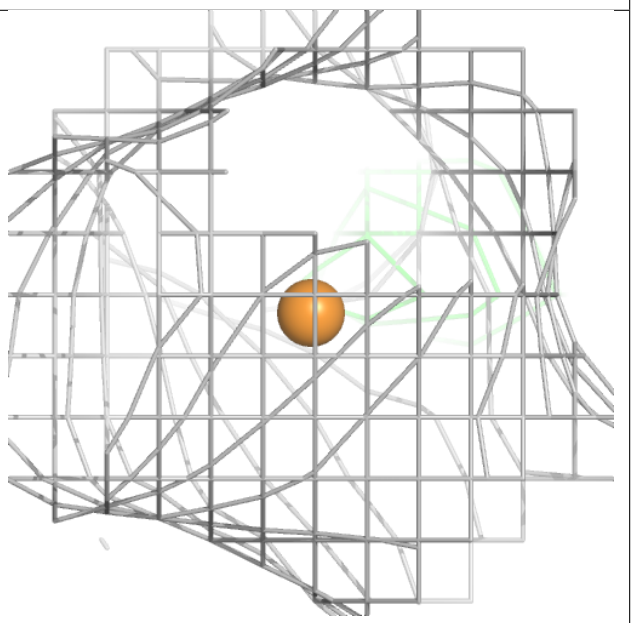


Electron density around CU H 702:

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

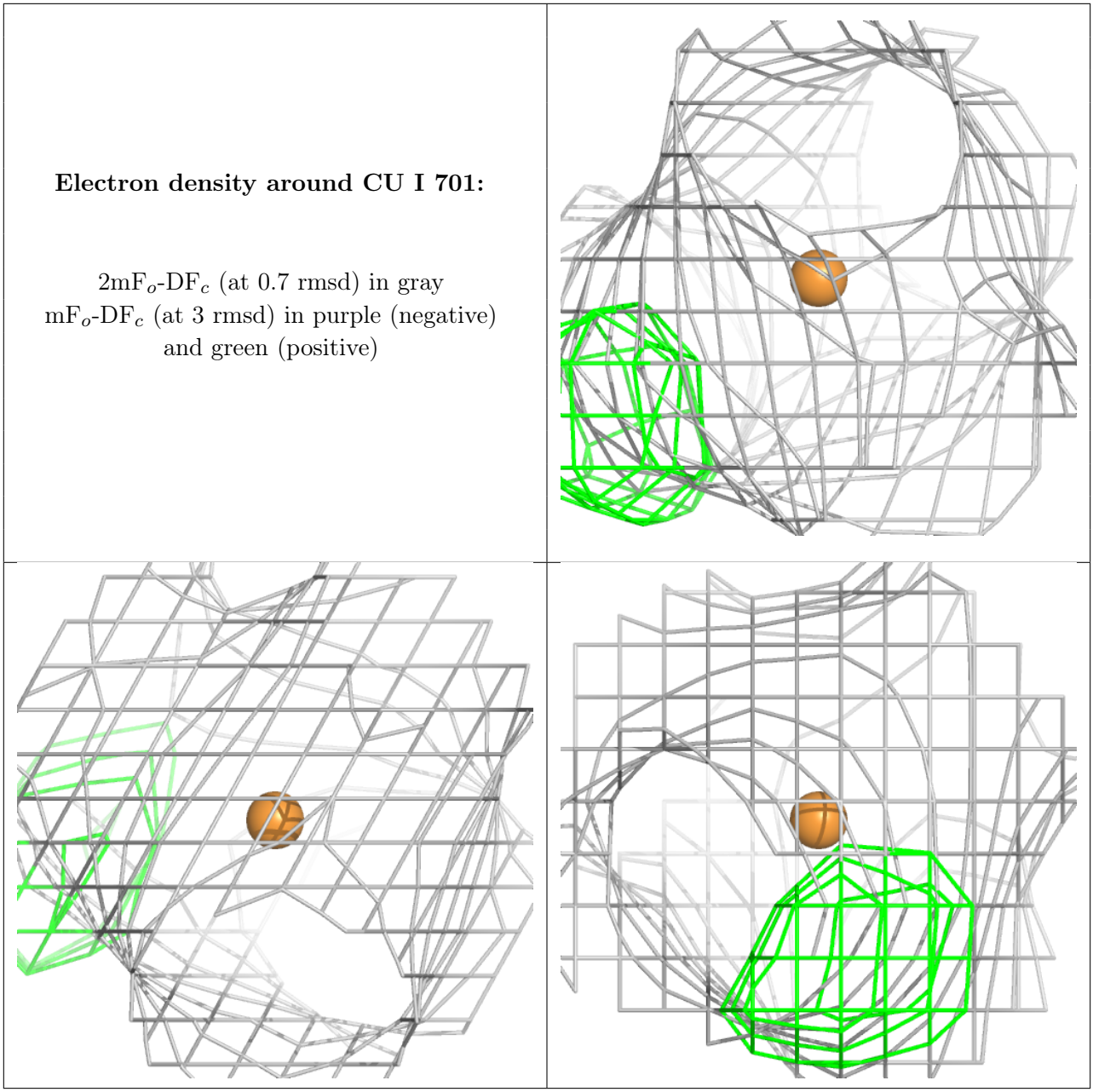






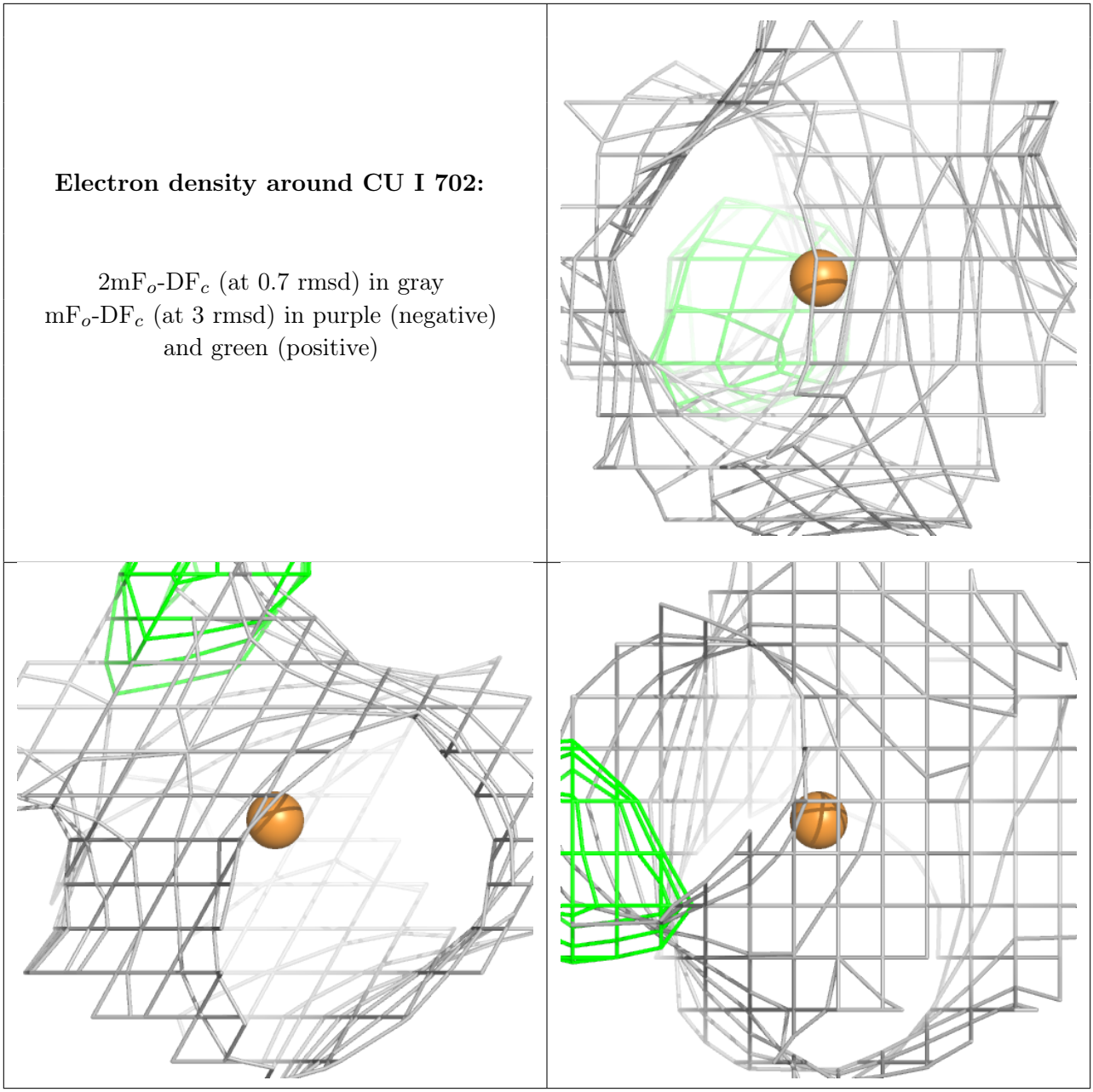
Electron density around CU I 701:

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



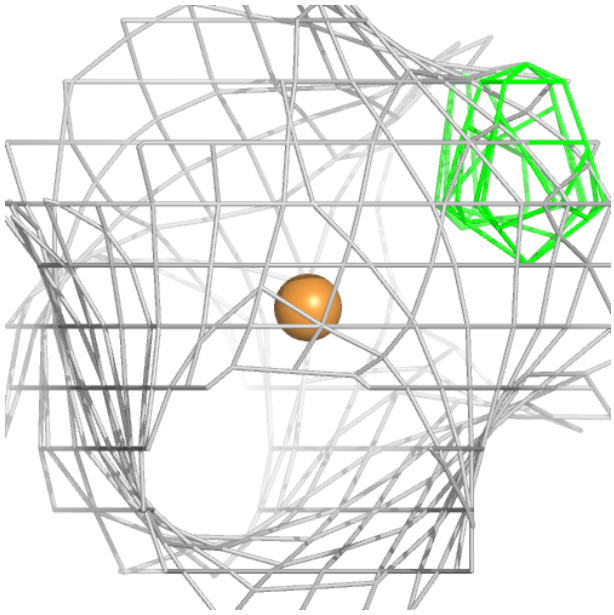
Electron density around CU I 702:

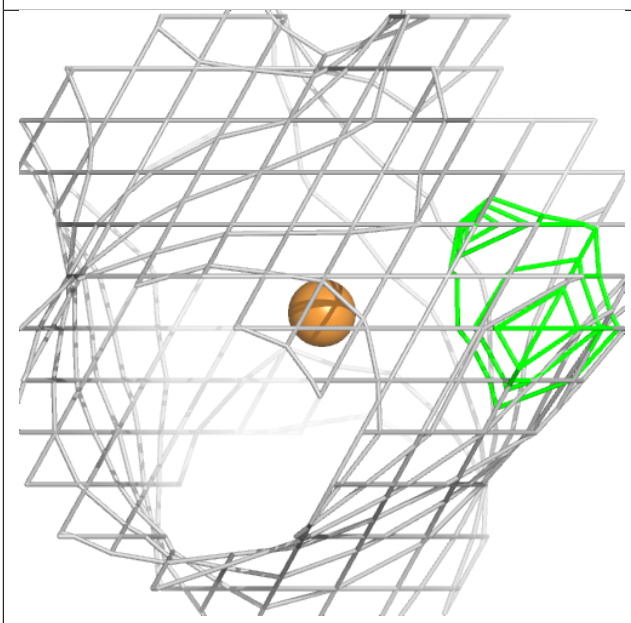
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

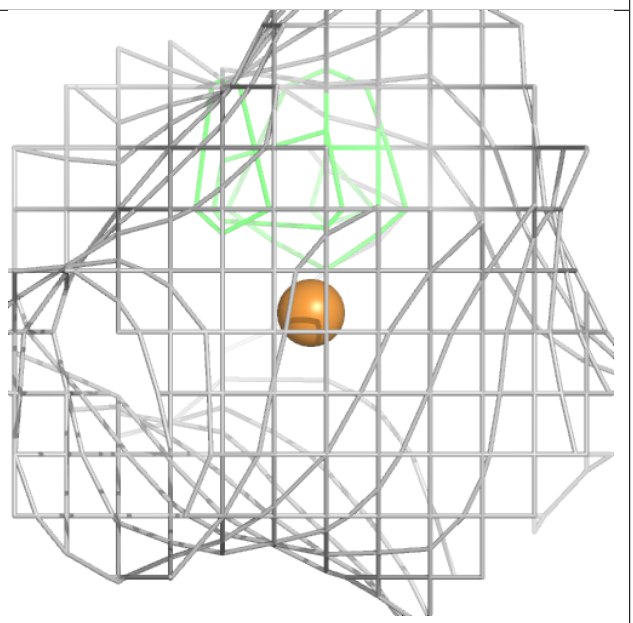


Electron density around CU J 701:

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

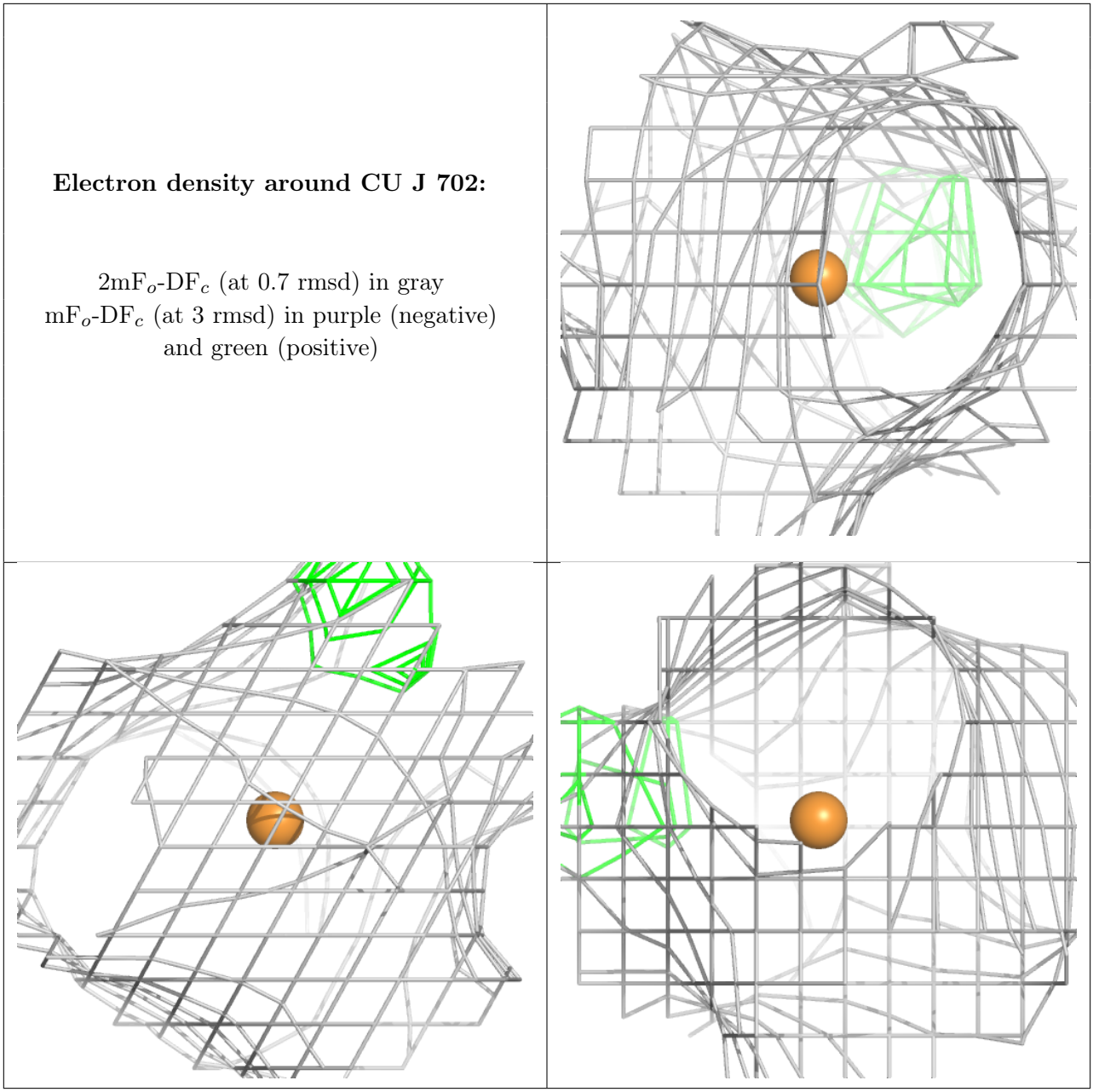






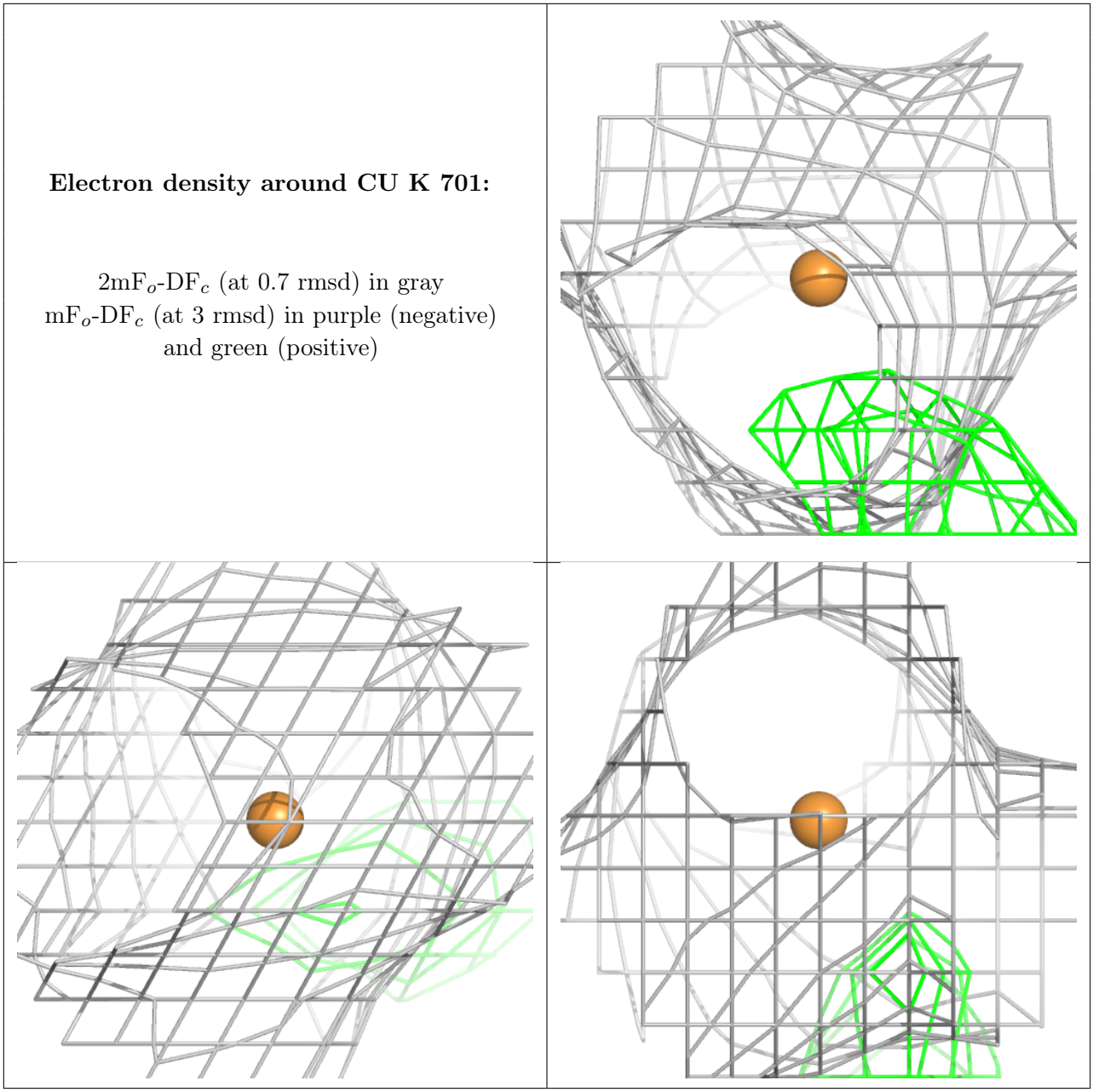
Electron density around CU J 702:

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



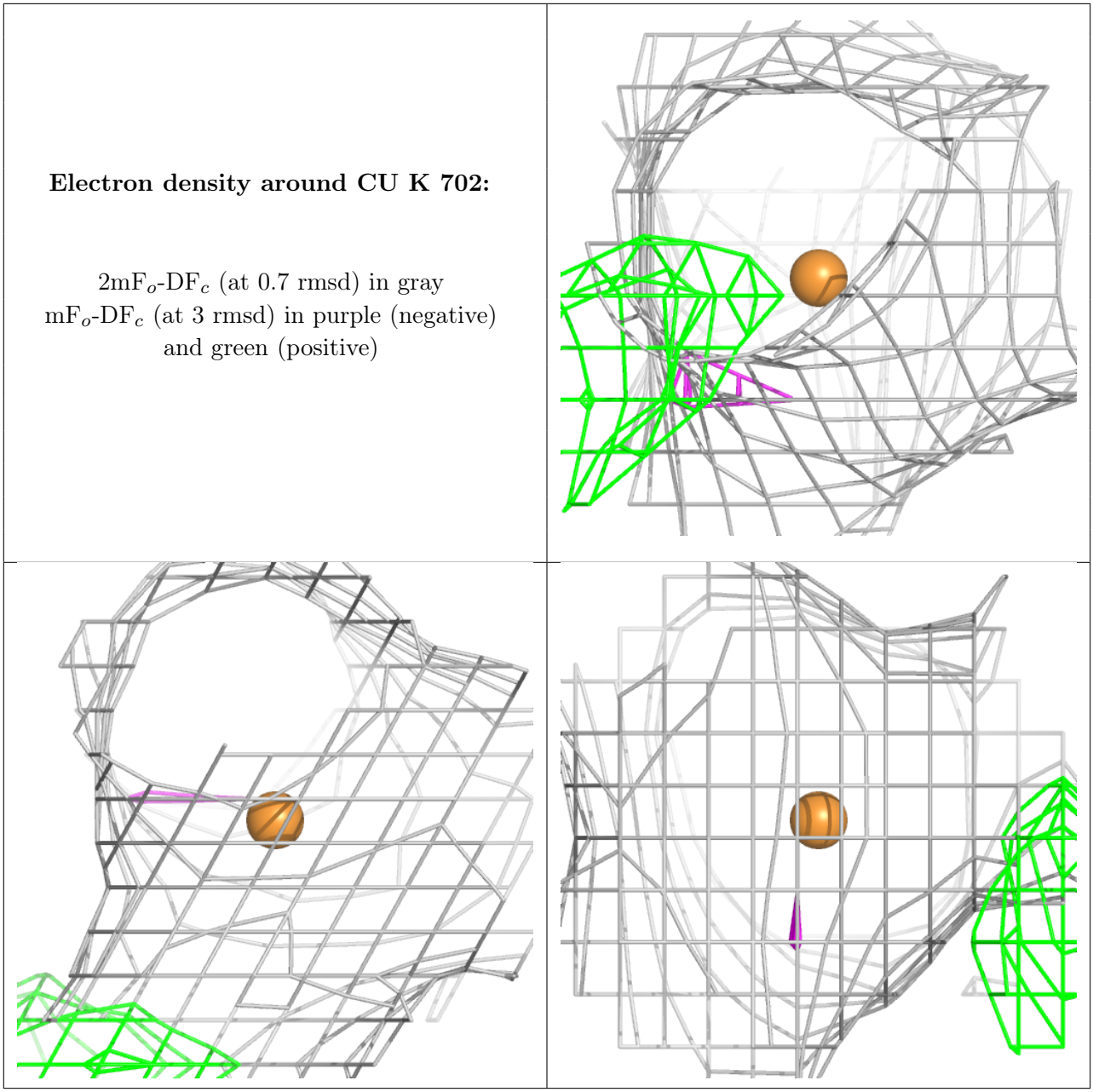
Electron density around CU K 701:

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



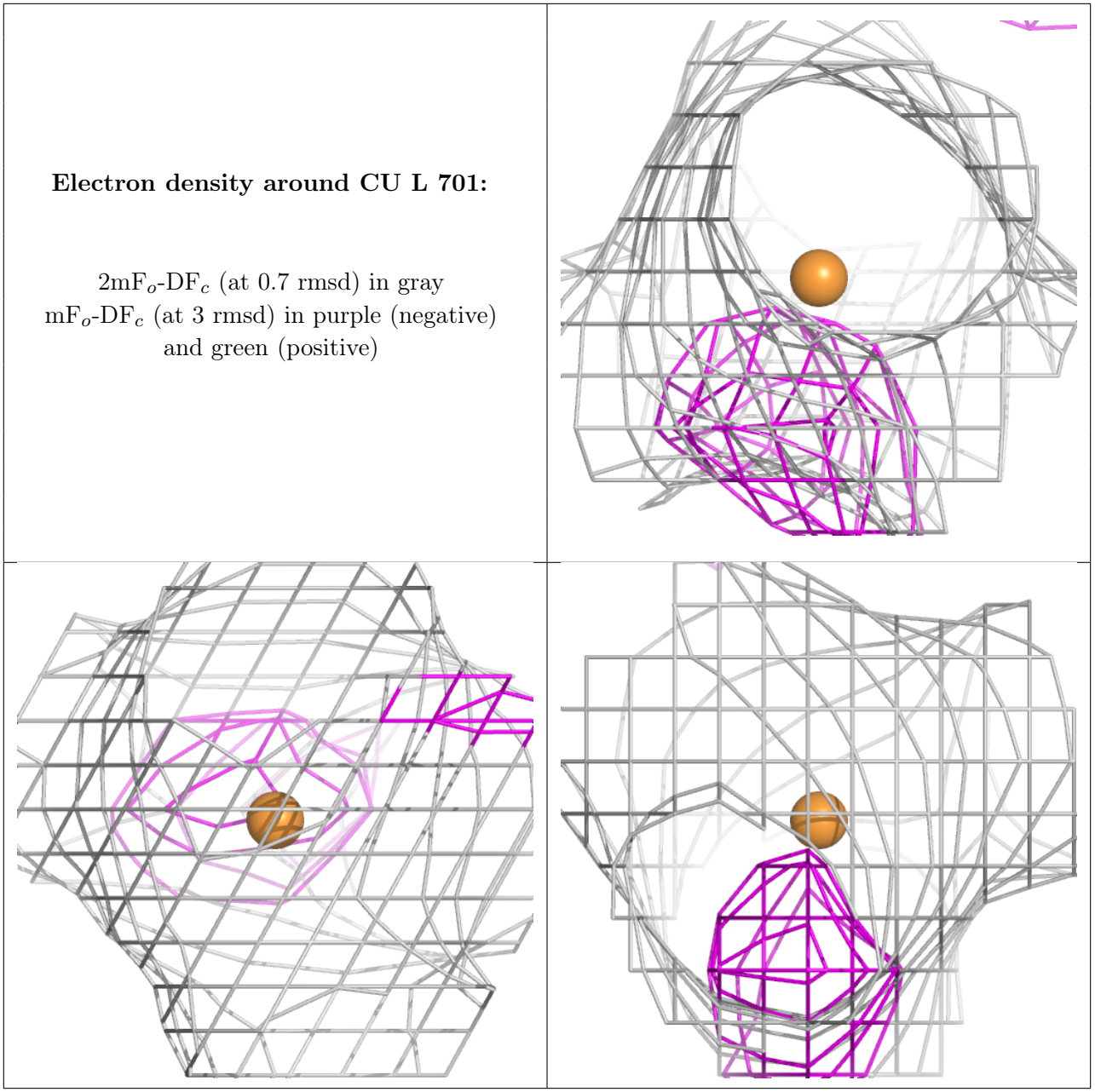
Electron density around CU K 702:

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



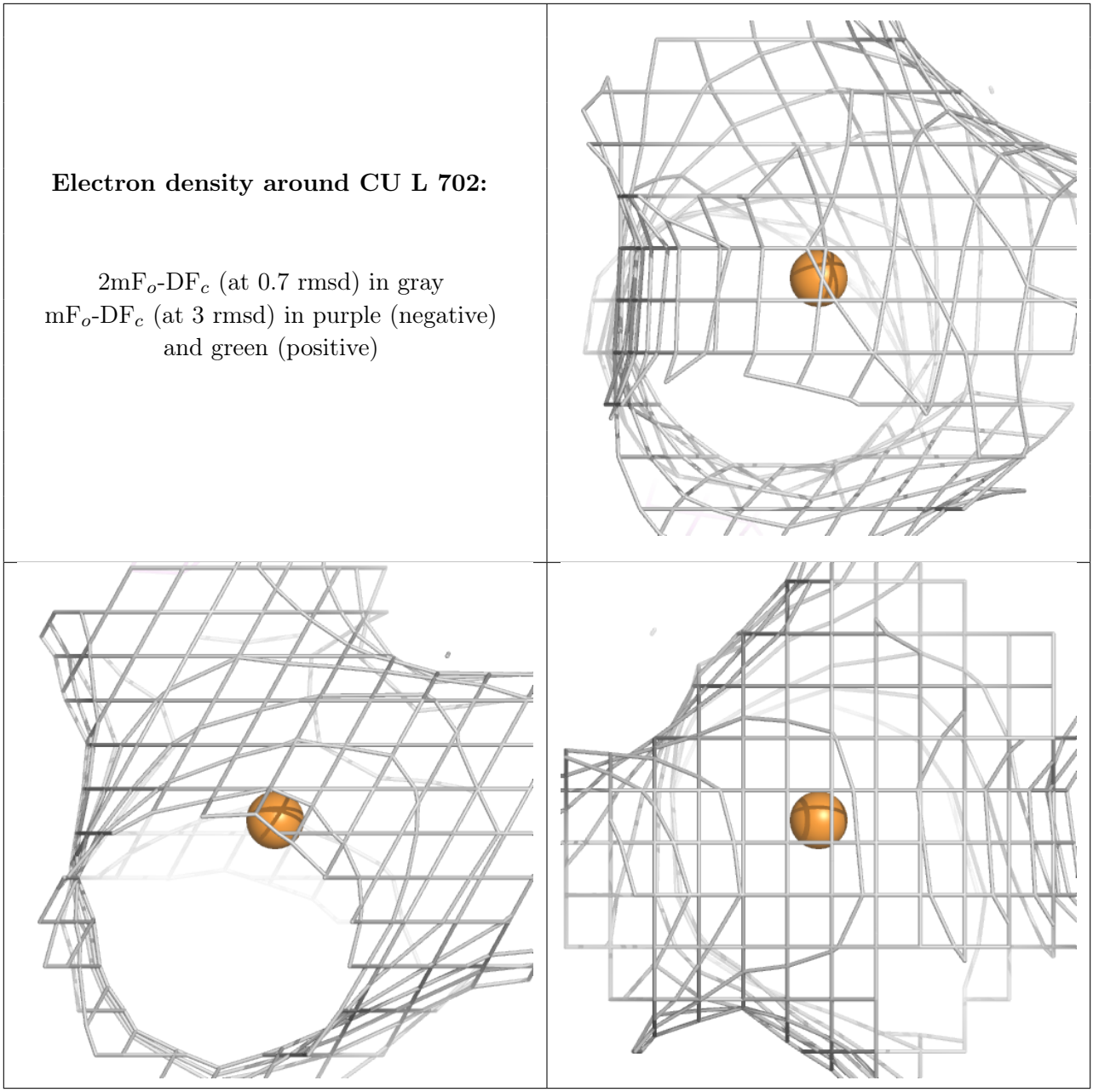
Electron density around CU L 701:

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



Electron density around CU L 702:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.