



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 7Z5P / pdb_00007z5p
Title : Bilirubin oxidase from *Bacillus pumilus*
Authors : Gihaz, S.; Herzallh, N.S.; Cohen, Y.; Bachar, O.; Fishman, A.; Yehezkeli, O.
Deposited on : 2022-03-09
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

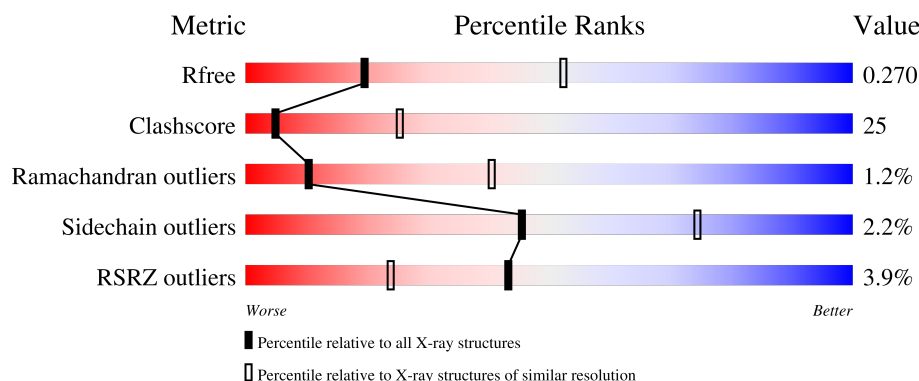
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	515	
1	B	515	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	A	604	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8243 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 Copper oxidase.

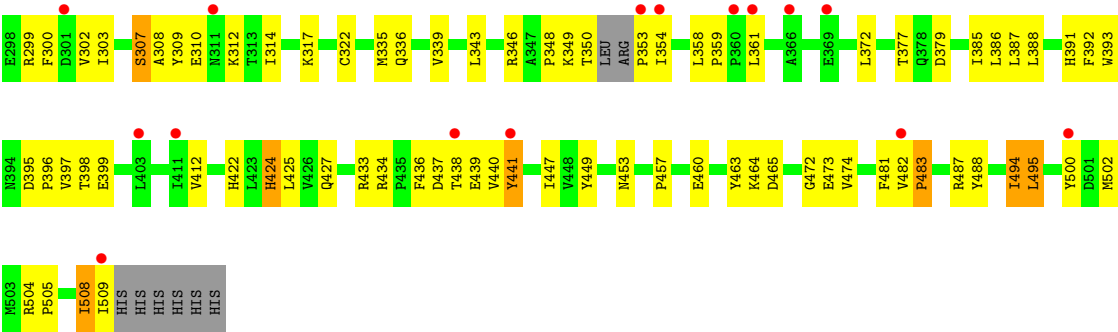
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	3	0	0
			4120	2643	709	755	13			
1	B	505	Total	C	N	O	S	1	0	0
			4115	2640	709	753	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510	HIS	-	expression tag	UNP A8FAG9
A	511	HIS	-	expression tag	UNP A8FAG9
A	512	HIS	-	expression tag	UNP A8FAG9
A	513	HIS	-	expression tag	UNP A8FAG9
A	514	HIS	-	expression tag	UNP A8FAG9
A	515	HIS	-	expression tag	UNP A8FAG9
B	510	HIS	-	expression tag	UNP A8FAG9
B	511	HIS	-	expression tag	UNP A8FAG9
B	512	HIS	-	expression tag	UNP A8FAG9
B	513	HIS	-	expression tag	UNP A8FAG9
B	514	HIS	-	expression tag	UNP A8FAG9
B	515	HIS	-	expression tag	UNP A8FAG9

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cu	0	0
			4	4		
2	B	4	Total	Cu	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.96Å 63.51Å 115.96Å 90.00° 124.57° 90.00°	Depositor
Resolution (Å)	59.22 – 2.99 59.22 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.1 (59.22-2.99) 98.4 (59.22-2.99)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.254 , 0.267 0.257 , 0.270	Depositor DCC
R_{free} test set	2405 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8243	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	0/4249	1.07	14/5793 (0.2%)
1	B	0.70	0/4245	1.02	9/5789 (0.2%)
All	All	0.70	0/8494	1.05	23/11582 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	288	HIS	N-CA-C	8.83	122.06	111.82
1	A	146	CYS	N-CA-C	8.17	120.55	108.14
1	A	440	VAL	CA-C-N	7.93	130.76	120.44
1	A	440	VAL	C-N-CA	7.93	130.76	120.44
1	A	394	ASN	N-CA-C	7.61	121.96	113.21
1	B	216	ASP	N-CA-C	-7.34	102.87	112.41
1	B	346	ARG	CA-C-N	-7.00	114.55	123.16
1	B	346	ARG	C-N-CA	-7.00	114.55	123.16
1	A	39	VAL	N-CA-CB	6.59	122.10	111.23
1	A	177	GLU	N-CA-C	-6.45	106.05	114.04
1	A	499	ASP	N-CA-C	6.12	120.01	112.54
1	B	424	HIS	CA-C-O	-5.65	115.32	121.87
1	A	4	GLU	N-CA-CB	5.64	118.70	109.95
1	A	307	SER	N-CA-C	5.48	117.96	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASN	N-CA-C	5.38	117.84	111.33
1	B	354	ILE	CA-C-N	-5.32	115.14	122.16
1	B	354	ILE	C-N-CA	-5.32	115.14	122.16
1	B	19	VAL	N-CA-C	-5.19	105.44	110.42
1	B	441	TYR	N-CA-C	-5.16	106.67	112.87
1	B	307	SER	N-CA-C	-5.13	102.79	110.23
1	A	218	ASP	N-CA-C	-5.13	105.79	113.89
1	A	405	SER	N-CA-C	5.08	117.26	110.35
1	A	92	HIS	CA-C-O	-5.01	116.18	121.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4120	0	3992	214	0
1	B	4115	0	3986	195	0
2	A	4	0	0	2	0
2	B	4	0	0	0	0
All	All	8243	0	7978	409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (409) 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:A:387:LEU:HD11	1:A:392:PHE:CE1	1.68	1.26
1:A:393:TRP:NE1	1:A:503:MET:HE2	1.57	1.16
1:A:117:PRO:CG	1:A:503:MET:HE1	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PRO:HG2	1:A:503:MET:HE1	1.12	1.06
1:A:489:VAL:HG11	1:A:503:MET:HE3	1.10	1.05
1:A:393:TRP:HE1	1:A:503:MET:CE	1.72	1.02
1:A:393:TRP:HE1	1:A:503:MET:HE2	0.82	0.98
1:A:401:PRO:HD2	1:A:507:ASP:O	1.64	0.96
1:B:3:LEU:HD22	1:B:40:HIS:HD2	1.28	0.96
1:A:117:PRO:HG2	1:A:503:MET:CE	1.95	0.95
1:A:489:VAL:HG11	1:A:503:MET:CE	1.97	0.94
1:A:387:LEU:HD11	1:A:392:PHE:HE1	1.10	0.93
1:A:489:VAL:CG1	1:A:503:MET:HE3	1.98	0.93
1:B:10:LEU:HD22	1:B:335:MET:HE1	1.50	0.93
1:A:309:TYR:O	1:A:339:VAL:HG21	1.68	0.93
1:A:243:LEU:HD23	1:A:337:PHE:CD1	2.04	0.92
1:B:213:THR:HG23	1:B:219:LEU:HD22	1.53	0.90
1:B:437:ASP:OD2	1:B:440:VAL:HG23	1.71	0.89
1:A:366:ALA:HB1	1:A:406:VAL:O	1.72	0.89
1:A:481:PHE:HD1	1:A:508:ILE:CD1	1.85	0.89
1:A:481:PHE:HD1	1:A:508:ILE:HD11	1.35	0.89
1:A:180:LEU:CD1	1:A:182:LEU:HD11	2.04	0.88
1:A:492:CYS:HG	2:A:604:CU:CU	0.54	0.87
1:A:387:LEU:CD1	1:A:392:PHE:CE1	2.56	0.86
1:A:163:TYR:CE1	1:A:228:PHE:CE2	2.64	0.84
1:B:105:HIS:CE1	1:B:422:HIS:CE1	2.66	0.83
1:A:147:THR:HG22	1:A:253:ARG:HD3	1.60	0.83
1:B:249:LYS:NZ	1:B:349:LYS:O	2.11	0.83
1:B:260:THR:HG23	1:B:494:ILE:HD13	1.60	0.83
1:B:3:LEU:HD22	1:B:40:HIS:CD2	2.15	0.82
1:A:492:CYS:SG	2:A:604:CU:CU	1.70	0.81
1:B:247:PRO:HG2	1:B:343:LEU:HD11	1.60	0.81
1:A:386:LEU:HB3	1:A:502:MET:HE3	1.64	0.80
1:B:105:HIS:CD2	1:B:149:TRP:HE1	2.00	0.79
1:B:131:PHE:HE2	1:B:487:ARG:NH1	1.80	0.79
1:B:44:PRO:HG2	1:B:202:GLY:HA3	1.62	0.79
1:B:7:VAL:CG1	1:B:40:HIS:HE1	1.94	0.79
1:B:386:LEU:HB3	1:B:502:MET:HE3	1.66	0.78
1:A:481:PHE:HB3	1:A:508:ILE:HD12	1.64	0.78
1:B:213:THR:CG2	1:B:219:LEU:HD22	2.13	0.78
1:A:219:LEU:HD23	1:A:220:PRO:O	1.84	0.77
1:B:39:VAL:HG12	1:B:239:VAL:HG23	1.65	0.77
1:B:103:HIS:CE1	1:B:424:HIS:CE1	2.72	0.77
1:B:377:THR:OG1	1:B:387:LEU:HD12	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TYR:HE1	1:A:172:ILE:HD11	1.49	0.76
1:A:437:ASP:O	1:A:438:THR:HG22	1.86	0.76
1:B:292:PHE:CD2	1:B:300:PHE:CE2	2.74	0.75
1:A:180:LEU:HD13	1:A:182:LEU:HD11	1.67	0.75
1:A:401:PRO:CD	1:A:507:ASP:O	2.33	0.75
1:A:491:HIS:HB3	1:A:503:MET:HG3	1.67	0.75
1:A:50:THR:OG1	1:A:54:SER:O	2.03	0.75
1:B:159:ARG:HA	1:B:495:LEU:HD13	1.68	0.74
1:A:243:LEU:HD23	1:A:337:PHE:HD1	1.50	0.74
1:A:286:PRO:CG	1:A:355:PHE:CE1	2.70	0.74
1:A:243:LEU:HD23	1:A:337:PHE:CE1	2.21	0.74
1:B:173:SER:OG	1:B:178:LYS:HE3	1.88	0.73
1:B:145:ALA:HB2	1:B:174:ASP:HB3	1.69	0.73
1:B:427:GLN:NE2	1:B:465:ASP:HB3	2.04	0.73
1:A:116:TYR:HH	1:A:393:TRP:HH2	1.37	0.73
1:B:159:ARG:HA	1:B:495:LEU:CD1	2.18	0.73
1:B:210:PRO:O	1:B:213:THR:OG1	2.06	0.73
1:B:177:GLU:HG3	1:B:282:PHE:HZ	1.53	0.73
1:B:109:THR:HG21	1:B:139:TYR:CD1	2.24	0.72
1:B:247:PRO:HG2	1:B:343:LEU:CD1	2.19	0.72
1:B:213:THR:CG2	1:B:219:LEU:CD2	2.69	0.71
1:B:361:LEU:HD12	1:B:361:LEU:O	1.90	0.71
1:A:481:PHE:CD1	1:A:508:ILE:CD1	2.73	0.71
1:B:8:ASP:OD1	1:B:41:ARG:HD2	1.91	0.70
1:A:207:PRO:HD3	1:A:228:PHE:CE1	2.26	0.70
1:A:351:LEU:C	1:A:351:LEU:HD13	2.17	0.70
1:B:177:GLU:HG3	1:B:282:PHE:CZ	2.26	0.70
1:A:286:PRO:HD3	1:A:355:PHE:CD1	2.26	0.70
1:A:116:TYR:OH	1:A:393:TRP:HH2	1.75	0.69
1:A:135:GLU:CD	1:A:135:GLU:H	2.00	0.69
1:A:458:LEU:HD23	1:A:461:GLN:OE1	1.92	0.69
1:A:481:PHE:CD1	1:A:508:ILE:HD11	2.25	0.69
1:B:436:PHE:O	1:B:438:THR:HG23	1.92	0.69
1:A:259:ASN:CG	1:A:495:LEU:HD12	2.17	0.69
1:B:438:THR:HG21	1:B:472:GLY:HA3	1.74	0.69
1:A:191:LEU:HD13	1:A:335:MET:HE1	1.74	0.68
1:A:147:THR:CG2	1:A:253:ARG:HD3	2.24	0.68
1:B:7:VAL:HG11	1:B:40:HIS:HE1	1.58	0.68
1:A:286:PRO:HG2	1:A:355:PHE:CE1	2.29	0.67
1:B:44:PRO:HG2	1:B:201:ASP:O	1.94	0.67
1:B:177:GLU:O	1:B:180:LEU:HD23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HG22	1:A:412:VAL:HB	1.75	0.67
1:A:227:PHE:HB2	1:A:260:THR:HG21	1.75	0.67
1:B:147:THR:HG22	1:B:253:ARG:HH11	1.60	0.67
1:B:213:THR:HG23	1:B:219:LEU:CD2	2.24	0.67
1:A:116:TYR:OH	1:A:393:TRP:CH2	2.47	0.66
1:A:95:GLU:HG3	1:A:95:GLU:O	1.95	0.66
1:B:8:ASP:OD1	1:B:41:ARG:CD	2.44	0.66
1:A:88:ILE:HD12	1:A:500:TYR:CD1	2.32	0.65
1:B:457:PRO:HD2	1:B:460:GLU:OE1	1.97	0.65
1:B:395:ASP:HB3	1:B:396:PRO:HD2	1.79	0.65
1:B:247:PRO:HD2	1:B:343:LEU:HD12	1.79	0.65
1:B:292:PHE:CE2	1:B:300:PHE:CD2	2.84	0.64
1:A:163:TYR:HH	1:A:228:PHE:HZ	1.45	0.64
1:A:209:ARG:HB2	1:A:210:PRO:CD	2.27	0.64
1:B:44:PRO:CG	1:B:201:ASP:C	2.71	0.64
1:B:434:ARG:HG2	1:B:449:TYR:CD1	2.31	0.64
1:A:457:PRO:HD2	1:A:460:GLU:OE1	1.97	0.63
1:B:44:PRO:HB2	1:B:45:PRO:HD2	1.80	0.63
1:B:438:THR:HG22	1:B:472:GLY:HA2	1.81	0.63
1:A:177:GLU:HG2	1:A:282:PHE:HZ	1.64	0.63
1:A:180:LEU:HD12	1:A:182:LEU:HD11	1.79	0.63
1:A:419:HIS:CE1	1:A:497:HIS:CE1	2.87	0.63
1:A:436:PHE:HA	1:A:449:TYR:HA	1.80	0.63
1:A:48:LEU:HD13	1:A:55:LEU:HD22	1.81	0.63
1:A:314:ILE:N	1:A:314:ILE:HD12	2.13	0.63
1:B:379:ASP:HB3	1:B:385:ILE:HD11	1.80	0.62
1:B:131:PHE:HE2	1:B:487:ARG:HH11	1.45	0.62
1:B:180:LEU:N	1:B:180:LEU:HD22	2.14	0.62
1:A:177:GLU:HG2	1:A:282:PHE:CZ	2.33	0.62
1:B:163:TYR:CE1	1:B:228:PHE:CE2	2.87	0.62
1:B:425:LEU:HD23	1:B:488:TYR:CE2	2.35	0.62
1:B:147:THR:HG22	1:B:253:ARG:HD3	1.82	0.62
1:A:145:ALA:HB2	1:A:174:ASP:CB	2.30	0.62
1:A:294:ILE:HD13	1:A:300:PHE:CD1	2.34	0.62
1:B:46:THR:O	1:B:48:LEU:HG	2.00	0.62
1:A:163:TYR:CZ	1:A:228:PHE:CZ	2.88	0.61
1:A:68:VAL:HB	1:A:139:TYR:HB2	1.83	0.61
1:A:247:PRO:HG2	1:A:343:LEU:HD21	1.81	0.61
1:B:145:ALA:HB2	1:B:174:ASP:CB	2.29	0.61
1:A:163:TYR:CE1	1:A:228:PHE:HE2	2.18	0.61
1:B:147:THR:CG2	1:B:253:ARG:HD3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLN:HE22	1:B:465:ASP:HB3	1.66	0.60
1:B:182:LEU:HD22	1:B:303:ILE:HD11	1.83	0.60
1:A:418:THR:O	1:A:469:ALA:O	2.19	0.60
1:A:425:LEU:HB2	1:A:488:TYR:CE2	2.35	0.60
1:B:105:HIS:HE1	1:B:422:HIS:CG	2.19	0.60
1:A:369:GLU:N	1:A:369:GLU:OE1	2.33	0.60
1:A:419:HIS:CE1	1:A:497:HIS:ND1	2.70	0.60
1:A:163:TYR:OH	1:A:228:PHE:HZ	1.84	0.60
1:A:412:VAL:HG13	1:A:474:VAL:HG22	1.84	0.60
1:A:88:ILE:HD12	1:A:500:TYR:CG	2.37	0.59
1:A:436:PHE:O	1:A:450:THR:HG23	2.01	0.59
1:B:7:VAL:CG1	1:B:40:HIS:CE1	2.81	0.59
1:B:155:MET:HE1	1:B:393:TRP:CD1	2.36	0.59
1:A:311:ASN:N	1:A:339:VAL:HG23	2.17	0.59
1:A:37:LEU:O	1:A:45:PRO:HA	2.02	0.59
1:B:39:VAL:HG11	1:B:198:PHE:CZ	2.38	0.59
1:B:44:PRO:CG	1:B:201:ASP:O	2.51	0.59
1:B:131:PHE:CE2	1:B:487:ARG:NH1	2.67	0.58
1:B:44:PRO:HB2	1:B:45:PRO:CD	2.34	0.58
1:A:207:PRO:HD3	1:A:228:PHE:HE1	1.66	0.58
1:B:434:ARG:HD2	1:B:453:ASN:ND2	2.18	0.58
1:A:245:VAL:HG23	1:A:339:VAL:HG12	1.84	0.58
1:B:261:ARG:HD3	1:B:263:TYR:CE1	2.39	0.58
1:A:219:LEU:CD2	1:A:220:PRO:O	2.50	0.58
1:A:163:TYR:HE1	1:A:228:PHE:HE2	1.51	0.58
1:B:44:PRO:CG	1:B:202:GLY:HA3	2.33	0.58
1:B:412:VAL:HG13	1:B:474:VAL:HG22	1.84	0.58
1:B:44:PRO:HG3	1:B:201:ASP:C	2.29	0.57
1:B:145:ALA:HB1	1:B:177:GLU:OE1	2.03	0.57
1:B:105:HIS:HD2	1:B:149:TRP:HE1	1.49	0.57
1:A:49:TRP:CD2	1:A:76:LEU:HD12	2.39	0.57
1:B:148:LEU:HD23	1:B:299:ARG:HH21	1.69	0.57
1:A:145:ALA:HB2	1:A:174:ASP:HB2	1.87	0.57
1:A:481:PHE:N	1:A:481:PHE:CD2	2.73	0.57
1:B:148:LEU:HD23	1:B:299:ARG:NH2	2.20	0.56
1:B:299:ARG:HH12	1:B:465:ASP:CG	2.13	0.56
1:B:49:TRP:CD2	1:B:76:LEU:HD12	2.40	0.56
1:B:105:HIS:CD2	1:B:149:TRP:NE1	2.73	0.56
1:B:189:ILE:HD12	1:B:189:ILE:N	2.20	0.56
1:A:209:ARG:HD2	1:A:213:THR:HG21	1.87	0.56
1:A:294:ILE:HD13	1:A:300:PHE:HD1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:HG11	1:B:40:HIS:CE1	2.39	0.56
1:A:209:ARG:HB2	1:A:210:PRO:HD3	1.87	0.55
1:A:485:SER:HB2	1:A:508:ILE:O	2.06	0.55
1:B:98:VAL:HG13	1:B:98:VAL:O	2.06	0.55
1:A:447:ILE:HD12	1:A:447:ILE:N	2.22	0.55
1:B:307:SER:O	1:B:308:ALA:HB3	2.07	0.55
1:B:310:GLU:HA	1:B:339:VAL:HG11	1.89	0.55
1:A:286:PRO:HG3	1:A:355:PHE:CE1	2.42	0.55
1:B:433:ARG:HD3	1:B:473:GLU:OE1	2.06	0.55
1:B:508:ILE:O	1:B:509:ILE:HG22	2.07	0.55
1:A:481:PHE:HB3	1:A:508:ILE:CD1	2.37	0.55
1:B:280:GLY:CA	1:B:427:GLN:OE1	2.56	0.55
1:A:105:HIS:CE1	1:A:422:HIS:CE1	2.95	0.54
1:A:387:LEU:HD21	1:A:501:ASP:HB3	1.90	0.54
1:B:148:LEU:HD12	1:B:172:ILE:CD1	2.38	0.54
1:B:177:GLU:C	1:B:180:LEU:HD23	2.32	0.54
1:A:508:ILE:O	1:A:508:ILE:HG22	2.08	0.54
1:B:209:ARG:CD	1:B:213:THR:HG21	2.38	0.54
1:A:243:LEU:HG	1:A:245:VAL:HG13	1.89	0.54
1:A:434:ARG:HG2	1:A:449:TYR:CD1	2.42	0.54
1:B:163:TYR:CE1	1:B:228:PHE:HE2	2.26	0.54
1:B:508:ILE:N	1:B:508:ILE:HD12	2.23	0.54
1:A:210:PRO:CG	1:A:219:LEU:HD11	2.38	0.54
1:A:25:GLN:OE1	1:A:69:LYS:NZ	2.36	0.53
1:A:286:PRO:HG3	1:A:355:PHE:CZ	2.43	0.53
1:B:103:HIS:CE1	1:B:424:HIS:NE2	2.76	0.53
1:B:44:PRO:HG2	1:B:201:ASP:C	2.33	0.53
1:A:447:ILE:HD12	1:A:447:ILE:H	1.72	0.53
1:B:438:THR:CG2	1:B:472:GLY:CA	2.87	0.53
1:A:88:ILE:HD11	1:A:224:ILE:HG21	1.90	0.53
1:B:189:ILE:HG22	1:B:191:LEU:CD1	2.39	0.53
1:A:379:ASP:HB3	1:A:385:ILE:HD11	1.91	0.53
1:B:40:HIS:HB3	1:B:43:LEU:HD21	1.91	0.53
1:B:44:PRO:HG2	1:B:202:GLY:CA	2.37	0.53
1:A:286:PRO:CD	1:A:355:PHE:CD1	2.92	0.52
1:B:279:ASP:OD2	1:B:464:LYS:HE2	2.09	0.52
1:A:391:HIS:CB	1:A:504:ARG:NH1	2.72	0.52
1:B:39:VAL:CG1	1:B:239:VAL:HG23	2.38	0.52
1:B:180:LEU:N	1:B:180:LEU:CD2	2.73	0.52
1:B:7:VAL:HG12	1:B:40:HIS:HE1	1.72	0.52
1:B:44:PRO:HD2	1:B:202:GLY:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:HG12	1:A:98:VAL:O	2.09	0.52
1:B:10:LEU:HD22	1:B:335:MET:CE	2.33	0.52
1:B:377:THR:O	1:B:385:ILE:N	2.32	0.52
1:B:397:VAL:HG22	1:B:505:PRO:HG2	1.90	0.52
1:A:273:ILE:HG23	1:A:302:VAL:HG11	1.92	0.52
1:A:387:LEU:HD11	1:A:392:PHE:CD1	2.36	0.52
1:B:273:ILE:HG23	1:B:302:VAL:HG11	1.92	0.52
1:A:219:LEU:HD23	1:A:220:PRO:N	2.25	0.51
1:B:148:LEU:O	1:B:170:TYR:N	2.39	0.51
1:B:43:LEU:HB2	1:B:44:PRO:HD2	1.92	0.51
1:A:305:ASP:OD1	1:A:307:SER:OG	2.26	0.51
1:B:184:LYS:HZ1	1:B:349:LYS:HZ1	1.57	0.51
1:B:105:HIS:HE1	1:B:422:HIS:ND1	2.09	0.51
1:A:170:TYR:CE1	1:A:172:ILE:HD11	2.38	0.51
1:A:209:ARG:CB	1:A:210:PRO:CD	2.88	0.51
1:A:315:THR:CG2	1:A:336:GLN:HE21	2.23	0.51
1:A:393:TRP:NE1	1:A:503:MET:CE	2.50	0.51
1:B:78:LEU:O	1:B:98:VAL:HG12	2.11	0.51
1:A:70:VAL:HG11	1:A:72:TRP:CE2	2.46	0.50
1:A:88:ILE:HD11	1:A:224:ILE:CG2	2.41	0.50
1:B:148:LEU:HD12	1:B:172:ILE:HD11	1.93	0.50
1:A:117:PRO:HG3	1:A:503:MET:HE1	1.83	0.50
1:A:163:TYR:CE1	1:A:228:PHE:CZ	3.00	0.50
1:B:184:LYS:HZ1	1:B:349:LYS:NZ	2.08	0.50
1:A:29:GLU:C	1:A:30:ILE:HD12	2.37	0.50
1:A:191:LEU:HD13	1:A:335:MET:CE	2.41	0.50
1:B:70:VAL:HG11	1:B:72:TRP:CE2	2.46	0.50
1:A:294:ILE:HD11	1:A:298:GLU:O	2.11	0.49
1:A:401:PRO:HG2	1:A:481:PHE:CD1	2.47	0.49
1:A:21:LYS:HG3	1:A:26:THR:HG22	1.95	0.49
1:A:219:LEU:HD23	1:A:219:LEU:C	2.37	0.49
1:B:105:HIS:NE2	1:B:297:ALA:HB1	2.27	0.49
1:A:418:THR:O	1:A:418:THR:HG22	2.11	0.49
1:B:387:LEU:HD22	1:B:391:HIS:O	2.13	0.49
1:B:269:ASN:ND2	1:B:314:ILE:HD13	2.28	0.49
1:A:398:THR:OG1	1:A:399:GLU:CD	2.56	0.49
1:A:180:LEU:HD12	1:A:182:LEU:CD1	2.43	0.49
1:B:105:HIS:CE1	1:B:422:HIS:ND1	2.81	0.49
1:B:398:THR:OG1	1:B:399:GLU:CD	2.56	0.49
1:A:28:TYR:HB3	1:A:30:ILE:CD1	2.43	0.48
1:A:351:LEU:C	1:A:351:LEU:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PHE:CD1	1:B:336:GLN:HB2	2.47	0.48
1:A:366:ALA:CB	1:A:406:VAL:HG12	2.44	0.48
1:B:163:TYR:CE1	1:B:196:ARG:HD3	2.48	0.48
1:A:148:LEU:HD12	1:A:170:TYR:CD1	2.47	0.48
1:B:209:ARG:HD3	1:B:213:THR:HG21	1.95	0.48
1:A:6:PHE:CD1	1:A:336:GLN:HB2	2.49	0.48
1:A:159:ARG:CZ	1:A:224:ILE:HD12	2.43	0.48
1:A:239:VAL:O	1:A:240:TRP:C	2.56	0.48
1:B:285:ARG:NH1	1:B:286:PRO:O	2.46	0.48
1:B:441:TYR:HE1	1:B:447:ILE:CG2	2.27	0.48
1:B:441:TYR:HE1	1:B:447:ILE:HG22	1.78	0.48
1:A:163:TYR:CE1	1:A:196:ARG:HD3	2.48	0.47
1:A:362:ARG:O	1:A:362:ARG:HG3	2.13	0.47
1:B:239:VAL:O	1:B:240:TRP:C	2.57	0.47
1:A:207:PRO:HD3	1:A:228:PHE:CD1	2.49	0.47
1:A:3:LEU:CD2	1:A:239:VAL:HG11	2.44	0.47
1:A:182:LEU:HB3	1:A:183:PRO:CD	2.44	0.47
1:A:216:ASP:OD1	1:A:216:ASP:N	2.46	0.47
1:A:401:PRO:HG2	1:A:481:PHE:CE1	2.49	0.47
1:A:385:ILE:HG22	1:A:387:LEU:HG	1.95	0.47
1:A:403:LEU:H	1:A:509:ILE:C	2.23	0.47
1:B:38:LYS:HD2	1:B:40:HIS:O	2.15	0.47
1:A:481:PHE:N	1:A:481:PHE:HD2	2.11	0.47
1:B:105:HIS:CE1	1:B:422:HIS:NE2	2.83	0.47
1:B:195:ASP:HB3	1:B:261:ARG:HD2	1.97	0.47
1:B:438:THR:CG2	1:B:472:GLY:HA3	2.40	0.47
1:B:105:HIS:O	1:B:148:LEU:HD22	2.15	0.47
1:A:243:LEU:CD2	1:A:337:PHE:CE1	2.96	0.47
1:B:44:PRO:HD2	1:B:202:GLY:HA3	1.97	0.47
1:B:36:PHE:CE1	1:B:47:LYS:HB2	2.50	0.46
1:B:438:THR:HG21	1:B:472:GLY:CA	2.44	0.46
1:B:309:TYR:CB	1:B:314:ILE:HD11	2.45	0.46
1:B:353:PRO:O	1:B:353:PRO:HG2	2.15	0.46
1:B:155:MET:CE	1:B:393:TRP:CD1	2.98	0.46
1:B:309:TYR:O	1:B:312:LYS:HB2	2.14	0.46
1:B:109:THR:HG21	1:B:139:TYR:HD1	1.77	0.46
1:B:184:LYS:NZ	1:B:349:LYS:NZ	2.64	0.46
1:A:174:ASP:OD1	1:A:175:ALA:N	2.49	0.46
1:A:387:LEU:HD21	1:A:392:PHE:HD1	1.81	0.46
1:B:292:PHE:CE2	1:B:300:PHE:CE2	3.04	0.46
1:A:145:ALA:HB2	1:A:174:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:HG23	1:A:336:GLN:HE21	1.81	0.46
1:B:207:PRO:HB2	1:B:225:VAL:HG21	1.98	0.46
1:A:387:LEU:CD1	1:A:392:PHE:CD1	2.97	0.45
1:B:188:ASP:N	1:B:189:ILE:HD12	2.31	0.45
1:B:310:GLU:HA	1:B:339:VAL:CG1	2.46	0.45
1:B:379:ASP:HB3	1:B:385:ILE:CD1	2.45	0.45
1:B:385:ILE:HG12	1:B:500:TYR:CE2	2.51	0.45
1:A:195:ASP:HB3	1:A:261:ARG:HD2	1.98	0.45
1:B:438:THR:CG2	1:B:472:GLY:HA2	2.46	0.45
1:A:362:ARG:N	1:A:363:PRO:HD3	2.31	0.45
1:B:189:ILE:HG22	1:B:191:LEU:HD12	1.99	0.45
1:B:3:LEU:HD11	1:B:43:LEU:HD23	1.98	0.45
1:B:225:VAL:CG1	1:B:226:PRO:HD2	2.47	0.45
1:A:134:ARG:HH11	1:A:134:ARG:CG	2.30	0.45
1:B:398:THR:HG1	1:B:399:GLU:CD	2.25	0.45
1:A:210:PRO:HG2	1:A:219:LEU:HD11	1.98	0.45
1:A:24:ARG:O	1:A:67:LYS:HD2	2.17	0.45
1:A:245:VAL:CG2	1:A:339:VAL:HG12	2.47	0.44
1:A:273:ILE:O	1:A:289:HIS:HB2	2.17	0.44
1:A:393:TRP:O	1:A:393:TRP:CE3	2.70	0.44
1:B:387:LEU:HD22	1:B:391:HIS:C	2.41	0.44
1:A:49:TRP:CE2	1:A:76:LEU:HD12	2.51	0.44
1:A:297:ALA:HB2	1:A:493:HIS:CD2	2.51	0.44
1:B:163:TYR:HE1	1:B:228:PHE:HE2	1.64	0.44
1:B:176:PHE:O	1:B:180:LEU:CD2	2.65	0.44
1:B:434:ARG:NE	1:B:449:TYR:CG	2.85	0.44
1:A:366:ALA:CB	1:A:406:VAL:O	2.55	0.44
1:A:82:LEU:O	1:A:84:VAL:HG23	2.17	0.44
1:B:88:ILE:HG23	1:B:500:TYR:HB2	1.99	0.44
1:B:22:ASN:OD1	1:B:22:ASN:C	2.61	0.44
1:A:483:PRO:HG2	1:A:484:TYR:CE2	2.53	0.44
1:B:3:LEU:HB3	1:B:40:HIS:CD2	2.53	0.44
1:A:163:TYR:OH	1:A:228:PHE:CZ	2.65	0.44
1:A:260:THR:HA	1:A:494:ILE:HG23	1.99	0.44
1:A:421:ILE:O	1:A:466:THR:HA	2.17	0.44
1:B:49:TRP:CE2	1:B:76:LEU:HD12	2.53	0.43
1:A:22:ASN:OD1	1:A:24:ARG:N	2.51	0.43
1:A:41:ARG:HG3	1:A:42:ASP:OD1	2.19	0.43
1:A:148:LEU:HD12	1:A:170:TYR:HD1	1.83	0.43
1:B:392:PHE:O	1:B:504:ARG:NH1	2.51	0.43
1:A:387:LEU:CD2	1:A:501:ASP:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:HD3	1:A:473:GLU:OE2	2.19	0.43
1:A:3:LEU:HD23	1:A:239:VAL:HG11	1.98	0.43
1:A:30:ILE:HD12	1:A:30:ILE:N	2.33	0.43
1:A:366:ALA:HB2	1:A:406:VAL:HG12	1.99	0.43
1:A:286:PRO:CG	1:A:355:PHE:CD1	3.02	0.43
1:A:391:HIS:HB2	1:A:504:ARG:NH1	2.33	0.43
1:A:153:HIS:CE1	1:A:498:GLU:OE2	2.71	0.43
1:A:80:HIS:CE1	1:A:82:LEU:HB2	2.54	0.43
1:A:135:GLU:OE1	1:A:135:GLU:N	2.40	0.43
1:A:180:LEU:CB	1:A:182:LEU:HG	2.48	0.43
1:B:219:LEU:HD12	1:B:219:LEU:C	2.43	0.43
1:A:22:ASN:OD1	1:A:22:ASN:C	2.61	0.43
1:B:174:ASP:O	1:B:177:GLU:N	2.52	0.43
1:B:188:ASP:C	1:B:189:ILE:HD12	2.44	0.42
1:B:209:ARG:HD2	1:B:213:THR:HG21	2.01	0.42
1:B:309:TYR:HB3	1:B:314:ILE:HD11	2.00	0.42
1:B:388:LEU:HD21	1:B:502:MET:HG2	2.01	0.42
1:B:425:LEU:HD23	1:B:488:TYR:CZ	2.54	0.42
1:A:82:LEU:HB3	1:A:83:PRO:CD	2.49	0.42
1:B:101:VAL:HB	1:B:120:TRP:HA	2.02	0.42
1:B:140:PRO:HB2	1:B:142:HIS:CE1	2.54	0.42
1:B:32:MET:HB3	1:B:76:LEU:HD21	2.01	0.42
1:B:85:ASP:OD1	1:B:222:PRO:O	2.37	0.42
1:A:39:VAL:HG12	1:A:239:VAL:HG23	2.02	0.42
1:A:135:GLU:CD	1:A:135:GLU:N	2.72	0.42
1:A:101:VAL:HB	1:A:120:TRP:HA	2.02	0.42
1:B:44:PRO:CD	1:B:202:GLY:HA3	2.49	0.42
1:A:400:ASN:HA	1:A:507:ASP:O	2.19	0.42
1:B:32:MET:HE3	1:B:74:ASN:HA	2.02	0.42
1:B:385:ILE:HG12	1:B:500:TYR:CZ	2.54	0.42
1:A:27:TYR:CE2	1:A:29:GLU:HG3	2.55	0.42
1:A:297:ALA:CB	1:A:493:HIS:CD2	3.02	0.42
1:B:22:ASN:OD1	1:B:24:ARG:N	2.52	0.42
1:B:438:THR:O	1:B:438:THR:OG1	2.31	0.42
1:A:334:ILE:HG22	1:A:335:MET:HG2	2.00	0.42
1:A:398:THR:HG1	1:A:399:GLU:CD	2.26	0.42
1:A:210:PRO:CD	1:A:219:LEU:HD11	2.50	0.41
1:A:261:ARG:HD3	1:A:263:TYR:CE2	2.55	0.41
1:B:482:VAL:HA	1:B:483:PRO:HA	1.84	0.41
1:A:292:PHE:CD1	1:A:300:PHE:CE2	3.07	0.41
1:B:161:ASN:O	1:B:166:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HG22	1:B:219:LEU:CD2	2.46	0.41
1:A:294:ILE:HD12	1:A:298:GLU:HB2	2.02	0.41
1:A:311:ASN:H	1:A:339:VAL:HG23	1.85	0.41
1:A:391:HIS:HB2	1:A:504:ARG:HH11	1.86	0.41
1:B:49:TRP:CD2	1:B:76:LEU:CD1	3.04	0.41
1:A:180:LEU:HB3	1:A:182:LEU:HG	2.02	0.41
1:A:247:PRO:HG2	1:A:343:LEU:CD2	2.50	0.41
1:A:321:GLY:HA2	1:A:326:VAL:HG22	2.01	0.41
1:B:284:PRO:HB3	1:B:358:LEU:HB3	2.02	0.41
1:B:481:PHE:CD2	1:B:481:PHE:N	2.88	0.41
1:A:177:GLU:CD	1:A:177:GLU:C	2.88	0.41
1:A:435:PRO:HA	1:A:473:GLU:HA	2.03	0.41
1:B:280:GLY:HA3	1:B:427:GLN:OE1	2.21	0.41
1:A:312:LYS:O	1:A:339:VAL:HG22	2.20	0.41
1:A:339:VAL:HG23	1:A:339:VAL:O	2.21	0.41
1:A:369:GLU:O	1:A:369:GLU:HG2	2.20	0.41
1:A:388:LEU:HD21	1:A:502:MET:HG2	2.02	0.41
1:B:105:HIS:CE1	1:B:422:HIS:CD2	3.09	0.41
1:B:80:HIS:CE1	1:B:82:LEU:HB2	2.56	0.41
1:A:215:GLU:C	1:A:217:SER:H	2.29	0.40
1:B:289:HIS:O	1:B:290:GLN:HB2	2.21	0.40
1:B:359:PRO:HG2	1:B:463:TYR:OH	2.20	0.40
1:B:438:THR:HG22	1:B:472:GLY:CA	2.46	0.40
1:B:266:HIS:NE2	1:B:317:LYS:HB2	2.37	0.40
1:B:508:ILE:N	1:B:508:ILE:CD1	2.84	0.40
1:A:213:THR:O	1:A:213:THR:OG1	2.32	0.40
1:A:330:THR:OG1	1:A:331:ASP:N	2.54	0.40
1:A:402:ARG:HA	1:A:509:ILE:C	2.46	0.40
1:A:434:ARG:NH1	1:A:453:ASN:OD1	2.54	0.40
1:B:40:HIS:CD2	1:B:42:ASP:HB2	2.57	0.40
1:B:159:ARG:HA	1:B:495:LEU:HD12	1.99	0.40
1:A:128:THR:HG21	1:A:132:PHE:CD2	2.56	0.40
1:A:215:GLU:C	1:A:217:SER:N	2.80	0.40
1:A:312:LYS:H	1:A:339:VAL:CG2	2.34	0.40
1:B:106:GLY:HA3	1:B:148:LEU:HD22	2.03	0.40
1:B:190:PRO:O	1:B:191:LEU:HD12	2.21	0.40
1:B:425:LEU:HD13	1:B:425:LEU:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/515 (97%)	446 (89%)	46 (9%)	7 (1%)	9	36
1	B	499/515 (97%)	454 (91%)	40 (8%)	5 (1%)	12	45
All	All	998/1030 (97%)	900 (90%)	86 (9%)	12 (1%)	10	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	289	HIS
1	A	360	PRO
1	B	95	GLU
1	B	94	ASP
1	B	439	GLU
1	A	419	HIS
1	A	98	VAL
1	A	217	SER
1	B	348	PRO
1	A	84	VAL
1	B	483	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/462 (98%)	443 (98%)	10 (2%)	45	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	452/462 (98%)	442 (98%)	10 (2%)	45	74
All	All	905/924 (98%)	885 (98%)	20 (2%)	45	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	39	VAL
1	A	98	VAL
1	A	219	LEU
1	A	314	ILE
1	A	322	CYS
1	A	341	ARG
1	A	343	LEU
1	A	372	LEU
1	A	415	THR
1	B	43	LEU
1	B	113	SER
1	B	178	LYS
1	B	184	LYS
1	B	322	CYS
1	B	350	THR
1	B	372	LEU
1	B	494	ILE
1	B	495	LEU
1	B	508	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	199	GLN
1	A	468	GLN
1	A	470	HIS
1	B	2	ASN
1	B	40	HIS
1	B	105	HIS
1	B	144	GLN
1	B	470	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	505/515 (98%)	0.32	18 (3%)	46 26	62, 85, 136, 190	5 (0%)
1	B	505/515 (98%)	0.29	21 (4%)	40 22	49, 85, 134, 207	2 (0%)
All	All	1010/1030 (98%)	0.30	39 (3%)	43 24	49, 85, 136, 207	7 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	LEU	5.4
1	A	369	GLU	4.5
1	B	45	PRO	4.2
1	A	485	SER	3.8
1	B	41	ARG	3.8
1	A	431	ILE	3.8
1	B	438	THR	3.2
1	B	193	ILE	3.1
1	B	42	ASP	3.0
1	A	290	GLN	2.9
1	B	311	ASN	2.9
1	B	366	ALA	2.9
1	A	508	ILE	2.9
1	B	361	LEU	2.8
1	A	210	PRO	2.8
1	B	500	TYR	2.8
1	A	228	PHE	2.7
1	A	216	ASP	2.7
1	A	209	ARG	2.6
1	A	273	ILE	2.5
1	A	393	TRP	2.5
1	B	509	ILE	2.5
1	B	2	ASN	2.5
1	A	3	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	365	ARG	2.4
1	B	411	ILE	2.4
1	B	369	GLU	2.3
1	B	360	PRO	2.3
1	B	482	VAL	2.2
1	A	345	GLY	2.1
1	B	354	ILE	2.1
1	A	37	LEU	2.1
1	B	353	PRO	2.1
1	A	391	HIS	2.1
1	B	93	HIS	2.1
1	B	301	ASP	2.1
1	B	441	TYR	2.1
1	A	147	THR	2.0
1	A	438	THR	2.0

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

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

6.3 Carbohydrates [i](#)

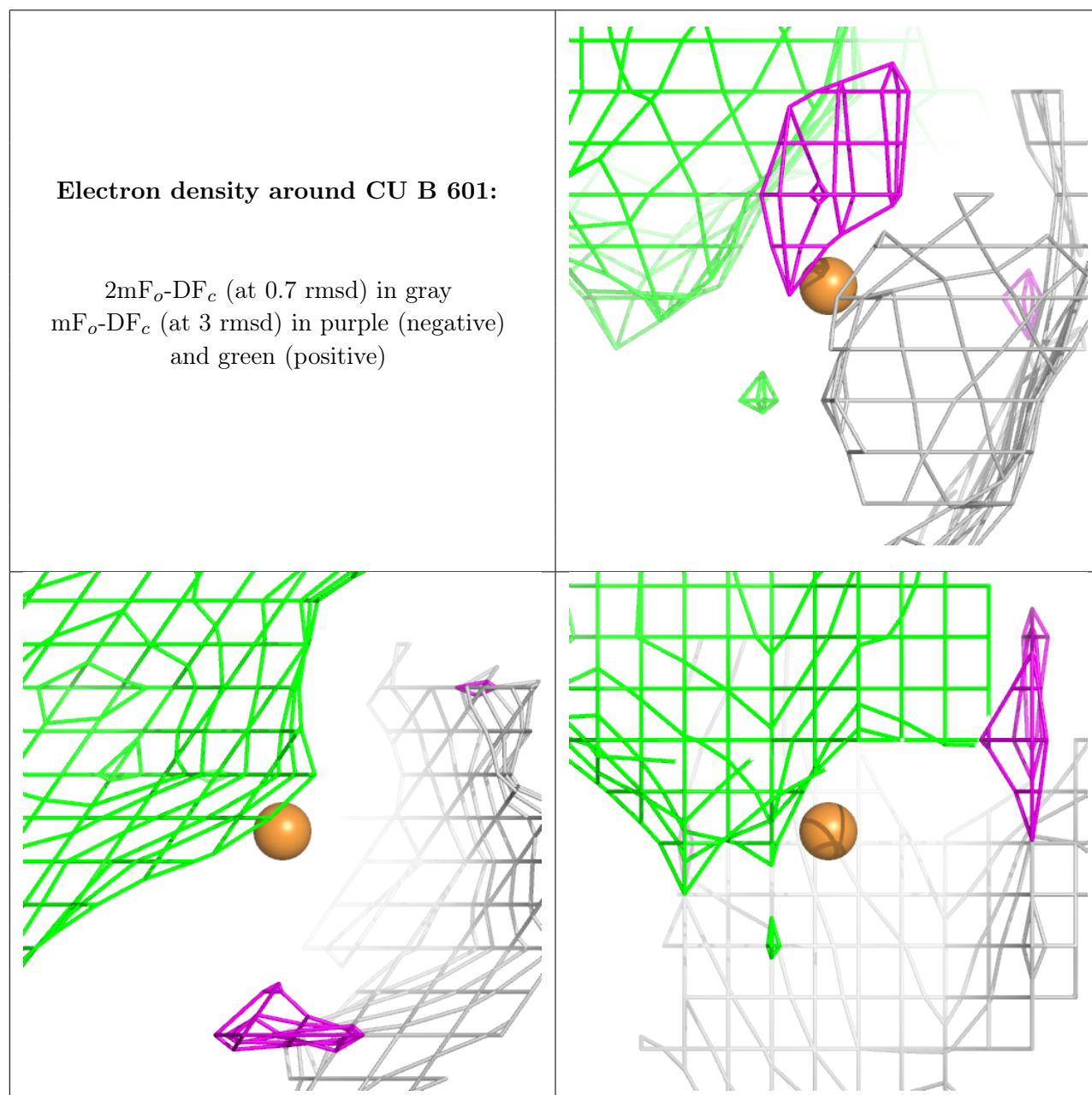
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

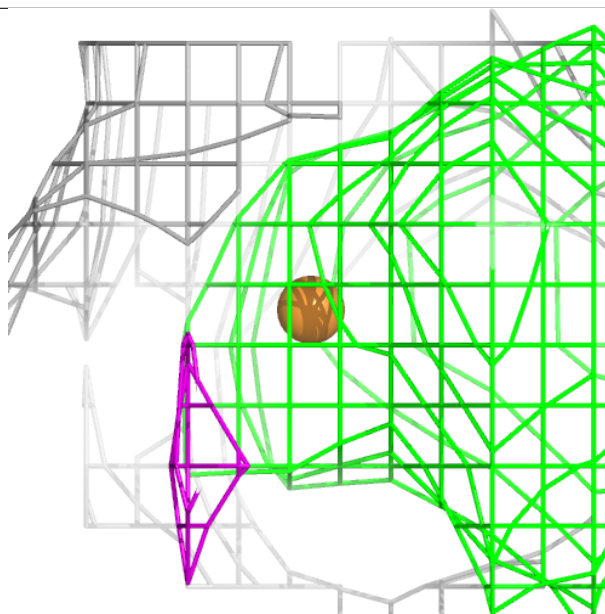
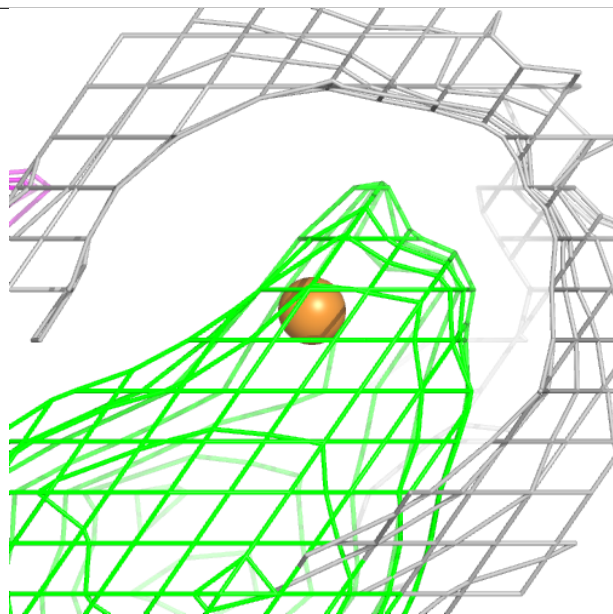
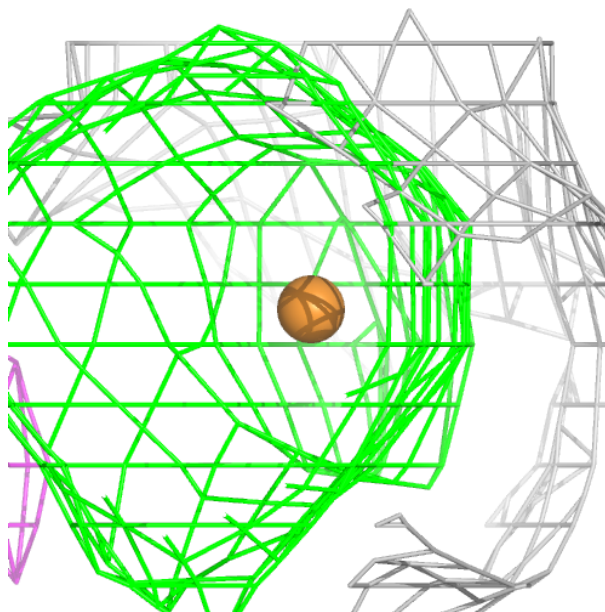
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU	B	601	1/1	0.88	0.09	114,114,114,114	0
2	CU	B	602	1/1	0.92	0.14	96,96,96,96	0
2	CU	A	602	1/1	0.93	0.12	96,96,96,96	0
2	CU	B	603	1/1	0.93	0.14	96,96,96,96	0
2	CU	A	603	1/1	0.95	0.07	96,96,96,96	0
2	CU	A	601	1/1	0.97	0.06	96,96,96,96	0
2	CU	B	604	1/1	0.97	0.06	107,107,107,107	0
2	CU	A	604	1/1	0.98	0.05	104,104,104,104	0

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



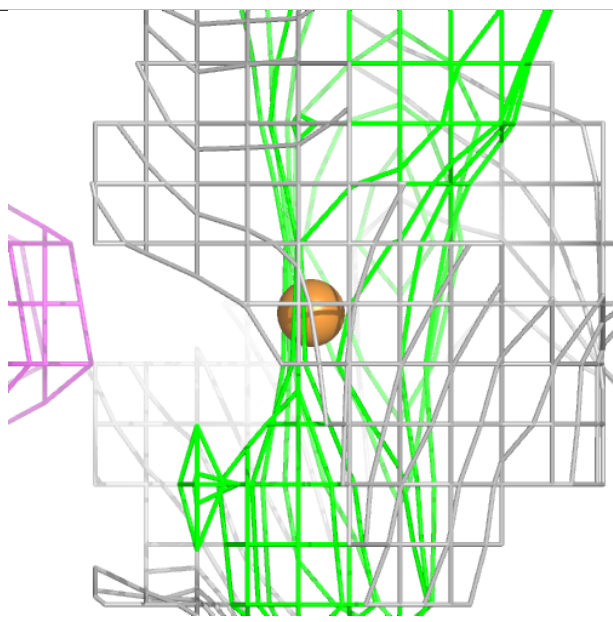
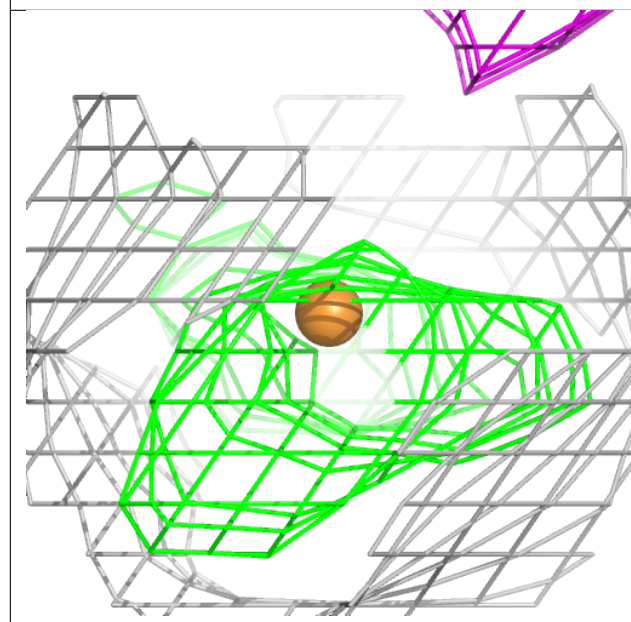
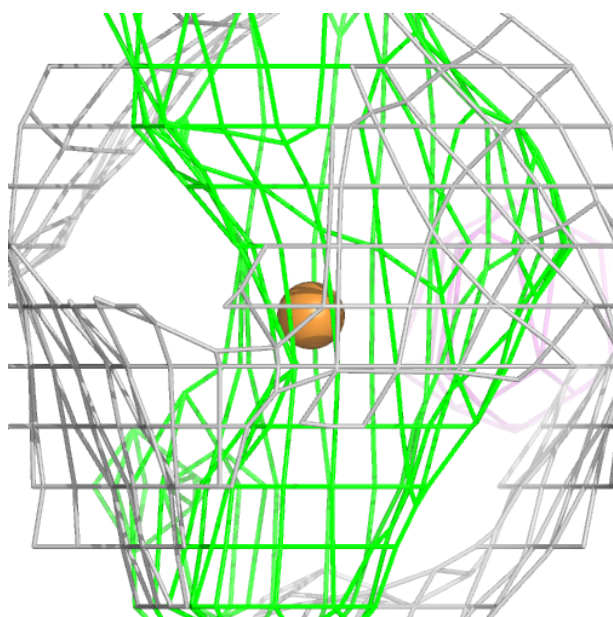
Electron density around CU B 602:

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



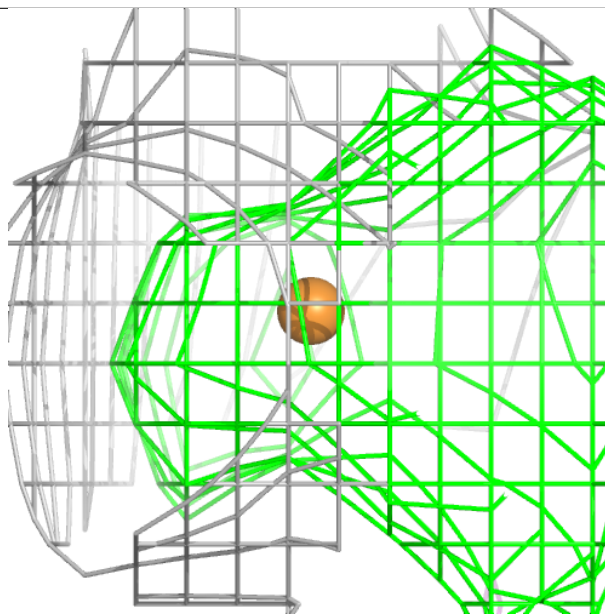
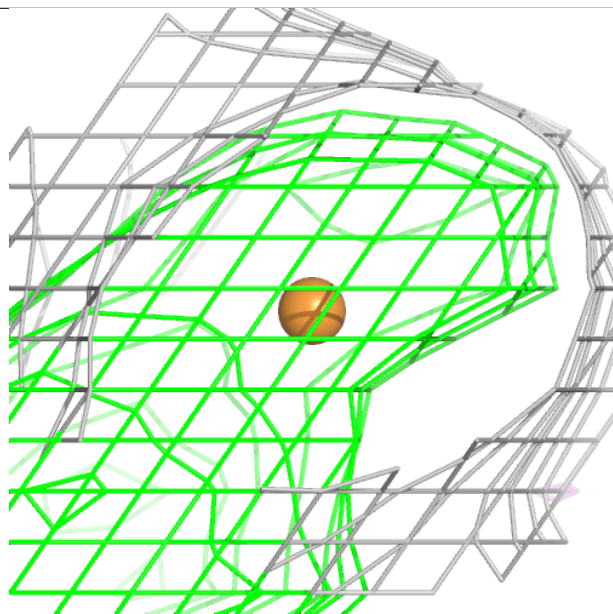
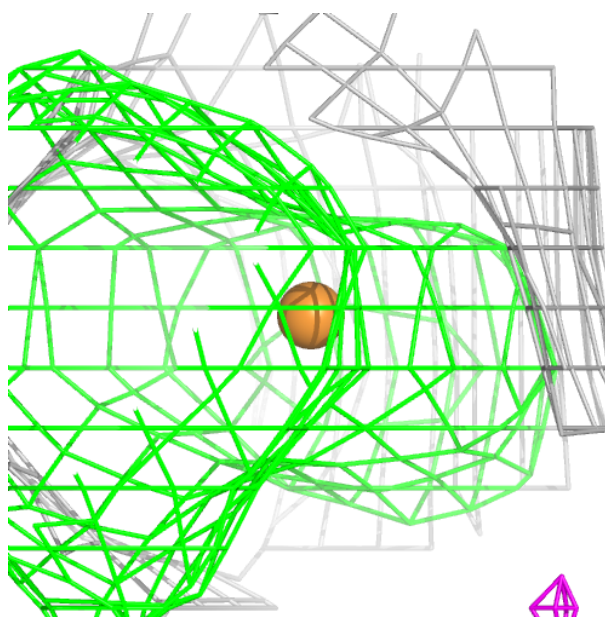
Electron density around CU A 602:

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



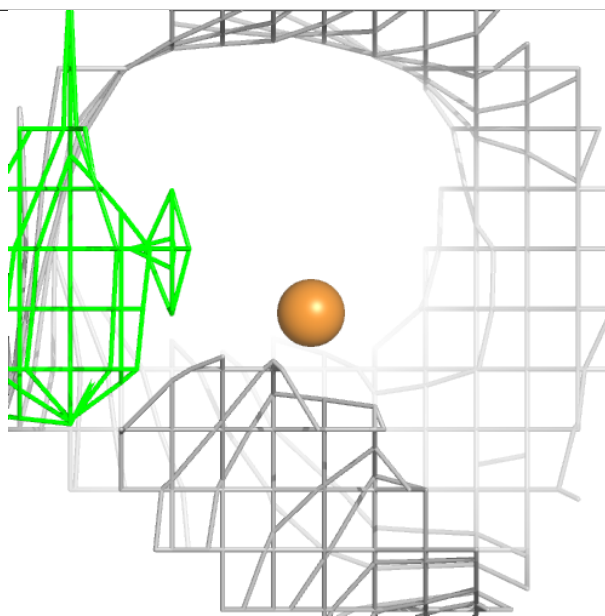
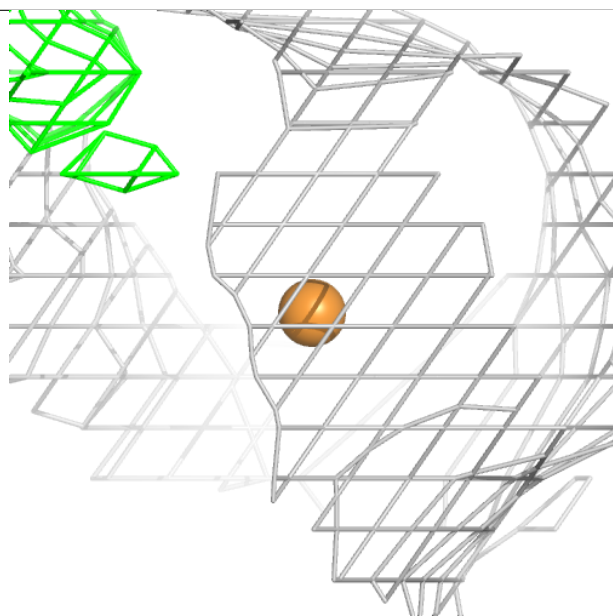
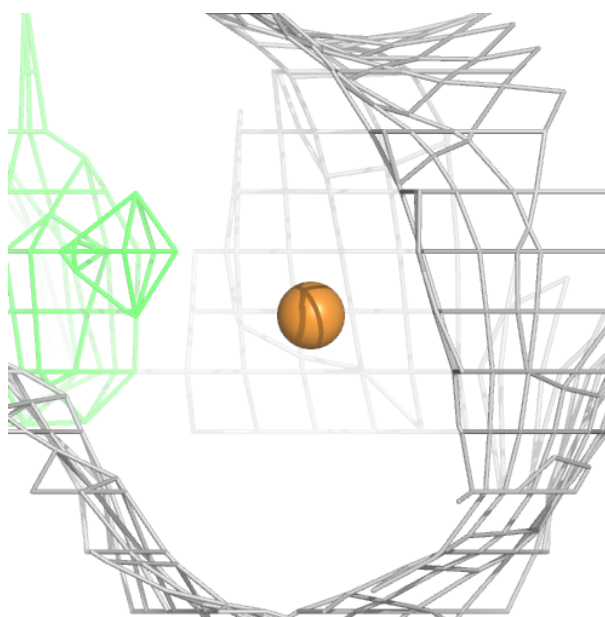
Electron density around CU B 603:

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



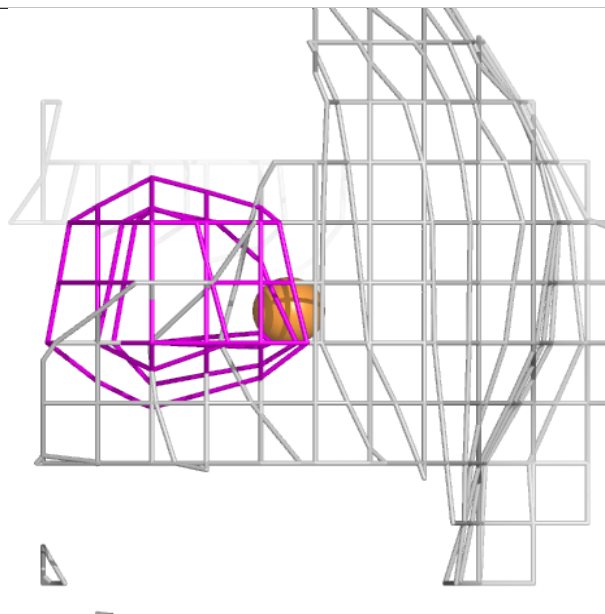
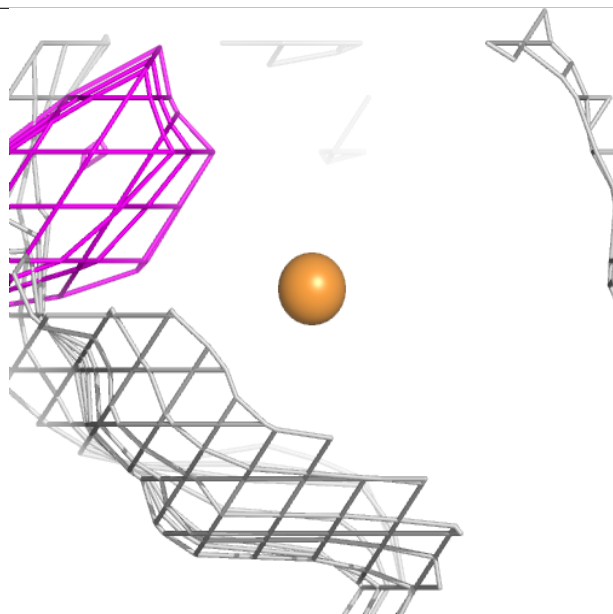
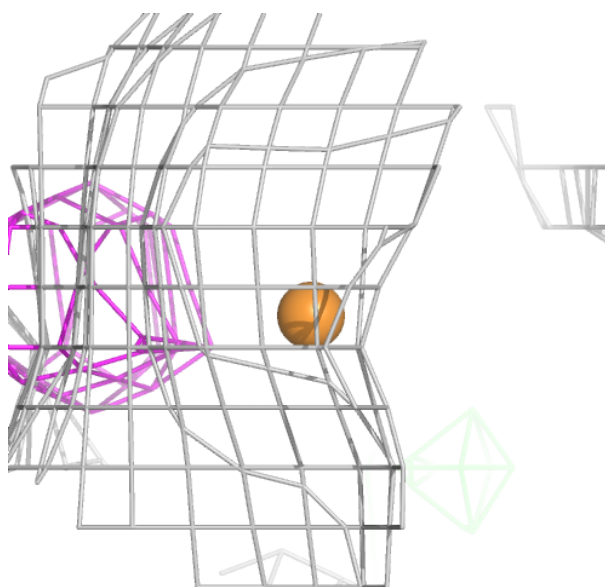
Electron density around CU A 603:

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



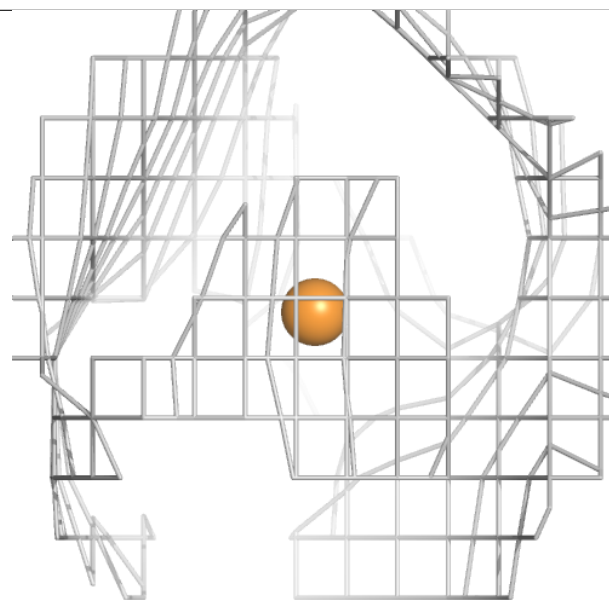
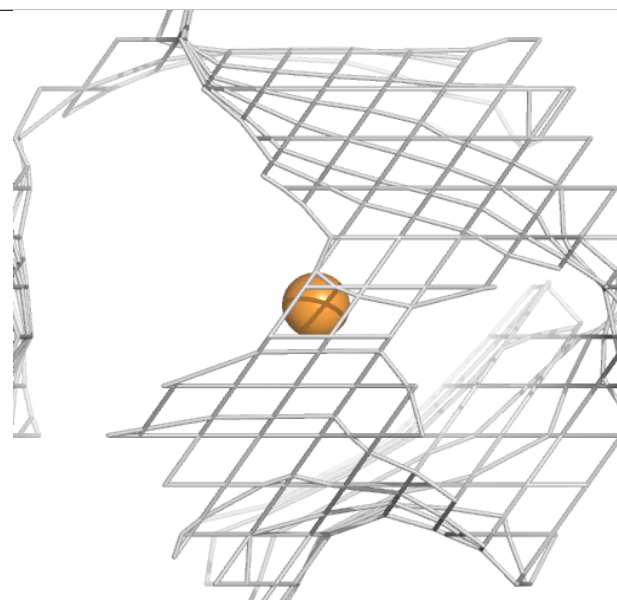
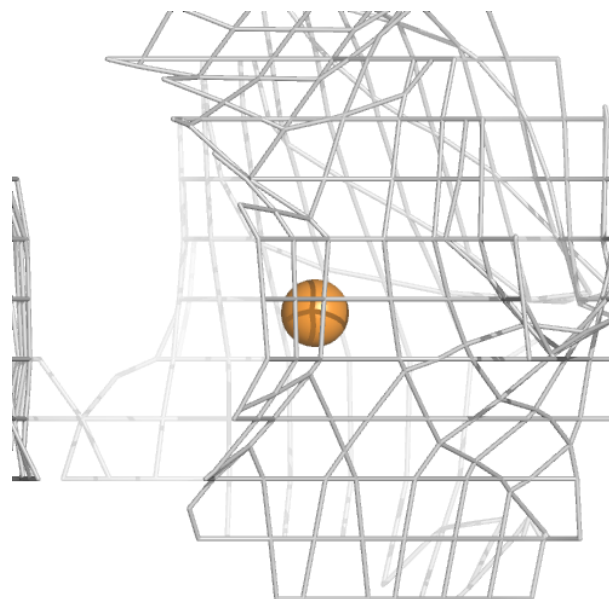
Electron density around CU A 601:

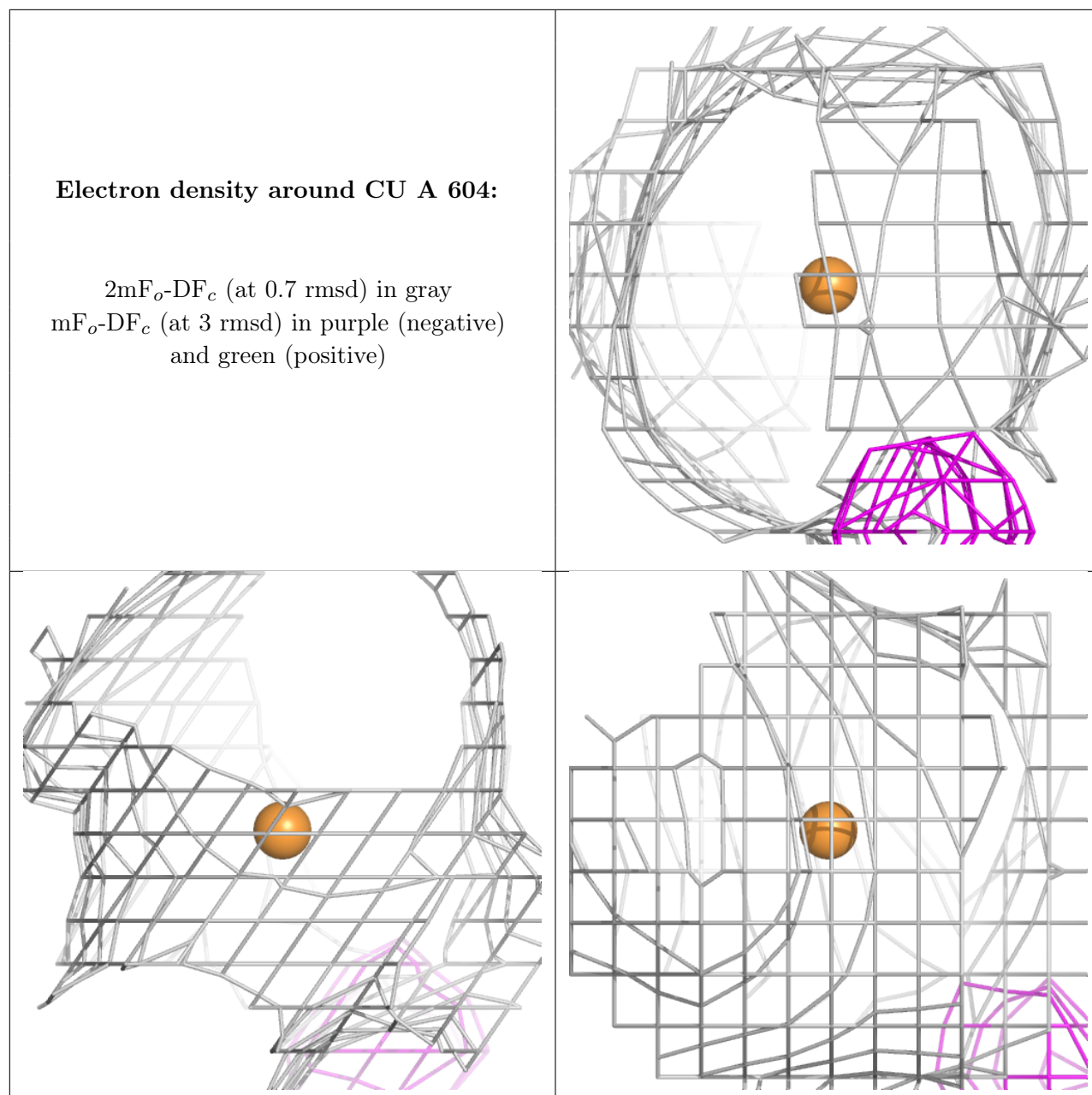
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU B 604:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.