Full wwPDB X-ray Structure Validation Report (i)

May 19, 2022 – 03:05 pm BST

PDB ID	:	7Z5P
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

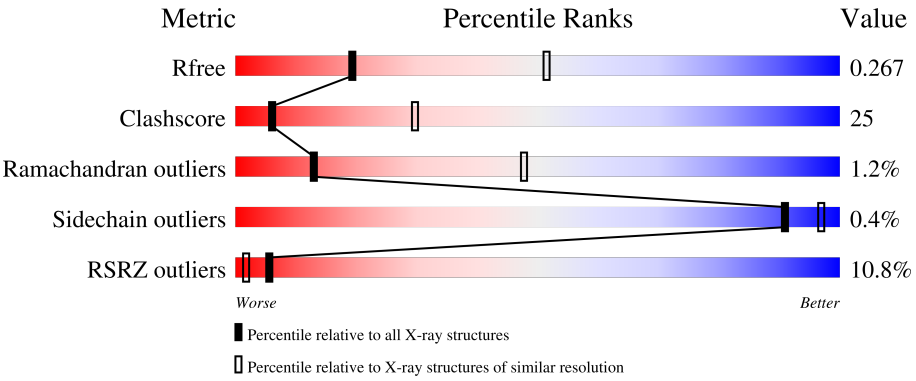
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	10% 63% 34%
1	B	515	11% 64% 33%

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 (i)

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 (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

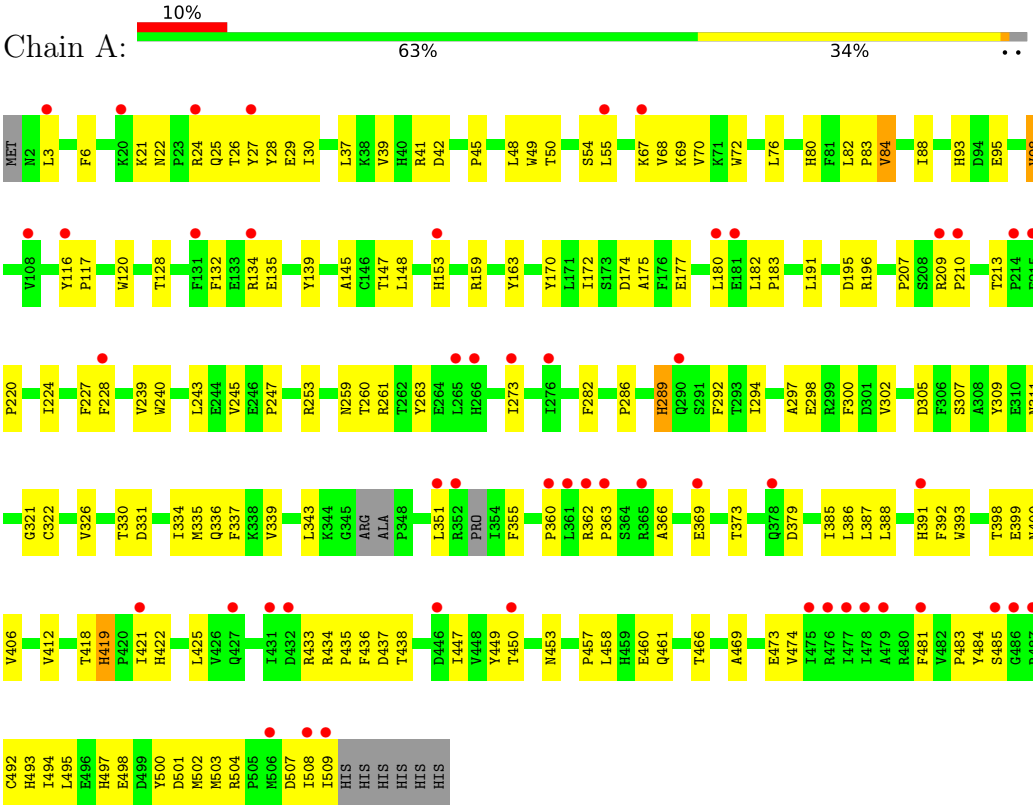
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cu	0	0
			4	4		
2	B	4	Total	Cu	0	0
			4	4		

3 Residue-property plots (i)

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

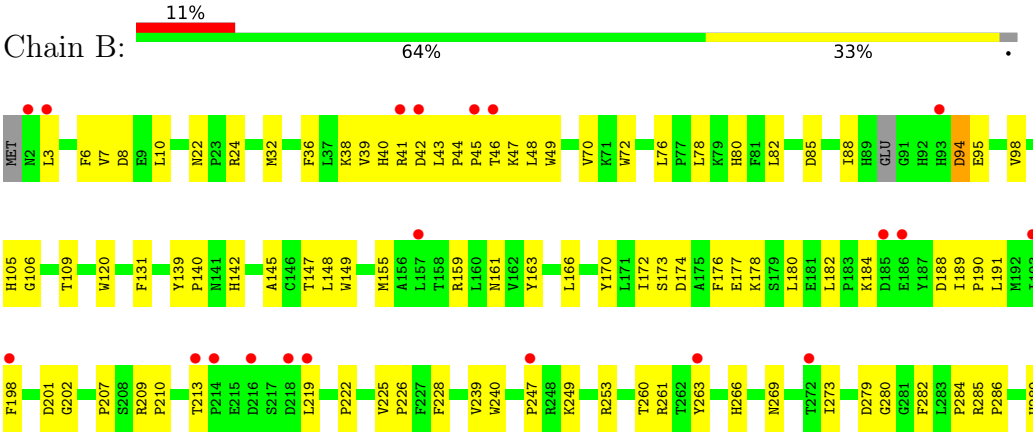
• Molecule 1: Copper oxidase

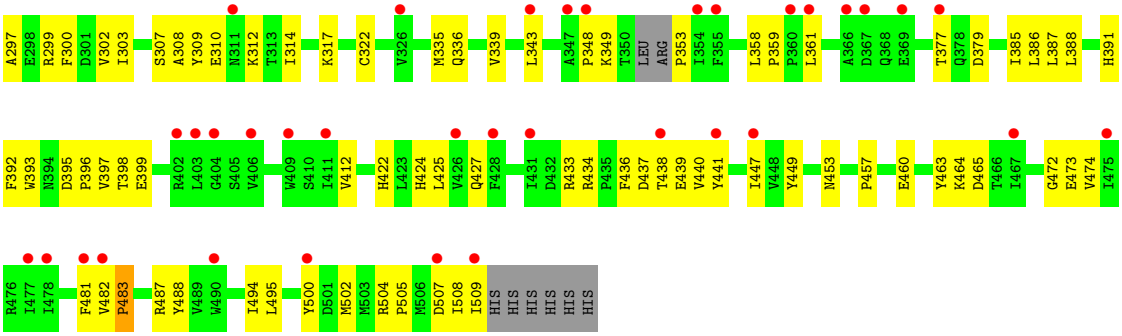
Chain A:



• Molecule 1: Copper oxidase

Chain B:




A297 E298 R299 F300 D301 V302 I303 S307 A308 Y309 E310 N311 K312 T313 I314 K317 C322 V326 M335 Q336 V339 L343 A347 P348 K349 T350 LEU ARG P353 I354 F355 L358 P359 P360 L361 A366 D367 Q368 E369 T377 Q378 D379 I385 L386 L387 L388 H391
F392 W393 N394 D395 P396 V397 T398 E399 R402 L403 G404 S405 V406 W409 S410 I411 V412 H422 L423 H424 L425 V426 Q427 F428 I431 D432 R433 R434 P435 F436 D437 T438 E439 V440 Y441 I447 V448 Y449 N453 P457 E460 Y463 K464 D465 T466 I467 G472 E473 V474 I475
R476 I477 I478 F481 V482 P483 R487 Y488 V489 W490 I494 L495 Y500 D501 M502 M503 R504 P505 M506 D507 I508 I509 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.60 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.254 , 0.267 0.254 , 0.267	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	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.*

[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: 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	0.45	0/4249	0.73	0/5793
1	B	0.45	0/4245	0.67	0/5789
All	All	0.45	0/8494	0.70	0/11582

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.

There are no bond angle outliers.

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	211	0
1	B	4115	0	3986	189	0
2	A	4	0	0	2	0
2	B	4	0	0	0	0
All	All	8243	0	7978	400	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 (400) 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:HE1	1:A:503:MET:HE2	1.15	1.07
1:A:117:PRO:HG2	1:A:503:MET:HE1	1.36	1.06
1:A:393:TRP:HE1	1:A:503:MET:CE	1.72	1.02
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: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: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:A:492:CYS:HG	2:A:604:CU:CU	0.52	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:489:VAL:HG11	1:A:503:MET:HE2	1.64	0.81
1:B:247:PRO:HG2	1:B:343:LEU:HD11	1.60	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:CG1	1:B:40:HIS:HE1	1.94	0.79
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
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:A:492:CYS:SG	2:A:604:CU:CU	1.70	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:A:393:TRP:NE1	1:A:503:MET:CE	2.50	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: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: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:B:438:THR:HG21	1:B:472:GLY:HA3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:489:VAL:HG11	1:A:503:MET:HE3	1.76	0.66
1:A:88:ILE:HD12	1:A:500:TYR:CD1	2.32	0.65
1:A:351:LEU:C	1:A:351:LEU:HD13	2.17	0.65
1:A:489:VAL:CG1	1:A:503:MET:HE2	2.25	0.65
1:A:117:PRO:CG	1:A:503:MET:CE	2.74	0.65
1:B:457:PRO:HD2	1:B:460:GLU:OE1	1.97	0.65
1:A:135:GLU:CD	1:A:135:GLU:H	2.00	0.65
1:A:259:ASN:CG	1:A:495:LEU:HD12	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:44:PRO:CG	1:B:201:ASP:C	2.71	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:10:LEU:HD22	1:B:335:MET:CE	2.33	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:117:PRO:HG2	1:A:503:MET:HE3	1.86	0.57
1:B:148:LEU:HD23	1:B:299:ARG:NH2	2.20	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
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: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:191:LEU:HD13	1:A:335:MET:HE1	1.90	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:A:393:TRP:NE1	1:A:503:MET:HE2	2.01	0.53
1:A:447:ILE:HD12	1:A:447:ILE:H	1.72	0.53
1:B:10:LEU:HD22	1:B:335:MET:HE1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:98:VAL:HG12	1:A:98:VAL:O	2.09	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:44:PRO:HG3	1:B:201:ASP:C	2.29	0.52
1:B:273:ILE:HG23	1:B:302:VAL:HG11	1.92	0.52
1:B:299:ARG:HH12	1:B:465:ASP:CG	2.13	0.51
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:117:PRO:CG	1:A:503:MET:HE1	2.24	0.51
1:A:386:LEU:HD12	1:A:502:MET:HE3	1.93	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:418:THR:O	1:A:418:THR:HG22	2.11	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:117:PRO:CG	1:A:503:MET:HE3	2.40	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:163:TYR:CE1	1:A:228:PHE:CZ	3.00	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:B:105:HIS:NE2	1:B:297:ALA:HB1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:C	1:B:180:LEU:HD23	2.32	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: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:A:28:TYR:HB3	1:A:30:ILE:CD1	2.43	0.48
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:44:PRO:HG2	1:B:201:ASP:C	2.33	0.48
1:B:155:MET:HE1	1:B:393:TRP:CD1	2.48	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LEU:HD12	1:B:502:MET:HE3	1.96	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
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:29:GLU:C	1:A:30:ILE:HD12	2.37	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:A:219:LEU:HD23	1:A:219:LEU:C	2.37	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:B:10:LEU:HD22	1:B:335:MET:HE3	1.99	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: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:398:THR:OG1	1:A:399:GLU:CD	2.56	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:398:THR:OG1	1:B:399:GLU:CD	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:VAL:O	1:A:240:TRP:C	2.56	0.43
1:B:239:VAL:O	1:B:240:TRP:C	2.57	0.43
1:A:387:LEU:CD2	1:A:501:ASP:HB3	2.48	0.43
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:174:ASP:O	1:B:177:GLU:N	2.52	0.43
1:A:351:LEU:C	1:A:351:LEU:CD1	2.86	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:A:403:LEU:H	1:A:509:ILE:C	2.23	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: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:213:THR:O	1:A:213:THR:OG1	2.32	0.42
1:A:400:ASN:HA	1:A:507:ASP:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:184:LYS:HZ1	1:B:349:LYS:HZ1	1.67	0.42
1:B:184:LYS:HZ1	1:B:349:LYS:NZ	2.16	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
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: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:A:305:ASP:OD1	1:A:307:SER:OG	2.26	0.41
1:B:80:HIS:CE1	1:B:82:LEU:HB2	2.56	0.41
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:330:THR:OG1	1:A:331:ASP:N	2.54	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:312:LYS:H	1:A:339:VAL:CG2	2.34	0.40
1:A:393:TRP:NE1	1:A:503:MET:HE1	2.35	0.40
1:B:106:GLY:HA3	1:B:148:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PRO:O	1:B:191:LEU:HD12	2.21	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%)	11	43
1	B	499/515 (97%)	454 (91%)	40 (8%)	5 (1%)	15	53
All	All	998/1030 (97%)	900 (90%)	86 (9%)	12 (1%)	13	48

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%)	451 (100%)	2 (0%)	91	97
1	B	452/462 (98%)	450 (100%)	2 (0%)	91	97
All	All	905/924 (98%)	901 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ASP
1	A	322	CYS
1	B	322	CYS
1	B	507	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	419	HIS
1	B	2	ASN
1	B	40	HIS
1	B	105	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 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	505/515 (98%)	0.71	54 (10%)	6 2	62, 85, 136, 190	5 (0%)
1	B	505/515 (98%)	0.71	55 (10%)	5 2	49, 86, 134, 207	2 (0%)
All	All	1010/1030 (98%)	0.71	109 (10%)	5 2	49, 85, 135, 207	7 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	ARG	8.8
1	A	369	GLU	8.1
1	B	438	THR	7.1
1	B	403	LEU	7.0
1	B	93	HIS	6.9
1	A	431	ILE	6.1
1	B	213	THR	5.7
1	B	41	ARG	5.6
1	B	366	ALA	5.5
1	A	485	SER	5.4
1	A	508	ILE	5.2
1	B	369	GLU	5.2
1	B	361	LEU	5.0
1	B	219	LEU	4.8
1	B	348	PRO	4.7
1	A	352	ARG	4.6
1	B	214	PRO	4.3
1	A	273	ILE	4.2
1	B	45	PRO	4.1
1	B	218	ASP	4.0
1	A	478	ILE	3.9
1	A	450	THR	3.9
1	B	482	VAL	3.6
1	B	326	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	507	ASP	3.6
1	B	402	ARG	3.6
1	A	481	PHE	3.5
1	A	290	GLN	3.4
1	B	409	TRP	3.3
1	A	131	PHE	3.3
1	A	228	PHE	3.3
1	A	432	ASP	3.3
1	A	506	MET	3.2
1	B	490	TRP	3.2
1	B	477	ILE	3.2
1	B	186	GLU	3.2
1	B	311	ASN	3.2
1	A	180	LEU	3.1
1	B	360	PRO	3.1
1	B	216	ASP	3.1
1	B	411	ILE	3.1
1	A	134	ARG	3.0
1	A	487	ARG	3.0
1	A	210	PRO	3.0
1	B	428	PHE	2.9
1	A	363	PRO	2.9
1	B	478	ILE	2.9
1	A	391	HIS	2.8
1	B	347	ALA	2.8
1	A	181	GLU	2.8
1	A	215	GLU	2.8
1	A	476	ARG	2.8
1	B	354	ILE	2.8
1	B	500	TYR	2.8
1	A	67	LYS	2.7
1	A	365	ARG	2.7
1	B	193	ILE	2.7
1	A	351	LEU	2.7
1	B	355	PHE	2.7
1	B	475	ILE	2.7
1	A	446	ASP	2.6
1	A	276	ILE	2.6
1	A	477	ILE	2.6
1	A	427	GLN	2.5
1	A	3	LEU	2.5
1	A	108	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	LEU	2.5
1	B	377	THR	2.5
1	A	20	LYS	2.5
1	A	402	ARG	2.5
1	B	42	ASP	2.5
1	B	406	VAL	2.4
1	B	3	LEU	2.4
1	B	367	ASP	2.4
1	B	441	TYR	2.4
1	B	431	ILE	2.4
1	A	214	PRO	2.4
1	A	55	LEU	2.4
1	A	475	ILE	2.3
1	B	426	VAL	2.3
1	A	361	LEU	2.3
1	B	509	ILE	2.3
1	B	198	PHE	2.3
1	B	185	ASP	2.3
1	B	247	PRO	2.3
1	B	263	TYR	2.2
1	A	421	ILE	2.2
1	A	209	ARG	2.2
1	B	272	THR	2.2
1	B	404	GLY	2.2
1	B	46	THR	2.2
1	A	490	TRP	2.2
1	A	265	LEU	2.2
1	B	481	PHE	2.2
1	A	378	GLN	2.1
1	A	266	HIS	2.1
1	A	509	ILE	2.1
1	B	2	ASN	2.1
1	A	218	ASP	2.1
1	A	153	HIS	2.1
1	A	116	TYR	2.1
1	B	343	LEU	2.1
1	A	486	GLY	2.1
1	A	24	ARG	2.1
1	B	447	ILE	2.1
1	A	360	PRO	2.1
1	A	479	ALA	2.0
1	A	27	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	467	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

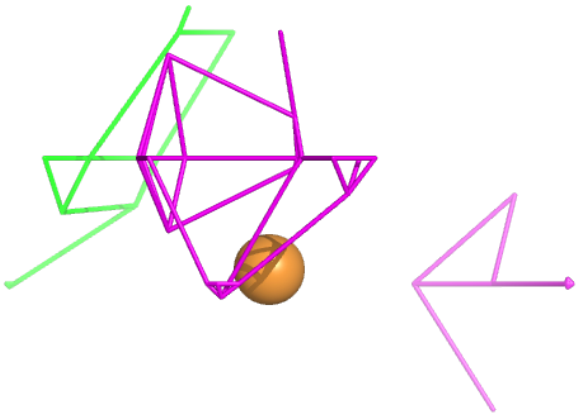
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

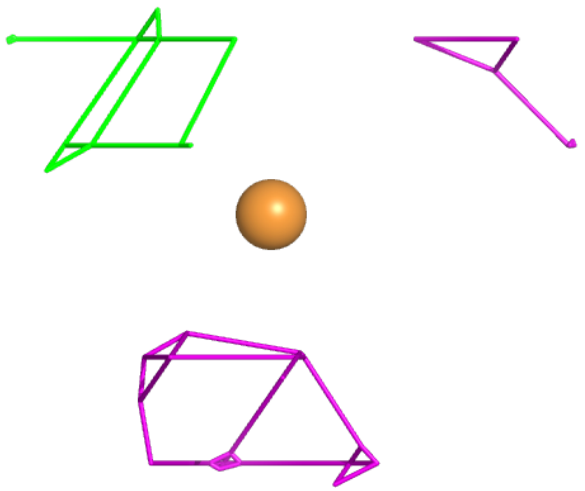
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	B	601	1/1	0.73	0.18	114,114,114,114	0
2	CU	B	604	1/1	0.81	0.08	107,107,107,107	0
2	CU	B	603	1/1	0.87	0.28	96,96,96,96	0
2	CU	B	602	1/1	0.88	0.27	96,96,96,96	0
2	CU	A	601	1/1	0.89	0.07	96,96,96,96	0
2	CU	A	602	1/1	0.91	0.22	96,96,96,96	0
2	CU	A	603	1/1	0.94	0.17	96,96,96,96	0
2	CU	A	604	1/1	0.95	0.06	104,104,104,104	0

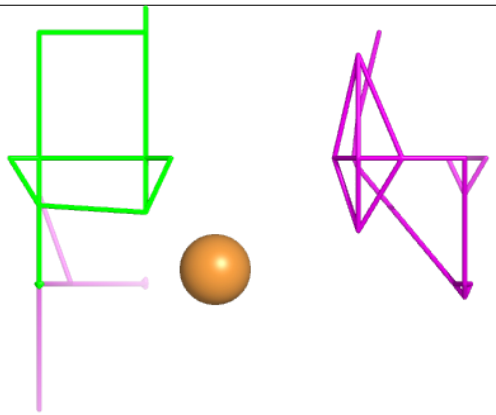
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CU B 601:

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

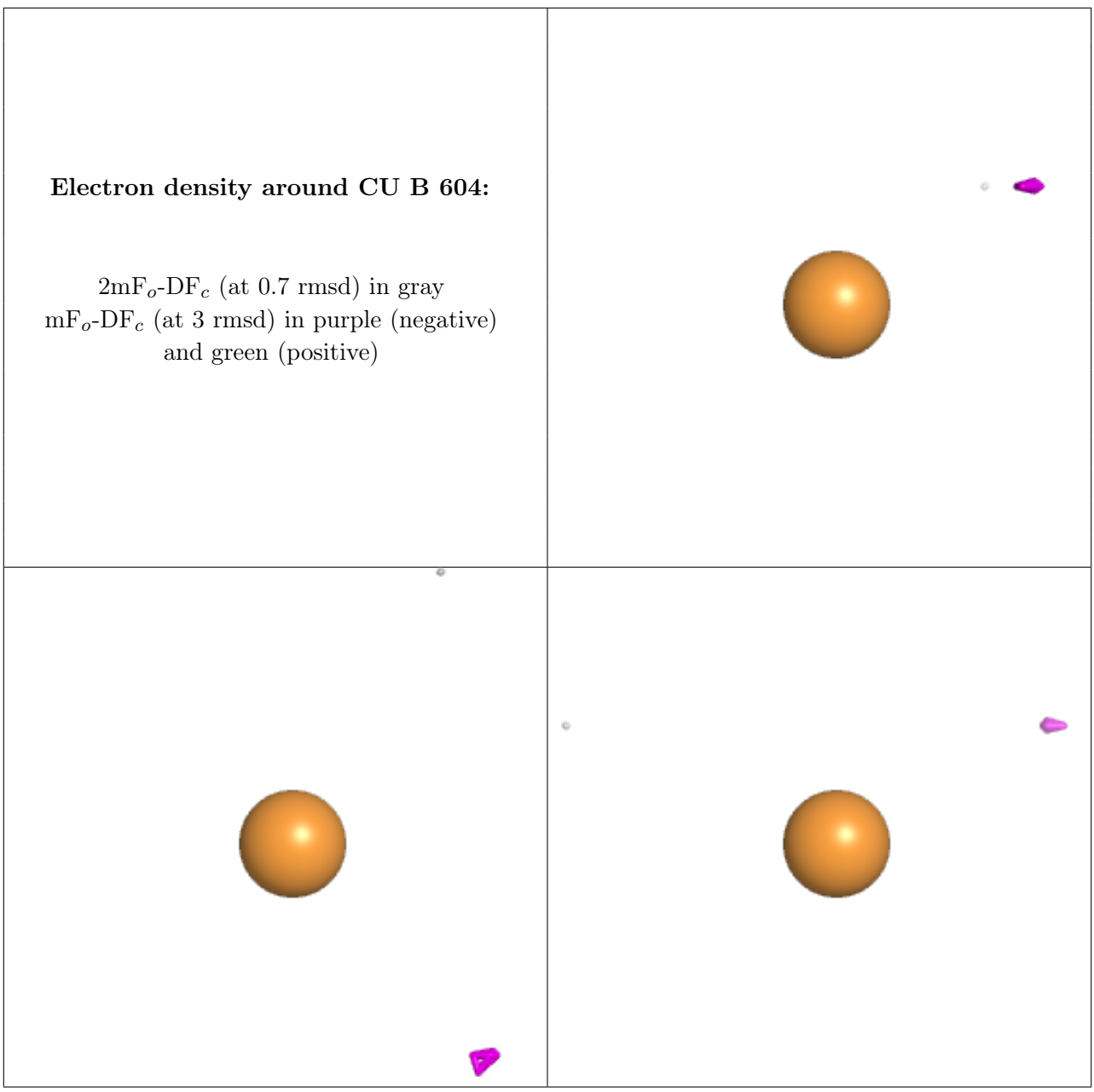






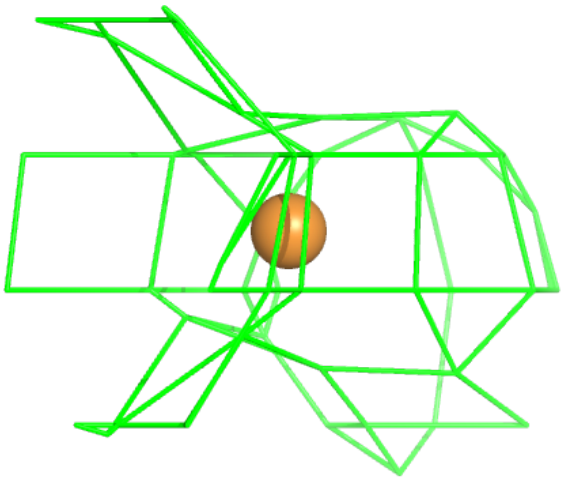
Electron density around CU B 604:

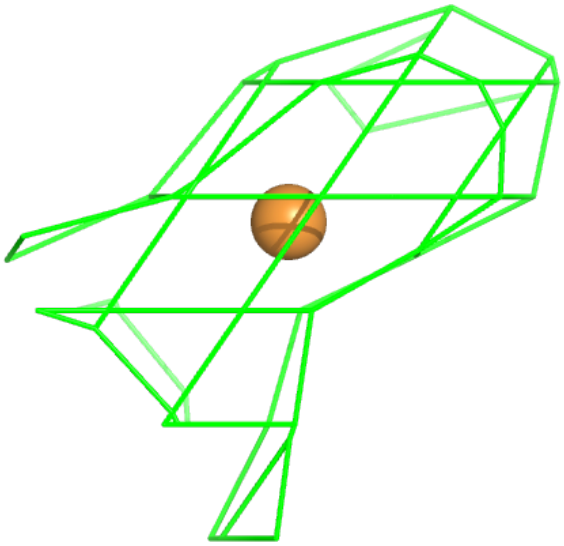
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

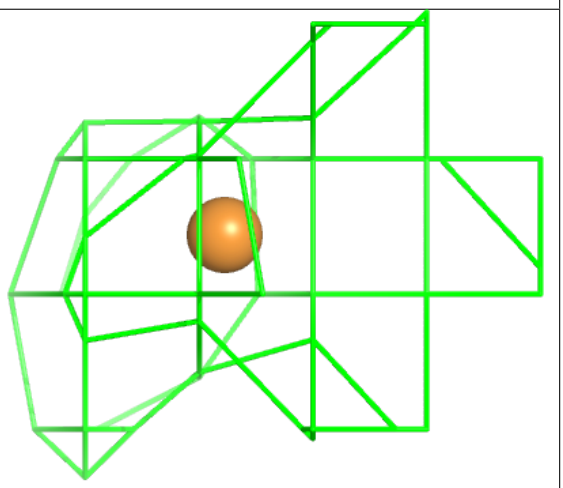


Electron density around CU B 603:

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

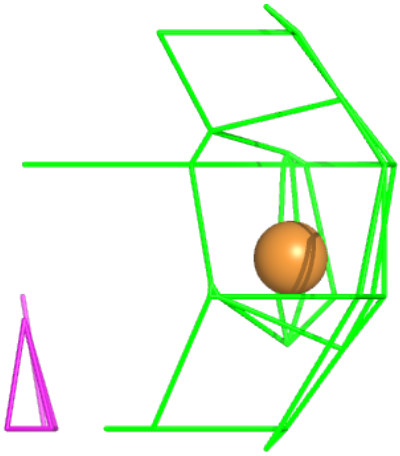


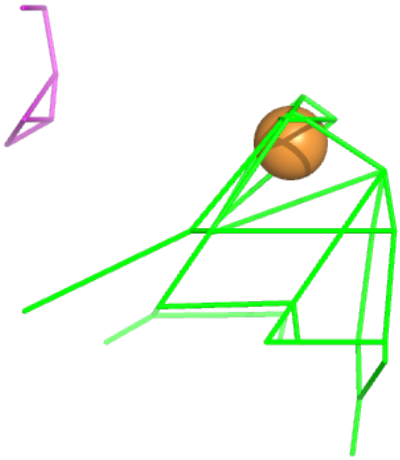


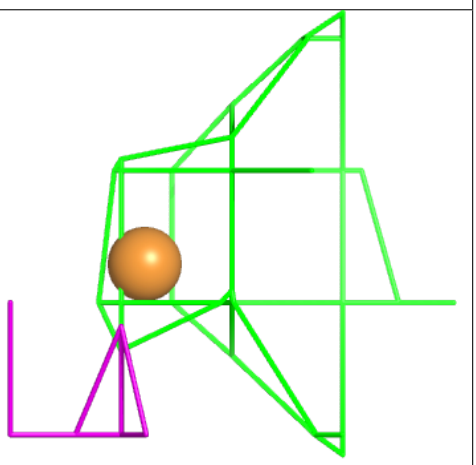


Electron density around CU B 602:

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

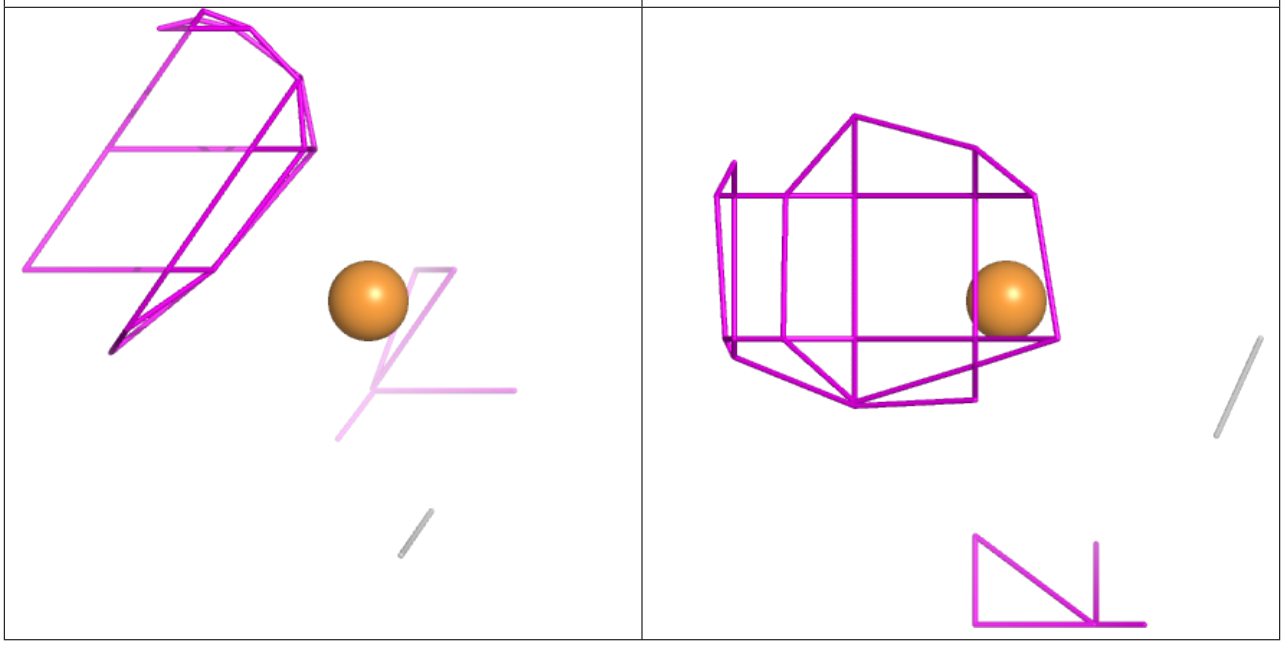






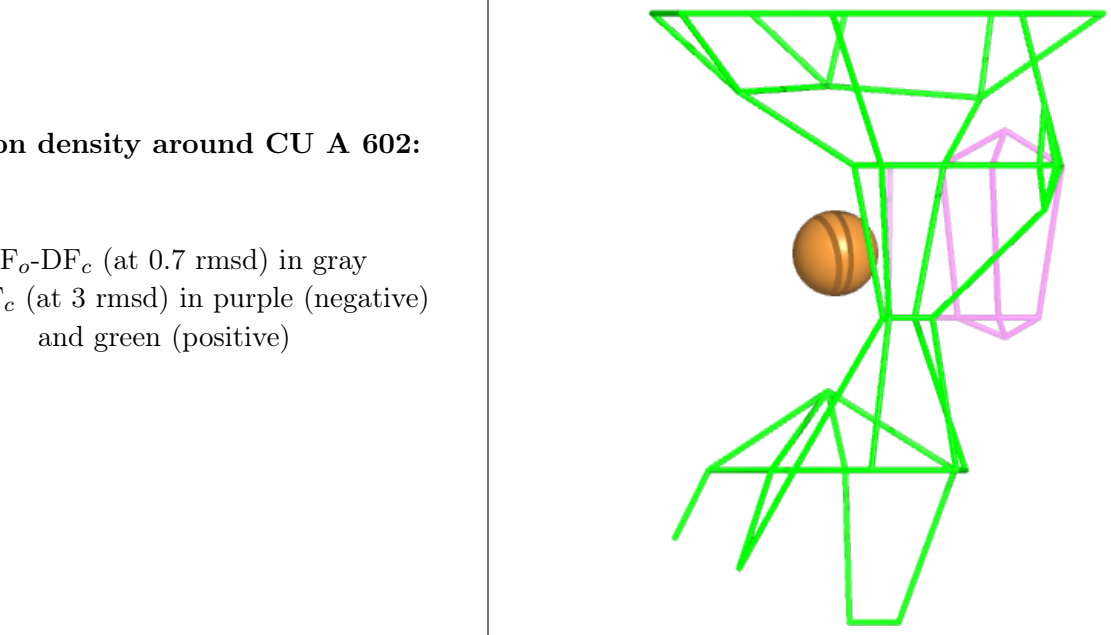
Electron density around CU A 601:

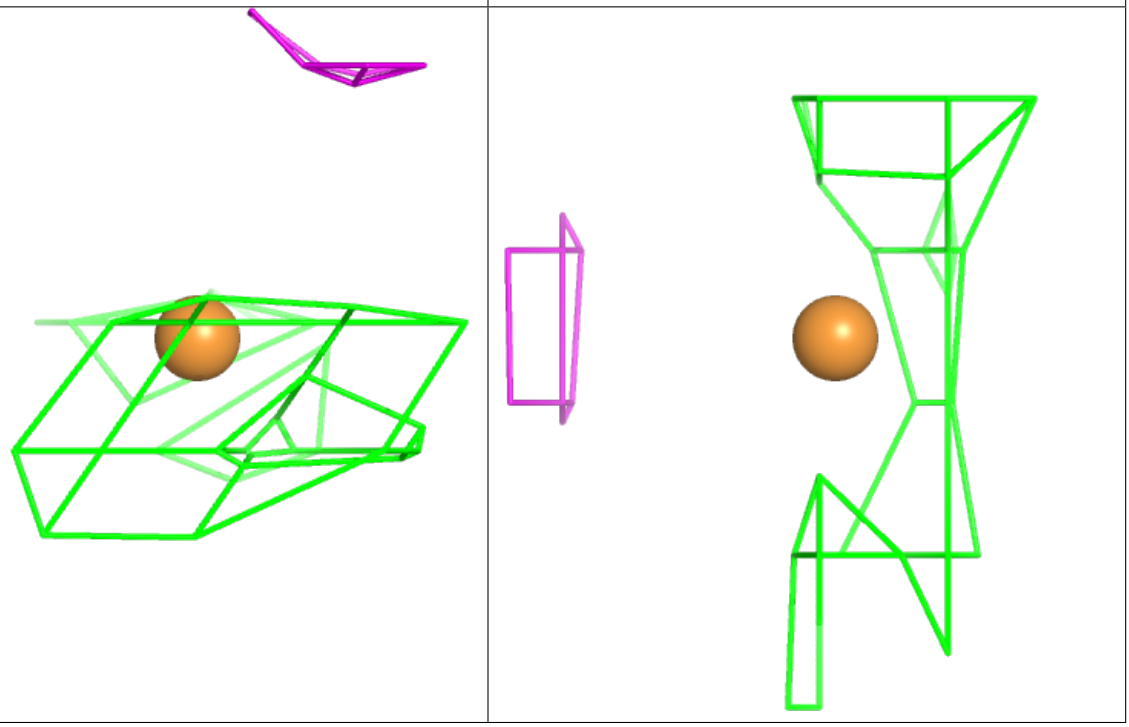
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CU A 602:

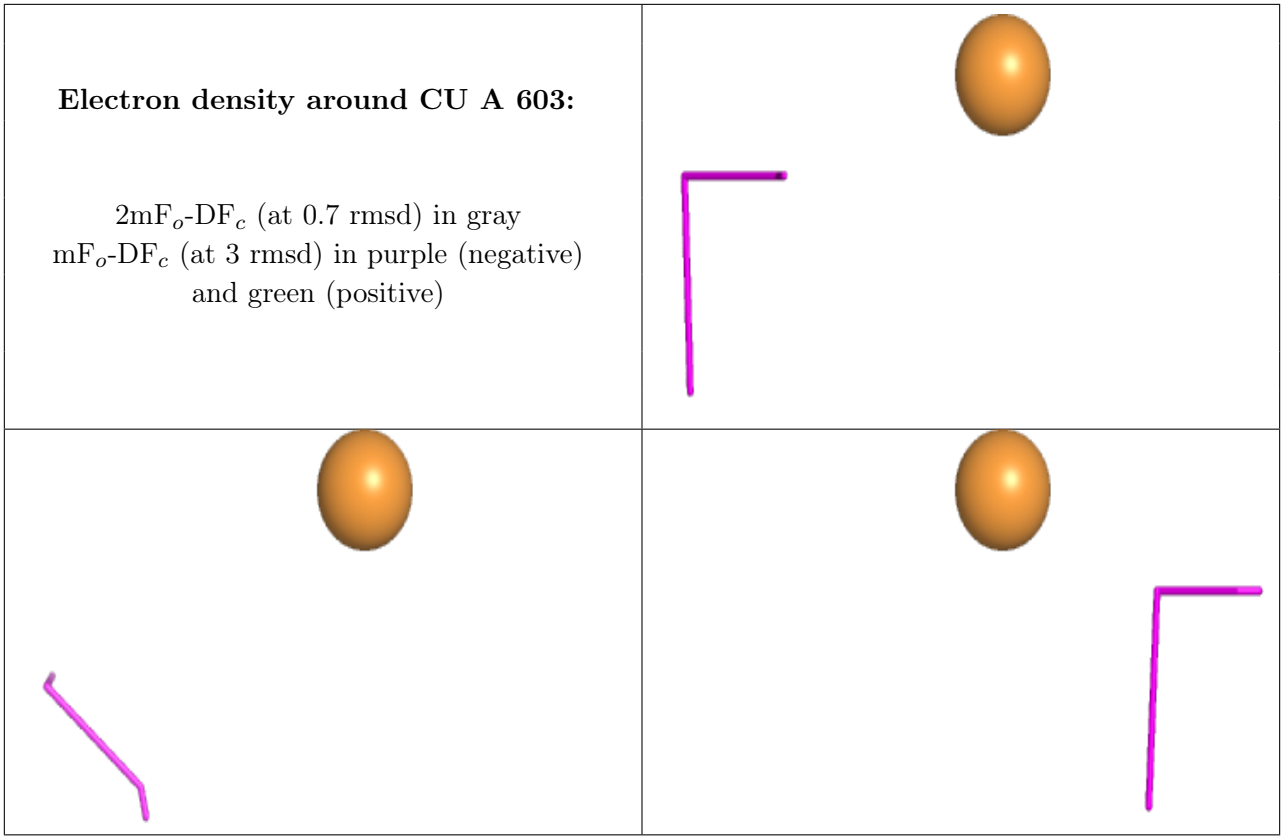
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





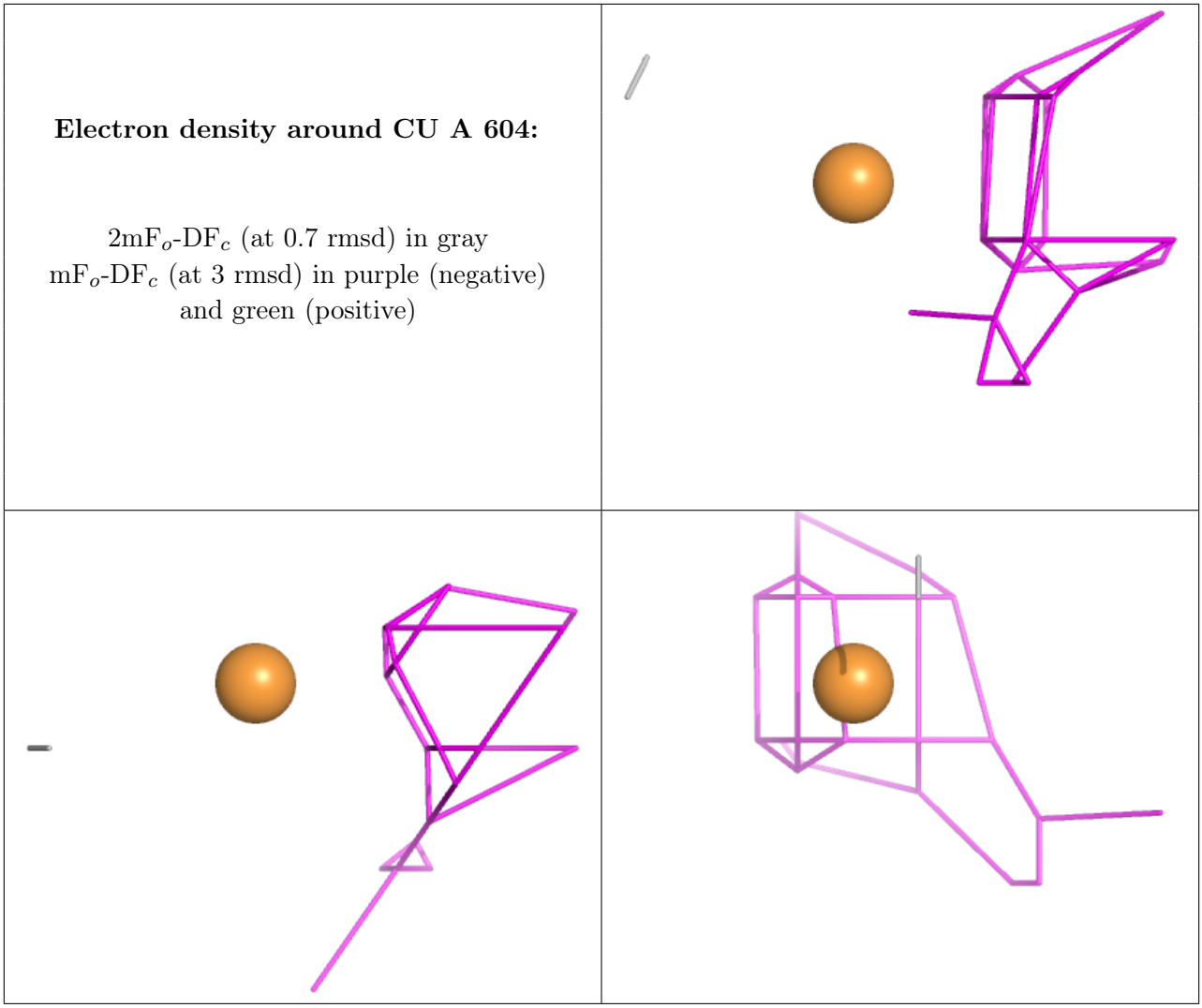
Electron density around CU A 603:

$2mF_o$-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 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.