Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:23 PM JST

PDB ID	:	7Y1W
Title	:	Controlling fibrosis using compound with novel binding mode to prolyl-tRNA synthetase 1
Authors	:	Kim, S.; Yoon, I.; Son, J.; Park, S.; Hwang, K.Y.
Deposited on	:	2022-06-09
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

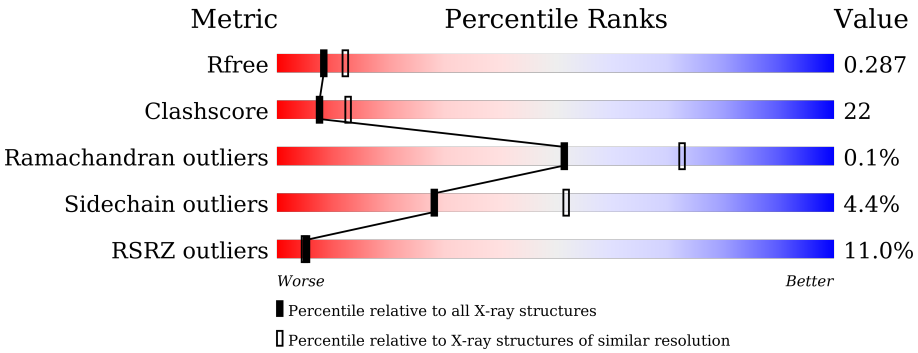
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	498	7% 59% 36%
1	B	498	15% 54% 40%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7862 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.

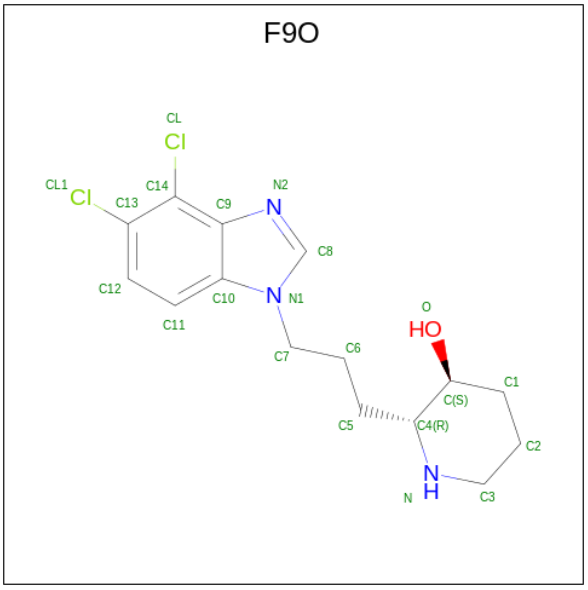
- Molecule 1 is a protein called Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3874	2482	654	713	25			
1	B	483	Total	C	N	O	S	0	1	0
			3874	2481	652	716	25			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

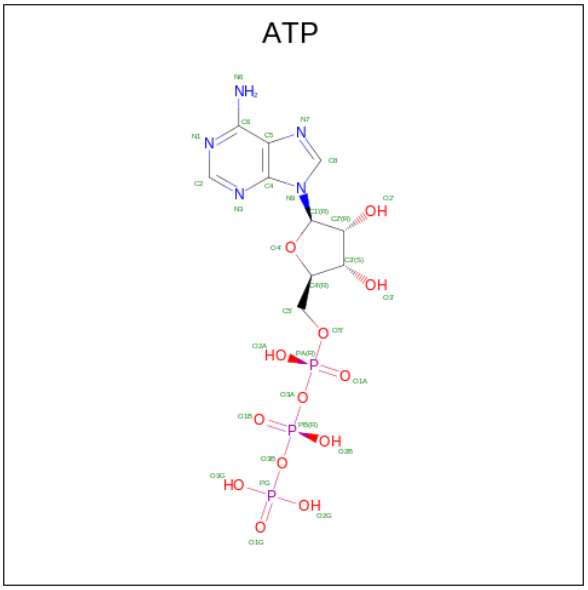
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2R,3S)-2-[3-[4,5-bis(chloranyl)benzimidazol-1-yl]propyl]piperidin-3-ol (three-letter code: F9O) (formula: $C_{15}H_{19}Cl_2N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			21	15	2	3	1		
3	B	1	Total	C	Cl	N	O	0	0
			21	15	2	3	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

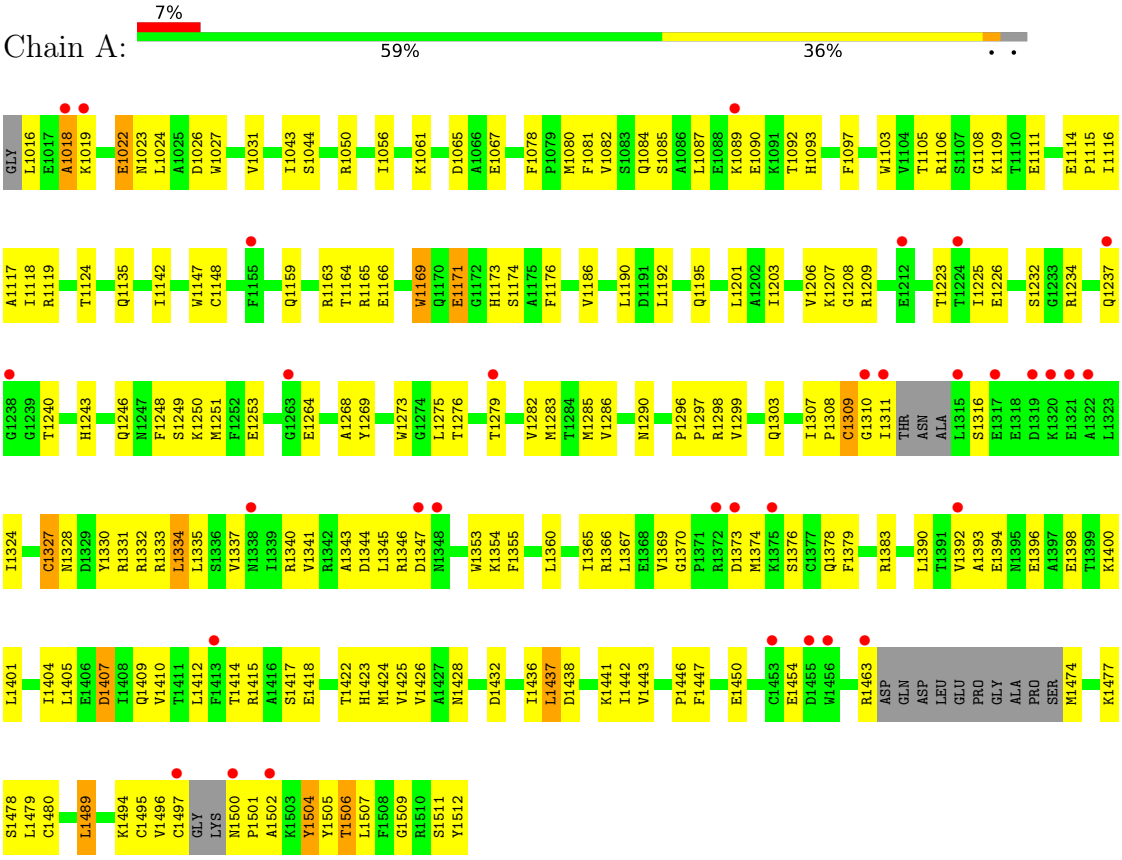
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	10	Total	O	0	0
			10	10		

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.

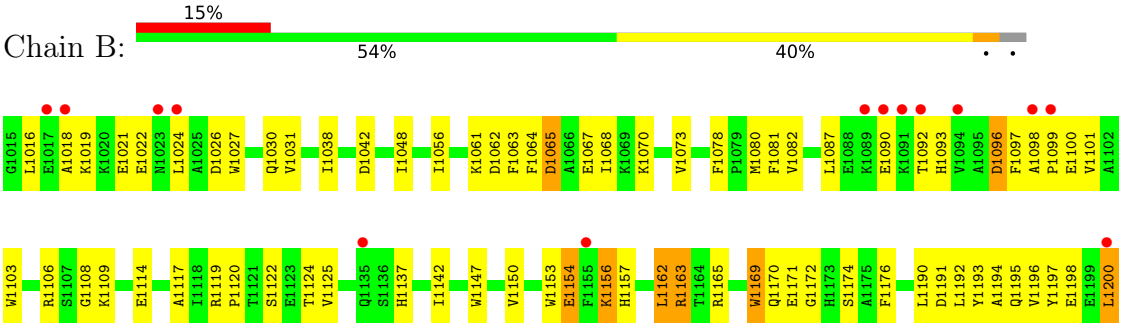
• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

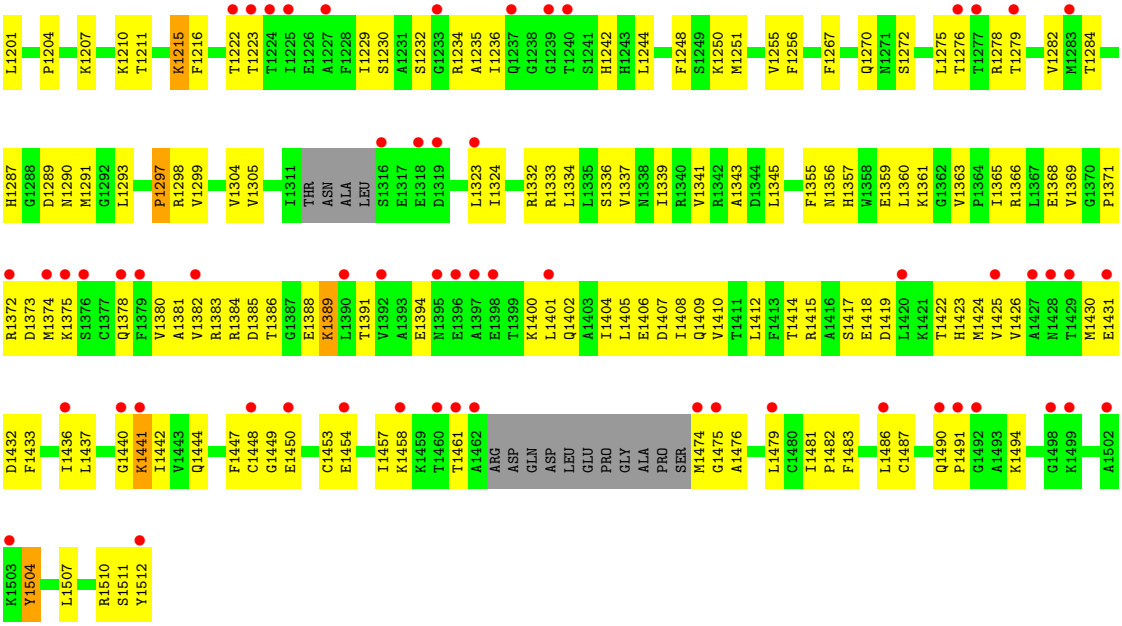
Chain A:



• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain B:




L1201 P1204 K1207 K1210 T1211 K1215 F1216 T1222 T1223 T1224 I1225 E1226 A1227 F1228 I1229 S1230 A1231 S1232 G1233 R1234 A1235 I1236 Q1237 G1238 G1239 T1240 S1241 H1242 H1243 L1244 F1248 S1249 K1250 M1251 V1255 F1256 F1267 Q1270 N1271 S1272 L1275 T1276 T1277 R1278 T1279 V1282 M1283 T1284
H1287 G1288 D1289 N1290 M1291 G1292 L1293 P1297 R1298 V1299 V1304 V1305 T1311 THR ASN ALA LEU S1316 E1317 E1318 D1319 L1323 I1324 R1332 R1333 L1334 L1335 S1336 V1337 N1338 I1339 R1340 V1341 R1342 A1343 D1344 L1345 F1355 N1356 H1357 W1358 E1359 L1360 K1361 G1362 V1363 P1364 I1365 R1366 L1367 E1368 V1369 G1370 P1371
R1372 D1373 M1374 K1375 S1376 C1377 Q1378 F1379 V1380 A1381 V1382 R1383 R1384 D1385 T1386 G1387 E1388 K1389 L1390 T1391 V1392 A1393 E1394 N1395 E1396 A1397 E1398 T1399 K1400 L1401 Q1402 A1403 I1404 L1405 E1406 D1407 I1408 Q1409 V1410 T1411 L1412 F1413 T1414 R1415 A1416 S1417 E1418 D1419 L1420 K1421 T1422 H1423 M1424 V1425 V1426 A1427 N1428 T1429 M1430 E1431
D1432 F1433 I1436 L1437 G1440 K1441 I1442 V1443 Q1444 F1447 C1448 G1449 E1450 C1453 E1454 I1457 K1458 K1459 T1460 T1461 A1462 ARG ASP GLN ASP LEU GLU PRO GLY ALA PRO SER M1474 G1475 A1476 L1479 C1480 I1481 P1482 F1483 L1486 C1487 Q1490 P1491 G1492 A1493 K1494 G1498 K1499 A1502
K1503 Y1504 L1507 R1510 S1511 Y1512

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.56Å 92.15Å 86.73Å 90.00° 108.77° 90.00°	Depositor
Resolution (Å)	33.22 – 2.50 33.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.1 (33.22-2.50) 88.2 (33.22-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4438	Depositor
R, R_{free}	0.229 , 0.289 0.230 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (6.15%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: ZN, F9O, ATP, MG

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	0.42	0/3965	0.73	6/5364 (0.1%)
1	B	0.40	0/3969	0.79	8/5371 (0.1%)
All	All	0.41	0/7934	0.76	14/10735 (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	B	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1441	LYS	CD-CE-NZ	-6.68	96.33	111.70
1	A	1275	LEU	CA-CB-CG	6.61	130.51	115.30
1	A	1327	CYS	CA-CB-SG	-6.40	102.48	114.00
1	B	1097	PHE	C-N-CA	-6.25	106.07	121.70
1	A	1309	CYS	N-CA-C	6.07	127.40	111.00
1	A	1018	ALA	C-N-CA	6.03	136.77	121.70
1	A	1022	GLU	N-CA-C	5.97	127.11	111.00
1	B	1431	GLU	CA-CB-CG	5.71	125.96	113.40
1	B	1298	ARG	CA-CB-CG	5.68	125.89	113.40
1	B	1162	LEU	CA-CB-CG	-5.65	102.31	115.30
1	B	1096	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	1297	PRO	C-N-CA	-5.50	107.95	121.70
1	A	1022	GLU	N-CA-CB	-5.32	101.03	110.60
1	B	1096	ASP	CB-CG-OD1	-5.21	113.61	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1098	ALA	Peptide
1	B	1154	GLU	Peptide
1	B	1482	PRO	Peptide

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	3874	0	3840	152	1
1	B	3874	0	3831	195	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0
4	A	31	0	12	0	0
5	A	2	0	0	0	0
6	A	27	0	0	8	0
6	B	10	0	0	5	0
All	All	7862	0	7683	341	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (341) 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:1497:CYS:HG	1:A:1500:ASN:N	1.50	1.08
1:A:1022:GLU:HG3	1:A:1023:ASN:H	1.23	1.00
1:B:1016:LEU:HD11	1:B:1031:VAL:HG22	1.50	0.93
1:B:1305:VAL:HG23	1:B:1363:VAL:HG11	1.56	0.86
1:B:1432:ASP:O	1:B:1436:ILE:N	2.10	0.84
1:A:1298:ARG:H	1:A:1409:GLN:HE22	1.23	0.84
1:B:1339:ILE:HD11	1:B:1402:GLN:HG2	1.59	0.83
1:B:1156:LYS:O	6:B:1701:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1068:ILE:HD12	1:B:1073:VAL:HG21	1.63	0.81
1:A:1297:PRO:HB3	1:A:1405:LEU:HD22	1.62	0.81
1:B:1474:MET:HA	1:B:1510:ARG:HH12	1.44	0.81
1:A:1309:CYS:SG	1:A:1310:GLY:N	2.54	0.80
1:B:1383:ARG:HG3	1:B:1388:GLU:HB3	1.66	0.78
1:A:1309:CYS:HB2	1:A:1311:ILE:HD13	1.66	0.78
1:B:1210:LYS:HB2	1:B:1215:LYS:HB3	1.64	0.77
1:A:1497:CYS:SG	1:A:1500:ASN:N	2.57	0.77
1:B:1230:SER:OG	1:B:1419:ASP:OD2	2.03	0.75
1:A:1423:HIS:HA	1:A:1441:LYS:HE3	1.67	0.75
1:B:1378:GLN:HE21	1:B:1391:THR:HB	1.51	0.74
1:B:1191:ASP:OD1	1:B:1207:LYS:NZ	2.14	0.72
1:B:1402:GLN:O	1:B:1406:GLU:HG3	1.89	0.71
1:A:1378:GLN:HG3	1:A:1379:PHE:H	1.55	0.71
1:A:1454:GLU:OE1	1:A:1478:SER:OG	2.05	0.71
1:B:1423:HIS:HD2	1:B:1440:GLY:O	1.73	0.70
1:A:1393:ALA:HB3	1:A:1396:GLU:HB2	1.73	0.70
1:B:1021:GLU:OE1	1:B:1290:ASN:ND2	2.25	0.70
1:A:1108:GLY:HA3	1:B:1099:PRO:HA	1.75	0.69
1:B:1109:LYS:NZ	6:B:1704:HOH:O	2.24	0.69
1:B:1424:MET:HG3	1:B:1442:ILE:HG13	1.74	0.69
1:A:1428:ASN:ND2	6:A:1705:HOH:O	2.24	0.69
1:B:1458:LYS:HG3	1:B:1475:GLY:HA3	1.74	0.69
1:A:1264:GLU:OE1	6:A:1702:HOH:O	2.10	0.68
1:A:1092:THR:HG23	1:A:1248:PHE:HE2	1.58	0.68
1:A:1309:CYS:SG	1:A:1311:ILE:N	2.63	0.68
1:B:1419:ASP:O	1:B:1422:THR:OG1	2.12	0.67
1:B:1433:PHE:HA	1:B:1436:ILE:HB	1.75	0.67
1:B:1108:GLY:O	6:B:1702:HOH:O	2.12	0.67
1:B:1216:PHE:H	1:B:1222:THR:HG21	1.59	0.66
1:A:1093:HIS:HB2	1:A:1097:PHE:HD2	1.60	0.66
1:B:1019:LYS:HB3	1:B:1290:ASN:HD21	1.61	0.66
1:A:1253:GLU:O	6:A:1703:HOH:O	2.13	0.66
1:A:1392:VAL:HG21	1:A:1400:LYS:HG2	1.77	0.66
1:B:1304:VAL:HB	1:B:1341:VAL:HG23	1.77	0.66
1:A:1027:TRP:O	1:A:1031:VAL:HG23	1.95	0.66
1:A:1087:LEU:HA	1:A:1124:THR:HG21	1.78	0.65
1:B:1250:LYS:HG2	1:B:1267:PHE:CD2	2.32	0.65
1:A:1333:ARG:NH1	1:A:1398:GLU:OE2	2.28	0.65
1:A:1022:GLU:OE2	1:A:1027:TRP:HB2	1.97	0.65
1:B:1372:ARG:HG3	1:B:1372:ARG:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1400:LYS:O	1:B:1404:ILE:HG13	1.96	0.65
1:A:1479:LEU:HD12	1:A:1507:LEU:HD22	1.80	0.64
1:A:1298:ARG:H	1:A:1409:GLN:NE2	1.95	0.64
1:A:1022:GLU:HG3	1:A:1023:ASN:N	2.05	0.62
1:A:1022:GLU:CG	1:A:1023:ASN:H	2.01	0.62
1:A:1195:GLN:NE2	6:A:1706:HOH:O	2.24	0.61
1:B:1163:ARG:NH1	1:B:1512:TYR:HD2	1.99	0.61
1:A:1347:ASP:OD2	6:A:1704:HOH:O	2.16	0.61
1:B:1082:VAL:HG12	1:B:1125:VAL:HG23	1.82	0.61
1:B:1082:VAL:HG12	1:B:1125:VAL:CG2	2.30	0.61
1:A:1135:GLN:NE2	6:A:1708:HOH:O	2.33	0.60
1:A:1018:ALA:HB1	1:A:1022:GLU:OE2	2.01	0.60
1:B:1236:ILE:HD11	1:B:1278:ARG:NH1	2.16	0.60
1:B:1236:ILE:CD1	1:B:1512:TYR:HB2	2.31	0.60
1:B:1360:LEU:HD12	1:B:1360:LEU:H	1.66	0.60
1:A:1016:LEU:HD22	1:A:1360:LEU:HD21	1.83	0.60
1:B:1333:ARG:NH2	1:B:1394:GLU:O	2.35	0.59
1:B:1410:VAL:O	1:B:1414:THR:HG23	2.01	0.59
1:B:1474:MET:CA	1:B:1510:ARG:HH12	2.15	0.59
1:B:1450:GLU:OE1	1:B:1450:GLU:N	2.35	0.59
1:A:1061:LYS:O	1:A:1065:ASP:HB2	2.02	0.59
1:A:1303:GLN:HE21	1:A:1340:ARG:H	1.50	0.59
1:A:1392:VAL:HG21	1:A:1400:LYS:CG	2.32	0.59
1:B:1418:GLU:O	1:B:1422:THR:HG23	2.03	0.58
1:B:1430:MET:HA	1:B:1433:PHE:HB3	1.85	0.58
1:B:1194:ALA:O	1:B:1198:GLU:HB2	2.02	0.58
1:B:1433:PHE:O	1:B:1437:LEU:N	2.35	0.58
1:A:1437:LEU:HD11	1:A:1509:GLY:HA2	1.84	0.58
1:B:1190:LEU:HD23	1:B:1207:LYS:HG2	1.85	0.58
1:A:1324:ILE:O	1:A:1328:ASN:ND2	2.36	0.58
1:B:1090[B]:GLU:HG3	1:B:1251:MET:HB3	1.85	0.57
1:B:1026:ASP:O	1:B:1030:GLN:HG2	2.04	0.57
1:A:1169:TRP:HB3	1:A:1276:THR:HG22	1.86	0.57
1:A:1344:ASP:OD1	1:A:1346:ARG:HG3	2.04	0.57
1:A:1164:THR:HG22	1:A:1165:ARG:N	2.20	0.57
1:A:1446:PRO:HD3	1:A:1505:TYR:HE1	1.69	0.57
1:B:1021:GLU:CD	1:B:1021:GLU:H	2.07	0.57
1:B:1063:PHE:CE2	1:B:1196:VAL:HG12	2.41	0.56
1:A:1249:SER:OG	1:A:1268:ALA:N	2.39	0.56
1:A:1027:TRP:CE2	1:A:1031:VAL:HG21	2.41	0.56
1:B:1101:VAL:HG22	1:B:1120:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:THR:O	1:A:1418:GLU:HG2	2.06	0.56
1:A:1504:TYR:CD1	1:A:1506:THR:HG22	2.41	0.56
1:A:1337:VAL:HG21	1:A:1398:GLU:HB3	1.88	0.56
1:B:1024:LEU:CD2	1:B:1232:SER:HB3	2.35	0.56
1:B:1255:VAL:HG12	1:B:1267:PHE:CD1	2.40	0.56
1:A:1050:ARG:HG2	1:A:1050:ARG:HH11	1.71	0.56
1:A:1447:PHE:HZ	1:A:1454:GLU:HB2	1.70	0.56
1:B:1204:PRO:HG2	1:B:1417:SER:HA	1.88	0.56
1:B:1368:GLU:HB2	1:B:1380:VAL:CG1	2.35	0.55
1:A:1424:MET:SD	1:A:1507:LEU:HD11	2.46	0.55
1:B:1255:VAL:HG12	1:B:1267:PHE:HD1	1.71	0.55
1:B:1407:ASP:O	1:B:1410:VAL:HG22	2.05	0.55
1:A:1208:GLY:HA3	1:A:1480:CYS:SG	2.47	0.55
1:A:1203:ILE:HD13	1:A:1282:VAL:HG12	1.89	0.55
1:B:1430:MET:O	1:B:1433:PHE:N	2.39	0.55
1:A:1142:ILE:O	1:A:1174:SER:HA	2.07	0.55
1:A:1308:PRO:HA	1:A:1369:VAL:O	2.07	0.55
1:B:1426:VAL:HG21	1:B:1487:CYS:SG	2.47	0.55
1:A:1090:GLU:HB3	1:A:1251:MET:SD	2.47	0.54
1:B:1190:LEU:HD22	1:B:1223:THR:CG2	2.37	0.54
1:B:1368:GLU:HB2	1:B:1380:VAL:HG13	1.89	0.54
1:A:1164:THR:HG22	1:A:1165:ARG:H	1.72	0.54
1:A:1412:LEU:HD23	1:A:1415:ARG:HD3	1.88	0.54
1:A:1308:PRO:HD3	1:A:1327:CYS:SG	2.48	0.54
1:A:1190:LEU:HD21	1:A:1207:LYS:HG2	1.90	0.53
1:A:1082:VAL:HG13	1:A:1117:ALA:HB3	1.90	0.53
1:B:1276:THR:O	1:B:1279:THR:HG23	2.08	0.53
1:B:1385:ASP:OD1	1:B:1386:THR:N	2.41	0.53
1:B:1216:PHE:HD2	1:B:1242:HIS:HD1	1.57	0.53
1:B:1087:LEU:HD13	1:B:1124:THR:HG21	1.90	0.53
1:B:1061:LYS:HG3	1:B:1147:TRP:CZ2	2.44	0.53
1:B:1150:VAL:HG21	1:B:1169:TRP:CE2	2.44	0.53
1:B:1284:THR:HG23	1:B:1293:LEU:CD2	2.38	0.53
1:A:1084:GLN:OE1	1:A:1115:PRO:HD2	2.09	0.53
1:B:1190:LEU:CD2	1:B:1207:LYS:HG2	2.39	0.52
1:B:1356:ASN:O	1:B:1360:LEU:HD12	2.09	0.52
1:A:1494:LYS:HA	1:A:1501:PRO:HA	1.91	0.52
1:A:1418:GLU:O	1:A:1422:THR:HG23	2.10	0.52
1:A:1106:ARG:NE	1:A:1108:GLY:O	2.30	0.52
1:A:1246:GLN:O	1:A:1250:LYS:HG2	2.09	0.52
1:A:1400:LYS:O	1:A:1404:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1147:TRP:CE3	1:B:1170:GLN:HB3	2.44	0.52
1:B:1150:VAL:HG21	1:B:1169:TRP:CZ2	2.45	0.52
1:B:1142:ILE:O	1:B:1174:SER:HA	2.10	0.52
1:A:1393:ALA:HB3	1:A:1396:GLU:CB	2.39	0.51
1:A:1474:MET:N	6:A:1710:HOH:O	2.44	0.51
1:B:1090[A]:GLU:HG2	1:B:1251:MET:HB3	1.92	0.51
1:B:1355:PHE:CE1	1:B:1368:GLU:HG2	2.46	0.51
1:A:1186:VAL:HG21	1:A:1243:HIS:HB2	1.92	0.51
1:A:1383:ARG:NH1	1:A:1404:ILE:HG23	2.25	0.51
1:A:1080:MET:HA	1:A:1119:ARG:NH1	2.25	0.51
1:A:1365:ILE:HD12	1:A:1405:LEU:HG	1.91	0.51
1:B:1365:ILE:HD12	1:B:1405:LEU:HG	1.93	0.51
1:A:1019:LYS:O	1:A:1022:GLU:OE2	2.29	0.50
1:A:1022:GLU:CG	1:A:1023:ASN:N	2.71	0.50
1:B:1447:PHE:CZ	1:B:1454:GLU:HB2	2.47	0.50
1:A:1333:ARG:NH2	1:A:1394:GLU:O	2.26	0.50
1:B:1211:THR:HG22	1:B:1481:ILE:HD11	1.92	0.50
1:B:1287:HIS:CD2	1:B:1412:LEU:HD12	2.47	0.50
1:A:1450:GLU:N	1:A:1450:GLU:OE1	2.44	0.50
1:A:1237:GLN:NE2	1:A:1240:THR:HG22	2.27	0.50
1:B:1063:PHE:HE2	1:B:1196:VAL:HG12	1.75	0.50
1:B:1163:ARG:O	1:B:1163:ARG:HG2	2.12	0.50
1:B:1432:ASP:HB3	1:B:1436:ILE:HG12	1.94	0.50
1:A:1159:GLN:HE22	1:A:1512:TYR:HE2	1.58	0.50
1:B:1371:PRO:HA	1:B:1374:MET:HE2	1.94	0.50
1:B:1170:GLN:HE21	1:B:1275:LEU:N	2.10	0.49
1:A:1307:ILE:HD12	1:A:1366:ARG:HG3	1.93	0.49
1:B:1378:GLN:NE2	1:B:1391:THR:HB	2.25	0.49
1:B:1425:VAL:HG22	1:B:1426:VAL:H	1.77	0.49
1:A:1016:LEU:HD21	1:A:1290:ASN:O	2.12	0.49
1:A:1019:LYS:N	1:A:1022:GLU:OE1	2.45	0.49
1:A:1332:ARG:HA	1:A:1335:LEU:HD12	1.94	0.49
1:A:1067:GLU:HG3	1:A:1192:LEU:HD22	1.95	0.49
1:B:1406:GLU:O	1:B:1410:VAL:HG13	2.12	0.49
1:B:1414:THR:HA	1:B:1417:SER:HB2	1.94	0.49
1:B:1018:ALA:HB3	1:B:1027:TRP:HA	1.95	0.49
1:B:1100:GLU:HG2	1:B:1154:GLU:HA	1.94	0.49
1:B:1156:LYS:HG2	1:B:1157:HIS:H	1.77	0.49
1:B:1090[A]:GLU:CG	1:B:1251:MET:HB3	2.42	0.49
1:B:1343:ALA:HB1	1:B:1345:LEU:HD21	1.95	0.49
1:B:1382:VAL:HA	1:B:1388:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1444:GLN:OE1	1:B:1486:LEU:HB2	2.13	0.49
1:A:1119:ARG:NH2	1:A:1148:CYS:HB2	2.28	0.48
1:B:1324:ILE:HG23	1:B:1345:LEU:HD13	1.94	0.48
1:A:1203:ILE:HD11	1:A:1283:MET:HA	1.94	0.48
1:B:1067:GLU:HA	1:B:1070:LYS:HE3	1.94	0.48
1:B:1234:ARG:HB3	1:B:1511:SER:HA	1.95	0.48
1:A:1085:SER:O	1:A:1089:LYS:HB2	2.14	0.48
1:B:1019:LYS:HA	1:B:1290:ASN:OD1	2.14	0.48
1:A:1346:ARG:NH2	1:A:1353:TRP:CZ3	2.82	0.48
1:A:1378:GLN:NE2	1:A:1393:ALA:HA	2.29	0.48
1:B:1474:MET:HG3	1:B:1510:ARG:HH22	1.78	0.48
1:B:1490:GLN:OE1	1:B:1490:GLN:HA	2.13	0.48
1:A:1080:MET:HG2	1:A:1118:ILE:HG23	1.94	0.48
1:B:1082:VAL:CG2	1:B:1117:ALA:HB3	2.43	0.48
1:B:1372:ARG:HD2	1:B:1375:LYS:HD2	1.95	0.48
1:B:1447:PHE:HE2	1:B:1457:ILE:HD12	1.79	0.48
1:B:1056:ILE:HD12	1:B:1299:VAL:HG22	1.96	0.47
1:B:1479:LEU:HD21	1:B:1511:SER:HB2	1.95	0.47
1:B:1090[B]:GLU:CG	1:B:1251:MET:HB3	2.44	0.47
1:B:1193:TYR:O	1:B:1196:VAL:HG22	2.14	0.47
1:B:1355:PHE:CE1	1:B:1366:ARG:HD3	2.49	0.47
1:A:1203:ILE:HG12	1:A:1286:VAL:HG21	1.96	0.47
1:A:1346:ARG:NH2	1:A:1353:TRP:HZ3	2.11	0.47
1:B:1106:ARG:NE	6:B:1702:HOH:O	2.46	0.47
1:B:1090[B]:GLU:HB3	1:B:1251:MET:SD	2.55	0.47
1:B:1424:MET:HA	1:B:1442:ILE:O	2.15	0.47
1:A:1346:ARG:HH21	1:A:1353:TRP:HZ3	1.63	0.47
1:A:1425:VAL:HG22	1:A:1426:VAL:H	1.80	0.47
1:B:1197:TYR:OH	1:B:1279:THR:HG22	2.14	0.47
1:B:1235:ALA:HB3	1:B:1479:LEU:HD13	1.97	0.47
1:B:1405:LEU:O	1:B:1408:ILE:HG22	2.13	0.47
1:B:1236:ILE:HG21	1:B:1282:VAL:HG11	1.96	0.47
1:A:1330:TYR:OH	1:A:1379:PHE:HD2	1.98	0.46
1:B:1216:PHE:HB2	1:B:1242:HIS:CE1	2.51	0.46
1:B:1278:ARG:O	1:B:1282:VAL:HG13	2.16	0.46
1:A:1250:LYS:HB3	1:A:1250:LYS:HE2	1.62	0.46
1:B:1232:SER:HB2	1:B:1234:ARG:HE	1.79	0.46
1:A:1061:LYS:HA	1:A:1147:TRP:CH2	2.51	0.46
1:B:1365:ILE:HD13	1:B:1401:LEU:HD22	1.98	0.46
1:B:1423:HIS:CD2	1:B:1440:GLY:O	2.62	0.46
1:B:1449:GLY:HA2	1:B:1504:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:LEU:O	1:B:1287:HIS:HE1	1.99	0.46
1:B:1448:CYS:HB3	1:B:1450:GLU:OE1	2.16	0.46
1:B:1481:ILE:HD13	1:B:1504:TYR:CZ	2.50	0.46
1:B:1490:GLN:HB3	1:B:1491:PRO:HD2	1.97	0.46
1:A:1043:ILE:HD13	1:B:1081:PHE:HB3	1.98	0.46
1:A:1078:PHE:CD2	1:B:1048:ILE:HG12	2.51	0.46
1:B:1229:ILE:HG12	1:B:1234:ARG:O	2.16	0.46
1:B:1453:CYS:O	1:B:1457:ILE:HG13	2.16	0.46
1:A:1190:LEU:HD22	1:A:1223:THR:HG21	1.97	0.45
1:B:1248:PHE:HB2	1:B:1270:GLN:HE21	1.81	0.45
1:B:1355:PHE:CD1	1:B:1366:ARG:HD3	2.51	0.45
1:B:1424:MET:HE3	1:B:1486:LEU:HD11	1.98	0.45
1:B:1461:THR:HG21	1:B:1476:ALA:HB3	1.99	0.45
1:A:1024:LEU:CD2	1:A:1232:SER:HB3	2.47	0.45
1:A:1108:GLY:CA	1:B:1099:PRO:HA	2.45	0.45
1:B:1027:TRP:O	1:B:1031:VAL:HG23	2.16	0.45
1:B:1381:ALA:O	1:B:1389:LYS:HA	2.16	0.45
1:A:1337:VAL:HG12	1:A:1337:VAL:O	2.16	0.45
1:B:1229:ILE:HD11	1:B:1512:TYR:HE1	1.82	0.45
1:B:1458:LYS:HB2	1:B:1476:ALA:O	2.15	0.45
1:A:1373:ASP:O	1:A:1376:SER:HB3	2.17	0.45
1:B:1337:VAL:HG12	1:B:1337:VAL:O	2.17	0.45
1:A:1022:GLU:H	1:A:1022:GLU:HG2	1.40	0.45
1:A:1207:LYS:HG3	1:A:1225:ILE:HG22	1.99	0.45
1:A:1442:ILE:HD12	1:A:1507:LEU:HD21	1.98	0.44
1:B:1087:LEU:HG	1:B:1093:HIS:HE1	1.82	0.44
1:B:1436:ILE:HD13	1:B:1441:LYS:NZ	2.31	0.44
1:A:1436:ILE:HD11	1:A:1443:VAL:CG2	2.47	0.44
1:A:1201:LEU:HD11	1:A:1279:THR:OG1	2.18	0.44
1:A:1355:PHE:CE1	1:A:1366:ARG:HD3	2.52	0.44
1:B:1297:PRO:HG3	1:B:1408:ILE:CG2	2.47	0.44
1:A:1331:ARG:HG3	1:A:1341:VAL:HG13	2.00	0.44
1:B:1190:LEU:HD22	1:B:1223:THR:HG22	1.99	0.44
1:B:1383:ARG:HH11	1:B:1404:ILE:HG23	1.82	0.44
1:A:1163:ARG:NH2	1:A:1512:TYR:OXT	2.49	0.44
1:B:1190:LEU:HD13	1:B:1223:THR:HG22	1.99	0.44
1:B:1334:LEU:HD21	1:B:1401:LEU:CD1	2.48	0.44
1:B:1401:LEU:HD23	1:B:1401:LEU:HA	1.74	0.44
1:B:1447:PHE:HZ	1:B:1454:GLU:HB2	1.82	0.44
1:A:1378:GLN:OE1	1:A:1393:ALA:HA	2.18	0.44
1:A:1392:VAL:HG21	1:A:1400:LYS:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1491:PRO:O	6:B:1703:HOH:O	2.20	0.44
1:A:1176:PHE:N	1:A:1269:TYR:O	2.45	0.43
1:A:1303:GLN:NE2	1:A:1340:ARG:H	2.14	0.43
1:B:1323:LEU:HD13	1:B:1374:MET:SD	2.58	0.43
1:B:1447:PHE:CE2	1:B:1457:ILE:HD12	2.53	0.43
1:B:1507:LEU:HD12	1:B:1507:LEU:HA	1.90	0.43
1:A:1169:TRP:CB	1:A:1276:THR:HG22	2.47	0.43
1:A:1489:LEU:HD11	1:A:1502:ALA:HB3	2.00	0.43
1:B:1458:LYS:O	1:B:1461:THR:OG1	2.36	0.43
1:A:1171:GLU:HG3	1:A:1173:HIS:CD2	2.53	0.43
1:B:1061:LYS:O	1:B:1065:ASP:HB2	2.18	0.43
1:B:1244:LEU:HD13	1:B:1248:PHE:CD1	2.53	0.43
1:A:1067:GLU:HB3	1:A:1192:LEU:HD13	2.00	0.43
1:A:1119:ARG:HH21	1:A:1148:CYS:HB2	1.84	0.43
1:B:1163:ARG:NH1	1:B:1512:TYR:CD2	2.84	0.43
1:B:1174:SER:HB2	1:B:1176:PHE:CE1	2.53	0.43
1:A:1056:ILE:HG23	1:A:1299:VAL:CG1	2.49	0.43
1:A:1190:LEU:CD2	1:A:1207:LYS:HG2	2.48	0.43
1:A:1334:LEU:HD11	1:A:1341:VAL:HG21	2.01	0.43
1:B:1064:PHE:O	1:B:1068:ILE:HG12	2.19	0.43
1:B:1090[A]:GLU:HB3	1:B:1251:MET:SD	2.58	0.43
1:B:1232:SER:CB	1:B:1234:ARG:HE	2.31	0.43
1:B:1355:PHE:HE1	1:B:1368:GLU:HG2	1.82	0.43
1:A:1050:ARG:NH1	6:A:1714:HOH:O	2.52	0.42
1:A:1192:LEU:O	1:A:1195:GLN:HB2	2.18	0.42
1:A:1367:LEU:HD12	1:A:1401:LEU:HD11	2.00	0.42
1:B:1056:ILE:HG23	1:B:1299:VAL:HG21	2.00	0.42
1:B:1357:HIS:O	1:B:1361:LYS:HG3	2.19	0.42
1:B:1196:VAL:O	1:B:1200:LEU:HB2	2.20	0.42
1:A:1169:TRP:CD1	1:A:1169:TRP:C	2.93	0.42
1:B:1038:ILE:HA	1:B:1048:ILE:O	2.19	0.42
1:A:1024:LEU:HD21	1:A:1285:MET:CE	2.50	0.42
1:A:1105:THR:HG23	1:A:1111:GLU:OE2	2.18	0.42
1:A:1331:ARG:O	1:A:1334:LEU:HD12	2.18	0.42
1:B:1078:PHE:HD2	1:B:1125:VAL:HG12	1.84	0.42
1:B:1137:HIS:HB3	1:B:1256:PHE:CD2	2.54	0.42
1:A:1081:PHE:HB3	1:A:1116:ILE:CG2	2.49	0.42
1:A:1479:LEU:HD12	1:A:1507:LEU:CD2	2.49	0.42
1:B:1215:LYS:HB2	1:B:1222:THR:HG23	2.02	0.42
1:B:1279:THR:O	1:B:1282:VAL:HG22	2.20	0.42
1:A:1206:VAL:HG22	1:A:1226:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:ALA:HB1	1:A:1345:LEU:HD21	2.01	0.42
1:B:1162:LEU:HD23	1:B:1162:LEU:HA	1.80	0.42
1:B:1291:MET:HE2	1:B:1291:MET:HB3	1.85	0.42
1:A:1103:TRP:HB2	1:B:1106:ARG:HG3	2.02	0.41
1:A:1407:ASP:HA	1:A:1410:VAL:HG22	2.02	0.41
1:A:1495:CYS:SG	1:A:1496:VAL:N	2.93	0.41
1:B:1103:TRP:CZ3	1:B:1117:ALA:HB2	2.54	0.41
1:B:1169:TRP:CZ2	1:B:1171:GLU:HG3	2.54	0.41
1:B:1333:ARG:O	1:B:1336:SER:OG	2.38	0.41
1:B:1474:MET:C	1:B:1510:ARG:HH22	2.24	0.41
1:A:1171:GLU:HG3	1:A:1173:HIS:NE2	2.35	0.41
1:A:1166:GLU:OE2	1:B:1080:MET:HE2	2.21	0.41
1:A:1296:PRO:HB3	1:A:1409:GLN:OE1	2.21	0.41
1:A:1370:GLY:O	1:A:1374:MET:N	2.53	0.41
1:A:1171:GLU:HG3	1:A:1173:HIS:HE2	1.85	0.41
1:A:1383:ARG:HH22	1:A:1407:ASP:HB3	1.86	0.41
1:A:1477:LYS:NZ	1:A:1511:SER:H	2.19	0.41
1:B:1284:THR:HG23	1:B:1293:LEU:HD21	2.02	0.41
1:B:1291:MET:O	1:B:1291:MET:HG2	2.21	0.41
1:B:1068:ILE:O	1:B:1073:VAL:HG22	2.20	0.41
1:B:1096:ASP:O	1:B:1099:PRO:HD2	2.21	0.41
1:B:1236:ILE:HG21	1:B:1282:VAL:CG1	2.51	0.41
1:A:1436:ILE:HD11	1:A:1443:VAL:HG21	2.03	0.41
1:B:1172:GLY:O	1:B:1272:SER:HA	2.20	0.41
1:B:1289:ASP:OD2	1:B:1384:ARG:NH1	2.33	0.41
1:B:1291:MET:HE1	1:B:1359:GLU:CD	2.41	0.41
1:A:1344:ASP:OD1	1:A:1354:LYS:HE2	2.21	0.41
1:B:1192:LEU:O	1:B:1195:GLN:HB2	2.20	0.41
1:B:1382:VAL:HG22	1:B:1389:LYS:HG3	2.03	0.41
1:A:1253:GLU:HA	1:A:1253:GLU:OE1	2.21	0.40
1:B:1122:SER:N	1:B:1171:GLU:OE2	2.49	0.40
1:B:1323:LEU:HD11	1:B:1369:VAL:HG13	2.04	0.40
1:A:1093:HIS:HB2	1:A:1097:PHE:CD2	2.48	0.40
1:A:1234:ARG:HB3	1:A:1511:SER:HA	2.03	0.40
1:A:1331:ARG:HG3	1:A:1341:VAL:CG1	2.51	0.40
1:A:1401:LEU:HA	1:A:1404:ILE:HD12	2.03	0.40
1:A:1425:VAL:HG22	1:A:1426:VAL:N	2.36	0.40
1:B:1019:LYS:O	1:B:1022:GLU:HB2	2.20	0.40
1:B:1356:ASN:CG	1:B:1360:LEU:HD11	2.41	0.40
1:A:1432:ASP:O	1:A:1436:ILE:HG23	2.22	0.40
1:B:1236:ILE:HD11	1:B:1278:ARG:HH12	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1242:HIS:CD2	1:B:1242:HIS:N	2.90	0.40
1:B:1457:ILE:O	1:B:1461:THR:HG23	2.22	0.40
1:B:1461:THR:HG21	1:B:1476:ALA:CB	2.51	0.40
1:B:1078:PHE:O	1:B:1119:ARG:NH2	2.55	0.40
1:B:1424:MET:CE	1:B:1486:LEU:HD11	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:LYS:O	1:B:1490:GLN:NE2[2_857]	2.08	0.12

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	474/498 (95%)	465 (98%)	8 (2%)	1 (0%)	47 68
1	B	478/498 (96%)	468 (98%)	10 (2%)	0	100 100
All	All	952/996 (96%)	933 (98%)	18 (2%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1316	SER

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	417/428 (97%)	400 (96%)	17 (4%)	30	55
1	B	416/428 (97%)	396 (95%)	20 (5%)	25	48
All	All	833/856 (97%)	796 (96%)	37 (4%)	28	52

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1026	ASP
1	A	1044	SER
1	A	1114	GLU
1	A	1169	TRP
1	A	1171	GLU
1	A	1209	ARG
1	A	1273	TRP
1	A	1334	LEU
1	A	1390	LEU
1	A	1407	ASP
1	A	1417	SER
1	A	1437	LEU
1	A	1438	ASP
1	A	1463	ARG
1	A	1489	LEU
1	A	1504	TYR
1	A	1506	THR
1	B	1042	ASP
1	B	1062	ASP
1	B	1065	ASP
1	B	1092	THR
1	B	1114	GLU
1	B	1153	TRP
1	B	1156	LYS
1	B	1163	ARG
1	B	1165	ARG
1	B	1169	TRP
1	B	1200	LEU
1	B	1215	LYS
1	B	1332	ARG
1	B	1373	ASP
1	B	1389	LYS
1	B	1409	GLN

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Mol	Chain	Res	Type
1	B	1415	ARG
1	B	1483	PHE
1	B	1494	LYS
1	B	1504	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1170	GLN
1	A	1237	GLN
1	A	1303	GLN
1	A	1409	GLN
1	B	1170	GLN
1	B	1287	HIS
1	B	1290	ASN
1	B	1378	GLN

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	F9O	A	1602	-	22,23,23	0.70	1 (4%)	20,32,32	1.98	2 (10%)
4	ATP	A	1603	5	26,33,33	0.60	0	31,52,52	0.92	2 (6%)
3	F9O	B	1602	-	22,23,23	0.73	0	20,32,32	0.91	1 (5%)

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	F9O	A	1602	-	-	2/6/17/17	0/3/3/3
4	ATP	A	1603	5	-	5/18/38/38	0/3/3/3
3	F9O	B	1602	-	-	3/6/17/17	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1602	F9O	C14-C9	-2.05	1.39	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1602	F9O	C3-N-C4	8.16	116.71	111.62
4	A	1603	ATP	C3'-C2'-C1'	2.59	104.88	100.98
3	B	1602	F9O	C5-C6-C7	-2.44	105.90	113.26
4	A	1603	ATP	C5-C6-N6	2.31	123.86	120.35
3	A	1602	F9O	C6-C5-C4	2.26	118.55	113.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1602	F9O	N-C4-C5-C6
3	B	1602	F9O	C-C4-C5-C6
4	A	1603	ATP	C5'-O5'-PA-O2A
3	A	1602	F9O	C5-C6-C7-N1
3	B	1602	F9O	C5-C6-C7-N1
4	A	1603	ATP	O4'-C4'-C5'-O5'
4	A	1603	ATP	C5'-O5'-PA-O1A
3	A	1602	F9O	C-C4-C5-C6

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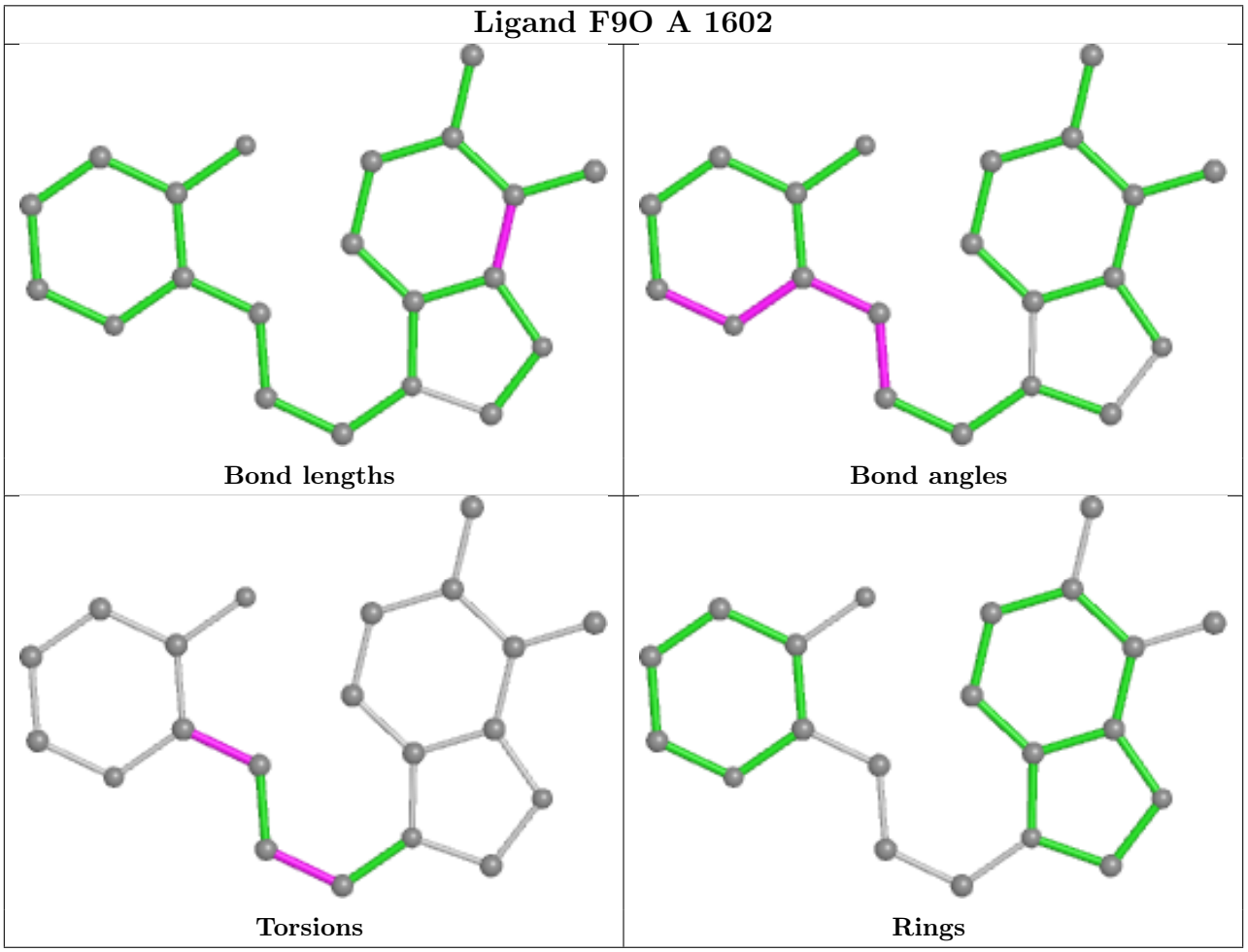
Mol	Chain	Res	Type	Atoms
4	A	1603	ATP	C3'-C4'-C5'-O5'
4	A	1603	ATP	C5'-O5'-PA-O3A

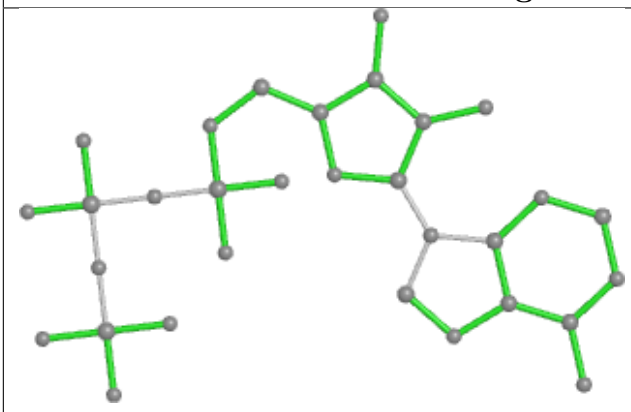
There are no ring outliers.

No monomer is involved in short contacts.

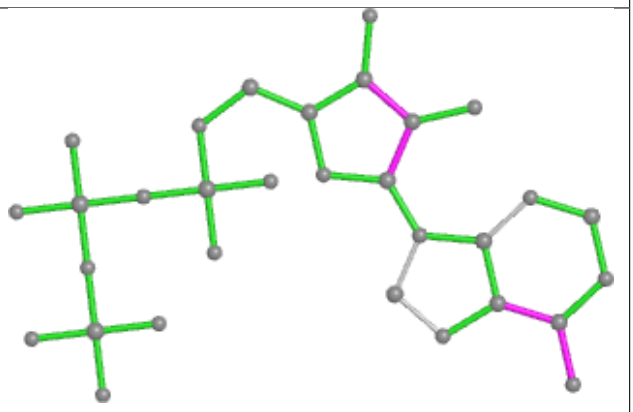
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



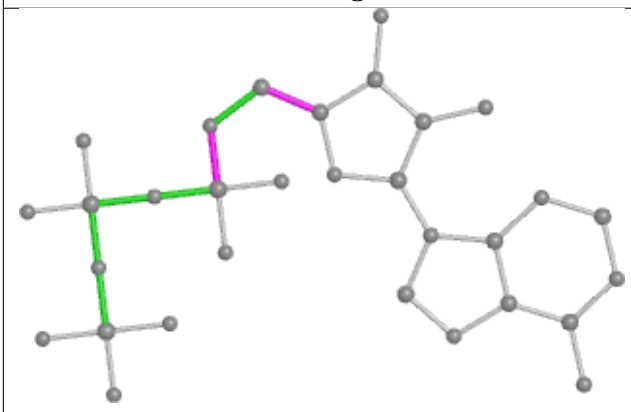
Ligand ATP A 1603



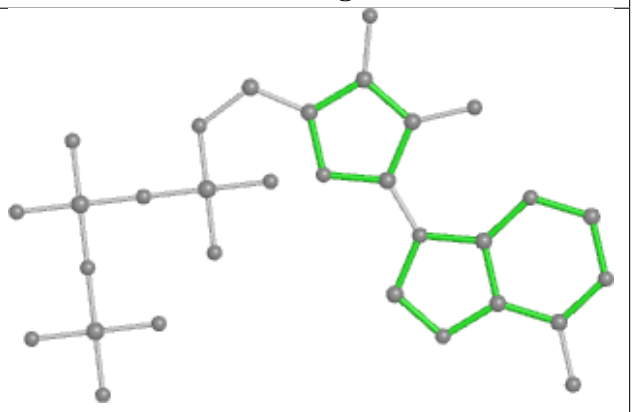
Bond lengths



Bond angles

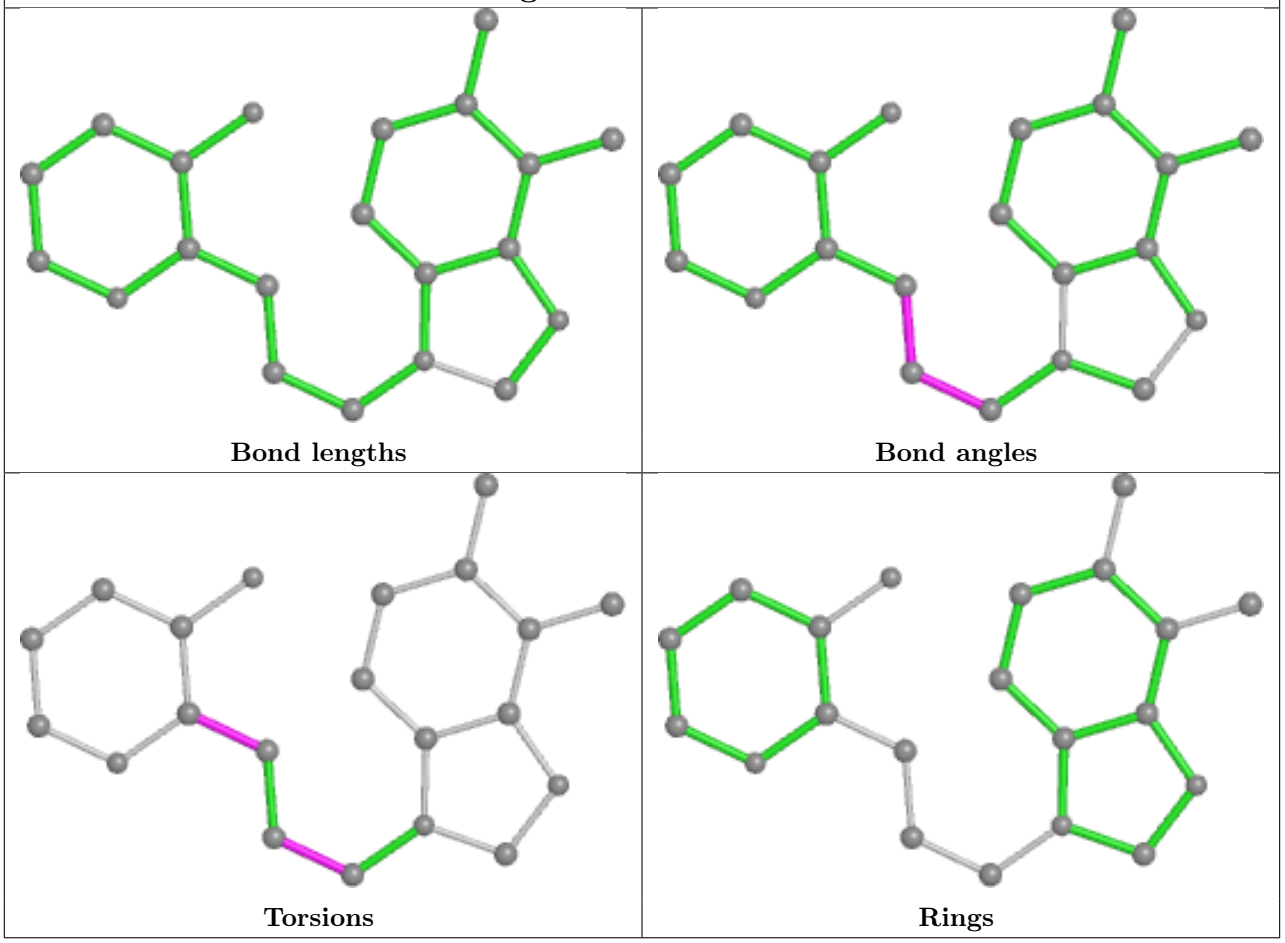


Torsions



Rings

Ligand F9O B 1602



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	482/498 (96%)	0.47	33 (6%) 17 17	34, 70, 108, 132	0
1	B	483/498 (96%)	0.87	73 (15%) 2 1	32, 80, 124, 138	0
All	All	965/996 (96%)	0.67	106 (10%) 5 5	32, 75, 120, 138	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1155	PHE	8.0
1	B	1091	LYS	7.0
1	A	1311	ILE	6.3
1	B	1092	THR	5.4
1	B	1316	SER	5.3
1	B	1440	GLY	5.3
1	A	1392	VAL	5.2
1	B	1094	VAL	5.0
1	B	1372	ARG	4.9
1	A	1497	CYS	4.8
1	B	1375	LYS	4.8
1	B	1397	ALA	4.7
1	B	1396	GLU	4.6
1	B	1461	THR	4.4
1	B	1378	GLN	4.4
1	B	1486	LEU	4.3
1	B	1023	ASN	4.3
1	B	1475	GLY	4.3
1	B	1017	GLU	4.1
1	B	1395	ASN	4.1
1	B	1474	MET	4.0
1	B	1502	ALA	4.0
1	A	1456	TRP	3.8
1	A	1310	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1372	ARG	3.7
1	B	1427	ALA	3.5
1	B	1098	ALA	3.5
1	A	1317	GLU	3.5
1	B	1392	VAL	3.5
1	B	1499	LYS	3.5
1	B	1429	THR	3.5
1	A	1463	ARG	3.5
1	A	1315	LEU	3.4
1	B	1454	GLU	3.4
1	A	1322	ALA	3.3
1	A	1019	LYS	3.2
1	B	1401	LEU	3.2
1	B	1379	PHE	3.1
1	B	1441	LYS	3.1
1	B	1090[A]	GLU	3.1
1	B	1318	GLU	3.1
1	B	1024	LEU	3.0
1	B	1425	VAL	3.0
1	B	1374	MET	2.9
1	B	1319	ASP	2.9
1	B	1323	LEU	2.9
1	A	1319	ASP	2.9
1	B	1498	GLY	2.9
1	A	1320	LYS	2.9
1	B	1512	TYR	2.9
1	B	1458	LYS	2.8
1	B	1376	SER	2.8
1	B	1276	THR	2.8
1	A	1224	THR	2.8
1	B	1222	THR	2.8
1	B	1462	ALA	2.8
1	A	1212	GLU	2.7
1	A	1321	GLU	2.7
1	B	1428	ASN	2.7
1	B	1492	GLY	2.7
1	B	1224	THR	2.6
1	B	1491	PRO	2.6
1	B	1503	LYS	2.6
1	A	1455	ASP	2.6
1	B	1089	LYS	2.6
1	A	1018	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1279	THR	2.5
1	A	1453	CYS	2.5
1	B	1135	GLN	2.5
1	A	1348	ASN	2.5
1	B	1283	MET	2.5
1	B	1436	ILE	2.4
1	B	1420	LEU	2.4
1	B	1237	GLN	2.4
1	B	1479	LEU	2.4
1	B	1431	GLU	2.4
1	B	1240	THR	2.4
1	B	1490	GLN	2.3
1	A	1347	ASP	2.3
1	A	1502	ALA	2.3
1	B	1099	PRO	2.3
1	B	1382	VAL	2.3
1	A	1338	ASN	2.3
1	A	1373	ASP	2.3
1	A	1238	GLY	2.3
1	A	1155	PHE	2.3
1	B	1223	THR	2.3
1	B	1018	ALA	2.2
1	B	1239	GLY	2.2
1	B	1448	CYS	2.2
1	B	1398	GLU	2.2
1	A	1413	PHE	2.2
1	B	1227	ALA	2.2
1	B	1460	THR	2.1
1	B	1390	LEU	2.1
1	A	1500	ASN	2.1
1	A	1237	GLN	2.1
1	B	1225	ILE	2.1
1	A	1263	GLY	2.1
1	B	1277	THR	2.1
1	B	1233	GLY	2.1
1	A	1375	LYS	2.1
1	B	1200	LEU	2.0
1	B	1450	GLU	2.0
1	A	1089	LYS	2.0
1	A	1279	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 monosaccharides in this entry.

6.4 Ligands (i)

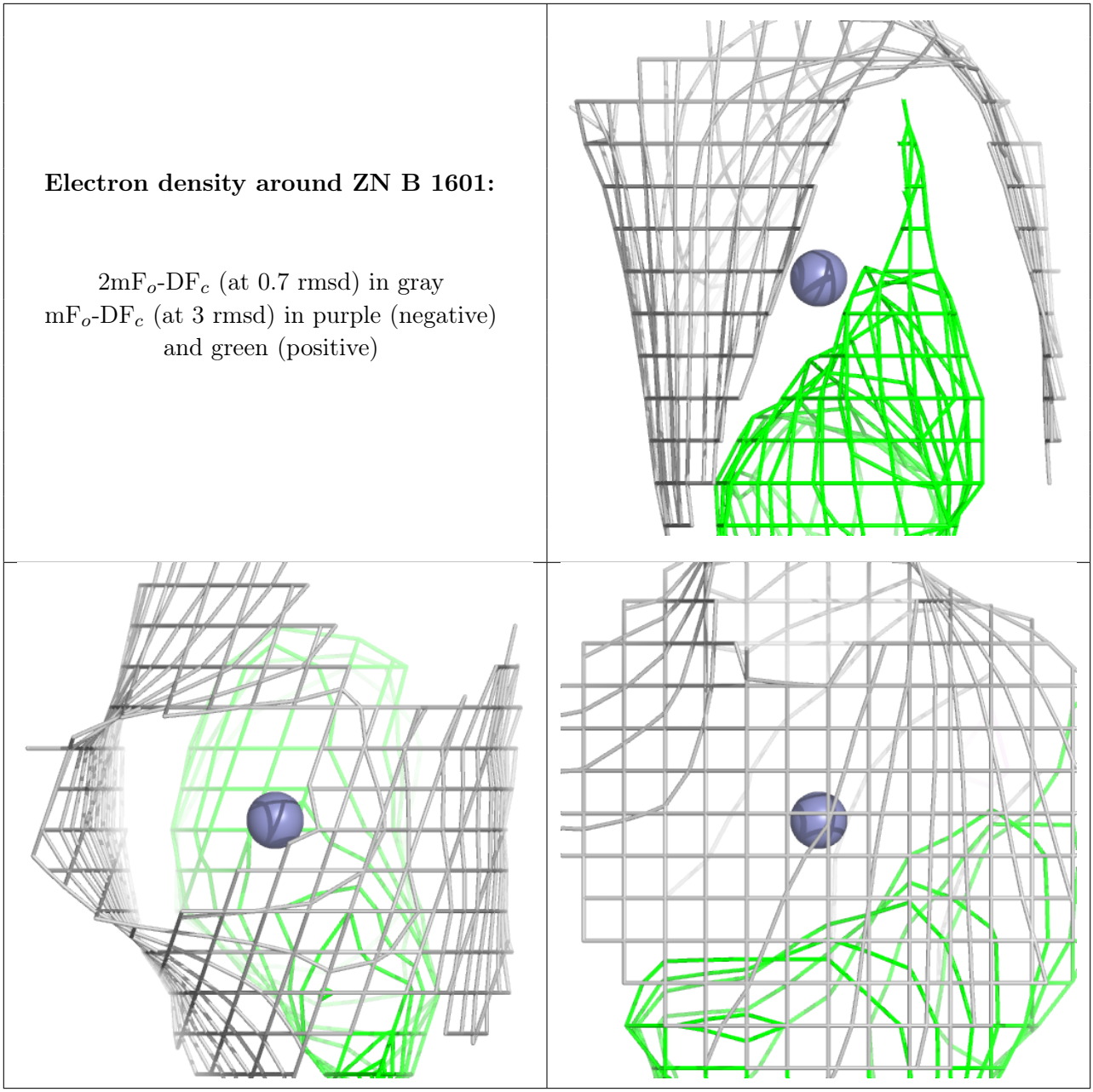
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ZN	B	1601	1/1	0.03	0.12	139,139,139,139	0
2	ZN	A	1601	1/1	0.86	0.08	116,116,116,116	0
5	MG	A	1605	1/1	0.88	0.81	86,86,86,86	0
3	F9O	B	1602	21/21	0.91	0.19	41,61,89,102	2
3	F9O	A	1602	21/21	0.91	0.21	35,63,89,108	0
4	ATP	A	1603	31/31	0.93	0.24	49,68,113,171	0
5	MG	A	1604	1/1	0.99	0.40	52,52,52,52	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.

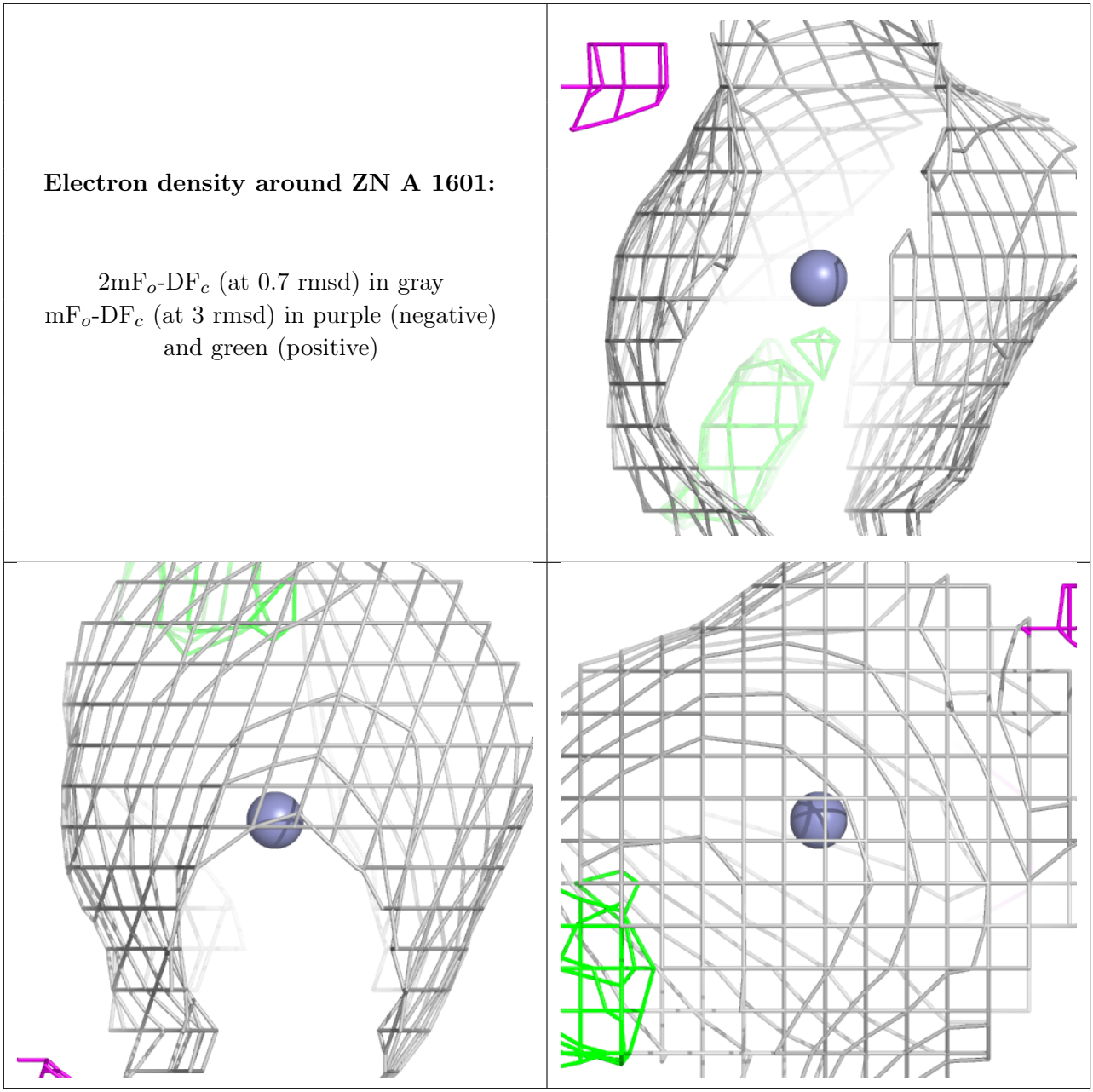
Electron density around ZN B 1601:

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



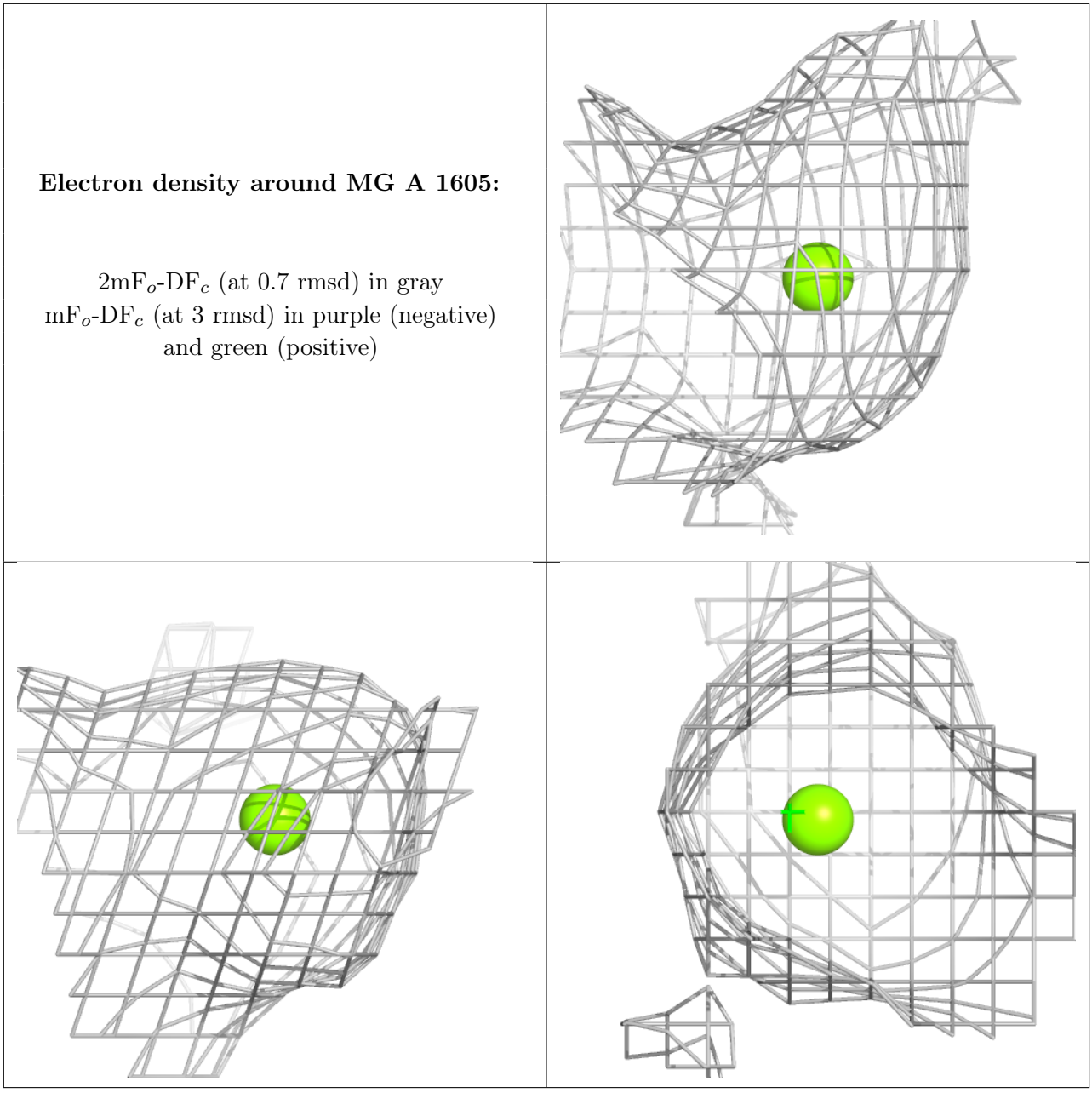
Electron density around ZN A 1601:

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



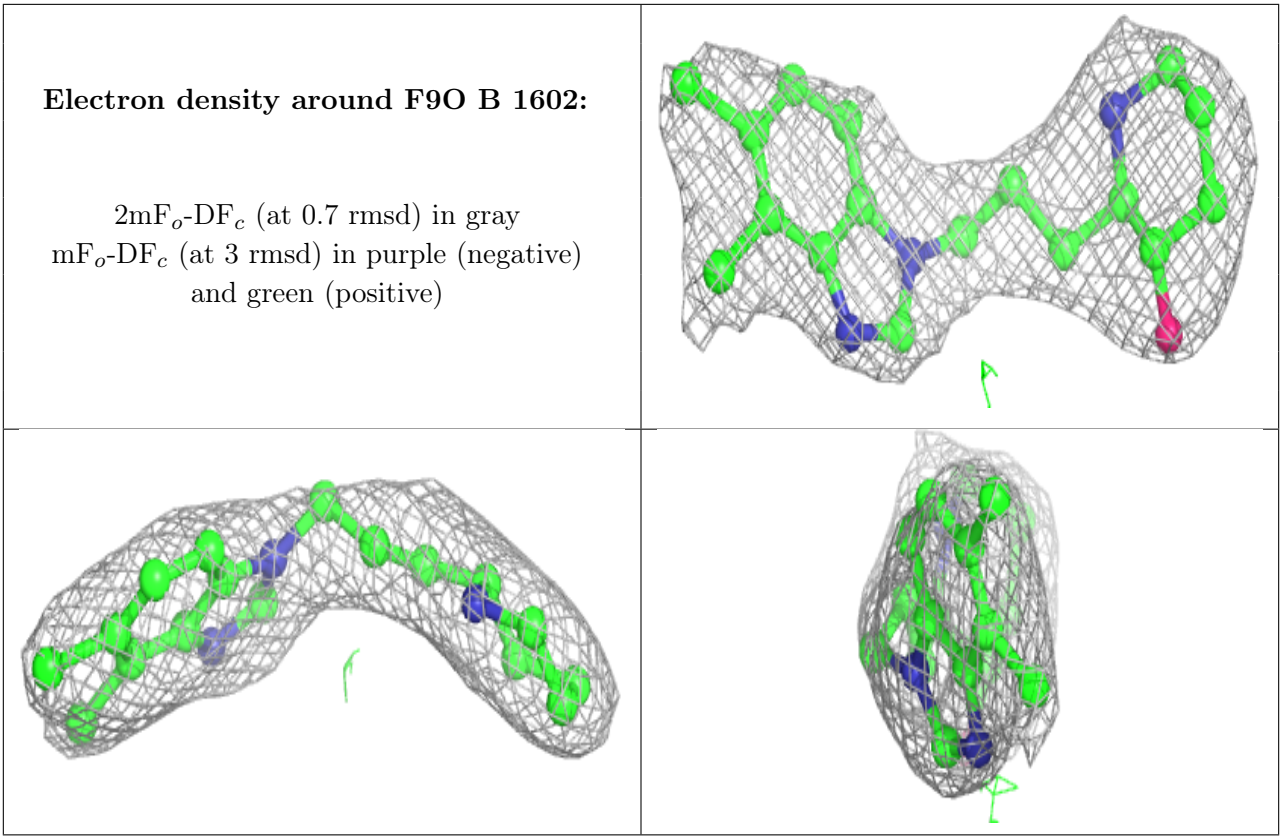
Electron density around MG A 1605:

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



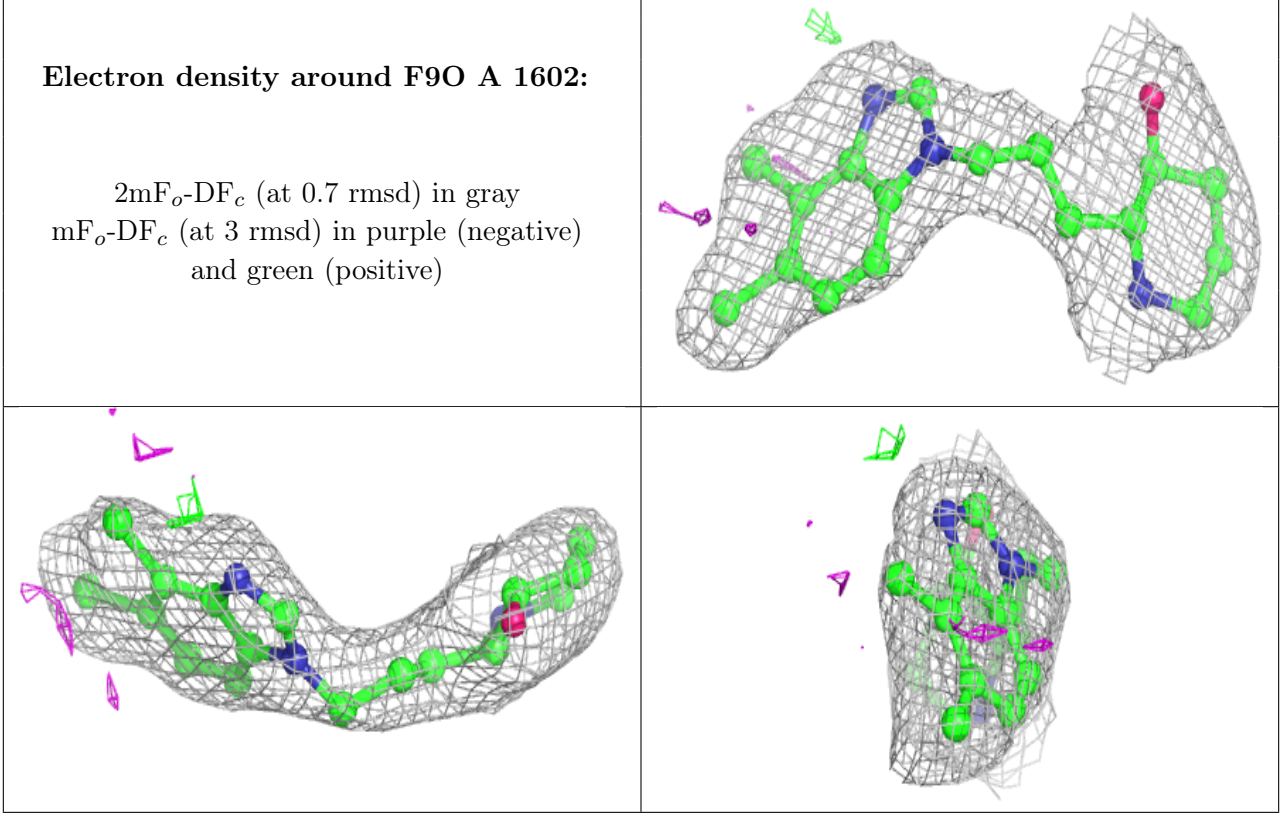
Electron density around F9O B 1602:

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



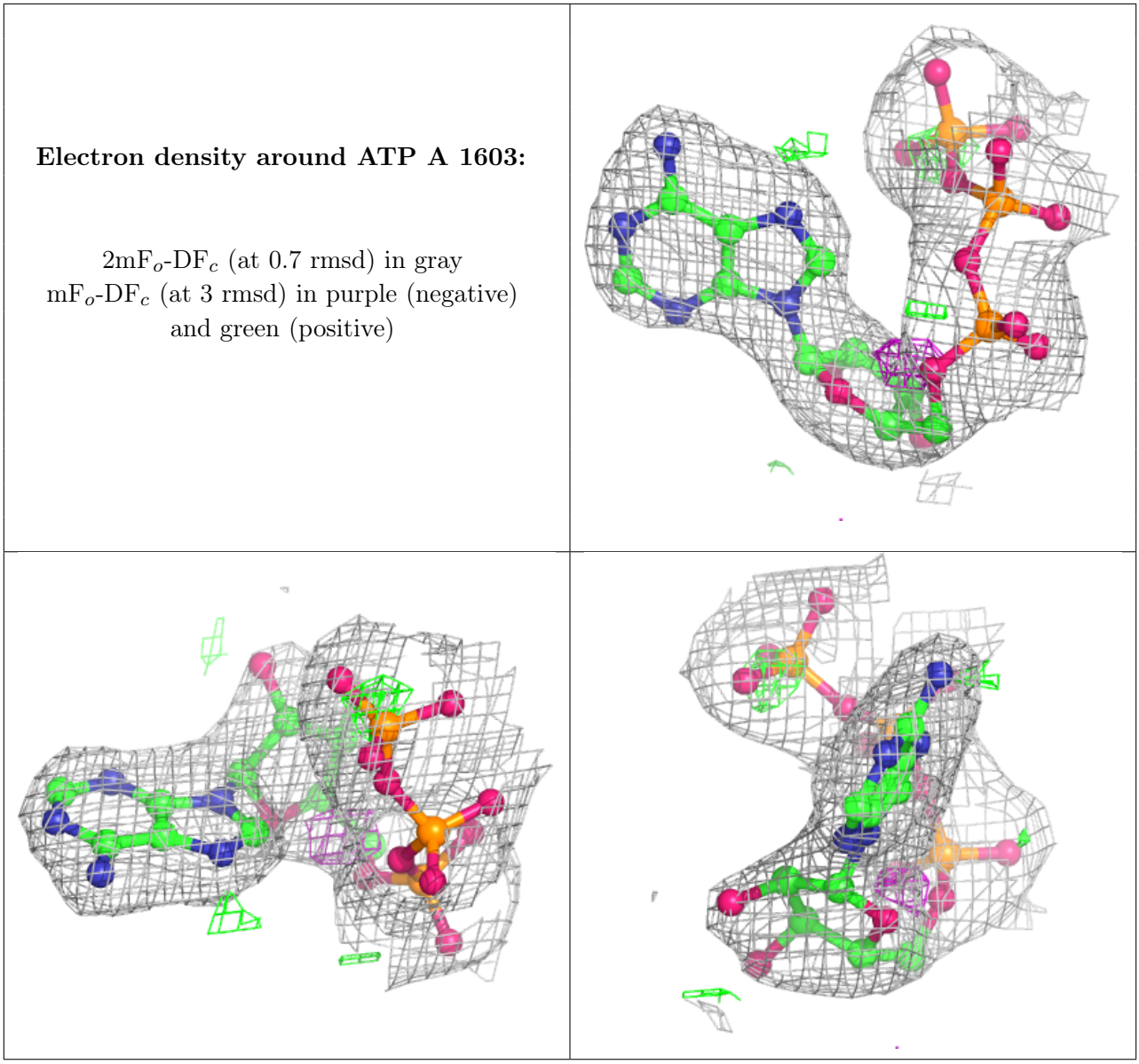
Electron density around F9O A 1602:

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



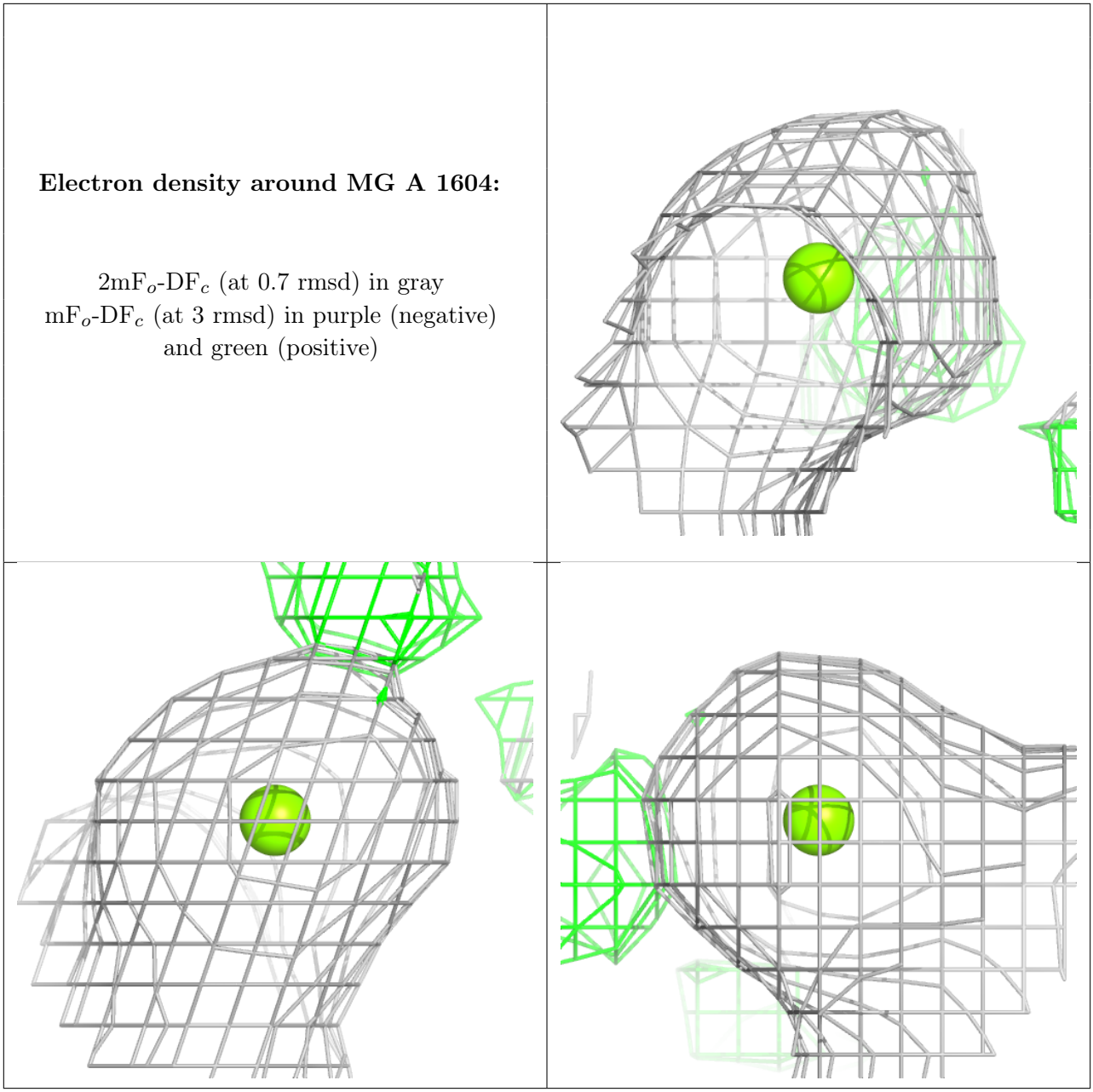
Electron density around ATP A 1603:

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



Electron density around MG A 1604:

$2mF_o$-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.