



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:36 PM UTC

PDB ID : 7OT3 / pdb_00007ot3
Title : Human Prolyl-tRNA Synthetase in Complex with L-proline and Compound 3b
Authors : Pang, L.; Zitko, J.; Strelkov, S.V.; Weeks, S.D.
Deposited on : 2021-06-09
Resolution : 2.53 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

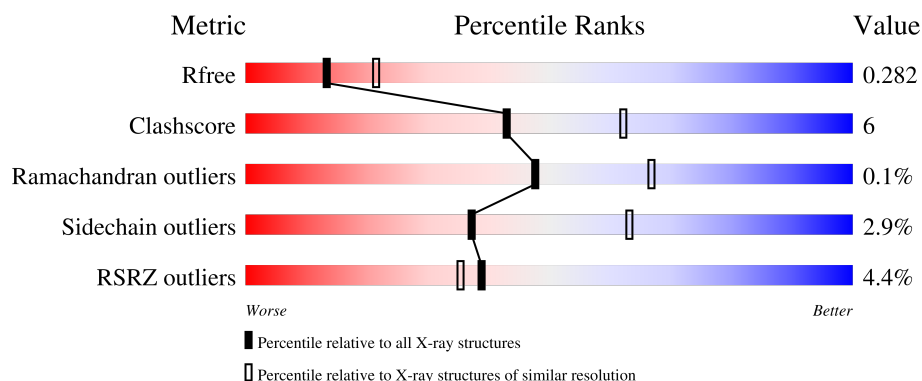
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 $\leq 5\%$. 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	512	 4% 81% 15% ..
1	B	512	 5% 77% 17% • 6%

2 Entry composition [i](#)

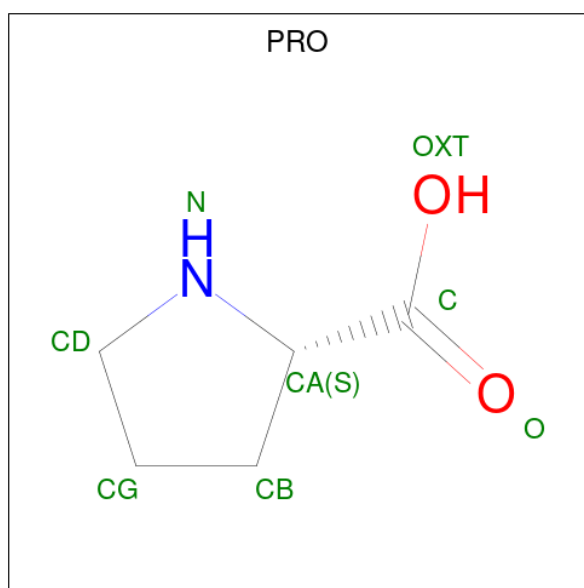
There are 6 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

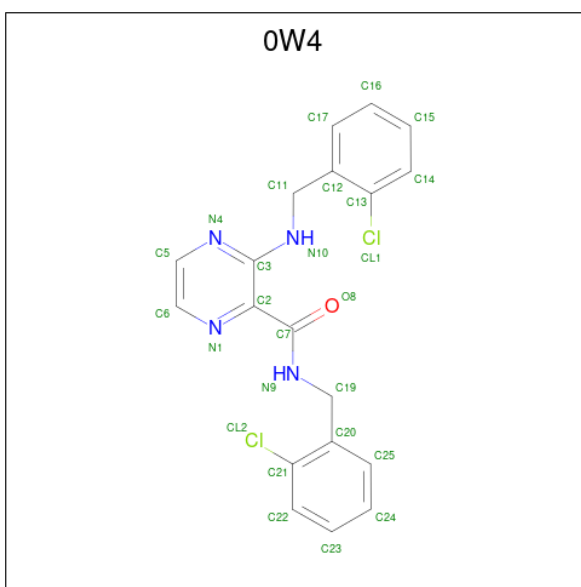
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3802	2434	641	702	25			
1	B	483	Total	C	N	O	S	0	0	0
			3679	2358	621	678	22			

- Molecule 2 is PROLINE (CCD ID: PRO) (formula: C₅H₉NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 3 is {N}-[(2-chlorophenyl)methyl]-3-[(2-chlorophenyl)methylamino]pyrazine-2-carboxamide (CCD ID: 0W4) (formula: C₁₉H₁₆Cl₂N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			26	19	2	4	1		
3	B	1	Total	C	Cl	N	O	0	0
			26	19	2	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Sr	0	0
			3	3		
5	B	1	Total	Sr	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		

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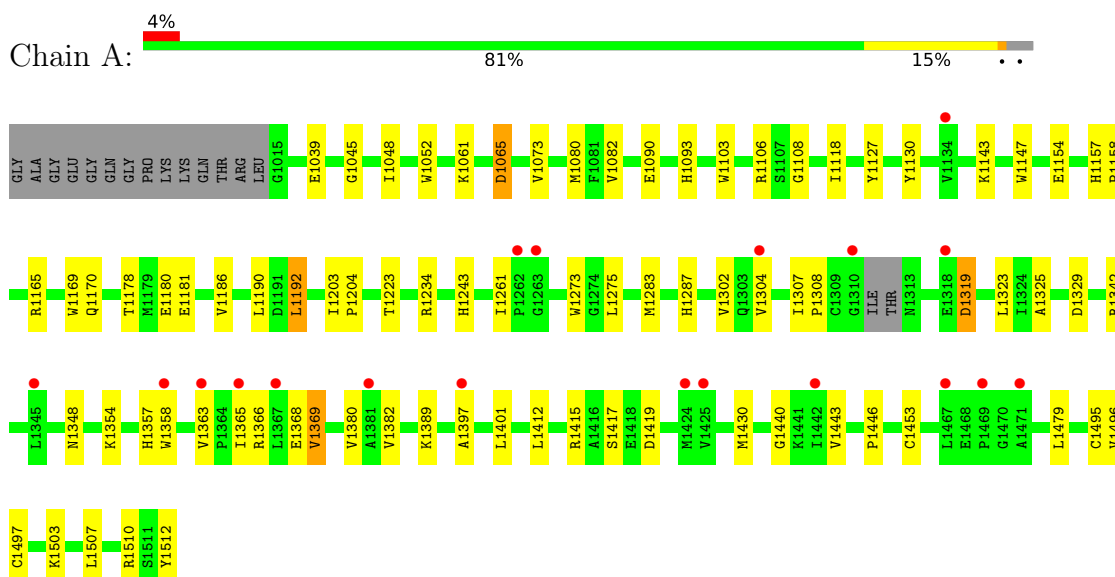
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	10	Total	O	0	0
			10	10		

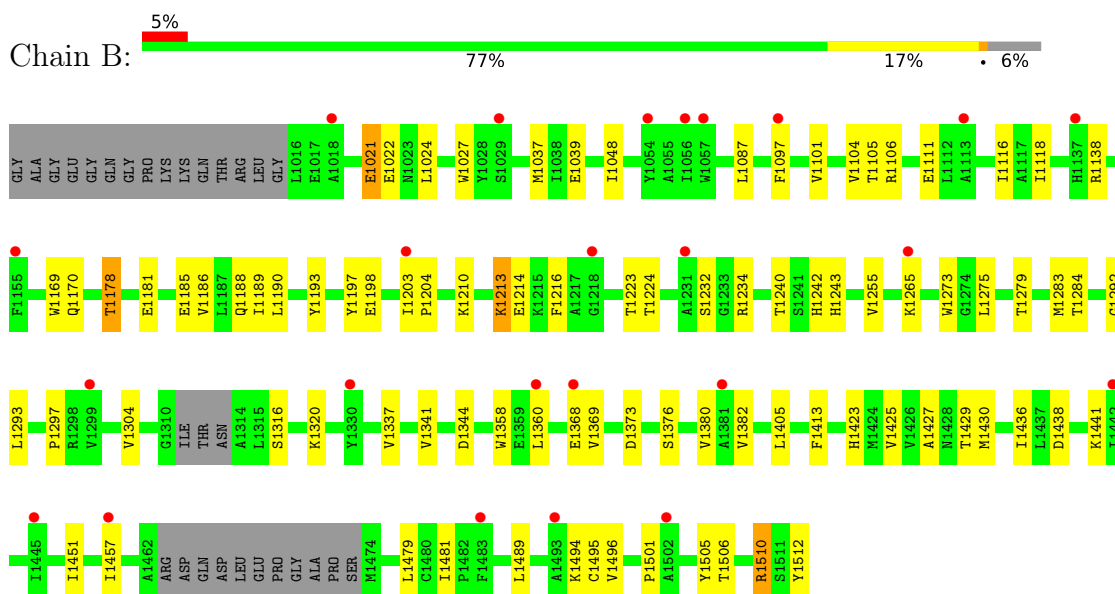
3 Residue-property plots

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.87Å 92.42Å 87.26Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	54.77 – 2.53 54.77 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.77-2.53) 99.1 (54.77-2.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.218 , 0.276 0.223 , 0.282	Depositor DCC
R_{free} test set	1888 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0W4, SR, ZN

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	0.09	0/3897	0.28	0/5309
1	B	0.08	0/3770	0.27	0/5141
All	All	0.08	0/7667	0.27	0/10450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3802	0	3588	45	0
1	B	3679	0	3448	47	0
2	A	8	0	7	0	0
2	B	8	0	7	0	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	0	0
All	All	7581	0	7050	90	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 6.

All (90) 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:B:1255:VAL:HG11	1:B:1265:LYS:HE3	1.61	0.79
1:A:1368:GLU:HB2	1:A:1380:VAL:HB	1.70	0.73
1:B:1234:ARG:HH21	1:B:1512:TYR:HA	1.55	0.71
1:B:1178:THR:HG23	1:B:1181:GLU:HB2	1.74	0.69
1:B:1427:ALA:HB2	1:B:1436:ILE:HD11	1.77	0.67
1:A:1382:VAL:HG22	1:A:1389:LYS:HG2	1.80	0.63
1:A:1302:VAL:HG11	1:A:1342:ARG:HB2	1.80	0.63
1:A:1103:TRP:HB2	1:B:1106:ARG:HG3	1.80	0.63
1:A:1319:ASP:OD1	1:A:1319:ASP:N	2.31	0.63
1:B:1495:CYS:SG	1:B:1496:VAL:N	2.72	0.63
1:B:1430:MET:HE1	1:B:1457:ILE:HG13	1.81	0.62
1:B:1481:ILE:HG12	1:B:1506:THR:HG22	1.84	0.58
1:A:1479:LEU:HD12	1:A:1507:LEU:HD22	1.84	0.58
1:B:1104:VAL:N	1:B:1116:ILE:O	2.35	0.58
1:A:1080:MET:HE2	1:A:1118:ILE:HG23	1.86	0.57
1:A:1154:GLU:O	1:A:1165:ARG:NH2	2.39	0.56
1:A:1204:PRO:HG3	1:A:1417:SER:HA	1.90	0.54
1:B:1292:GLY:HA3	1:B:1360:LEU:HA	1.90	0.54
1:B:1024:LEU:HA	1:B:1027:TRP:HB3	1.89	0.54
1:A:1170:GLN:HE21	1:A:1275:LEU:HB3	1.73	0.54
1:B:1344:ASP:OD2	1:B:1358:TRP:NE1	2.40	0.54
1:A:1190:LEU:HD22	1:A:1223:THR:HB	1.89	0.52
1:A:1090:GLU:HB3	1:A:1093:HIS:HB3	1.90	0.52
1:B:1284:THR:HG22	1:B:1293:LEU:HD11	1.91	0.52
1:A:1073:VAL:HG22	1:A:1143:LYS:HB3	1.90	0.52
1:A:1234:ARG:HH21	1:A:1512:TYR:HA	1.74	0.52
1:A:1366:ARG:HH21	1:A:1382:VAL:HG21	1.75	0.52
1:A:1430:MET:HG2	1:A:1496:VAL:HG12	1.93	0.50
1:B:1203:ILE:HD11	1:B:1283:MET:HA	1.93	0.50
1:B:1438:ASP:HA	1:B:1510:ARG:HH22	1.76	0.50
1:B:1489:LEU:HD13	1:B:1505:TYR:HE1	1.77	0.50
1:B:1316:SER:O	1:B:1320:LYS:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:GLY:HA2	1:A:1510:ARG:HH22	1.78	0.49
1:A:1118:ILE:HD11	1:B:1118:ILE:HD11	1.94	0.49
1:B:1429:THR:OG1	1:B:1430:MET:N	2.45	0.48
1:A:1354:LYS:HA	1:A:1357:HIS:HB3	1.95	0.48
1:A:1397:ALA:HA	1:A:1401:LEU:HD13	1.95	0.48
1:B:1024:LEU:HD11	1:B:1232:SER:HB2	1.96	0.48
1:A:1106:ARG:NH1	1:A:1108:GLY:O	2.48	0.47
1:B:1297:PRO:HB3	1:B:1405:LEU:HD22	1.97	0.47
1:A:1495:CYS:SG	1:A:1496:VAL:N	2.89	0.46
1:B:1198:GLU:HG2	1:B:1204:PRO:HA	1.96	0.46
1:A:1045:GLY:HA3	1:A:1165:ARG:HG3	1.98	0.45
1:A:1061:LYS:O	1:A:1065:ASP:HB2	2.17	0.45
1:B:1189:ILE:HG21	1:B:1273:TRP:CG	2.51	0.45
1:A:1052:TRP:HH2	1:A:1302:VAL:HG22	1.80	0.45
1:A:1415:ARG:NH1	1:A:1419:ASP:OD1	2.50	0.45
1:B:1193:TYR:HH	1:B:1273:TRP:HE3	1.65	0.45
1:A:1453:CYS:SG	1:A:1497:CYS:HB3	2.57	0.44
1:B:1368:GLU:HB2	1:B:1380:VAL:HG23	1.99	0.44
1:A:1308:PRO:HA	1:A:1369:VAL:HG23	1.98	0.44
1:A:1169:TRP:C	1:A:1169:TRP:CD1	2.96	0.44
1:B:1185:GLU:HA	1:B:1188:GLN:HG2	1.99	0.44
1:B:1224:THR:HB	1:B:1240:THR:HG22	1.99	0.44
1:B:1039:GLU:HB3	1:B:1048:ILE:HB	2.00	0.44
1:B:1105:THR:O	1:B:1111:GLU:HG3	2.18	0.43
1:B:1021:GLU:CD	1:B:1021:GLU:H	2.25	0.43
1:B:1210:LYS:HG3	1:B:1214:GLU:HB2	2.01	0.43
1:B:1037:MET:HE1	1:B:1284:THR:HG21	2.00	0.43
1:B:1170:GLN:HE21	1:B:1275:LEU:HB3	1.84	0.43
1:B:1373:ASP:HA	1:B:1376:SER:HB3	2.00	0.43
1:A:1127:TYR:HA	1:A:1130:TYR:HB2	2.01	0.42
1:A:1192:LEU:HD13	1:A:1192:LEU:HA	1.89	0.42
1:B:1213:LYS:HZ3	1:B:1213:LYS:HB3	1.84	0.42
1:A:1178:THR:HB	1:A:1181:GLU:HB2	2.01	0.42
1:B:1197:TYR:CZ	1:B:1279:THR:HG22	2.55	0.42
1:A:1446:PRO:O	1:A:1496:VAL:HG23	2.19	0.42
1:A:1147:TRP:CE3	1:A:1170:GLN:HB3	2.55	0.42
1:A:1325:ALA:O	1:A:1329:ASP:N	2.52	0.42
1:A:1397:ALA:O	1:A:1401:LEU:HB2	2.20	0.41
1:B:1198:GLU:HB3	1:B:1413:PHE:CZ	2.55	0.41
1:B:1304:VAL:O	1:B:1341:VAL:HA	2.20	0.41
1:B:1216:PHE:HB2	1:B:1242:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:ARG:NH2	1:A:1512:TYR:HA	2.34	0.41
1:B:1097:PHE:O	1:B:1101:VAL:HG23	2.20	0.41
1:B:1425:VAL:HG23	1:B:1436:ILE:HD12	2.02	0.41
1:A:1203:ILE:HD11	1:A:1283:MET:HA	2.03	0.41
1:B:1169:TRP:CD1	1:B:1169:TRP:C	2.99	0.41
1:B:1186:VAL:HG21	1:B:1243:HIS:HB2	2.03	0.41
1:A:1157:HIS:HA	1:A:1158:PRO:HD3	1.95	0.41
1:A:1287:HIS:ND1	1:A:1412:LEU:HD12	2.36	0.41
1:A:1358:TRP:O	1:A:1363:VAL:HG12	2.21	0.41
1:B:1190:LEU:HD22	1:B:1223:THR:HB	2.03	0.41
1:A:1186:VAL:HG21	1:A:1243:HIS:HB2	2.03	0.41
1:A:1503:LYS:HE2	1:A:1503:LYS:HB3	1.91	0.41
1:A:1039:GLU:HB3	1:A:1048:ILE:HB	2.04	0.40
1:B:1423:HIS:CD2	1:B:1441:LYS:HG3	2.56	0.40
1:B:1494:LYS:HA	1:B:1501:PRO:HA	2.02	0.40
1:A:1304:VAL:HG22	1:A:1365:ILE:HB	2.02	0.40
1:B:1138:ARG:H	1:B:1138:ARG:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	492/512 (96%)	484 (98%)	8 (2%)	0	100	100
1	B	477/512 (93%)	458 (96%)	18 (4%)	1 (0%)	43	62
All	All	969/1024 (95%)	942 (97%)	26 (3%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1022	GLU

5.3.2 Protein sidechains ⓘ

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	381/437 (87%)	369 (97%)	12 (3%)	35	60
1	B	364/437 (83%)	354 (97%)	10 (3%)	39	65
All	All	745/874 (85%)	723 (97%)	22 (3%)	37	62

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ASP
1	A	1082	VAL
1	A	1180	GLU
1	A	1192	LEU
1	A	1261	ILE
1	A	1273	TRP
1	A	1307	ILE
1	A	1319	ASP
1	A	1323	LEU
1	A	1348	ASN
1	A	1369	VAL
1	A	1443	VAL
1	B	1021	GLU
1	B	1087	LEU
1	B	1178	THR
1	B	1213	LYS
1	B	1337	VAL
1	B	1369	VAL
1	B	1382	VAL
1	B	1451	ILE
1	B	1479	LEU
1	B	1510	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1170	GLN
1	A	1247	ASN
1	A	1266	GLN
1	A	1395	ASN
1	A	1500	ASN
1	B	1023	ASN
1	B	1093	HIS
1	B	1135	GLN
1	B	1157	HIS
1	B	1170	GLN
1	B	1246	GLN
1	B	1247	ASN
1	B	1356	ASN
1	B	1444	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
2	PRO	B	1601	-	8,8,8	0.90	1 (12%)	10,10,10	1.40	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	0W4	B	1602	-	28,28,28	0.18	0	34,37,37	0.28	0
2	PRO	A	1601	-	8,8,8	0.89	1 (12%)	10,10,10	1.42	2 (20%)
3	0W4	A	1602	-	28,28,28	0.19	0	34,37,37	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PRO	B	1601	-	-	0/4/11/11	0/1/1/1
3	0W4	B	1602	-	-	4/14/14/14	0/3/3/3
2	PRO	A	1601	-	-	0/4/11/11	0/1/1/1
3	0W4	A	1602	-	-	1/14/14/14	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1601	PRO	OXT-C	-2.25	1.23	1.30
2	A	1601	PRO	OXT-C	-2.21	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	PRO	OXT-C-O	-2.73	117.89	124.08
2	B	1601	PRO	OXT-C-O	-2.69	117.97	124.08
2	A	1601	PRO	OXT-C-CA	2.23	121.07	113.51
2	B	1601	PRO	OXT-C-CA	2.19	120.92	113.51

There are no chirality outliers.

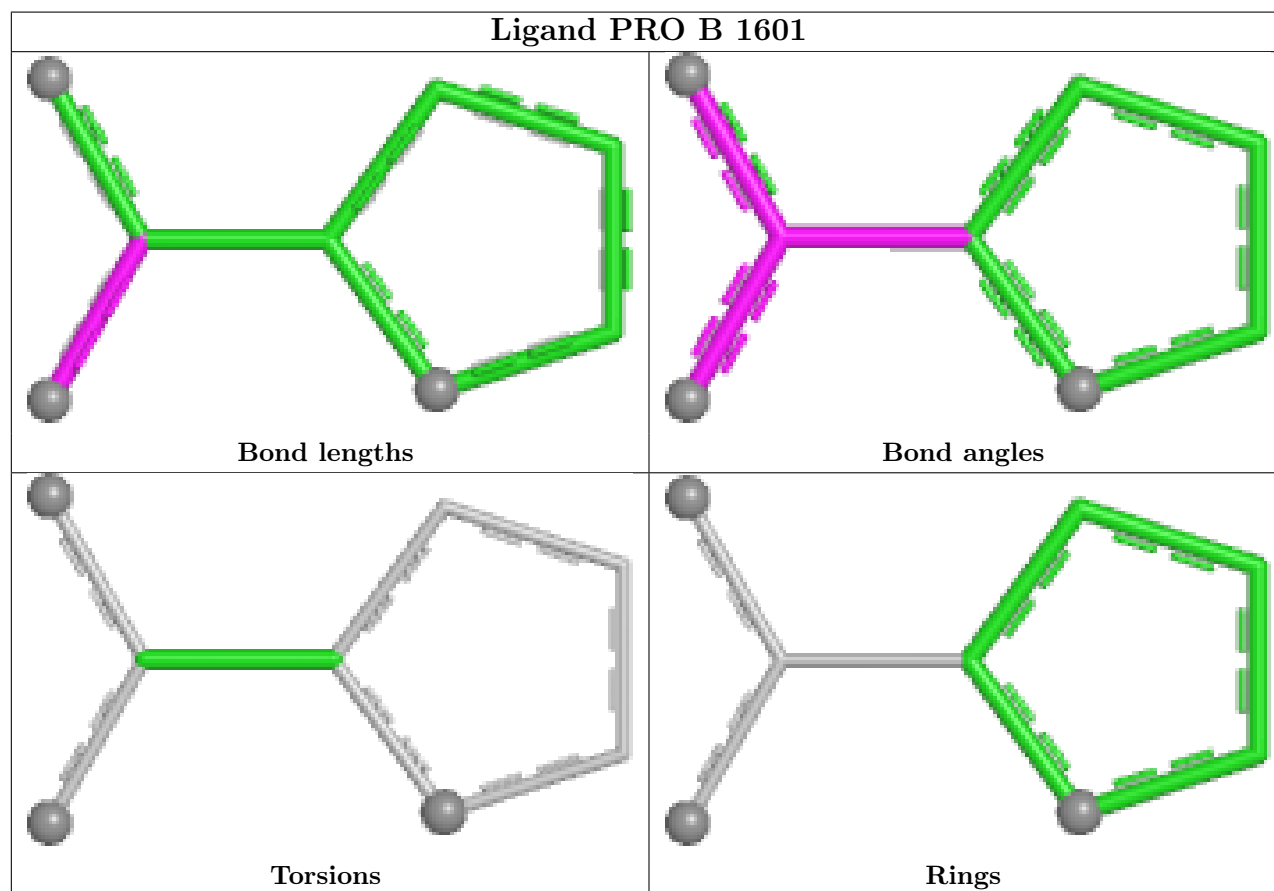
All (5) torsion outliers are listed below:

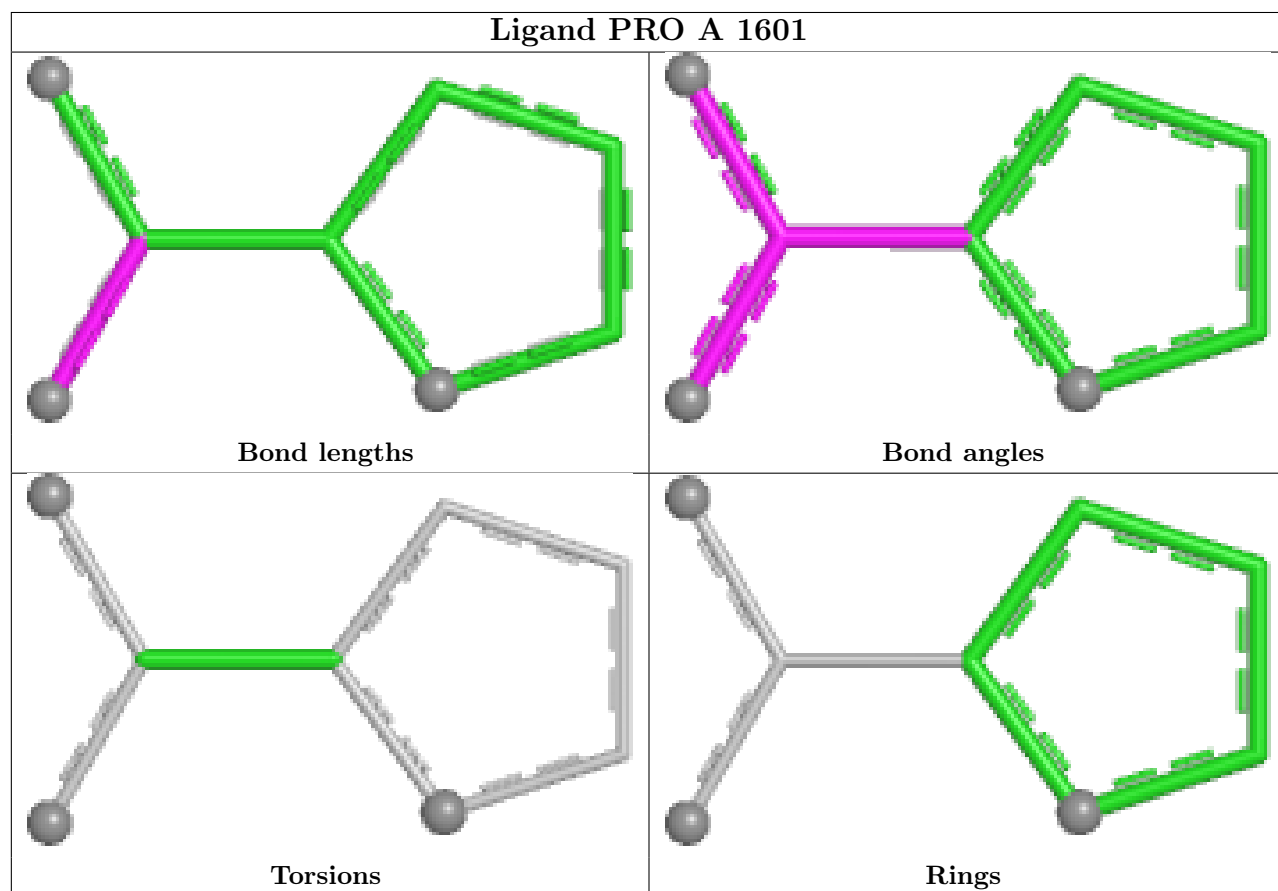
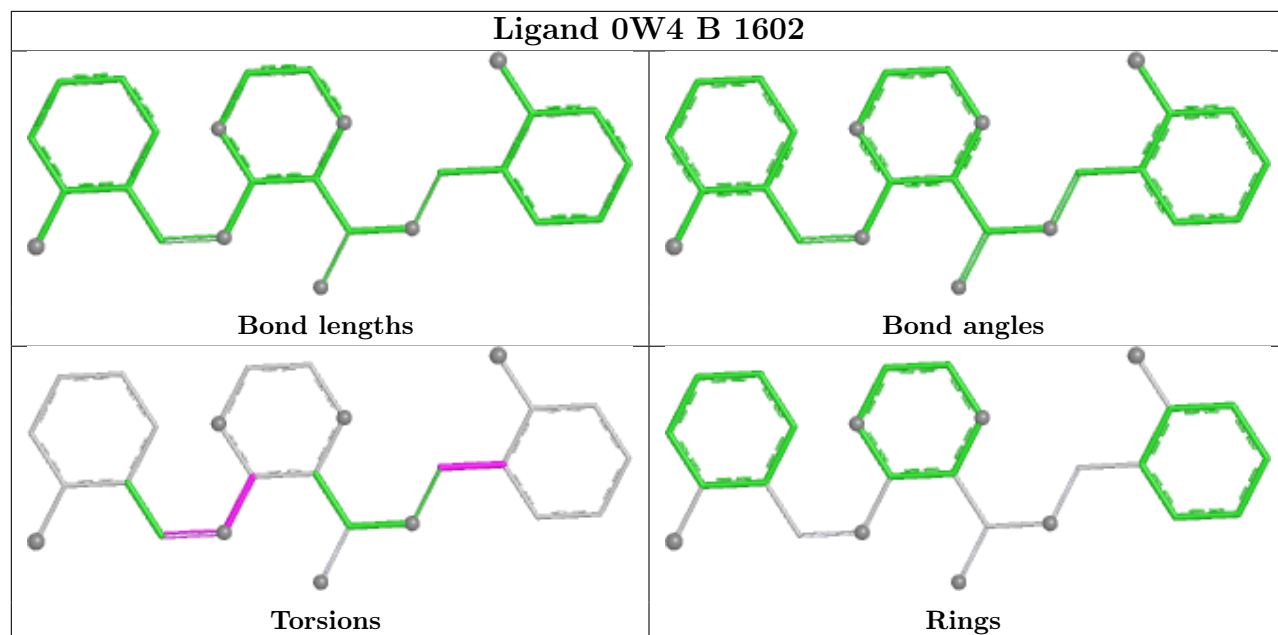
Mol	Chain	Res	Type	Atoms
3	B	1602	0W4	C2-C3-N10-C11
3	B	1602	0W4	C12-C11-N10-C3
3	B	1602	0W4	N4-C3-N10-C11
3	A	1602	0W4	N9-C19-C20-C21
3	B	1602	0W4	N9-C19-C20-C21

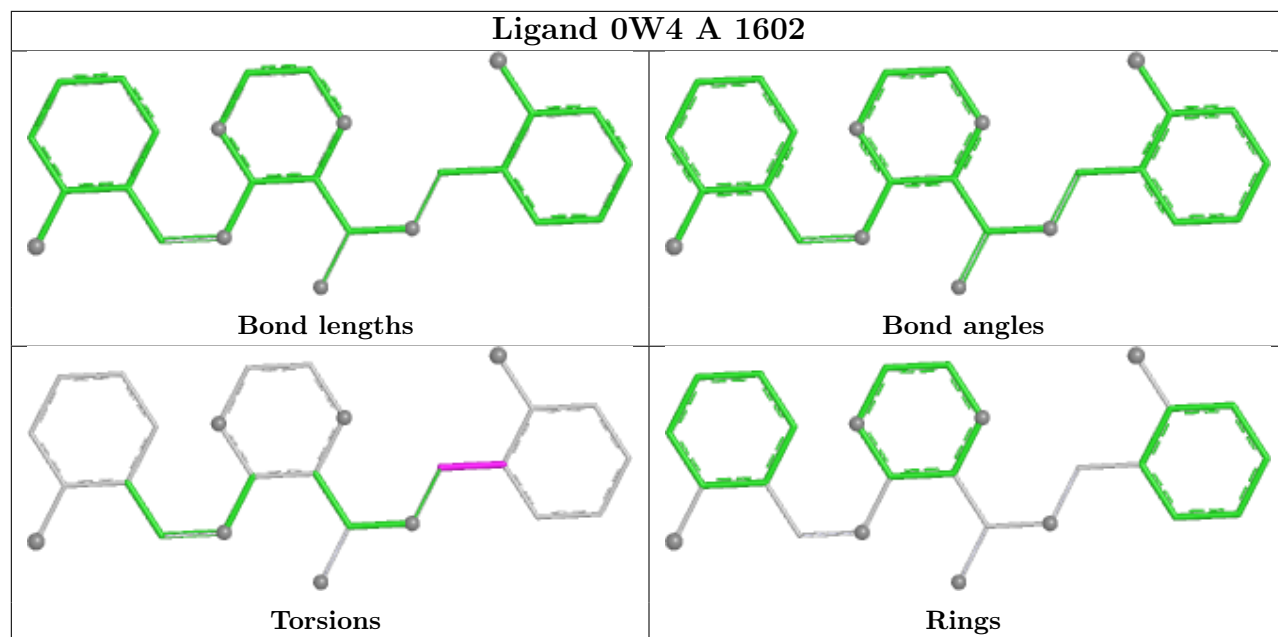
There are no ring outliers.

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 than 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.







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	496/512 (96%)	0.30	19 (3%)	44	40	56, 105, 171, 350	0
1	B	483/512 (94%)	0.48	24 (4%)	34	31	60, 122, 182, 238	0
All	All	979/1024 (95%)	0.39	43 (4%)	39	35	56, 113, 179, 350	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1299	VAL	4.4
1	B	1155	PHE	4.0
1	A	1442	ILE	3.8
1	B	1054	TYR	3.7
1	B	1330	TYR	3.5
1	B	1057	TRP	3.5
1	A	1397	ALA	3.4
1	A	1358	TRP	3.3
1	B	1203	ILE	3.3
1	B	1231	ALA	3.1
1	A	1304	VAL	3.0
1	B	1493	ALA	2.9
1	B	1360	LEU	2.9
1	B	1442	ILE	2.8
1	A	1365	ILE	2.8
1	A	1134	VAL	2.8
1	A	1367	LEU	2.7
1	A	1469	PRO	2.7
1	A	1381	ALA	2.7
1	B	1457	ILE	2.7
1	A	1262	PRO	2.6
1	A	1318	GLU	2.6
1	A	1467	LEU	2.5
1	A	1425	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1018	ALA	2.5
1	B	1029	SER	2.5
1	B	1137	HIS	2.5
1	A	1471	ALA	2.4
1	B	1113	ALA	2.4
1	B	1445	ILE	2.3
1	A	1345	LEU	2.3
1	B	1097	PHE	2.3
1	A	1263	GLY	2.2
1	A	1310	GLY	2.2
1	B	1502	ALA	2.2
1	B	1056	ILE	2.2
1	A	1424	MET	2.1
1	B	1483	PHE	2.1
1	A	1363	VAL	2.1
1	B	1381	ALA	2.1
1	B	1218	GLY	2.0
1	B	1265	LYS	2.0
1	B	1368	GLU	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.

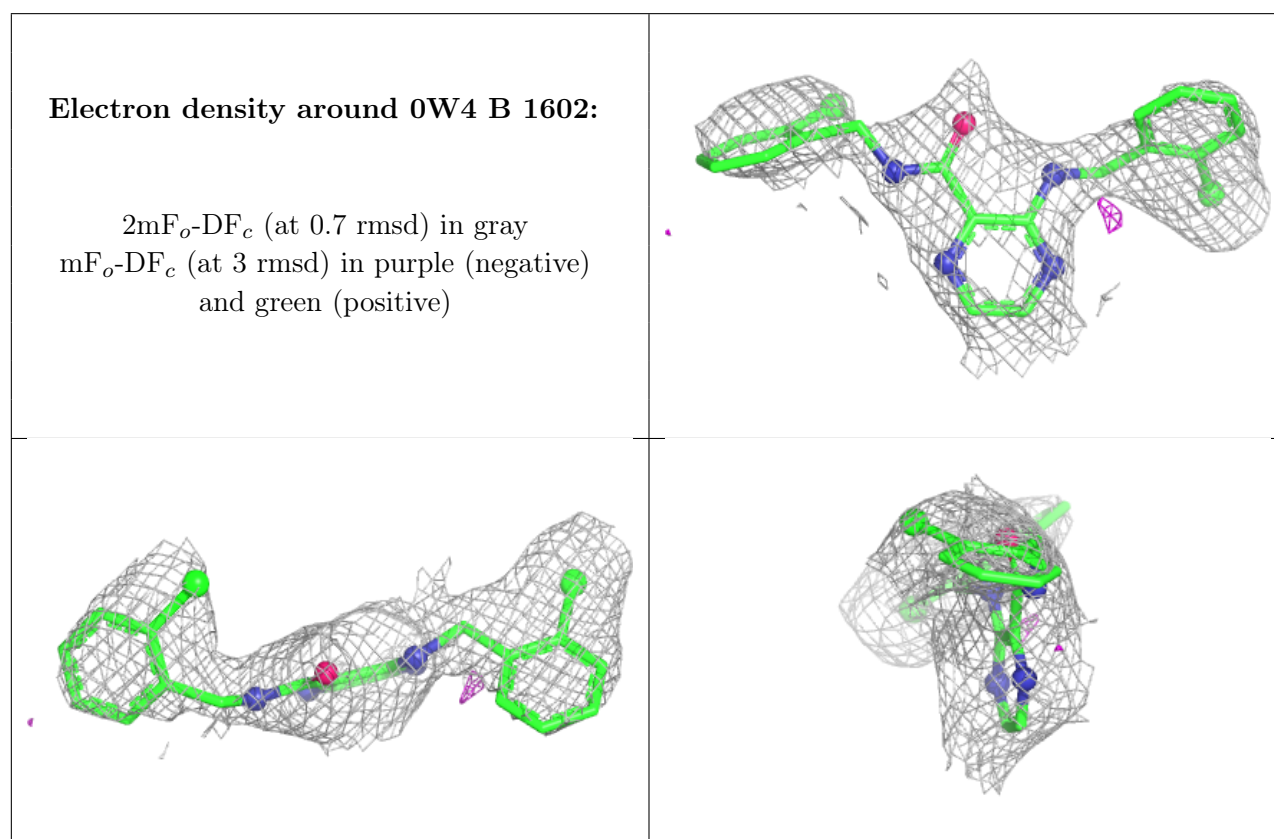
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SR	B	1604	1/1	0.75	0.13	256,256,256,256	0
5	SR	A	1604	1/1	0.87	0.09	184,184,184,184	0
5	SR	A	1605	1/1	0.88	0.11	233,233,233,233	0
5	SR	A	1606	1/1	0.90	0.11	237,237,237,237	0

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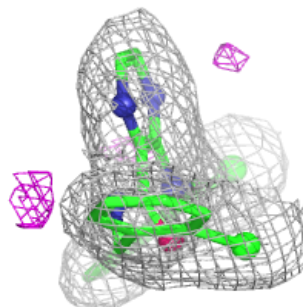
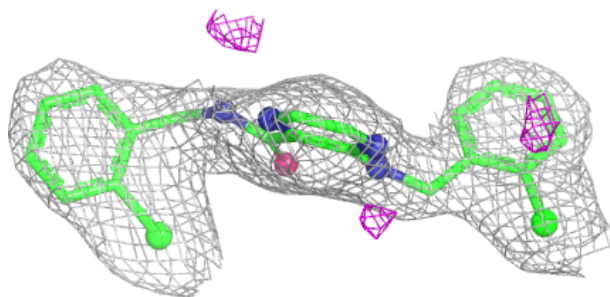
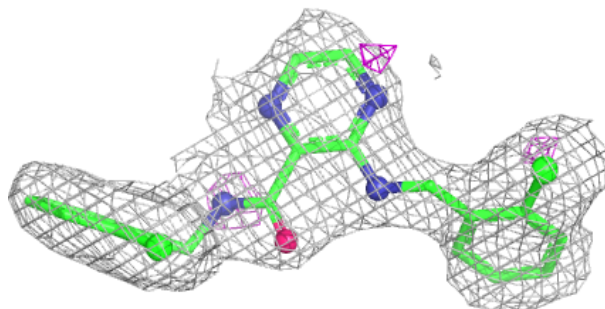
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OW4	B	1602	26/26	0.91	0.10	89,108,135,144	0
3	OW4	A	1602	26/26	0.93	0.09	62,83,100,108	0
2	PRO	B	1601	8/8	0.95	0.11	73,80,86,89	0
4	ZN	B	1603	1/1	0.95	0.06	172,172,172,172	0
2	PRO	A	1601	8/8	0.95	0.11	60,70,90,91	0
4	ZN	A	1603	1/1	0.97	0.06	118,118,118,118	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.

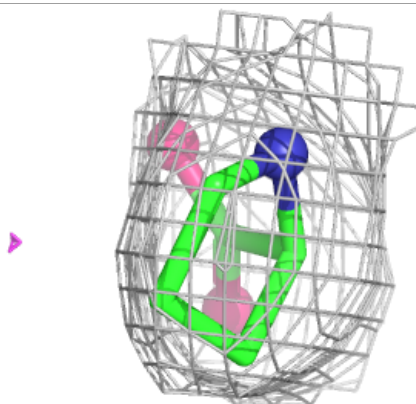
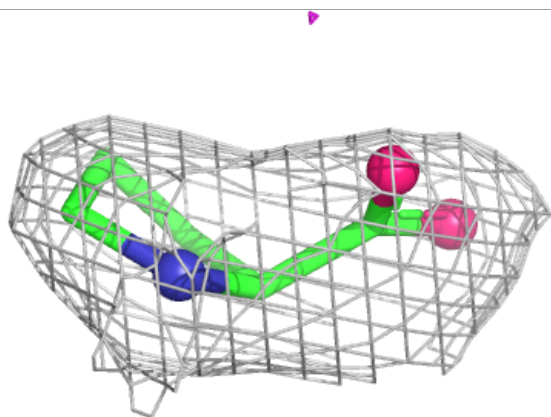
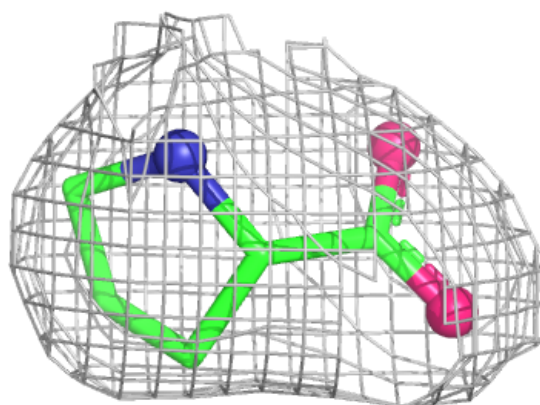


Electron density around OW4 A 1602:

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

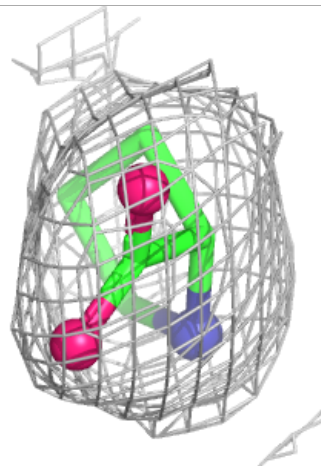
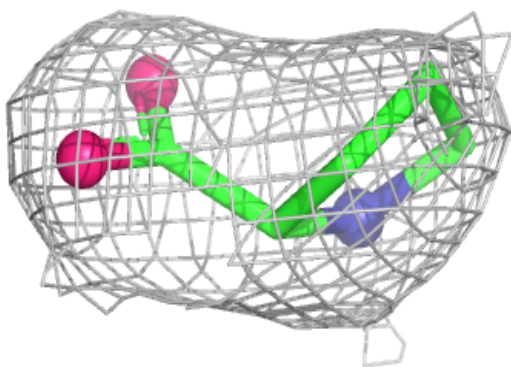
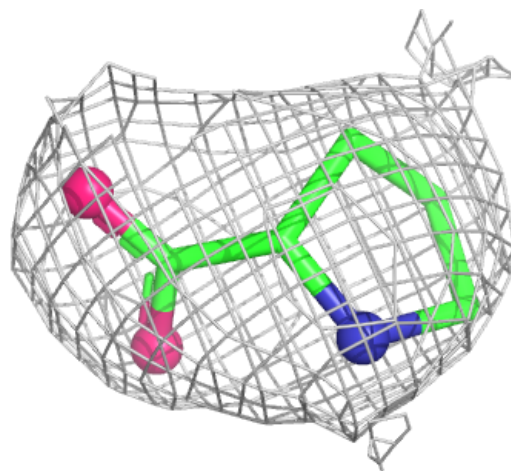
**Electron density around PRO B 1601:**

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



Electron density around PRO 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.