



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:47 PM UTC

PDB ID : 8YTK / pdb_00008ytk
Title : Crystal structure of human prolyl-tRNA synthetase in complex with inhibitor
Authors : Luo, Z.; Zhou, H.
Deposited on : 2024-03-26
Resolution : 2.55 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

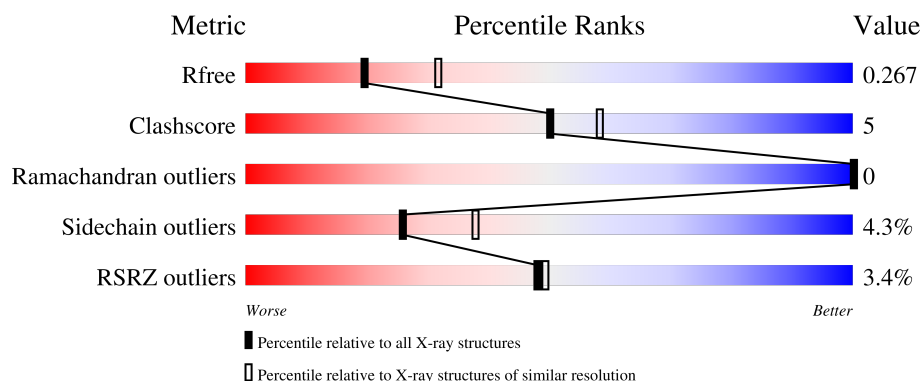
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

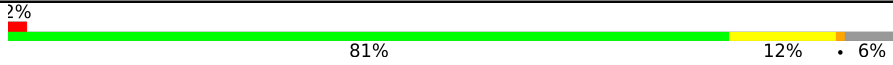
The reported resolution of this entry is 2.55 Å.

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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	524	
1	B	524	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7532 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	494	Total	C	N	O	S	0	0	0
			3817	2462	634	700	21			
1	B	464	Total	C	N	O	S	0	0	0
			3545	2282	589	652	22			

There are 28 discrepancies between the modelled and reference sequences:

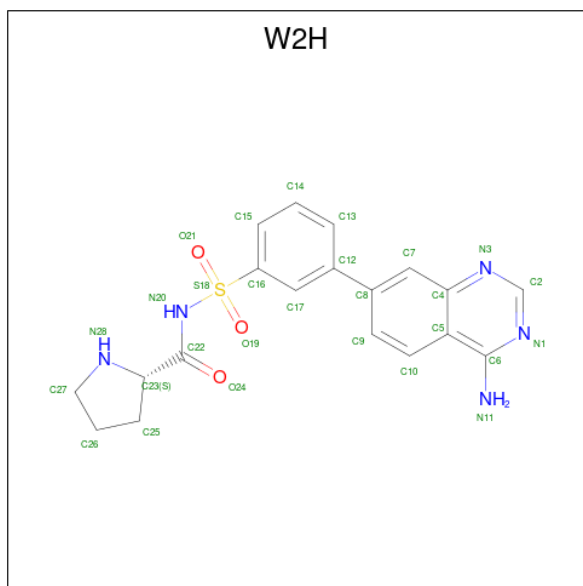
Chain	Residue	Modelled	Actual	Comment	Reference
A	989	MET	-	initiating methionine	UNP P07814
A	990	GLY	-	expression tag	UNP P07814
A	991	SER	-	expression tag	UNP P07814
A	992	SER	-	expression tag	UNP P07814
A	993	HIS	-	expression tag	UNP P07814
A	994	HIS	-	expression tag	UNP P07814
A	995	HIS	-	expression tag	UNP P07814
A	996	HIS	-	expression tag	UNP P07814
A	997	HIS	-	expression tag	UNP P07814
A	998	HIS	-	expression tag	UNP P07814
A	999	SER	-	expression tag	UNP P07814
A	1000	SER	-	expression tag	UNP P07814
A	1001	HIS	-	expression tag	UNP P07814
A	1002	MET	-	expression tag	UNP P07814
B	989	MET	-	initiating methionine	UNP P07814
B	990	GLY	-	expression tag	UNP P07814
B	991	SER	-	expression tag	UNP P07814
B	992	SER	-	expression tag	UNP P07814
B	993	HIS	-	expression tag	UNP P07814
B	994	HIS	-	expression tag	UNP P07814
B	995	HIS	-	expression tag	UNP P07814
B	996	HIS	-	expression tag	UNP P07814
B	997	HIS	-	expression tag	UNP P07814
B	998	HIS	-	expression tag	UNP P07814
B	999	SER	-	expression tag	UNP P07814

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	SER	-	expression tag	UNP P07814
B	1001	HIS	-	expression tag	UNP P07814
B	1002	MET	-	expression tag	UNP P07814

- Molecule 2 is (2 {S})- {N}-[3-(4-azanylquinazolin-7-yl)phenyl]sulfonylpyrrolidine-2-carboxamide (CCD ID: W2H) (formula: C₁₉H₁₉N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	5	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	44	Total	O	0	0
			44	44		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 92.16Å 86.62Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	46.12 – 2.55 46.12 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.12-2.55) 99.5 (46.12-2.55)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.49 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.250 (Not available) , 0.267	Depositor DCC
R_{free} test set	1797 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: EDO, W2H

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	0.47	0/3912	0.90	1/5324 (0.0%)
1	B	0.46	0/3629	0.89	0/4938
All	All	0.46	0/7541	0.90	1/10262 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	GLU	CB-CA-C	6.04	119.98	110.19

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	3817	0	3652	45	0
1	B	3545	0	3325	32	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
3	A	8	0	12	2	0
3	B	4	0	6	0	0
4	A	58	0	0	0	0
4	B	44	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7532	0	6995	76	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 5.

All (76) 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:1430:MET:HE2	1:A:1456:TRP:CZ3	2.00	0.96
1:B:1400:LYS:O	1:B:1404:ILE:HG13	1.84	0.76
1:B:1383:ARG:NH1	1:B:1407:ASP:OD2	2.26	0.68
1:B:1090:GLU:OE2	1:B:1218:GLY:HA2	1.94	0.66
1:A:1210:LYS:HE2	1:A:1224:THR:HG21	1.79	0.64
1:B:1453:CYS:O	1:B:1457:ILE:HG13	1.99	0.63
1:B:1065:ASP:OD2	1:B:1069:LYS:HE2	2.00	0.62
1:B:1430:MET:HE2	1:B:1456:TRP:CZ3	2.36	0.60
1:A:1219:GLY:HA2	1:A:1244:LEU:HA	1.85	0.58
1:A:1430:MET:HE2	1:A:1456:TRP:CH2	2.39	0.58
1:B:1355:PHE:O	1:B:1359:GLU:HB2	2.04	0.57
1:A:1344:ASP:OD2	1:A:1354:LYS:HG2	2.05	0.56
1:A:1430:MET:CE	1:A:1456:TRP:CH2	2.88	0.56
1:A:1500:ASN:HB2	1:A:1501:PRO:HD2	1.88	0.55
1:A:1090:GLU:HG3	1:A:1093:HIS:HB3	1.89	0.55
1:A:1368:GLU:HB2	1:A:1380:VAL:HB	1.87	0.54
1:A:1098:ALA:N	1:A:1099:PRO:HD2	2.23	0.52
1:B:1359:GLU:OE1	1:B:1366:ARG:NH1	2.42	0.52
1:A:1168:LEU:HD22	3:A:1602:EDO:H22	1.90	0.52
1:B:1203:ILE:HD11	1:B:1283:MET:HA	1.91	0.52
1:A:1430:MET:CE	1:A:1456:TRP:CZ3	2.84	0.52
1:A:1494:LYS:HA	1:A:1501:PRO:HA	1.93	0.51
1:B:1224:THR:HB	1:B:1240:THR:HG22	1.93	0.51
1:A:1250:LYS:HA	1:A:1267:PHE:CE1	2.46	0.51
1:A:1465:GLN:OE1	1:A:1510:ARG:NH2	2.44	0.49
1:B:1172:GLY:O	1:B:1272:SER:HA	2.12	0.49
1:A:1080:MET:SD	1:B:1080:MET:SD	3.11	0.49
1:B:1424:MET:HA	1:B:1442:ILE:O	2.13	0.48
1:A:1082:VAL:HB	1:A:1125:VAL:HG22	1.96	0.48
1:A:1024:LEU:CD2	1:A:1232:SER:HB3	2.44	0.48
1:A:1061:LYS:HD2	1:A:1147:TRP:CE3	2.49	0.48
1:A:1430:MET:HG2	1:A:1496:VAL:HB	1.95	0.47
1:A:1169:TRP:C	1:A:1169:TRP:CD1	2.93	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:ILE:HD11	1:A:1283:MET:HA	1.95	0.47
1:A:1213:LYS:NZ	1:A:1455:ASP:OD1	2.37	0.47
1:B:1452:ASP:HA	1:B:1455:ASP:HB2	1.96	0.47
1:B:1045:GLY:HA3	1:B:1165:ARG:HD3	1.97	0.47
1:B:1299:VAL:HG13	1:B:1299:VAL:O	2.14	0.46
1:B:1147:TRP:CE3	1:B:1170:GLN:HB3	2.50	0.46
1:A:1147:TRP:CE3	1:A:1170:GLN:HB3	2.51	0.46
1:A:1097:PHE:O	1:A:1101:VAL:HG23	2.16	0.45
1:B:1038:ILE:HD11	1:B:1161:PHE:CZ	2.51	0.45
1:A:1127:TYR:N	1:A:1128:PRO:CD	2.80	0.45
1:A:1222:THR:HG23	1:A:1242:HIS:ND1	2.32	0.45
1:A:1061:LYS:NZ	3:A:1602:EDO:O1	2.50	0.44
1:B:1342:ARG:NH1	4:B:1701:HOH:O	2.33	0.44
1:A:1061:LYS:O	1:A:1065:ASP:HB2	2.18	0.44
1:A:1326:LYS:HD3	1:A:1326:LYS:HA	1.81	0.44
1:A:1404:ILE:O	1:A:1408:ILE:HG13	2.18	0.43
1:B:1061:LYS:O	1:B:1065:ASP:HB2	2.18	0.43
1:A:1446:PRO:HB3	1:A:1489:LEU:HD11	1.99	0.43
1:A:1429:THR:HG1	1:A:1432:ASP:H	1.66	0.43
1:B:1127:TYR:N	1:B:1128:PRO:CD	2.82	0.43
1:B:1304:VAL:HG22	1:B:1365:ILE:HB	2.00	0.43
1:A:1366:ARG:NH2	1:A:1368:GLU:OE1	2.46	0.43
1:A:1430:MET:HE3	1:A:1456:TRP:CH2	2.54	0.43
1:A:1465:GLN:HB2	1:A:1510:ARG:HH22	1.82	0.43
1:B:1201:LEU:HB3	1:B:1203:ILE:HD12	2.02	0.42
1:A:1169:TRP:HB2	1:A:1275:LEU:O	2.19	0.42
1:A:1344:ASP:CG	1:A:1354:LYS:HE2	2.44	0.42
1:B:1071:LEU:O	1:B:1143:LYS:HE3	2.20	0.42
1:A:1027:TRP:O	1:A:1031:VAL:HG23	2.20	0.42
1:A:1222:THR:HG23	1:A:1242:HIS:HD1	1.84	0.41
1:B:1090:GLU:OE2	1:B:1218:GLY:CA	2.67	0.41
1:A:1169:TRP:CB	1:A:1276:THR:HG22	2.51	0.41
1:A:1400:LYS:O	1:A:1404:ILE:HG13	2.20	0.41
1:A:1078:PHE:CE2	1:A:1126:MET:HA	2.56	0.41
1:A:1465:GLN:HB2	1:A:1510:ARG:NH2	2.35	0.41
1:B:1101:VAL:CG1	1:B:1117:ALA:HB1	2.51	0.41
1:B:1106:ARG:HB3	1:B:1111:GLU:HA	2.02	0.41
1:B:1229:ILE:HD12	1:B:1512:TYR:CE1	2.55	0.41
1:B:1407:ASP:O	1:B:1411:THR:OG1	2.34	0.41
1:B:1445:ILE:C	1:B:1505:TYR:HD1	2.28	0.41
1:A:1169:TRP:HB3	1:A:1276:THR:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:TRP:CB	1:B:1276:THR:HG22	2.52	0.40
1:B:1228:PHE:CE2	1:B:1230:SER:HA	2.56	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	490/524 (94%)	479 (98%)	11 (2%)	0	100	100
1	B	452/524 (86%)	445 (98%)	7 (2%)	0	100	100
All	All	942/1048 (90%)	924 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	382/450 (85%)	366 (96%)	16 (4%)	26	38
1	B	346/450 (77%)	331 (96%)	15 (4%)	26	38
All	All	728/900 (81%)	697 (96%)	31 (4%)	26	38

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ASP
1	A	1090	GLU
1	A	1169	TRP
1	A	1209	ARG
1	A	1272	SER
1	A	1273	TRP
1	A	1326	LYS
1	A	1341	VAL
1	A	1342	ARG
1	A	1348	ASN
1	A	1359	GLU
1	A	1430	MET
1	A	1443	VAL
1	A	1453	CYS
1	A	1491	PRO
1	A	1504	TYR
1	B	1089	LYS
1	B	1090	GLU
1	B	1165	ARG
1	B	1169	TRP
1	B	1170	GLN
1	B	1273	TRP
1	B	1299	VAL
1	B	1324	ILE
1	B	1336	SER
1	B	1374	MET
1	B	1395	ASN
1	B	1417	SER
1	B	1428	ASN
1	B	1457	ILE
1	B	1504	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1023	ASN
1	A	1145	ASN
1	A	1157	HIS
1	A	1170	GLN
1	A	1195	GLN
1	A	1246	GLN
1	A	1270	GLN
1	A	1271	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1348	ASN
1	A	1395	ASN
1	B	1378	GLN
1	B	1428	ASN

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](#)

5 ligands are modelled in this entry.

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	W2H	B	1601	-	31,31,31	0.30	0	43,45,45	0.52	1 (2%)
3	EDO	B	1602	-	3,3,3	0.07	0	2,2,2	0.07	0
3	EDO	A	1602	-	3,3,3	0.09	0	2,2,2	0.17	0
3	EDO	A	1603	-	3,3,3	0.12	0	2,2,2	0.31	0
2	W2H	A	1601	-	31,31,31	0.34	0	43,45,45	0.51	1 (2%)

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	W2H	B	1601	-	-	9/19/26/26	0/4/4/4
3	EDO	B	1602	-	-	0/1/1/1	-
3	EDO	A	1602	-	-	1/1/1/1	-
3	EDO	A	1603	-	-	1/1/1/1	-
2	W2H	A	1601	-	-	4/19/26/26	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	W2H	C10-C5-C6	2.14	125.93	123.01
2	B	1601	W2H	C10-C5-C6	2.13	125.92	123.01

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1601	W2H	N20-C22-C23-C25
2	B	1601	W2H	O24-C22-C23-C25
2	A	1601	W2H	C17-C16-S18-O21
2	B	1601	W2H	C17-C16-S18-O21
2	A	1601	W2H	C15-C16-S18-O21
2	B	1601	W2H	C15-C16-S18-O21
2	A	1601	W2H	C17-C16-S18-N20
2	A	1601	W2H	C15-C16-S18-N20
2	B	1601	W2H	C17-C16-S18-N20
2	B	1601	W2H	N20-C22-C23-N28
2	B	1601	W2H	C15-C16-S18-N20
2	B	1601	W2H	O24-C22-C23-N28
3	A	1603	EDO	O1-C1-C2-O2
2	B	1601	W2H	C22-N20-S18-O19
3	A	1602	EDO	O1-C1-C2-O2

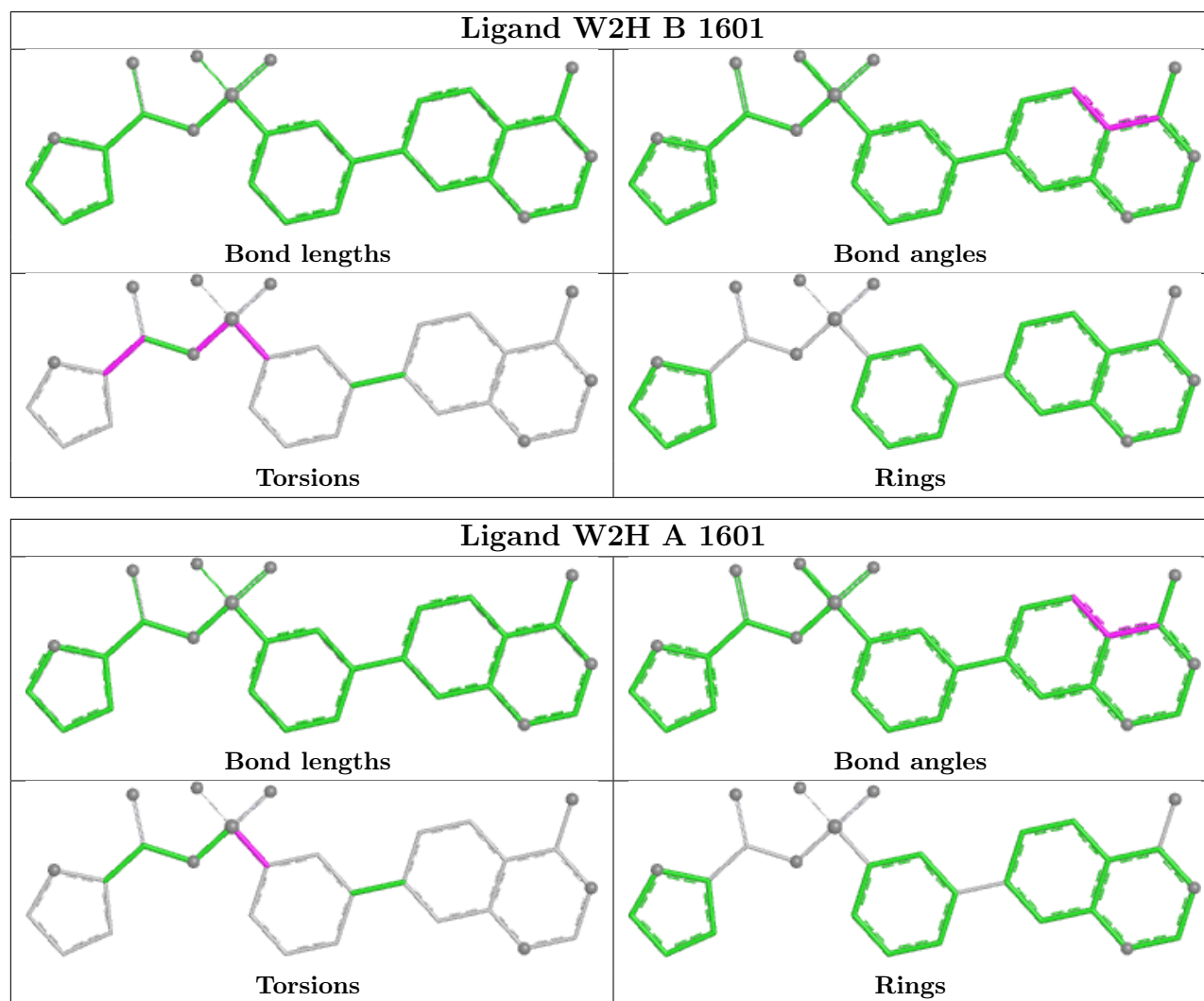
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	EDO	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	494/524 (94%)	0.10	8 (1%) 70 72	26, 44, 69, 89	1 (0%)
1	B	464/524 (88%)	0.35	25 (5%) 31 31	28, 52, 86, 97	1 (0%)
All	All	958/1048 (91%)	0.22	33 (3%) 48 49	26, 47, 81, 97	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1448	CYS	5.0
1	B	1453	CYS	4.8
1	B	1322	ALA	4.8
1	B	1500	ASN	4.5
1	A	1448	CYS	4.3
1	A	1030	GLN	3.3
1	A	1497	CYS	3.0
1	B	1431	GLU	3.0
1	B	1018	ALA	2.9
1	B	1433	PHE	2.9
1	B	1218	GLY	2.8
1	A	1453	CYS	2.8
1	B	1495	CYS	2.8
1	B	1429	THR	2.7
1	B	1449	GLY	2.6
1	A	1315	LEU	2.6
1	B	1368	GLU	2.6
1	B	1310	GLY	2.5
1	B	1451	ILE	2.4
1	B	1030	GLN	2.4
1	A	1437	LEU	2.3
1	B	1475	GLY	2.3
1	B	1503	LYS	2.3
1	B	1436	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1437	LEU	2.3
1	A	1022	GLU	2.1
1	B	1446	PRO	2.1
1	A	1449	GLY	2.1
1	B	1447	PHE	2.1
1	B	1496	VAL	2.1
1	B	1356	ASN	2.0
1	B	1445	ILE	2.0
1	B	1291	MET	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](#)

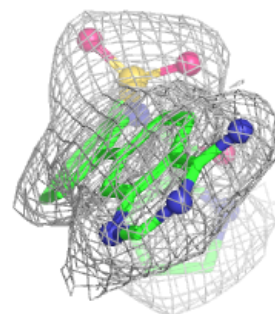
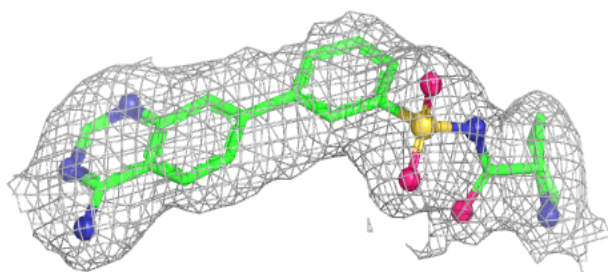
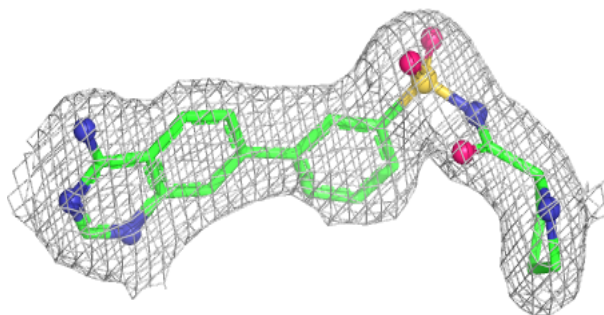
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	EDO	A	1603	4/4	0.84	0.17	51,54,55,55	0
3	EDO	B	1602	4/4	0.88	0.13	42,42,43,44	0
3	EDO	A	1602	4/4	0.89	0.18	41,44,44,45	0
2	W2H	B	1601	28/28	0.95	0.08	30,31,32,32	0
2	W2H	A	1601	28/28	0.97	0.07	25,27,28,29	0

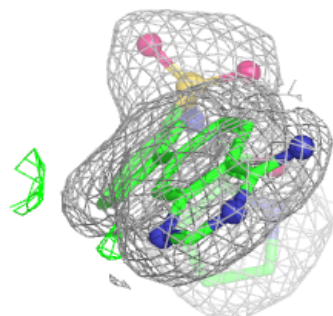
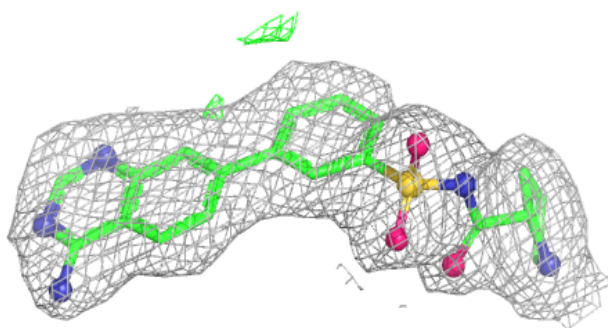
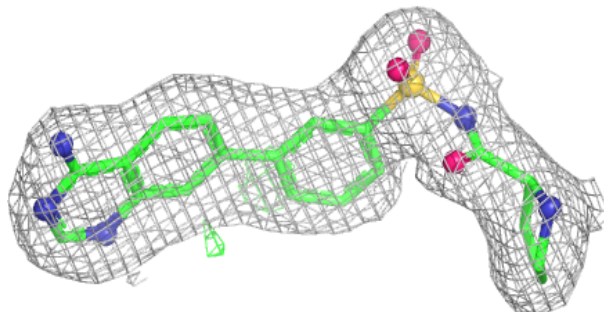
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W2H 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 W2H 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.