Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 02:32 PM JST

PDB ID	:	8YTK
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)

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

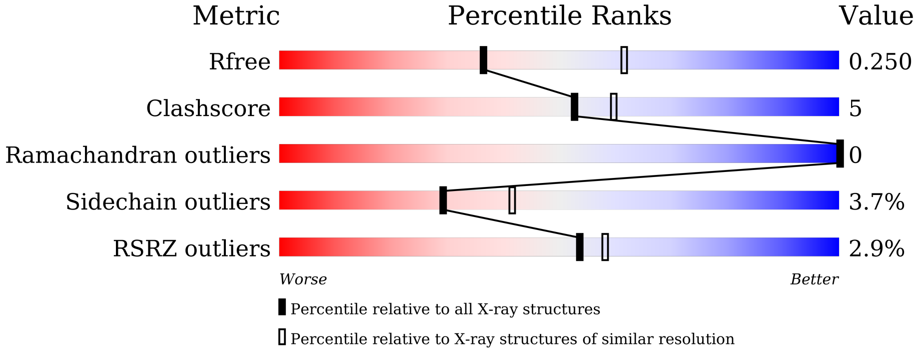
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance

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

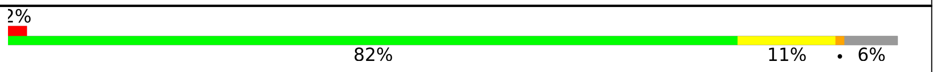
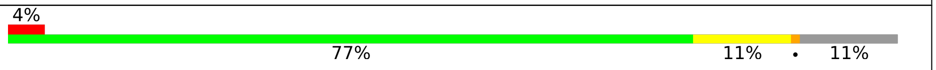
The reported resolution of this entry is 2.55 Å.

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}	164625	1685 (2.58-2.54)
Clashscore	180529	1779 (2.58-2.54)
Ramachandran outliers	177936	1766 (2.58-2.54)
Sidechain outliers	177891	1766 (2.58-2.54)
RSRZ outliers	164620	1685 (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 <=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 (i)

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 3817	C 2462	N 634	O 700	S 21	0	0	0
1	B	464	Total 3545	C 2282	N 589	O 652	S 22	0	0	0

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

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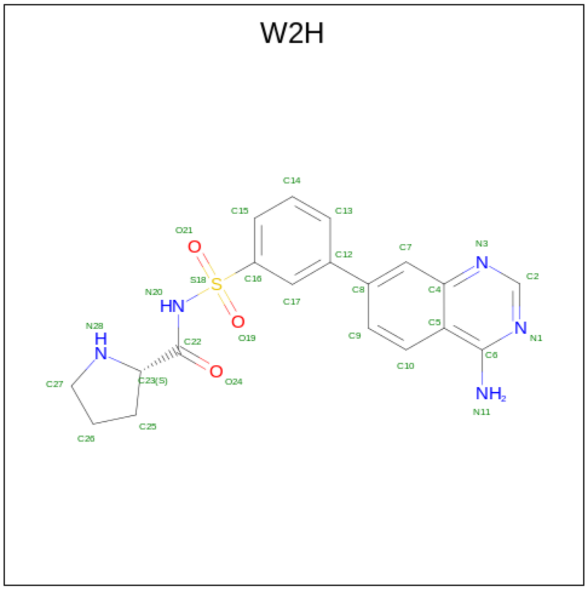
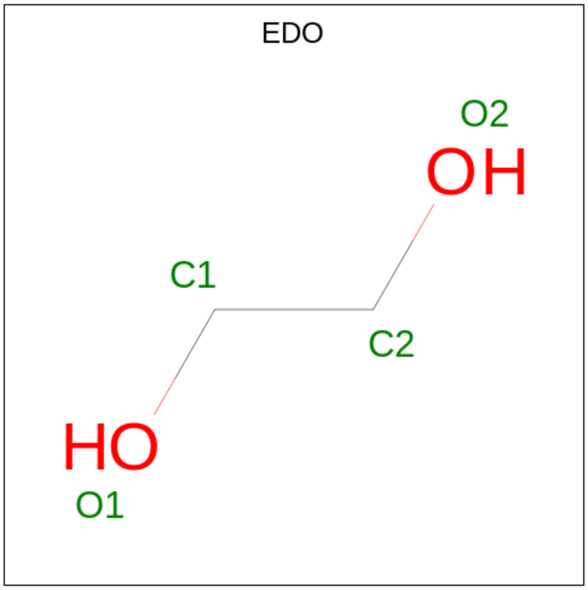
Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	SER	-	expression tag	UNP P07814
B	1001	HIS	-	expression tag	UNP P07814
B	1002	MET	-	expression tag	UNP P07814

- Molecule 2 is (2 {S})- {N}-[3-(4-azanylquinazolin-7-yl)phenyl]sulfonylpyrrolidine-2-carboxamide (three-letter code: W2H) (formula: $C_{19}H_{19}N_5O_3S$) (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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

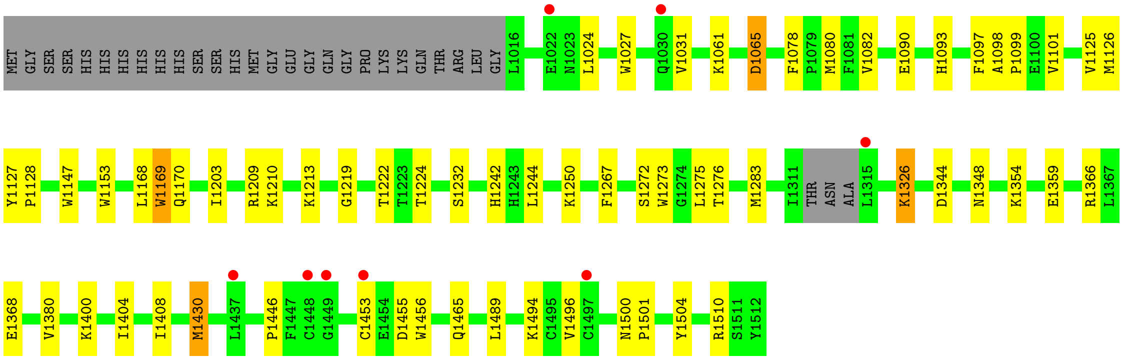
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total O 58 58	0	0
4	B	44	Total O 44 44	0	0

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.

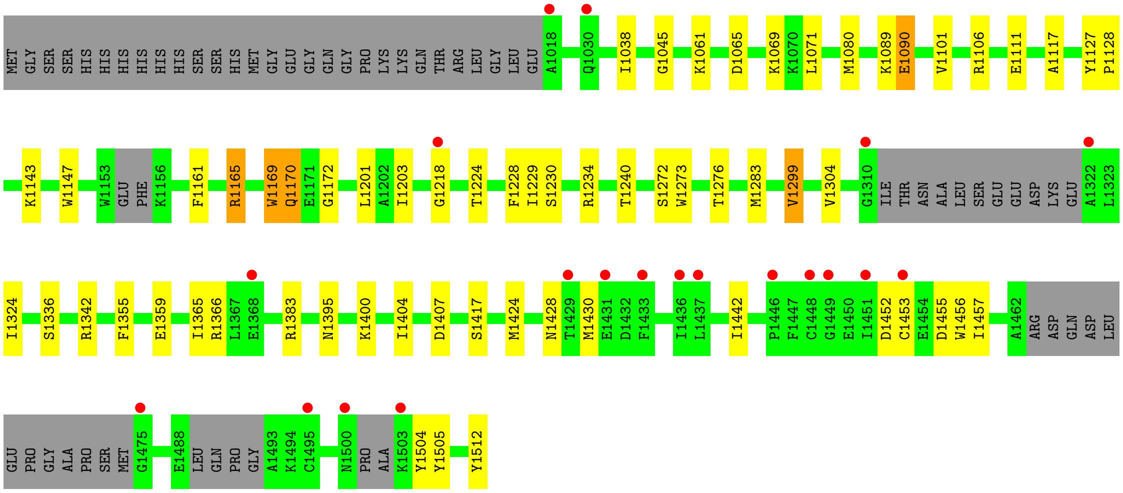
- Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain A:



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

Chain B:



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
$< I/\sigma(I) >$ [1]	6.49 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.250 0.204 , 0.250	Depositor DCC
R_{free} test set	1809 reflections (5.19%)	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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

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[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: 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	0.30	0/3912	0.60	0/5324
1	B	0.29	0/3629	0.58	0/4938
All	All	0.30	0/7541	0.59	0/10262

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 ⓘ

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	41	0
1	B	3545	0	3325	30	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
All	All	7532	0	6995	70	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 (70) 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	2.12	0.85
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:A:1430:MET:HE3	1:A:1456:TRP:CH2	2.35	0.62
1:A:1219:GLY:HA2	1:A:1244:LEU:HA	1.85	0.58
1:A:1430:MET:CE	1:A:1456:TRP:CZ3	2.84	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: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:B:1430:MET:HE2	1:B:1456:TRP:CZ3	2.50	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1169:TRP:C	1:A:1169:TRP:CD1	2.93	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: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:A:1169:TRP:HB3	1:A:1276:THR:HG22	2.02	0.40
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 ⓘ

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	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 ⓘ

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%)	370 (97%)	12 (3%)	35	49
1	B	346/450 (77%)	331 (96%)	15 (4%)	25	36
All	All	728/900 (81%)	701 (96%)	27 (4%)	29	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ASP
1	A	1153	TRP
1	A	1169	TRP
1	A	1209	ARG
1	A	1272	SER
1	A	1273	TRP
1	A	1326	LYS
1	A	1348	ASN
1	A	1359	GLU
1	A	1430	MET
1	A	1453	CYS
1	A	1504	TYR
1	B	1089	LYS
1	B	1090	GLU
1	B	1165	ARG

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Mol	Chain	Res	Type
1	B	1169	TRP
1	B	1170	GLN
1	B	1234	ARG
1	B	1273	TRP
1	B	1299	VAL
1	B	1324	ILE
1	B	1336	SER
1	B	1395	ASN
1	B	1417	SER
1	B	1428	ASN
1	B	1504	TYR
1	B	1505	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1023	ASN
1	A	1145	ASN
1	A	1170	GLN
1	A	1348	ASN
1	A	1395	ASN
1	B	1378	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\|Z\| > 2$
3	EDO	A	1602	-	3,3,3	0.09	0	2,2,2	0.24	0
3	EDO	B	1602	-	3,3,3	0.07	0	2,2,2	0.09	0
2	W2H	B	1601	-	31,31,31	0.29	0	43,45,45	0.51	1 (2%)
3	EDO	A	1603	-	3,3,3	0.12	0	2,2,2	0.39	0
2	W2H	A	1601	-	31,31,31	0.34	0	43,45,45	0.49	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
3	EDO	A	1602	-	-	1/1/1/1	-
3	EDO	B	1602	-	-	0/1/1/1	-
2	W2H	B	1601	-	-	9/19/26/26	0/4/4/4
3	EDO	A	1603	-	-	1/1/1/1	-
2	W2H	A	1601	-	-	5/19/26/26	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(^{o})	Ideal(^{o})
2	A	1601	W2H	C10-C5-C6	2.01	125.93	122.98
2	B	1601	W2H	C10-C5-C6	2.00	125.92	122.98

There are no chirality outliers.

All (16) 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

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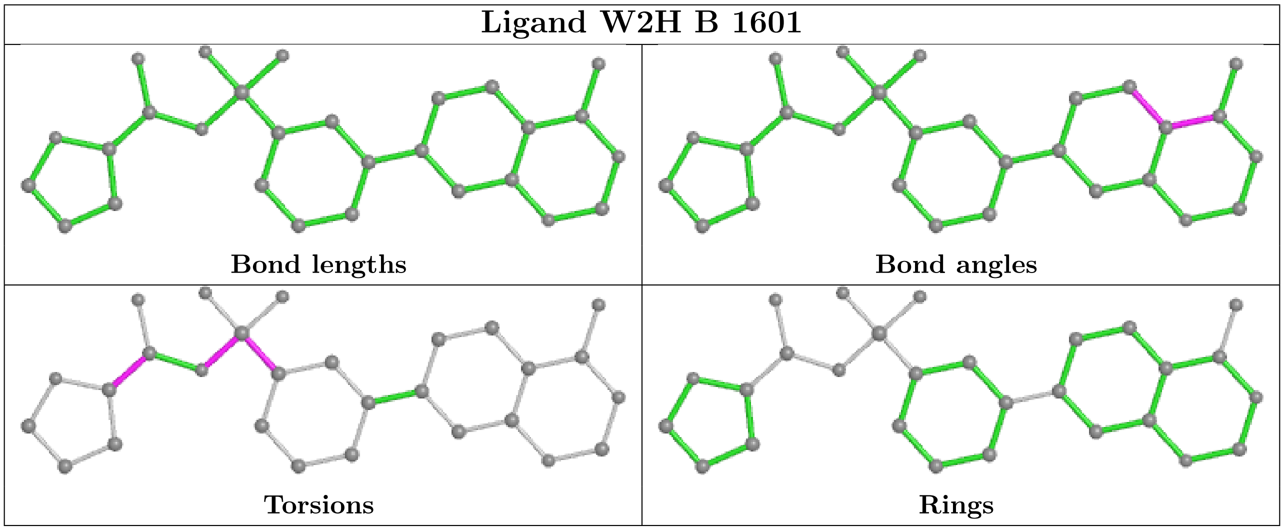
Mol	Chain	Res	Type	Atoms
2	A	1601	W2H	C15-C16-S18-O21
2	B	1601	W2H	C17-C16-S18-O21
2	B	1601	W2H	C15-C16-S18-O21
2	A	1601	W2H	C17-C16-S18-N20
2	A	1601	W2H	C15-C16-S18-N20
2	B	1601	W2H	C17-C16-S18-N20
2	B	1601	W2H	C15-C16-S18-N20
2	B	1601	W2H	N20-C22-C23-N28
2	B	1601	W2H	O24-C22-C23-N28
2	B	1601	W2H	C22-N20-S18-O19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

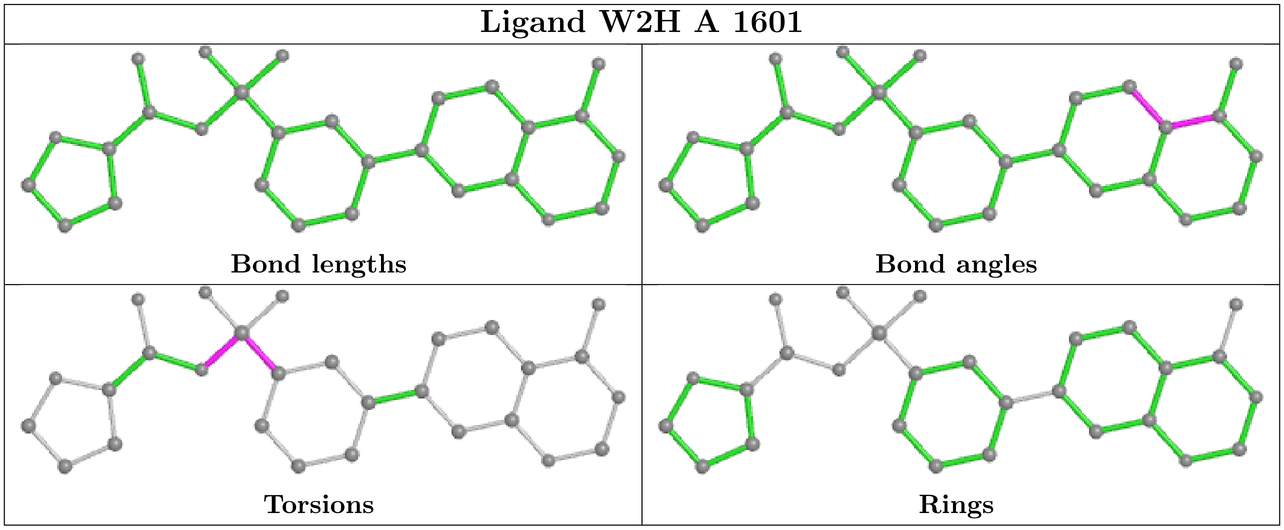
There are no ring outliers.

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 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.





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%)	-0.01	8 (1%)	70	74	26, 44, 69, 89	1 (0%)
1	B	464/524 (88%)	0.25	20 (4%)	40	45	28, 52, 86, 97	1 (0%)
All	All	958/1048 (91%)	0.12	28 (2%)	54	58	26, 47, 81, 97	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1448	CYS	4.9
1	B	1322	ALA	4.8
1	B	1453	CYS	4.7
1	B	1500	ASN	4.5
1	A	1448	CYS	4.1
1	A	1030	GLN	3.3
1	B	1431	GLU	3.0
1	B	1018	ALA	2.9
1	A	1497	CYS	2.8
1	B	1218	GLY	2.8
1	B	1433	PHE	2.7
1	A	1453	CYS	2.6
1	B	1495	CYS	2.6
1	B	1368	GLU	2.6
1	B	1429	THR	2.6
1	B	1449	GLY	2.6
1	A	1315	LEU	2.5
1	B	1310	GLY	2.5
1	B	1451	ILE	2.4
1	B	1030	GLN	2.3
1	B	1503	LYS	2.3
1	A	1437	LEU	2.2
1	B	1475	GLY	2.2
1	B	1436	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1437	LEU	2.2
1	A	1022	GLU	2.1
1	B	1446	PRO	2.0
1	A	1449	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

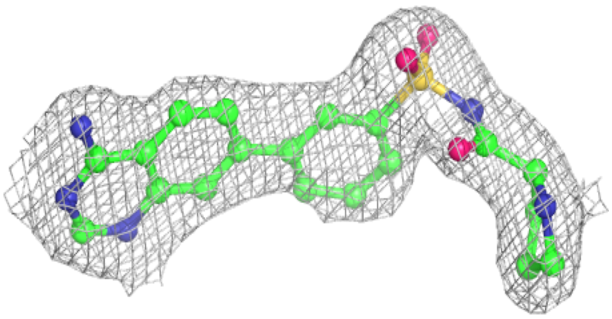
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q$<$ 0.9' lists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

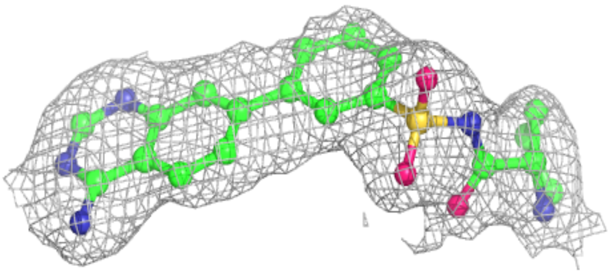
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	1603	4/4	0.84	0.17	51,54,55,55	0
3	EDO	B	1602	4/4	0.88	0.13	42,42,43,44	0
3	EDO	A	1602	4/4	0.89	0.18	41,44,44,45	0
2	W2H	B	1601	28/28	0.95	0.08	30,31,32,32	0
2	W2H	A	1601	28/28	0.97	0.07	25,27,28,29	0

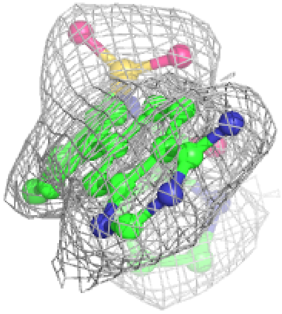
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight $>$ 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

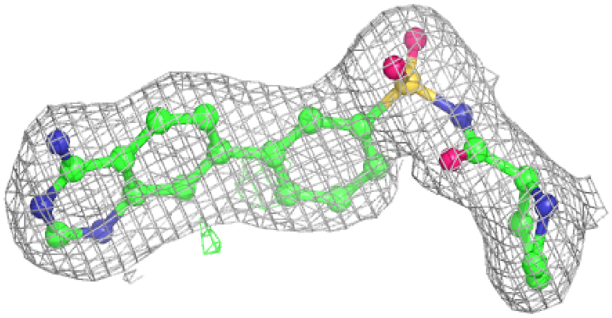


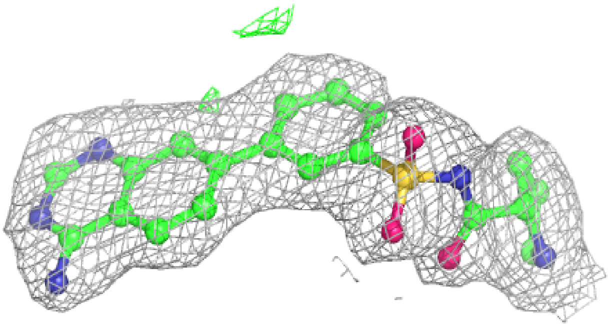


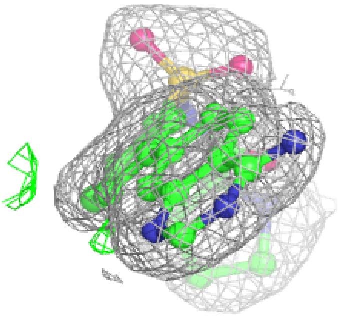


Electron density around W2H A 1601:

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 ⓘ

There are no such residues in this entry.