Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:31 PM EDT

PDB ID	:	5VAD
Title	:	Crystal structure of human Prolyl-tRNA synthetase (PRS) in complex with inhibitor
Authors	:	Okada, K.; Skene, R.J.
Deposited on	:	2017-03-24
Resolution	:	2.36 Å(reported)

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

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

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

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

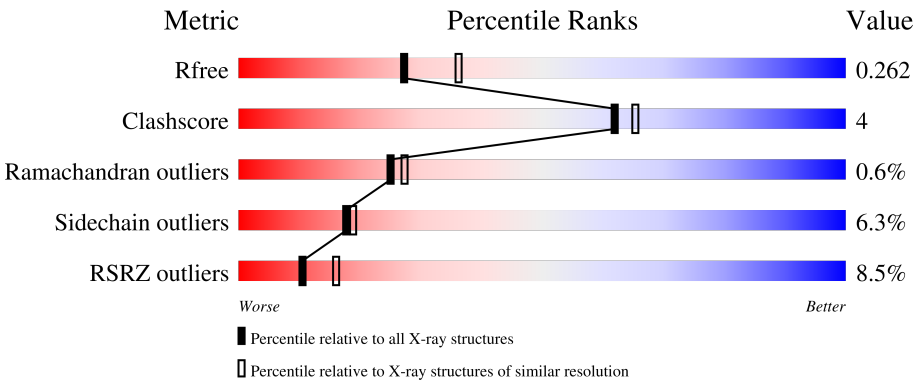
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	516	6% 80% 12% • 7%
1	B	516	9% 77% 14% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7849 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.

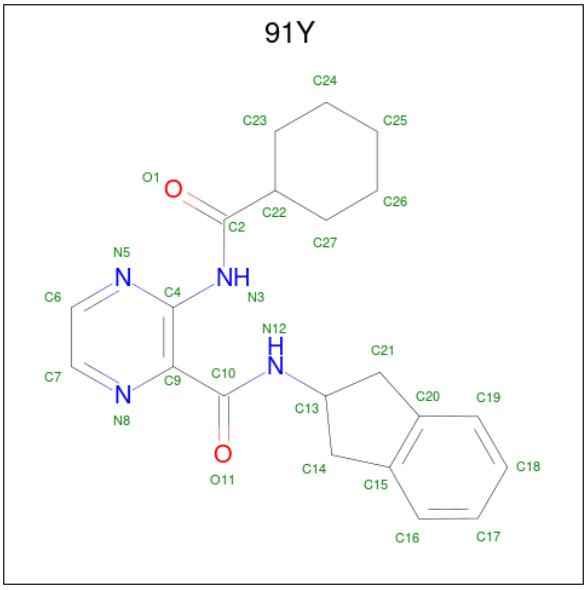
- Molecule 1 is a protein called Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3815	2445	641	704	25	0	0	0
1	B	482	3820	2448	642	705	25	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	997	GLY	-	expression tag	UNP P07814
B	997	GLY	-	expression tag	UNP P07814

- Molecule 2 is 3-[(cyclohexanecarbonyl)amino]-N-(2,3-dihydro-1H-inden-2-yl)pyrazine-2-carboxamide (three-letter code: 91Y) (formula: $C_{21}H_{24}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	27	21	4	2	0	0

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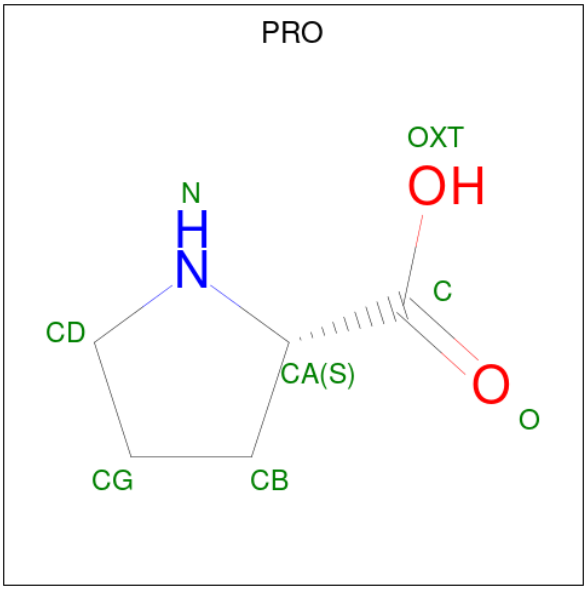
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	27	21	4	2	0	0

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

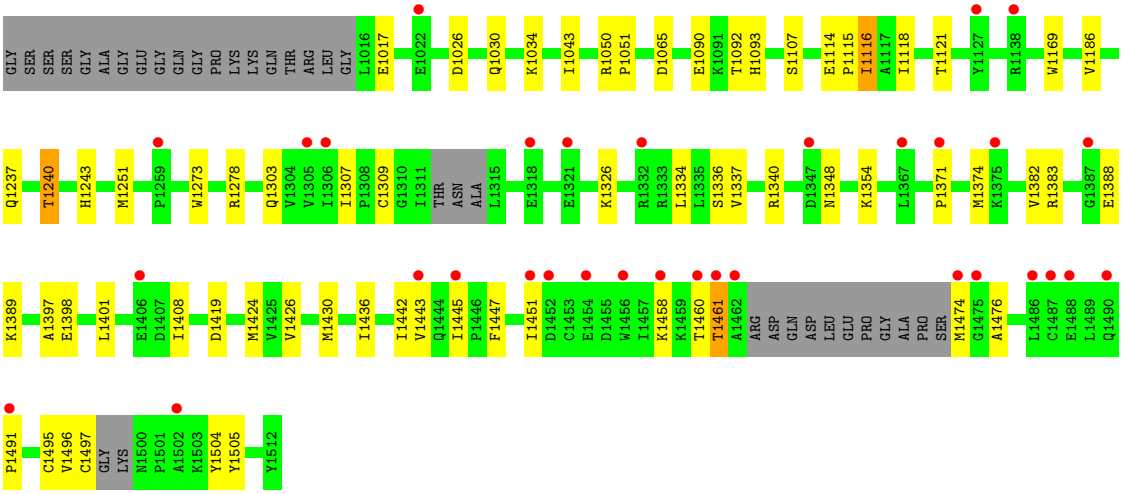
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	73	73	73	0	0
5	B	69	69	69	0	0

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.

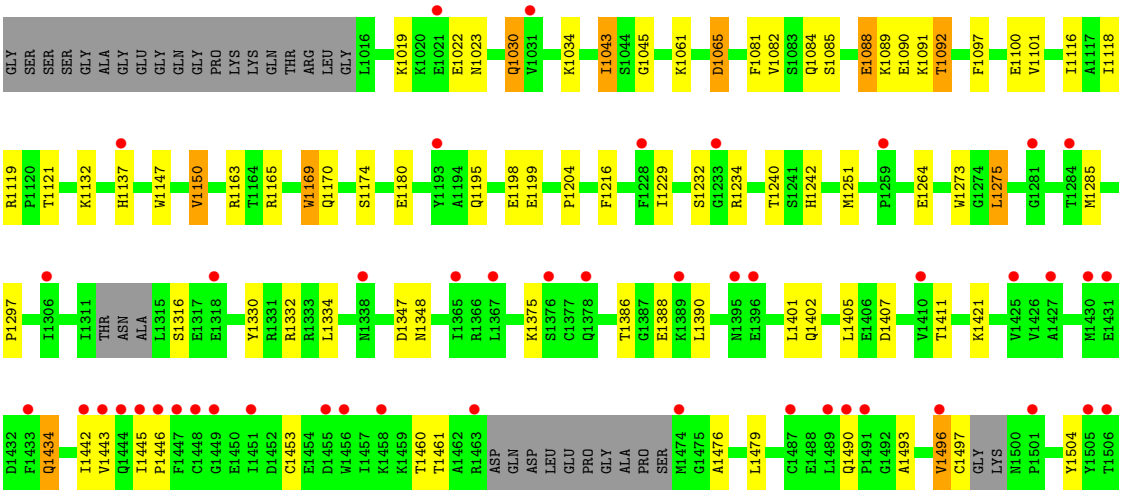
• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain A:



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

Chain B:



L1507
F1508
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	71.09Å 92.28Å 84.83Å 90.00° 111.18° 90.00°	Depositor
Resolution (Å)	19.93 – 2.36 19.93 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.93-2.36) 99.4 (19.93-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.262 0.196 , 0.262	Depositor DCC
R_{free} test set	2113 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.4	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	0.96	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 91Y, 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	0.66	0/3906	0.78	1/5296 (0.0%)
1	B	0.62	0/3911	0.76	0/5303
All	All	0.64	0/7817	0.77	1/10599 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1278	ARG	NE-CZ-NH2	-6.77	116.92	120.30

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	3815	0	3727	31	0
1	B	3820	0	3730	40	0
2	A	27	0	0	0	0
2	B	27	0	0	0	0
3	A	8	0	7	1	0
3	B	8	0	7	1	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	73	0	0	0	0
5	B	69	0	0	2	0
All	All	7849	0	7471	67	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 4.

All (67) 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:1237:GLN:NE2	1:A:1240:THR:HG23	1.93	0.83
1:B:1453:CYS:SG	4:B:1603:ZN:ZN	1.78	0.71
1:B:1085:SER:O	1:B:1089:LYS:HB2	1.93	0.69
1:A:1116:ILE:HG12	1:B:1043:ILE:HD12	1.76	0.67
1:B:1121:THR:HG1	3:B:1602:PRO:N	1.94	0.66
1:A:1237:GLN:NE2	1:A:1240:THR:CG2	2.61	0.63
1:B:1030:GLN:HG3	1:B:1034:LYS:HE2	1.81	0.63
1:B:1119:ARG:HG2	1:B:1150:VAL:HG22	1.81	0.63
1:A:1495:CYS:SG	1:A:1496:VAL:N	2.74	0.61
1:B:1232:SER:HB3	1:B:1234:ARG:HB2	1.83	0.61
1:B:1334:LEU:HD21	1:B:1401:LEU:HD12	1.82	0.61
1:A:1461:THR:CG2	1:A:1476:ALA:H	2.15	0.59
1:B:1479:LEU:HD12	1:B:1507:LEU:HG	1.85	0.58
1:A:1121:THR:HG1	3:A:1602:PRO:N	2.00	0.58
1:A:1017:GLU:HB3	1:A:1030:GLN:HE22	1.69	0.57
1:B:1251:MET:HG2	5:B:1763:HOH:O	2.05	0.57
1:B:1461:THR:HG23	1:B:1476:ALA:H	1.69	0.56
1:B:1407:ASP:O	1:B:1411:THR:OG1	2.17	0.56
1:B:1163:ARG:HD2	1:B:1512:TYR:HD1	1.70	0.56
1:B:1030:GLN:HG2	5:B:1706:HOH:O	2.06	0.55
1:A:1307:ILE:HG23	1:A:1354:LYS:HD2	1.88	0.55
1:A:1382:VAL:HG22	1:A:1389:LYS:HG2	1.88	0.55
1:A:1461:THR:HG21	1:A:1476:ALA:HB3	1.91	0.51
1:A:1118:ILE:HD11	1:B:1118:ILE:HD11	1.93	0.51
1:A:1090:GLU:HG3	1:A:1093:HIS:HB3	1.94	0.50
1:B:1445:ILE:HB	1:B:1496:VAL:HG21	1.94	0.49
1:A:1237:GLN:HE22	1:A:1240:THR:CG2	2.25	0.48
1:B:1097:PHE:O	1:B:1100:GLU:HG2	2.13	0.48
1:B:1195:GLN:O	1:B:1199:GLU:HB2	2.13	0.48
1:B:1442:ILE:HD12	1:B:1507:LEU:HD11	1.94	0.48
1:A:1426:VAL:HG13	1:A:1505:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:LEU:HD21	1:A:1401:LEU:HD12	1.95	0.47
1:A:1043:ILE:HD12	1:B:1116:ILE:HG12	1.96	0.47
1:B:1061:LYS:O	1:B:1065:ASP:HB2	2.14	0.47
1:B:1045:GLY:HA3	1:B:1165:ARG:HD2	1.96	0.47
1:B:1330:TYR:O	1:B:1334:LEU:HG	2.14	0.46
1:B:1461:THR:CG2	1:B:1476:ALA:H	2.28	0.46
1:B:1084:GLN:O	1:B:1088:GLU:HG3	2.15	0.46
1:A:1050:ARG:HB3	1:A:1051:PRO:HD2	1.96	0.46
1:A:1030:GLN:O	1:A:1034:LYS:HB2	2.16	0.45
1:B:1198:GLU:HG2	1:B:1204:PRO:HA	1.98	0.45
1:B:1453:CYS:SG	1:B:1497:CYS:SG	3.15	0.45
1:A:1186:VAL:HG21	1:A:1243:HIS:HB2	1.99	0.44
1:A:1309:CYS:O	1:A:1371:PRO:HD3	2.16	0.44
1:B:1119:ARG:HG2	1:B:1150:VAL:CG2	2.47	0.44
1:A:1430:MET:HB2	1:A:1496:VAL:HG13	1.98	0.44
1:B:1297:PRO:HB3	1:B:1405:LEU:HD22	2.00	0.43
1:B:1081:PHE:HB3	1:B:1116:ILE:CG2	2.48	0.43
1:B:1434:GLN:HE22	1:B:1461:THR:HA	1.82	0.43
1:A:1326:LYS:HG2	1:A:1374:MET:HG3	2.00	0.43
1:A:1447:PHE:HA	1:A:1495:CYS:SG	2.58	0.43
1:B:1446:PRO:HG2	1:B:1496:VAL:HG23	2.01	0.43
1:B:1490:GLN:HB2	1:B:1493:ALA:HB2	2.00	0.43
1:A:1445:ILE:O	1:A:1505:TYR:HA	2.18	0.42
1:A:1348:ASN:HD22	1:A:1348:ASN:N	2.16	0.42
1:A:1383:ARG:HG2	1:A:1408:ILE:HD11	2.01	0.42
1:A:1424:MET:HA	1:A:1442:ILE:O	2.19	0.42
1:A:1303:GLN:HG3	1:A:1340:ARG:HB2	2.01	0.42
1:B:1170:GLN:HE21	1:B:1275:LEU:HB3	1.85	0.42
1:B:1022:GLU:HG3	1:B:1023:ASN:H	1.85	0.41
1:A:1114:GLU:HA	1:A:1115:PRO:HD2	1.86	0.41
1:A:1337:VAL:HG21	1:A:1398:GLU:HB3	2.02	0.41
1:B:1147:TRP:CE3	1:B:1170:GLN:HB3	2.55	0.41
1:A:1107:SER:HA	1:B:1101:VAL:O	2.21	0.41
1:B:1229:ILE:HG23	1:B:1285:MET:HB3	2.03	0.41
1:B:1216:PHE:HB2	1:B:1242:HIS:CE1	2.57	0.40
1:B:1150:VAL:HG21	1:B:1169:TRP:CZ2	2.57	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	473/516 (92%)	459 (97%)	12 (2%)	2 (0%)	34	38
1	B	474/516 (92%)	447 (94%)	23 (5%)	4 (1%)	19	20
All	All	947/1032 (92%)	906 (96%)	35 (4%)	6 (1%)	25	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1388	GLU
1	B	1496	VAL
1	A	1491	PRO
1	A	1397	ALA
1	B	1092	THR
1	B	1264	GLU

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	404/440 (92%)	384 (95%)	20 (5%)	24	28
1	B	404/440 (92%)	373 (92%)	31 (8%)	13	12
All	All	808/880 (92%)	757 (94%)	51 (6%)	18	19

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1026	ASP
1	A	1065	ASP
1	A	1092	THR
1	A	1116	ILE
1	A	1169	TRP
1	A	1240	THR
1	A	1251	MET
1	A	1273	TRP
1	A	1336	SER
1	A	1388	GLU
1	A	1419	ASP
1	A	1436	ILE
1	A	1443	VAL
1	A	1451	ILE
1	A	1458	LYS
1	A	1460	THR
1	A	1461	THR
1	A	1474	MET
1	A	1497	CYS
1	A	1504	TYR
1	B	1019	LYS
1	B	1030	GLN
1	B	1043	ILE
1	B	1065	ASP
1	B	1082	VAL
1	B	1088	GLU
1	B	1090	GLU
1	B	1091	LYS
1	B	1092	THR
1	B	1132	LYS
1	B	1137	HIS
1	B	1150	VAL
1	B	1169	TRP
1	B	1174	SER
1	B	1180	GLU
1	B	1240	THR
1	B	1273	TRP
1	B	1275	LEU
1	B	1316	SER
1	B	1332	ARG
1	B	1347	ASP
1	B	1348	ASN
1	B	1375	LYS

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Mol	Chain	Res	Type
1	B	1386	THR
1	B	1390	LEU
1	B	1402	GLN
1	B	1421	LYS
1	B	1434	GLN
1	B	1443	VAL
1	B	1460	THR
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	1195	GLN
1	A	1237	GLN
1	A	1348	ASN
1	A	1423	HIS
1	B	1030	GLN
1	B	1170	GLN
1	B	1434	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 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
3	PRO	B	1602	-	8,8,8	0.72	0	10,10,10	1.38	2 (20%)
2	91Y	A	1601	-	30,30,30	0.66	0	35,41,41	1.46	7 (20%)
3	PRO	A	1602	-	8,8,8	0.80	0	10,10,10	1.52	2 (20%)
2	91Y	B	1601	-	30,30,30	0.73	0	35,41,41	1.55	7 (20%)

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	PRO	B	1602	-	-	2/4/11/11	0/1/1/1
2	91Y	A	1601	-	-	2/16/32/32	0/4/4/4
3	PRO	A	1602	-	-	0/4/11/11	0/1/1/1
2	91Y	B	1601	-	-	2/16/32/32	0/4/4/4

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	91Y	C9-C4-N5	-3.88	118.17	121.97
2	B	1601	91Y	C9-C4-N5	-3.80	118.25	121.97
3	A	1602	PRO	OXT-C-O	-3.05	117.17	124.09
2	B	1601	91Y	C22-C2-N3	2.77	119.09	115.02
2	B	1601	91Y	C4-C9-N8	-2.61	119.23	121.68
3	B	1602	PRO	OXT-C-CA	2.47	121.60	113.40
2	A	1601	91Y	C6-N5-C4	2.44	121.61	116.77
2	B	1601	91Y	C6-N5-C4	2.43	121.58	116.77
2	B	1601	91Y	C7-N8-C9	2.39	121.36	116.83
3	A	1602	PRO	OXT-C-CA	2.39	121.34	113.40
2	A	1601	91Y	C22-C2-N3	2.33	118.45	115.02
2	B	1601	91Y	C15-C14-C13	2.26	104.95	102.76
2	A	1601	91Y	C15-C14-C13	2.23	104.91	102.76
2	B	1601	91Y	O1-C2-N3	-2.19	119.21	123.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	91Y	C4-C9-N8	-2.19	119.63	121.68
3	B	1602	PRO	OXT-C-O	-2.18	119.13	124.09
2	A	1601	91Y	C7-N8-C9	2.12	120.83	116.83
2	A	1601	91Y	N3-C4-N5	2.06	122.73	117.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

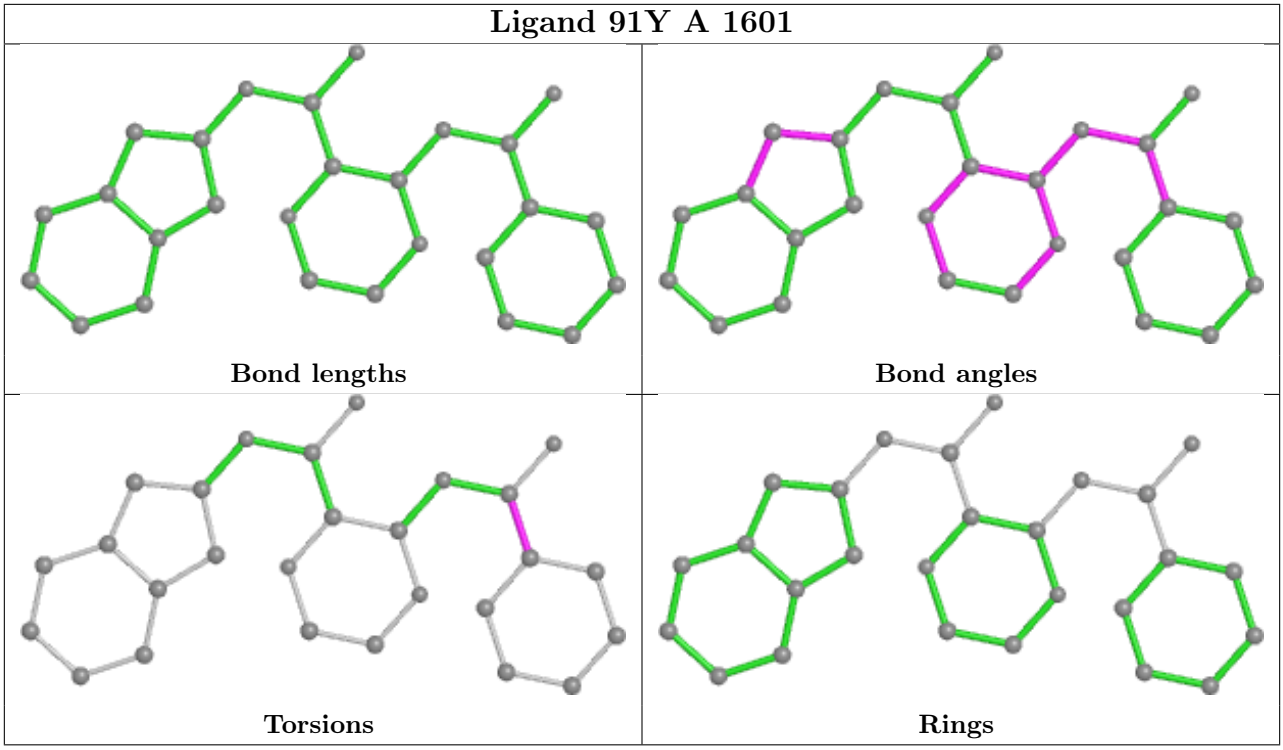
Mol	Chain	Res	Type	Atoms
2	B	1601	91Y	O1-C2-C22-C27
2	A	1601	91Y	N3-C2-C22-C27
2	B	1601	91Y	N3-C2-C22-C27
2	A	1601	91Y	O1-C2-C22-C27
3	B	1602	PRO	O-C-CA-CB
3	B	1602	PRO	OXT-C-CA-CB

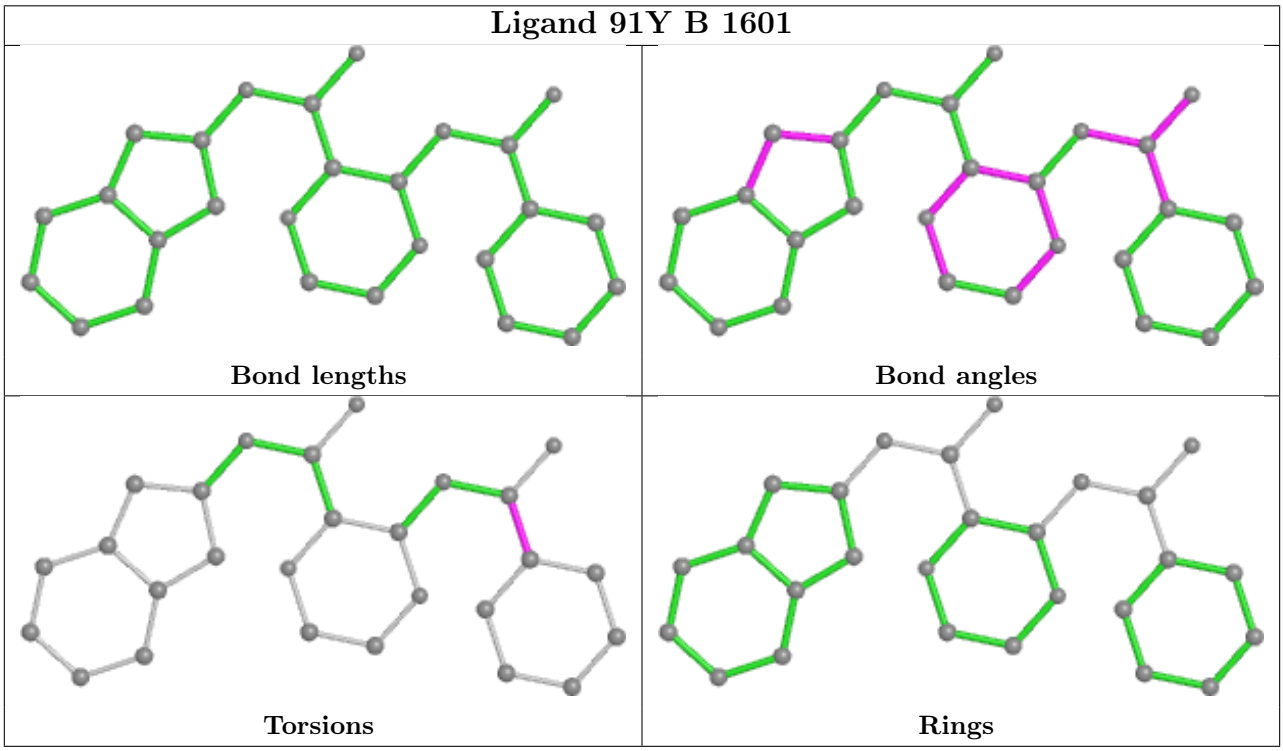
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1602	PRO	1	0
3	A	1602	PRO	1	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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	481/516 (93%)	0.24	33 (6%)	16	24	30, 69, 115, 145	4 (0%)
1	B	482/516 (93%)	0.42	49 (10%)	6	11	31, 74, 129, 158	5 (1%)
All	All	963/1032 (93%)	0.33	82 (8%)	10	16	30, 72, 124, 158	9 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1496	VAL	6.5
1	A	1259	PRO	6.4
1	A	1462	ALA	6.2
1	A	1367	LEU	5.4
1	A	1487	CYS	5.4
1	B	1443	VAL	5.0
1	B	1456	TRP	4.9
1	A	1491	PRO	4.9
1	B	1491	PRO	4.8
1	B	1396	GLU	4.8
1	B	1490	GLN	4.5
1	B	1487	CYS	4.4
1	B	1489	LEU	4.4
1	B	1446	PRO	4.1
1	A	1451	ILE	3.9
1	A	1460	THR	3.7
1	B	1376	SER	3.6
1	A	1486	LEU	3.3
1	A	1490	GLN	3.3
1	B	1367	LEU	3.3
1	A	1445	ILE	3.3
1	B	1447	PHE	3.3
1	B	1137	HIS	3.3
1	A	1371	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1445	ILE	3.2
1	A	1306	ILE	3.2
1	B	1430	MET	3.2
1	A	1321	GLU	3.1
1	B	1455	ASP	3.0
1	B	1508	PHE	3.0
1	A	1488	GLU	3.0
1	A	1138	ARG	2.9
1	B	1463	ARG	2.8
1	B	1474	MET	2.8
1	B	1451	ILE	2.8
1	A	1406	GLU	2.8
1	A	1458	LYS	2.8
1	A	1318	GLU	2.7
1	B	1433	PHE	2.7
1	A	1454	GLU	2.7
1	B	1507	LEU	2.7
1	B	1431	GLU	2.7
1	B	1378	GLN	2.7
1	B	1233	GLY	2.7
1	B	1338	ASN	2.6
1	A	1443	VAL	2.6
1	B	1425	VAL	2.5
1	B	1448	CYS	2.5
1	B	1427	ALA	2.5
1	B	1505	TYR	2.5
1	B	1458	LYS	2.4
1	B	1444	GLN	2.4
1	B	1501	PRO	2.4
1	A	1022	GLU	2.4
1	A	1474	MET	2.4
1	B	1259	PRO	2.4
1	A	1347	ASP	2.4
1	B	1021	GLU	2.4
1	B	1365	ILE	2.3
1	A	1502	ALA	2.3
1	A	1452	ASP	2.3
1	A	1461	THR	2.3
1	A	1456	TRP	2.3
1	B	1284	THR	2.3
1	B	1281	GLY	2.2
1	B	1318	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1127	TYR	2.2
1	B	1410	VAL	2.2
1	B	1193	TYR	2.2
1	B	1389	LYS	2.2
1	A	1387	GLY	2.2
1	A	1305	VAL	2.2
1	B	1228	PHE	2.2
1	B	1506	THR	2.1
1	B	1395	ASN	2.1
1	B	1031	VAL	2.1
1	B	1449	GLY	2.1
1	B	1306	ILE	2.1
1	A	1332	ARG	2.0
1	A	1375	LYS	2.0
1	B	1442	ILE	2.0
1	A	1475	GLY	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)

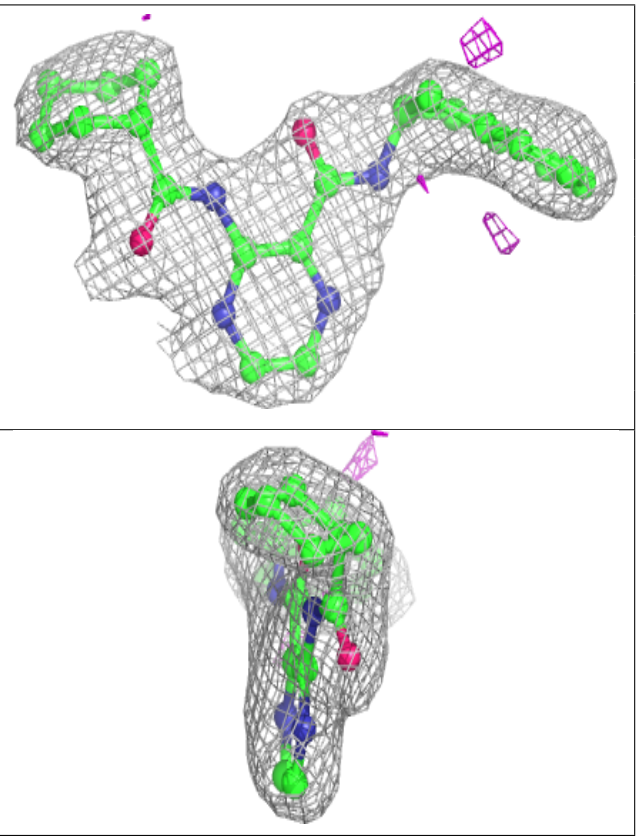
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

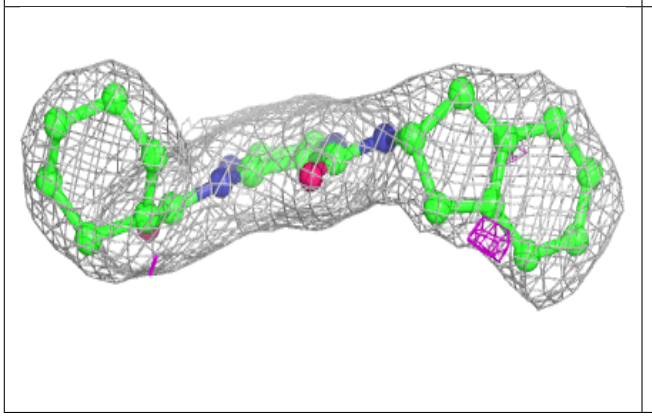
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PRO	A	1602	8/8	0.91	0.15	37,42,44,46	0
2	91Y	B	1601	27/27	0.95	0.12	43,50,53,55	0
2	91Y	A	1601	27/27	0.95	0.12	39,48,53,55	0
3	PRO	B	1602	8/8	0.95	0.12	42,48,53,56	0
4	ZN	B	1603	1/1	0.97	0.08	139,139,139,139	0
4	ZN	A	1603	1/1	0.98	0.06	102,102,102,102	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 91Y B 1601:

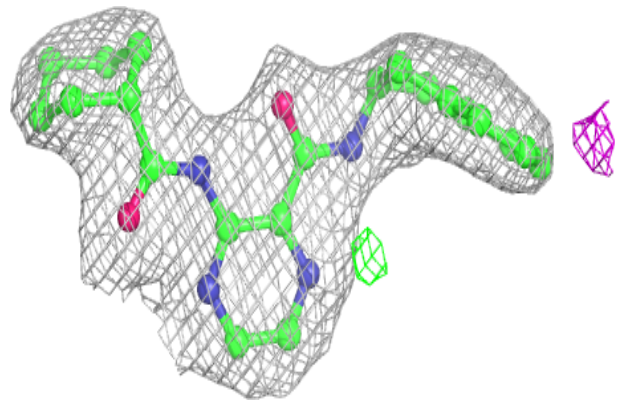
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

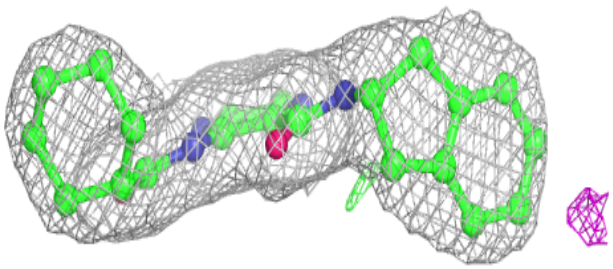


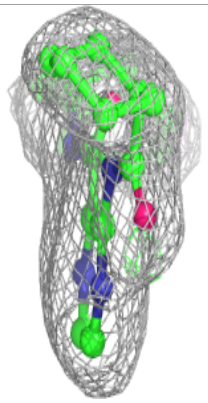


Electron density around 91Y A 1601:

$2mF_o$-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.