



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 09:46 PM EDT

PDB ID : 8D1T  
Title : Crystal structure of human USP30 in complex with a covalent inhibitor 552 and a Fab  
Authors : Song, X.; Butler, J.; Li, C.; Zhang, K.; Zhang, D.; Hao, Y.  
Deposited on : 2022-05-27  
Resolution : 2.94 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

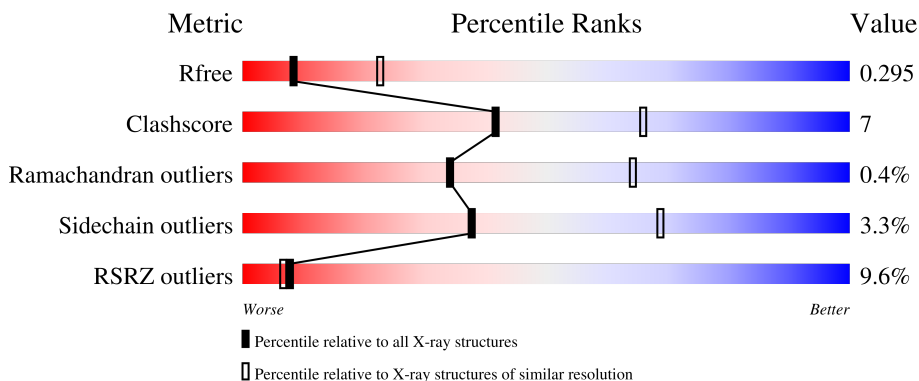
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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	349	 4% 76% 16% • 5%
2	H	222	 14% 68% 13% • 18%
3	L	214	 11% 78% 13% • 8%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5608 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 Ubiquitin carboxyl-terminal hydrolase 30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2657	1680	468	492	17	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP Q70CQ3
A	179	GLY	-	linker	UNP Q70CQ3
A	180	SER	-	linker	UNP Q70CQ3
A	181	GLY	-	linker	UNP Q70CQ3
A	182	SER	-	linker	UNP Q70CQ3
A	348	ASP	PHE	engineered mutation	UNP Q70CQ3
A	350	SER	MET	engineered mutation	UNP Q70CQ3
A	353	GLU	ILE	engineered mutation	UNP Q70CQ3
A	358	SER	-	linker	UNP Q70CQ3
A	359	ASN	-	linker	UNP Q70CQ3
A	360	ALA	-	linker	UNP Q70CQ3
A	503	LEU	-	expression tag	UNP Q70CQ3
A	504	GLU	-	expression tag	UNP Q70CQ3
A	505	VAL	-	expression tag	UNP Q70CQ3
A	506	LEU	-	expression tag	UNP Q70CQ3
A	507	PHE	-	expression tag	UNP Q70CQ3
A	508	GLN	-	expression tag	UNP Q70CQ3
A	509	GLY	-	expression tag	UNP Q70CQ3
A	510	PRO	-	expression tag	UNP Q70CQ3
A	511	HIS	-	expression tag	UNP Q70CQ3
A	512	HIS	-	expression tag	UNP Q70CQ3
A	513	HIS	-	expression tag	UNP Q70CQ3
A	514	HIS	-	expression tag	UNP Q70CQ3
A	515	HIS	-	expression tag	UNP Q70CQ3
A	516	HIS	-	expression tag	UNP Q70CQ3

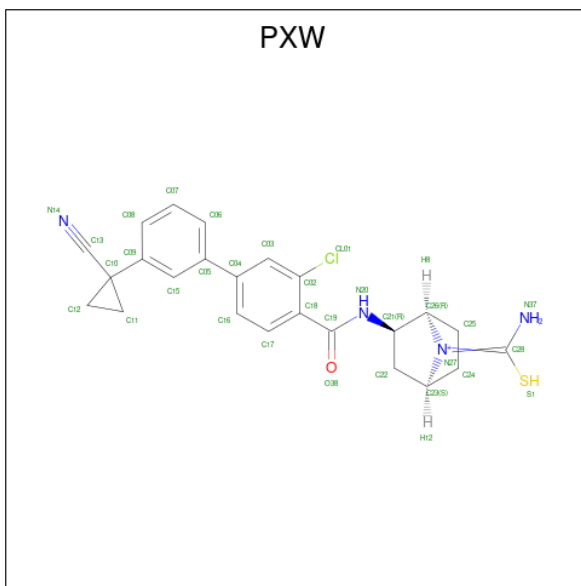
- Molecule 2 is a protein called mouse anti-huUSP30 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	183	1370	861	224	278	7	0	0	0

- Molecule 3 is a protein called mouse anti-huUSP30 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	197	1516	942	256	312	6	0	0	0

- Molecule 4 is (1R,2R,4S,7E)-7-[amino(sulfanyl)methylidene]-2-[[[(1P)-3-chloro-3'-(1-cyanocyclopropyl)[1,1'-biphenyl]-4-carbonyl]amino}-7-azabicyclo[2.2.1]heptan-7-ium (three-letter code: PXW) (formula: C<sub>24</sub>H<sub>24</sub>ClN<sub>4</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	30	24	1	4	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

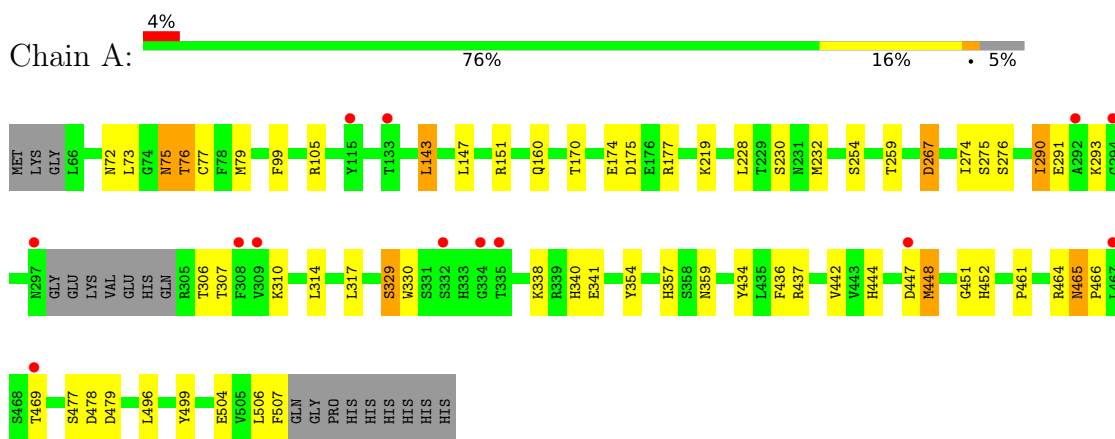
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0
7	H	8	Total O 8 8	0	0
7	L	5	Total O 5 5	0	0

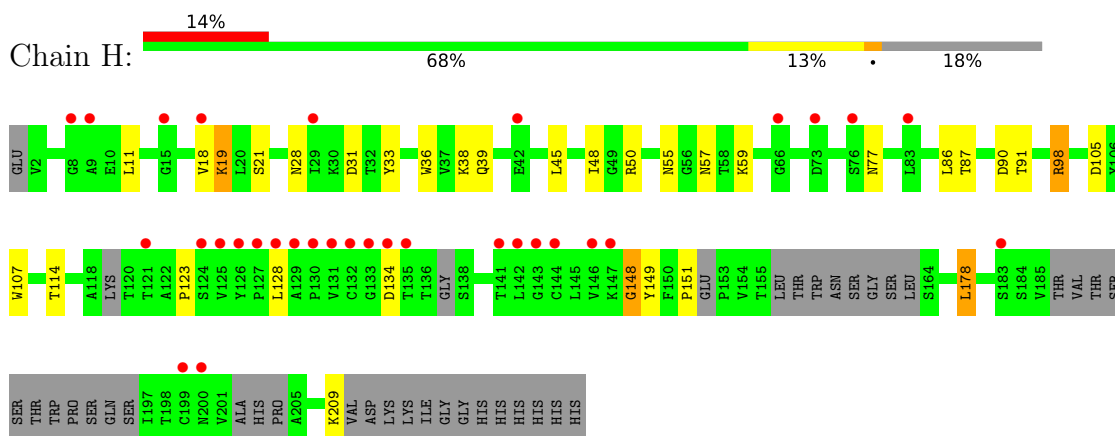
### 3 Residue-property plots

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.

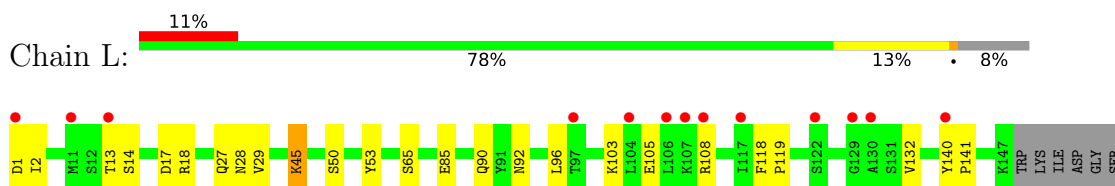
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 30

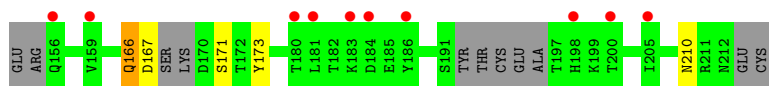


- Molecule 2: mouse anti-huUSP30 Fab heavy chain



- Molecule 3: mouse anti-huUSP30 Fab light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.88Å 71.72Å 148.63Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	40.70 – 2.94 40.70 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.70-2.94) 99.5 (40.70-2.94)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.95Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.236 , 0.294 0.237 , 0.295	Depositor DCC
$R_{free}$ test set	918 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, EDO, PXW

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	0.27	0/2728	0.54	2/3703 (0.1%)
2	H	0.27	0/1397	0.58	0/1900
3	L	0.28	0/1545	0.56	0/2094
All	All	0.27	0/5670	0.56	2/7697 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	73	LEU	CA-CB-CG	5.18	127.21	115.30

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	2657	0	2560	40	2
2	H	1370	0	1321	19	0
3	L	1516	0	1450	19	0
4	A	30	0	0	3	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	17	0	0	0	0
7	H	8	0	0	0	0
7	L	5	0	0	0	0
All	All	5608	0	5337	76	2

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 7.

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)
2:H:33:TYR:HD2	2:H:50:ARG:HD3	1.39	0.87
1:A:329:SER:O	4:A:601:PXW:C11	2.28	0.81
2:H:91:THR:HG23	2:H:114:THR:HA	1.62	0.81
3:L:2:ILE:HG21	3:L:90:GLN:HG2	1.64	0.80
2:H:31:ASP:HB2	2:H:98:ARG:HH22	1.52	0.74
1:A:177:ARG:NH2	1:A:219:LYS:O	2.24	0.71
3:L:85:GLU:HG3	3:L:103:LYS:HG2	1.75	0.69
1:A:75:ASN:HB3	1:A:160:GLN:OE1	1.94	0.67
1:A:314:LEU:HD13	1:A:317:LEU:HD21	1.76	0.66
1:A:72:ASN:ND2	1:A:77:CYS:SG	2.69	0.66
1:A:357:HIS:CD2	1:A:359:ASN:HD22	2.14	0.64
2:H:33:TYR:CD2	2:H:50:ARG:HD3	2.28	0.63
2:H:87:THR:N	2:H:90:ASP:OD2	2.27	0.62
1:A:329:SER:C	4:A:601:PXW:C11	2.69	0.61
1:A:170:THR:O	1:A:174:GLU:HG3	2.00	0.61
2:H:128:LEU:HB3	3:L:118:PHE:CD2	2.37	0.60
1:A:461:PRO:HG3	1:A:469:THR:HA	1.86	0.57
3:L:105:GLU:HG3	3:L:173:TYR:OH	2.05	0.56
1:A:290:ILE:HG22	1:A:291:GLU:HG2	1.90	0.54
1:A:77:CYS:HB3	1:A:478:ASP:OD1	2.08	0.54
2:H:28:ASN:HA	2:H:77:ASN:HD21	1.72	0.54
1:A:230:SER:HB3	1:A:310:LYS:HE2	1.91	0.53
3:L:140:TYR:HB3	3:L:141:PRO:HD3	1.89	0.53
1:A:341:GLU:N	1:A:341:GLU:OE2	2.42	0.52
3:L:108:ARG:HB2	3:L:140:TYR:CE2	2.45	0.51
1:A:105:ARG:HH21	1:A:105:ARG:HG3	1.75	0.51
2:H:19:LYS:HZ2	2:H:21:SER:HG	1.58	0.51
1:A:437:ARG:NH1	1:A:506:LEU:O	2.43	0.50
3:L:13:THR:HG22	3:L:105:GLU:O	2.11	0.50
2:H:148:GLY:HA2	2:H:178:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:OD1	1:A:76:THR:HG23	2.13	0.49
1:A:314:LEU:HD12	1:A:354:TYR:HB2	1.95	0.48
2:H:134:ASP:N	2:H:134:ASP:OD1	2.43	0.48
3:L:105:GLU:HG2	3:L:166:GLN:HE21	1.77	0.48
1:A:259:THR:HB	3:L:96:LEU:HD21	1.95	0.47
3:L:27:GLN:HG2	3:L:28:ASN:N	2.27	0.47
2:H:55:ASN:OD1	2:H:57:ASN:ND2	2.48	0.47
3:L:17:ASP:OD1	3:L:18:ARG:N	2.48	0.47
2:H:36:TRP:HB2	2:H:48:ILE:HD11	1.97	0.46
1:A:436:PHE:HB3	1:A:499:TYR:HB3	1.97	0.46
2:H:36:TRP:O	2:H:48:ILE:HG13	2.16	0.46
3:L:2:ILE:CG2	3:L:90:GLN:HG2	2.42	0.46
2:H:39:GLN:HG3	2:H:45:LEU:HG	1.99	0.45
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.98	0.45
1:A:276:SER:OG	1:A:310:LYS:O	2.28	0.44
1:A:447:ASP:O	1:A:451:GLY:N	2.49	0.44
1:A:338:LYS:HE2	1:A:444:HIS:ND1	2.32	0.44
3:L:29:VAL:C	3:L:92:ASN:HD22	2.20	0.43
3:L:45:LYS:HE2	3:L:45:LYS:HB2	1.75	0.43
1:A:232:MET:HE2	1:A:232:MET:HB3	1.87	0.43
3:L:85:GLU:CG	3:L:103:LYS:HG2	2.45	0.43
1:A:105:ARG:HG3	1:A:105:ARG:NH2	2.32	0.43
1:A:452:HIS:HE1	1:A:477:SER:OG	2.02	0.43
2:H:11:LEU:HD21	2:H:151:PRO:HB3	2.01	0.43
2:H:105:ASP:OD1	2:H:107:TRP:NE1	2.51	0.43
1:A:306:THR:HG22	1:A:307:THR:H	1.82	0.43
1:A:465:ASN:N	1:A:466:PRO:HD3	2.34	0.43
3:L:50:SER:HB3	3:L:53:TYR:CD1	2.54	0.42
1:A:267:ASP:OD1	1:A:267:ASP:N	2.52	0.42
1:A:143:LEU:O	1:A:147:LEU:HD23	2.19	0.42
1:A:338:LYS:HD3	1:A:340:HIS:NE2	2.34	0.42
3:L:2:ILE:HD13	3:L:2:ILE:HA	1.86	0.42
2:H:123:PRO:HD3	2:H:149:TYR:HB3	2.01	0.42
1:A:293:LYS:N	1:A:293:LYS:HD2	2.35	0.42
1:A:306:THR:HG22	1:A:307:THR:N	2.35	0.42
1:A:274:ILE:HD12	1:A:275:SER:N	2.34	0.41
1:A:506:LEU:HD12	1:A:507:PHE:H	1.84	0.41
1:A:448:MET:CE	4:A:601:PXW:CL01	3.06	0.41
3:L:119:PRO:HA	3:L:132:VAL:HG23	2.03	0.41
2:H:38:LYS:HB2	2:H:38:LYS:HE3	1.89	0.41
3:L:166:GLN:OE1	3:L:171:SER:OG	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD23	1:A:314:LEU:HD23	2.02	0.40
1:A:357:HIS:CD2	1:A:359:ASN:HB3	2.56	0.40
1:A:99:PHE:CE1	1:A:219:LYS:HB3	2.56	0.40
1:A:442:VAL:HB	1:A:496:LEU:HB2	2.03	0.40
1:A:504:GLU:HA	1:A:504:GLU:OE2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:OH	1:A:479:ASP:OD2[2_555]	2.07	0.13
1:A:175:ASP:OD1	1:A:464:ARG:NH1[1_655]	2.12	0.08

## 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	326/349 (93%)	310 (95%)	15 (5%)	1 (0%)	41	69
2	H	169/222 (76%)	156 (92%)	12 (7%)	1 (1%)	25	56
3	L	189/214 (88%)	174 (92%)	14 (7%)	1 (0%)	29	60
All	All	684/785 (87%)	640 (94%)	41 (6%)	3 (0%)	34	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	210	ASN
1	A	290	ILE
2	H	148	GLY

### 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	303/321 (94%)	293 (97%)	10 (3%)	38	69
2	H	154/188 (82%)	149 (97%)	5 (3%)	39	70
3	L	174/190 (92%)	168 (97%)	6 (3%)	37	68
All	All	631/699 (90%)	610 (97%)	21 (3%)	38	69

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	76	THR
1	A	79	MET
1	A	151	ARG
1	A	254	SER
1	A	267	ASP
1	A	329	SER
1	A	330	TRP
1	A	448	MET
1	A	465	ASN
2	H	19	LYS
2	H	59	LYS
2	H	98	ARG
2	H	178	LEU
2	H	209	LYS
3	L	1	ASP
3	L	14	SER
3	L	45	LYS
3	L	65	SER
3	L	166	GLN
3	L	167	ASP

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	114	GLN
1	A	268	HIS
1	A	357	HIS
1	A	452	HIS
2	H	77	ASN
3	L	92	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
4	PXW	A	601	1	28,34,35	4.49	12 (42%)	39,51,53	4.49	20 (51%)
6	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.35	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
4	PXW	A	601	1	-	0/18/48/50	0/6/5/5
6	EDO	A	603	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	PXW	C22-C21	-10.17	1.36	1.54
4	A	601	PXW	C25-C26	-9.83	1.31	1.52
4	A	601	PXW	C22-C23	-8.30	1.40	1.53
4	A	601	PXW	C21-N20	7.94	1.59	1.46
4	A	601	PXW	C10-C09	-7.48	1.48	1.53
4	A	601	PXW	C24-C23	-6.99	1.28	1.52
4	A	601	PXW	C19-N20	6.07	1.47	1.34
4	A	601	PXW	C25-C24	-4.37	1.42	1.54
4	A	601	PXW	C05-C04	-4.23	1.38	1.49
4	A	601	PXW	O38-C19	-4.22	1.14	1.23
4	A	601	PXW	C08-C09	-2.83	1.34	1.39
4	A	601	PXW	C17-C18	-2.20	1.36	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	PXW	C26-N27-C23	-19.39	87.12	111.46
4	A	601	PXW	C26-C21-N20	-8.82	100.52	113.09
4	A	601	PXW	C18-C19-N20	6.68	129.16	116.80
4	A	601	PXW	C25-C26-N27	-6.16	88.78	102.85
4	A	601	PXW	C23-N27-C28	5.82	133.02	123.85
4	A	601	PXW	C26-N27-C28	-5.79	115.01	123.81
4	A	601	PXW	O38-C19-C18	-5.54	110.89	121.01
4	A	601	PXW	C24-C23-N27	-5.05	91.38	102.80
4	A	601	PXW	C11-C10-C12	4.16	60.12	58.37
4	A	601	PXW	C22-C23-C24	-3.84	105.77	109.57
4	A	601	PXW	C21-N20-C19	-3.26	117.08	123.01
4	A	601	PXW	C25-C24-C23	3.09	108.70	104.06
4	A	601	PXW	C07-C08-C09	-3.08	117.52	120.76
4	A	601	PXW	C08-C09-C15	2.90	123.35	117.76
4	A	601	PXW	C22-C21-N20	2.78	118.33	112.39
4	A	601	PXW	C24-C25-C26	2.72	108.27	104.02
4	A	601	PXW	C22-C21-C26	2.58	108.46	104.02
4	A	601	PXW	C09-C10-C13	-2.55	109.35	114.27
4	A	601	PXW	C03-C02-CL01	-2.23	114.89	118.49
4	A	601	PXW	C04-C03-C02	-2.15	118.21	120.35

There are no chirality outliers.

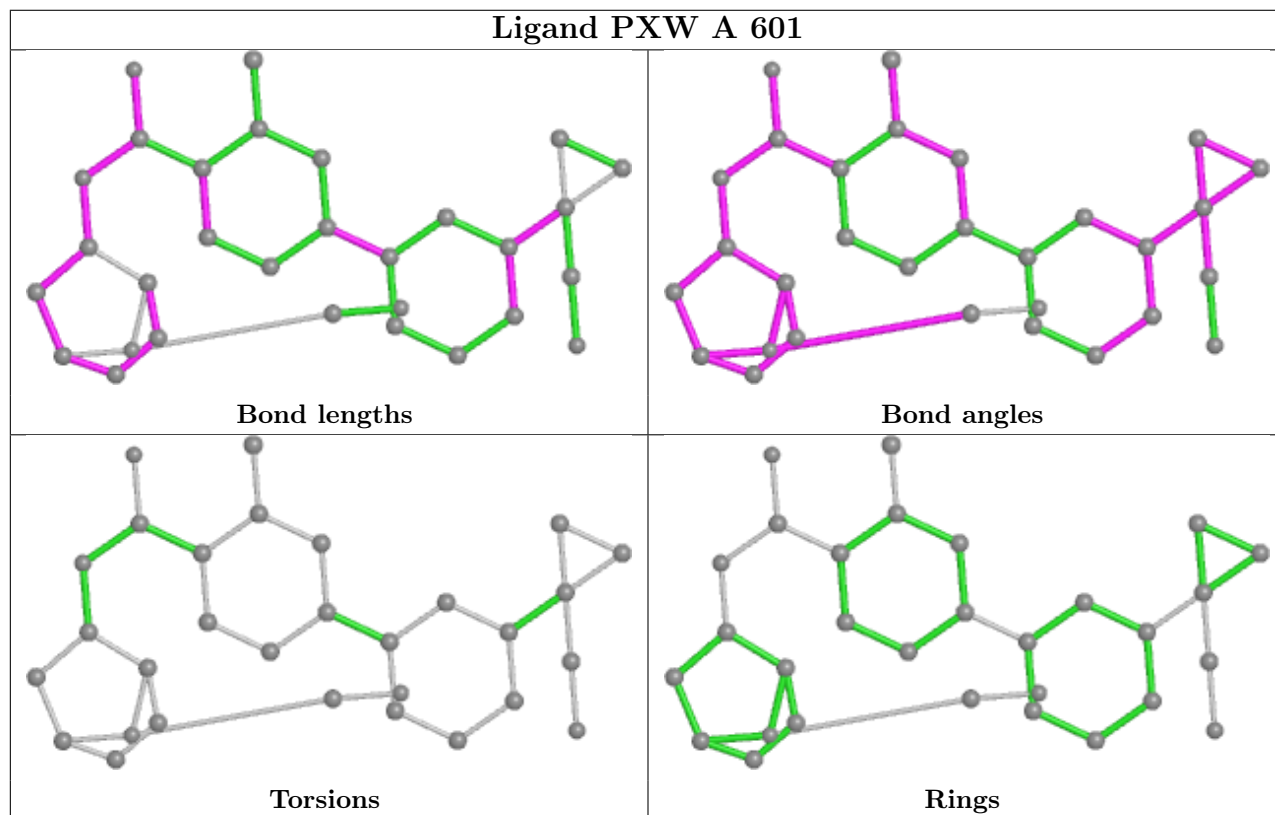
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	PXW	3	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	330/349 (94%)	0.47	13 (3%) 39 39	40, 67, 125, 140	0
2	H	183/222 (82%)	0.99	32 (17%) 1 1	69, 110, 146, 167	0
3	L	197/214 (92%)	0.76	23 (11%) 4 4	57, 111, 150, 153	0
All	All	710/785 (90%)	0.69	68 (9%) 8 7	40, 95, 142, 167	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	125	VAL	7.4
3	L	130	ALA	7.2
2	H	135	THR	6.1
3	L	205	ILE	5.9
1	A	297	ASN	5.6
2	H	124	SER	5.2
2	H	133	GLY	5.1
2	H	130	PRO	5.0
2	H	199	CYS	4.7
1	A	309	VAL	4.7
2	H	132	CYS	4.5
2	H	126	TYR	4.5
3	L	180	THR	4.2
1	A	292	ALA	4.1
3	L	129	GLY	4.1
2	H	134	ASP	4.0
2	H	129	ALA	4.0
2	H	142	LEU	4.0
2	H	131	VAL	3.9
2	H	128	LEU	3.9
1	A	294	GLY	3.9
3	L	106	LEU	3.8
3	L	108	ARG	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	186	TYR	3.8
2	H	15	GLY	3.7
2	H	144	CYS	3.4
1	A	334	GLY	3.4
3	L	140	TYR	3.3
3	L	200	THR	3.3
1	A	332	SER	3.3
2	H	183	SER	3.3
2	H	121	THR	3.2
3	L	1	ASP	2.9
2	H	9	ALA	2.9
1	A	133	THR	2.8
2	H	76	SER	2.8
2	H	83	LEU	2.7
1	A	467	LEU	2.7
1	A	335	THR	2.7
3	L	181	LEU	2.7
3	L	97	THR	2.7
3	L	117	ILE	2.6
1	A	308	PHE	2.6
3	L	183	LYS	2.5
2	H	143	GLY	2.5
2	H	146	VAL	2.5
2	H	73	ASP	2.4
2	H	29	ILE	2.4
2	H	66	GLY	2.4
2	H	42	GLU	2.3
3	L	13	THR	2.3
2	H	200	ASN	2.3
3	L	11	MET	2.3
2	H	18	VAL	2.3
3	L	104	LEU	2.3
3	L	159	VAL	2.3
3	L	122	SER	2.2
2	H	127	PRO	2.2
3	L	156	GLN	2.2
3	L	107	LYS	2.2
2	H	141	THR	2.2
1	A	447	ASP	2.2
2	H	147	LYS	2.1
2	H	8	GLY	2.1
3	L	198	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	469	THR	2.1
3	L	184	ASP	2.1
1	A	115	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

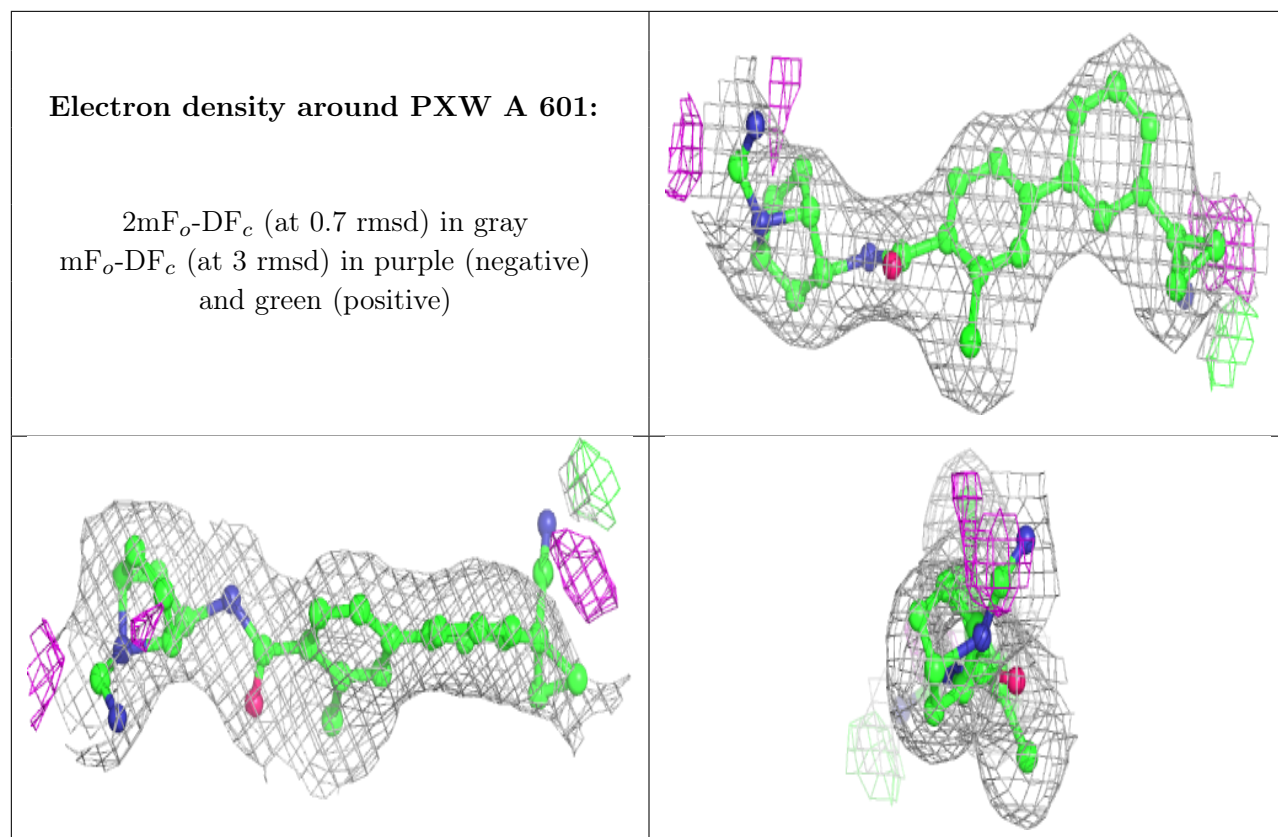
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	A	603	4/4	0.90	0.21	75,85,86,86	0
4	PXW	A	601	30/31	0.92	0.20	41,60,106,149	0
5	ZN	A	602	1/1	0.98	0.08	117,117,117,117	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.