



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 04:15 PM EDT

PDB ID : 7SVO  
Title : DPP8 IN COMPLEX WITH LIGAND ICeD-1  
Authors : Lammens, A.; Hollenstein, K.; Klein, D.J.  
Deposited on : 2021-11-19  
Resolution : 2.58 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 : 2.31.2  
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) : 2.31.2

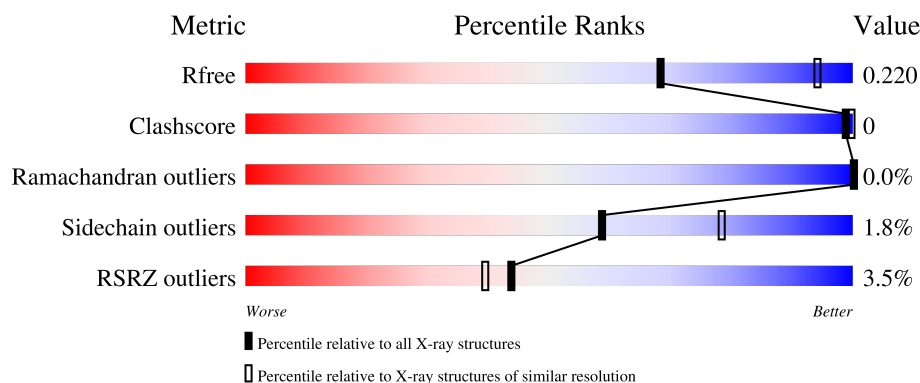
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	903	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	903	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	903	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21620 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.

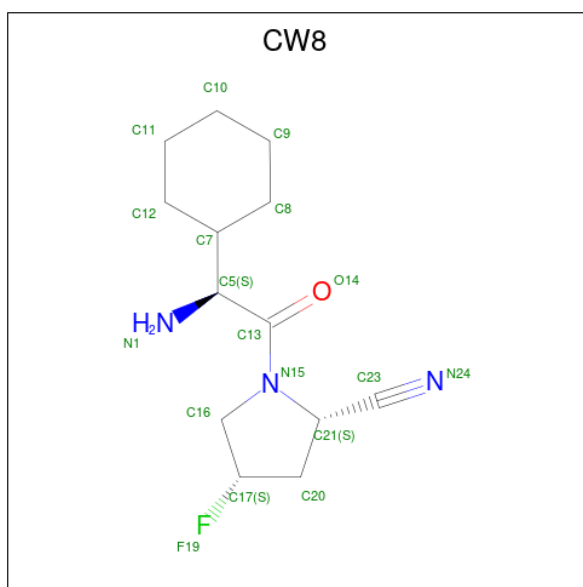
- Molecule 1 is a protein called Dipeptidyl peptidase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	848	Total	C	N	O	S	77	5	0
			6947	4459	1169	1290	29			
1	B	849	Total	C	N	O	S	89	7	0
			6970	4474	1172	1295	29			
1	C	840	Total	C	N	O	S	73	6	0
			6892	4423	1162	1280	27			

There are 15 discrepancies between the modelled and reference sequences:

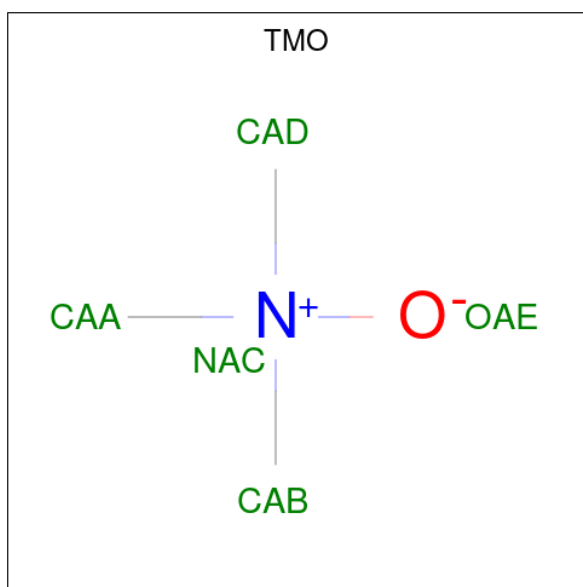
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q6V1X1
A	-3	ALA	-	expression tag	UNP Q6V1X1
A	-2	MET	-	expression tag	UNP Q6V1X1
A	-1	GLY	-	expression tag	UNP Q6V1X1
A	0	SER	-	expression tag	UNP Q6V1X1
B	-4	GLY	-	expression tag	UNP Q6V1X1
B	-3	ALA	-	expression tag	UNP Q6V1X1
B	-2	MET	-	expression tag	UNP Q6V1X1
B	-1	GLY	-	expression tag	UNP Q6V1X1
B	0	SER	-	expression tag	UNP Q6V1X1
C	-4	GLY	-	expression tag	UNP Q6V1X1
C	-3	ALA	-	expression tag	UNP Q6V1X1
C	-2	MET	-	expression tag	UNP Q6V1X1
C	-1	GLY	-	expression tag	UNP Q6V1X1
C	0	SER	-	expression tag	UNP Q6V1X1

- Molecule 2 is (2S,4S)-1-[(2S)-2-amino-2-cyclohexylacetyl]-4-fluoropyrrolidine-2-carbonitrile (three-letter code: CW8) (formula: C<sub>13</sub>H<sub>20</sub>FN<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			18	13	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			18	13	1	3	1		
2	C	1	Total	C	F	N	O	0	0
			18	13	1	3	1		

- Molecule 3 is trimethylamine oxide (three-letter code: TMO) (formula:  $C_3H_9NO$ ).



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

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

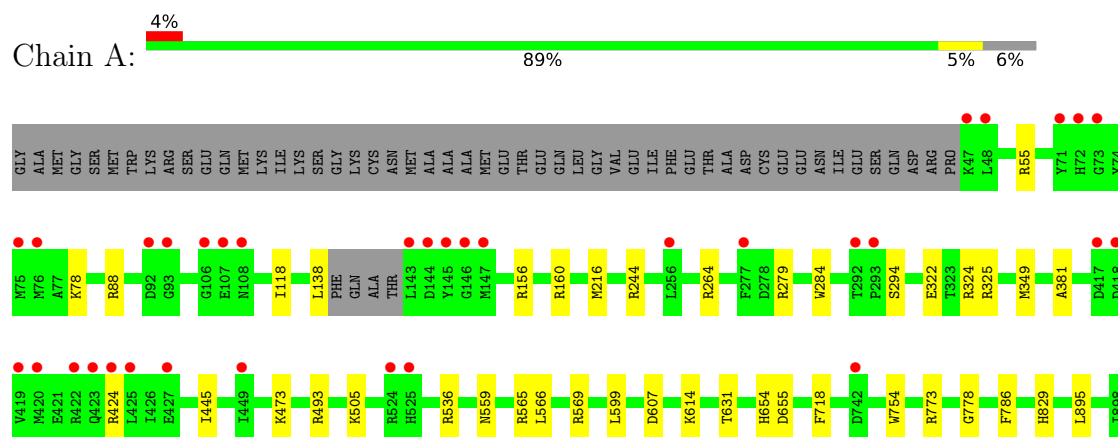
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	243	Total	O	0	0
			243	243		
4	C	259	Total	O	0	0
			259	259		

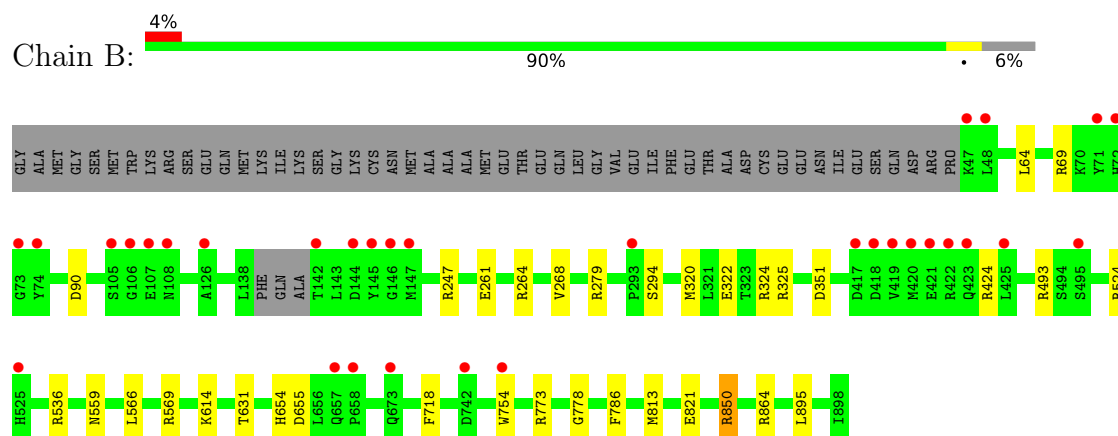
### 3 Residue-property plots [i](#)

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.

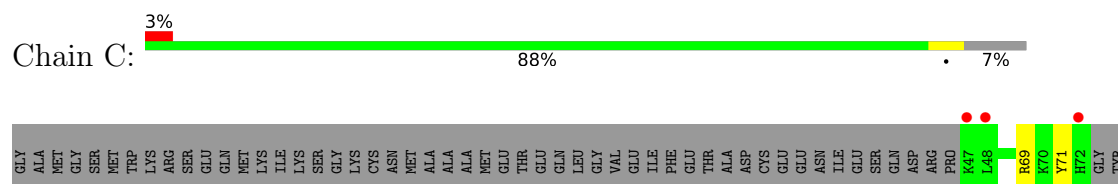
#### • Molecule 1: Dipeptidyl peptidase 8

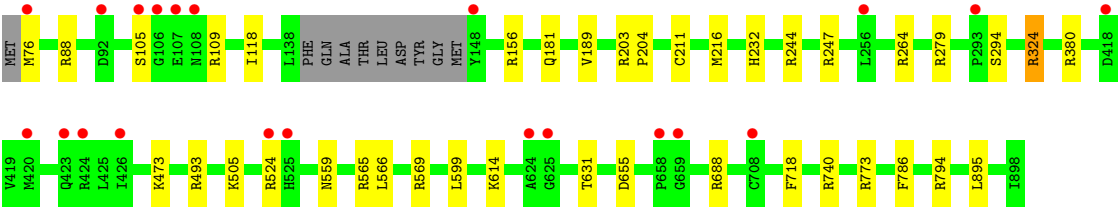


#### • Molecule 1: Dipeptidyl peptidase 8



#### • Molecule 1: Dipeptidyl peptidase 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.82Å 246.02Å 261.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.77 – 2.58 49.07 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (135.77-2.58) 97.5 (49.07-2.58)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.180 , 0.208 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	949 reflections (0.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CW8, TMO

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	0.74	3/7140 (0.0%)	0.92	14/9683 (0.1%)
1	B	0.74	0/7164	0.94	23/9718 (0.2%)
1	C	0.75	3/7083 (0.0%)	0.93	26/9607 (0.3%)
All	All	0.74	6/21387 (0.0%)	0.93	63/29008 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	LEU	CB-CG	6.97	1.72	1.52
1	C	505	LYS	CD-CE	-6.76	1.34	1.51
1	A	505	LYS	CD-CE	-6.05	1.36	1.51
1	C	71	TYR	CB-CG	5.55	1.59	1.51
1	C	76	MET	CB-CG	5.47	1.68	1.51
1	A	322	GLU	CD-OE2	5.42	1.31	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	850	ARG	NE-CZ-NH2	10.82	125.71	120.30
1	B	850	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	C	279	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	279	ARG	NE-CZ-NH2	-8.47	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	279	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	247	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	279	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	850	ARG	CD-NE-CZ	6.58	132.81	123.60
1	B	493	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	244	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	565	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	279	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	524	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	156	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	424	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	493	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	324	ARG	CG-CD-NE	6.22	124.86	111.80
1	C	324	ARG	CG-CD-NE	6.20	124.83	111.80
1	C	264	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	786	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	A	493	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	324	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	264	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	505	LYS	CG-CD-CE	5.93	129.70	111.90
1	B	69	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	493	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	324	ARG	CG-CD-NE	5.83	124.04	111.80
1	B	813	MET	CG-SD-CE	5.76	109.41	100.20
1	C	565	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	786	PHE	CB-CG-CD2	-5.72	116.79	120.80
1	C	324	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	524	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	88	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	351	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	55	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	156	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	740	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	264	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	247	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	247	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	90	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	C	688	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	786	PHE	CB-CG-CD1	5.38	124.56	120.80
1	C	380	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	69	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	569	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	786	PHE	CB-CG-CD1	5.22	124.46	120.80
1	C	493	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	493	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	569	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	794	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	247	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	109	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	786	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	C	203	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	524	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	607	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	160	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	864	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	569	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	565	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	850	ARG	Sidechain

## 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	6947	0	6753	5	0
1	B	6970	0	6772	4	0
1	C	6892	0	6699	7	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
3	A	10	0	18	0	0
3	B	30	0	54	0	0
3	C	15	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	200	0	0	1	0
4	B	243	0	0	0	1
4	C	259	0	0	0	0
All	All	21620	0	20323	16	1

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 0.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:O	1:B:614:LYS:HD3	2.11	0.50
1:A:754[A]:TRP:CE3	1:A:778:GLY:HA3	2.47	0.50
1:B:268[A]:VAL:HG23	1:B:268[A]:VAL:O	2.11	0.50
1:C:566:LEU:O	1:C:614:LYS:HD3	2.12	0.49
1:A:284:TRP:CZ2	1:A:381:ALA:HB3	2.50	0.47
1:C:181:GLN:HE22	1:C:216:MET:HE3	1.79	0.45
1:C:189:VAL:CG1	1:C:204:PRO:HA	2.47	0.45
1:C:181:GLN:HE22	1:C:216:MET:CE	2.29	0.45
1:A:566:LEU:O	1:A:614:LYS:HD3	2.18	0.44
1:B:320:MET:HG3	1:B:322[A]:GLU:OE2	2.18	0.43
1:A:244:ARG:NH2	4:A:1004:HOH:O	2.52	0.43
1:A:118:ILE:HD12	1:A:599:LEU:CD2	2.50	0.42
1:C:118:ILE:HD12	1:C:599:LEU:CD2	2.50	0.42
1:C:118:ILE:HD12	1:C:599:LEU:HD22	2.01	0.42
1:C:211:CYS:HB3	1:C:232:HIS:CD2	2.55	0.41
1:B:754[B]:TRP:CE3	1:B:778:GLY:HA3	2.55	0.41

All (1) 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)
4:B:1116:HOH:O	4:B:1116:HOH:O[4_555]	1.46	0.74

## 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	849/903 (94%)	826 (97%)	22 (3%)	1 (0%)	51	73
1	B	852/903 (94%)	827 (97%)	25 (3%)	0	100	100
1	C	840/903 (93%)	816 (97%)	24 (3%)	0	100	100
All	All	2541/2709 (94%)	2469 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	ILE

### 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	757/797 (95%)	740 (98%)	17 (2%)	52	74
1	B	760/797 (95%)	747 (98%)	13 (2%)	60	79
1	C	752/797 (94%)	742 (99%)	10 (1%)	69	85
All	All	2269/2391 (95%)	2229 (98%)	40 (2%)	59	78

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	88	ARG

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Mol	Chain	Res	Type
1	A	216	MET
1	A	294	SER
1	A	325	ARG
1	A	349	MET
1	A	424	ARG
1	A	473	LYS
1	A	536	ARG
1	A	559	ASN
1	A	631	THR
1	A	654	HIS
1	A	655	ASP
1	A	718	PHE
1	A	773	ARG
1	A	829	HIS
1	A	895	LEU
1	B	64	LEU
1	B	261	GLU
1	B	294	SER
1	B	325	ARG
1	B	536	ARG
1	B	559	ASN
1	B	631	THR
1	B	654	HIS
1	B	655	ASP
1	B	718	PHE
1	B	773	ARG
1	B	821	GLU
1	B	895	LEU
1	C	105	SER
1	C	294	SER
1	C	324	ARG
1	C	473	LYS
1	C	559	ASN
1	C	631	THR
1	C	655	ASP
1	C	718	PHE
1	C	773	ARG
1	C	895	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	173	GLN
1	A	258	ASN
1	A	882	HIS
1	B	173	GLN
1	B	258	ASN
1	C	173	GLN
1	C	181	GLN
1	C	234	ASN
1	C	882	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

14 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	TMO	A	903	-	4,4,4	6.31	1 (25%)	6,6,6	0.16	0
3	TMO	C	903	-	4,4,4	6.51	1 (25%)	6,6,6	0.16	0
3	TMO	B	905	-	4,4,4	6.19	1 (25%)	6,6,6	0.21	0
2	CW8	B	901	1	18,19,19	1.63	1 (5%)	18,26,26	8.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TMO	B	902	-	4,4,4	6.13	1 (25%)	6,6,6	0.23	0
3	TMO	A	902	-	4,4,4	6.34	1 (25%)	6,6,6	0.21	0
3	TMO	C	902	-	4,4,4	6.39	1 (25%)	6,6,6	0.18	0
2	CW8	A	901	1	18,19,19	1.49	2 (11%)	18,26,26	8.30	3 (16%)
3	TMO	B	904	-	4,4,4	6.24	1 (25%)	6,6,6	0.20	0
3	TMO	B	906	-	4,4,4	6.12	1 (25%)	6,6,6	0.23	0
3	TMO	B	907	-	4,4,4	6.07	1 (25%)	6,6,6	0.25	0
2	CW8	C	901	1	18,19,19	1.70	1 (5%)	18,26,26	8.26	2 (11%)
3	TMO	B	903	-	4,4,4	6.42	1 (25%)	6,6,6	0.19	0
3	TMO	C	904	-	4,4,4	6.26	1 (25%)	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CW8	B	901	1	-	0/12/34/34	0/2/2/2
2	CW8	A	901	1	-	0/12/34/34	0/2/2/2
2	CW8	C	901	1	-	0/12/34/34	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	TMO	OAE-NAC	-12.97	1.24	1.42
3	B	903	TMO	OAE-NAC	-12.82	1.25	1.42
3	C	902	TMO	OAE-NAC	-12.76	1.25	1.42
3	A	902	TMO	OAE-NAC	-12.64	1.25	1.42
3	A	903	TMO	OAE-NAC	-12.62	1.25	1.42
3	C	904	TMO	OAE-NAC	-12.51	1.25	1.42
3	B	904	TMO	OAE-NAC	-12.46	1.25	1.42
3	B	905	TMO	OAE-NAC	-12.35	1.25	1.42
3	B	906	TMO	OAE-NAC	-12.23	1.25	1.42
3	B	902	TMO	OAE-NAC	-12.22	1.25	1.42
3	B	907	TMO	OAE-NAC	-12.12	1.26	1.42
2	C	901	CW8	C23-N24	6.67	1.27	1.14
2	B	901	CW8	C23-N24	6.38	1.27	1.14
2	A	901	CW8	C23-N24	5.40	1.25	1.14
2	A	901	CW8	C5-C13	-2.24	1.50	1.53



All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	CW8	C21-C23-N24	-34.85	121.10	177.23
2	C	901	CW8	C21-C23-N24	-34.67	121.39	177.23
2	B	901	CW8	C21-C23-N24	-34.17	122.19	177.23
2	A	901	CW8	C13-C5-N1	-3.77	104.47	110.22
2	B	901	CW8	C13-C5-N1	-3.64	104.67	110.22
2	C	901	CW8	C13-C5-N1	-3.02	105.61	110.22
2	A	901	CW8	F19-C17-C16	2.06	112.05	108.62

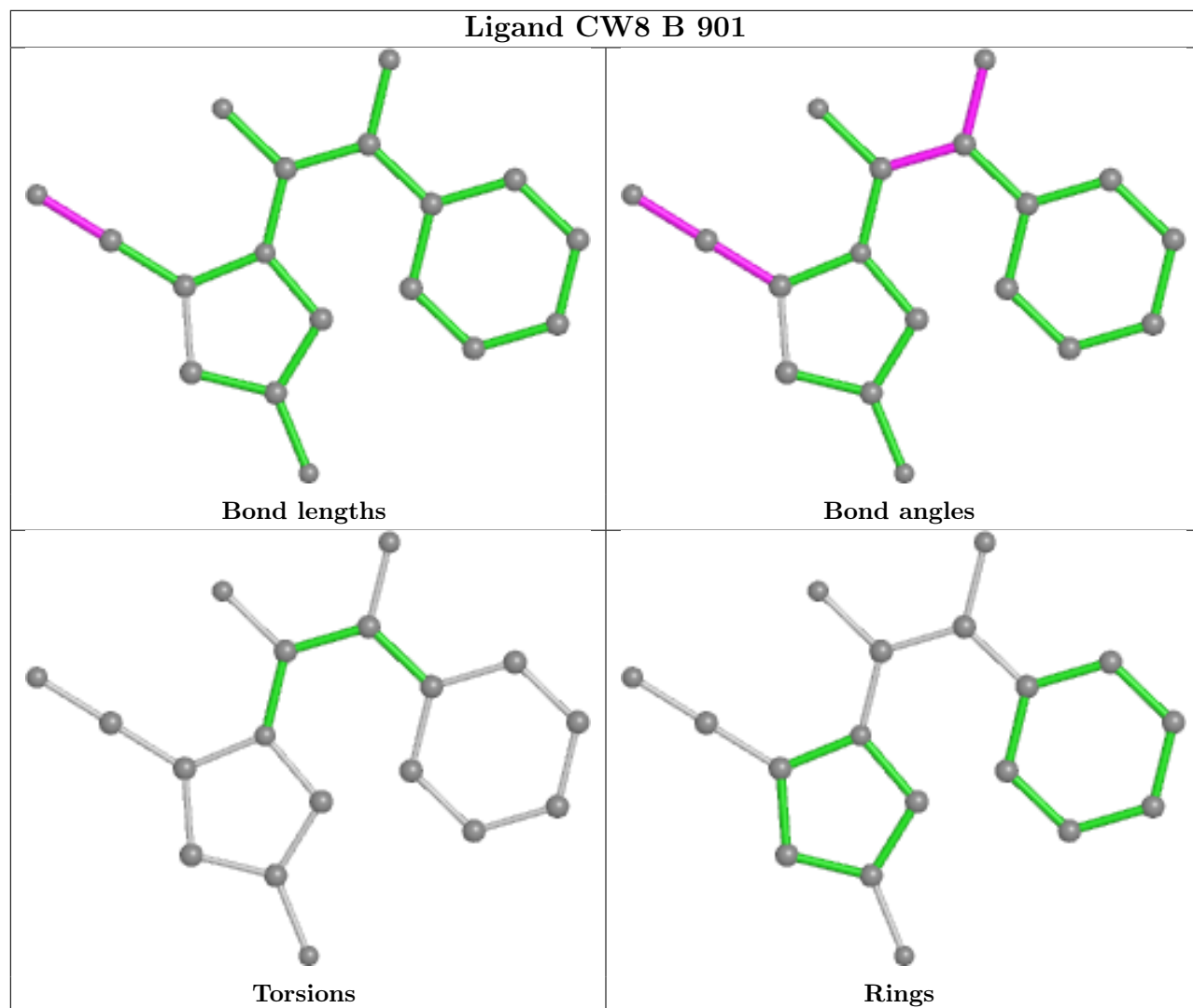
There are no chirality outliers.

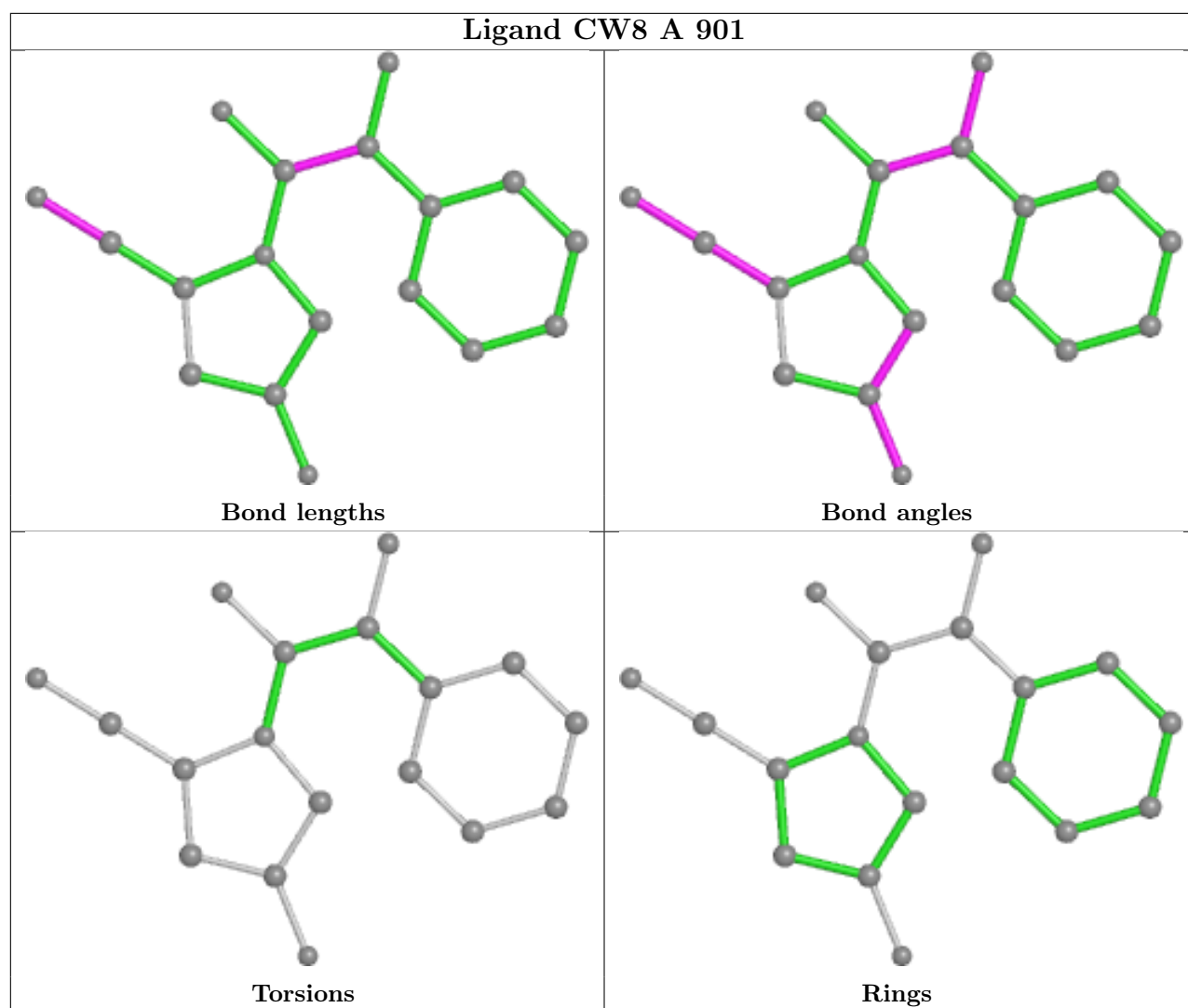
There are no torsion outliers.

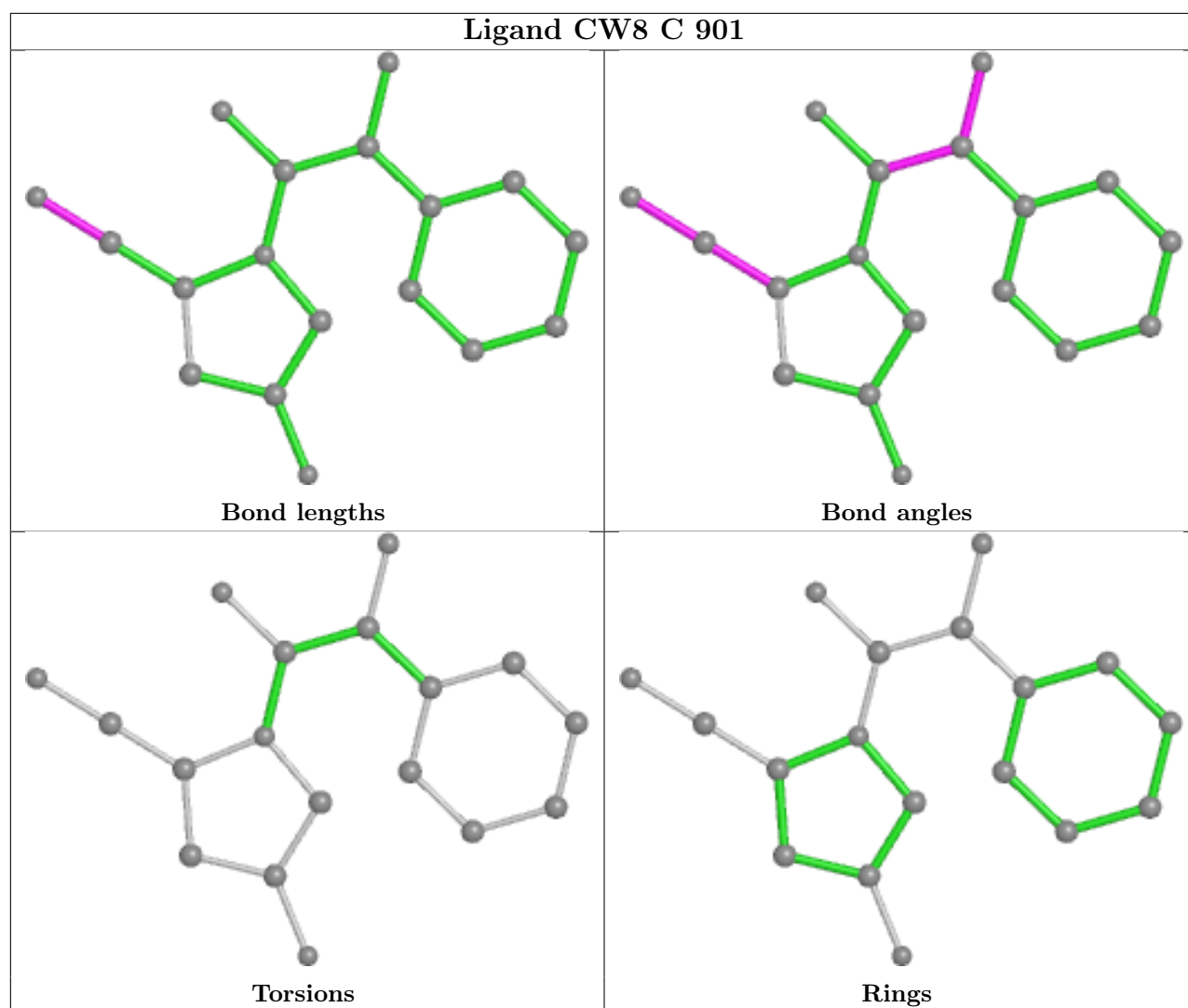
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	848/903 (93%)	0.10	34 (4%) 38 34	40, 60, 104, 180	27 (3%)
1	B	849/903 (94%)	0.06	32 (3%) 40 36	37, 58, 103, 190	33 (3%)
1	C	840/903 (93%)	0.06	24 (2%) 51 47	36, 57, 98, 157	30 (3%)
All	All	2537/2709 (93%)	0.07	90 (3%) 44 39	36, 58, 102, 190	90 (3%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	TYR	5.3
1	A	145	TYR	5.1
1	B	74	TYR	4.8
1	A	107	GLU	4.8
1	B	106	GLY	4.7
1	C	48	LEU	4.3
1	A	71	TYR	4.3
1	B	105	SER	4.2
1	A	147	MET	3.9
1	A	418	ASP	3.9
1	A	417	ASP	3.7
1	A	106	GLY	3.6
1	C	72	HIS	3.5
1	B	420	MET	3.5
1	A	144	ASP	3.4
1	A	108	ASN	3.4
1	B	419	VAL	3.4
1	B	142	THR	3.4
1	C	420	MET	3.4
1	A	424	ARG	3.3
1	C	107	GLU	3.3
1	C	256	LEU	3.3
1	B	293	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	72	HIS	3.3
1	A	449	ILE	3.3
1	A	48	LEU	3.2
1	B	418	ASP	3.2
1	C	106	GLY	3.2
1	C	625	GLY	3.2
1	B	47	LYS	3.2
1	A	143	LEU	3.2
1	B	73	GLY	3.1
1	B	48	LEU	3.1
1	A	524	ARG	3.0
1	B	525	HIS	3.0
1	C	293	PRO	3.0
1	B	108	ASN	2.9
1	A	277	PHE	2.9
1	A	420	MET	2.9
1	A	47	LYS	2.9
1	B	145	TYR	2.9
1	C	47	LYS	2.9
1	C	108	ASN	2.9
1	A	423	GLN	2.9
1	B	107	GLU	2.8
1	B	72	HIS	2.8
1	B	658	PRO	2.8
1	A	419	VAL	2.7
1	B	425	LEU	2.7
1	C	105	SER	2.7
1	C	525	HIS	2.6
1	B	422	ARG	2.6
1	A	73	GLY	2.5
1	B	146	GLY	2.5
1	A	293	PRO	2.5
1	C	423	GLN	2.5
1	B	147	MET	2.5
1	B	495	SER	2.5
1	A	76	MET	2.5
1	B	417	ASP	2.5
1	B	754[A]	TRP	2.4
1	C	426	ILE	2.4
1	C	708	CYS	2.4
1	A	292	THR	2.4
1	A	525	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	425	LEU	2.4
1	A	146	GLY	2.3
1	B	657[A]	GLN	2.3
1	C	424	ARG	2.3
1	B	144	ASP	2.3
1	A	75	MET	2.3
1	C	76	MET	2.3
1	B	423	GLN	2.3
1	C	624	ALA	2.2
1	C	659	GLY	2.2
1	A	422	ARG	2.2
1	B	126	ALA	2.2
1	C	658	PRO	2.1
1	A	92	ASP	2.1
1	C	524	ARG	2.1
1	A	256	LEU	2.1
1	B	742	ASP	2.1
1	C	92	ASP	2.1
1	B	673	GLN	2.1
1	C	418	ASP	2.1
1	A	427	GLU	2.0
1	B	421	GLU	2.0
1	A	93	GLY	2.0
1	C	148	TYR	2.0
1	A	742	ASP	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 ⓘ

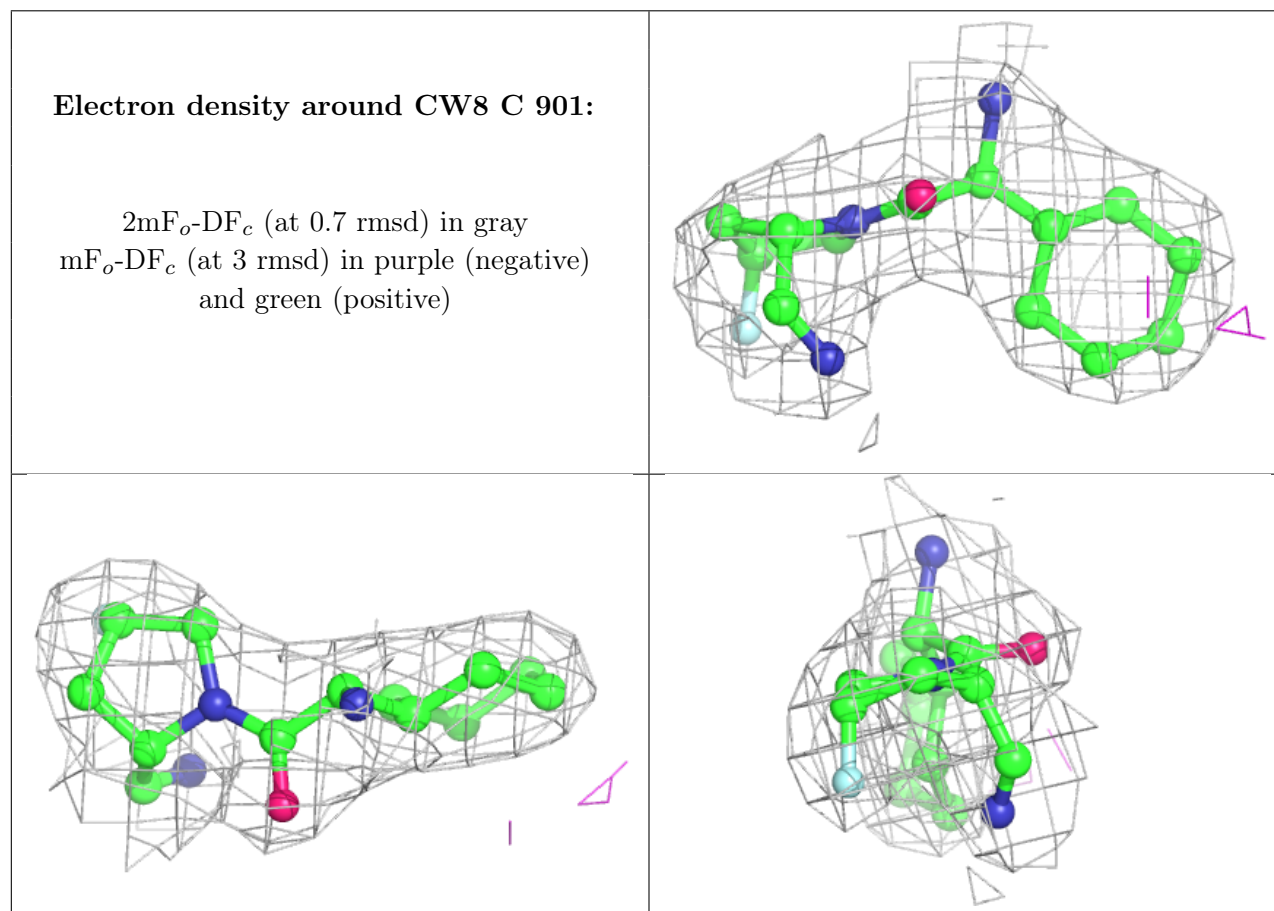
There are no monosaccharides in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
3	TMO	B	904	5/5	0.82	0.34	108,110,145,156	0
3	TMO	B	907	5/5	0.90	0.96	94,95,121,129	0
3	TMO	A	903	5/5	0.91	0.29	86,94,102,116	0
3	TMO	C	904	5/5	0.92	0.86	81,108,120,131	0
3	TMO	B	903	5/5	0.94	0.35	89,96,118,121	0
3	TMO	C	902	5/5	0.94	0.17	73,74,91,101	0
3	TMO	B	905	5/5	0.94	0.23	79,122,135,139	0
3	TMO	A	902	5/5	0.95	0.25	93,97,114,130	0
2	CW8	C	901	18/18	0.96	0.24	28,40,45,46	0
3	TMO	B	906	5/5	0.97	0.20	80,92,117,119	0
3	TMO	C	903	5/5	0.97	0.16	67,86,96,101	0
2	CW8	B	901	18/18	0.97	0.28	38,43,46,50	0
2	CW8	A	901	18/18	0.98	0.24	32,45,52,53	0
3	TMO	B	902	5/5	0.98	0.23	74,81,91,95	0

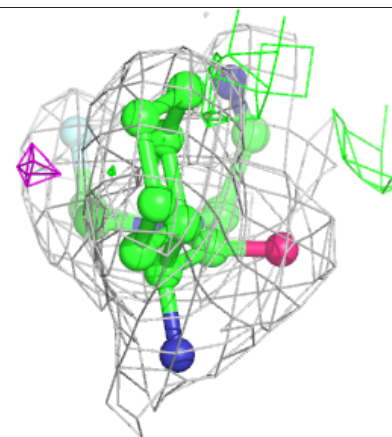
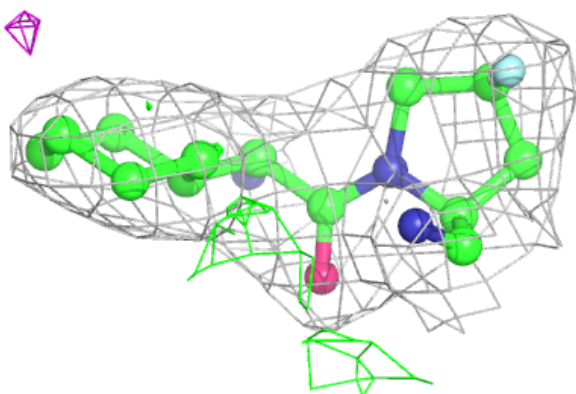
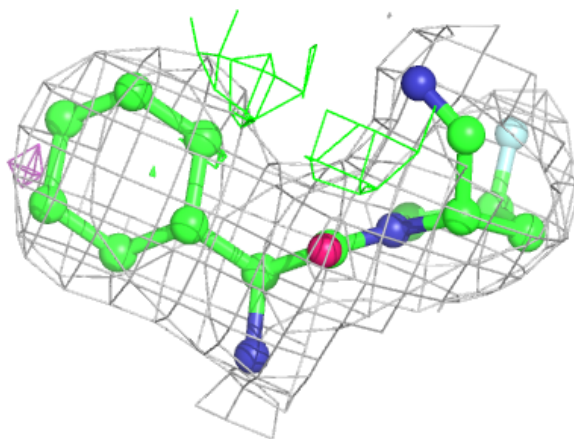
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



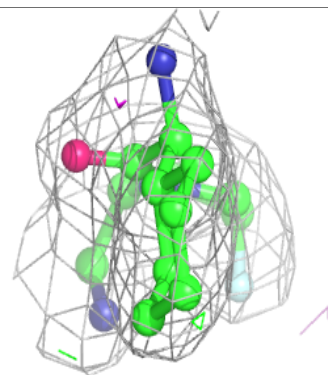
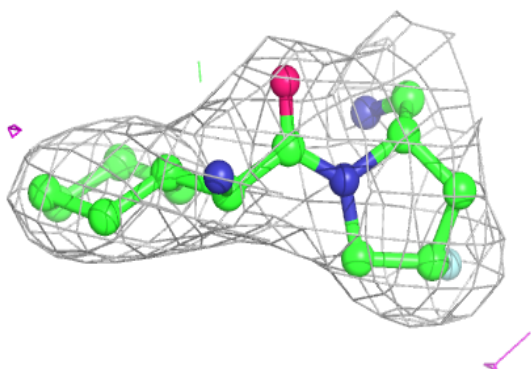
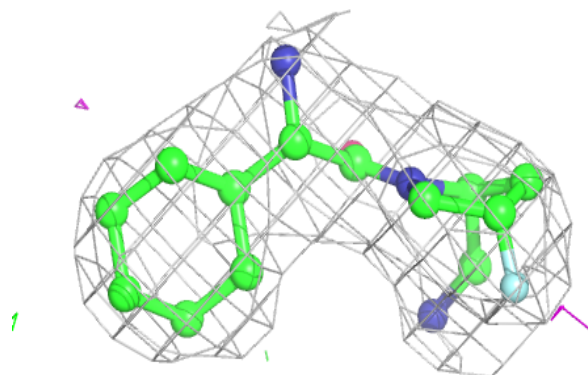


**Electron density around CW8 B 901:**

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

**Electron density around CW8 A 901:**

$2mF_o-DF_c$  (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.