



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 AM UTC

PDB ID : 7SVN / pdb_00007svn
Title : DPP9 IN COMPLEX WITH LIGAND ICeD-1
Authors : Lammens, A.; Hollenstein, K.; Klein, D.J.
Deposited on : 2021-11-19
Resolution : 2.78 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

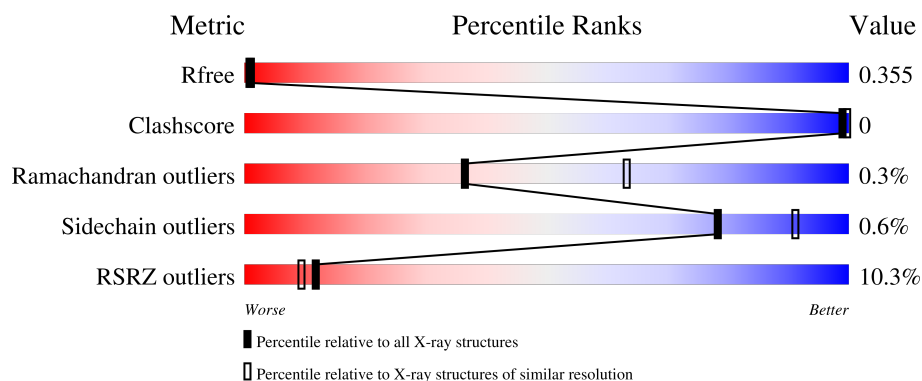
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	869	9% 93% 5%
1	B	869	9% 93% 5%
1	C	869	11% 93% 5%
1	D	869	10% 92% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27476 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 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	825	Total	C	N	O	S	170	1	0
			6702	4308	1144	1222	28			
1	B	822	Total	C	N	O	S	187	1	0
			6680	4299	1140	1213	28			
1	C	829	Total	C	N	O	S	157	2	0
			6743	4337	1153	1225	28			
1	D	827	Total	C	N	O	S	147	2	0
			6732	4330	1151	1223	28			

There are 24 discrepancies between the modelled and reference sequences:

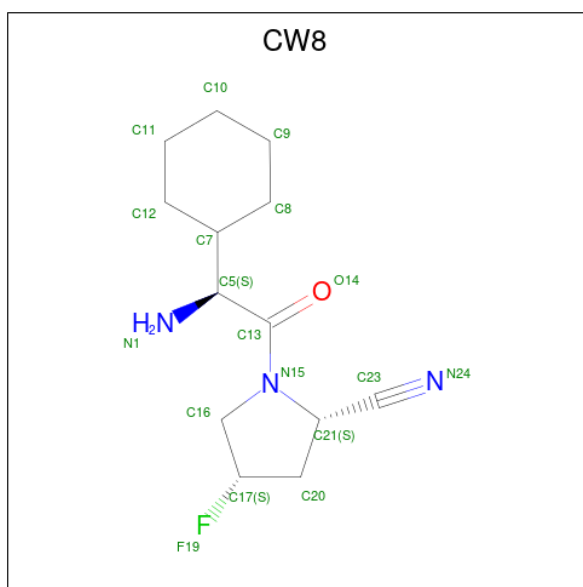
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is (2S,4S)-1-[(2S)-2-amino-2-cyclohexylacetyl]-4-fluoropyrrolidine-2-carbonitrile (CCD ID: CW8) (formula: C₁₃H₂₀FN₃O) (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		
2	D	1	Total	C	F	N	O	0	0
			18	13	1	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	125	Total	O	0	0
			125	125		
3	C	113	Total	O	0	0
			113	113		

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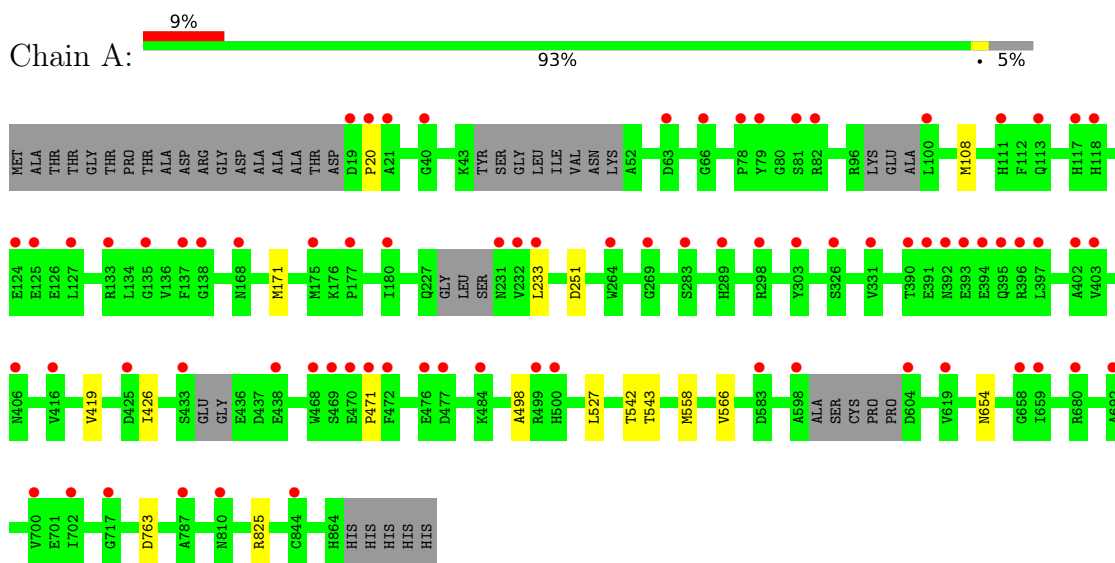
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	147	Total	O	0	0
			147	147		

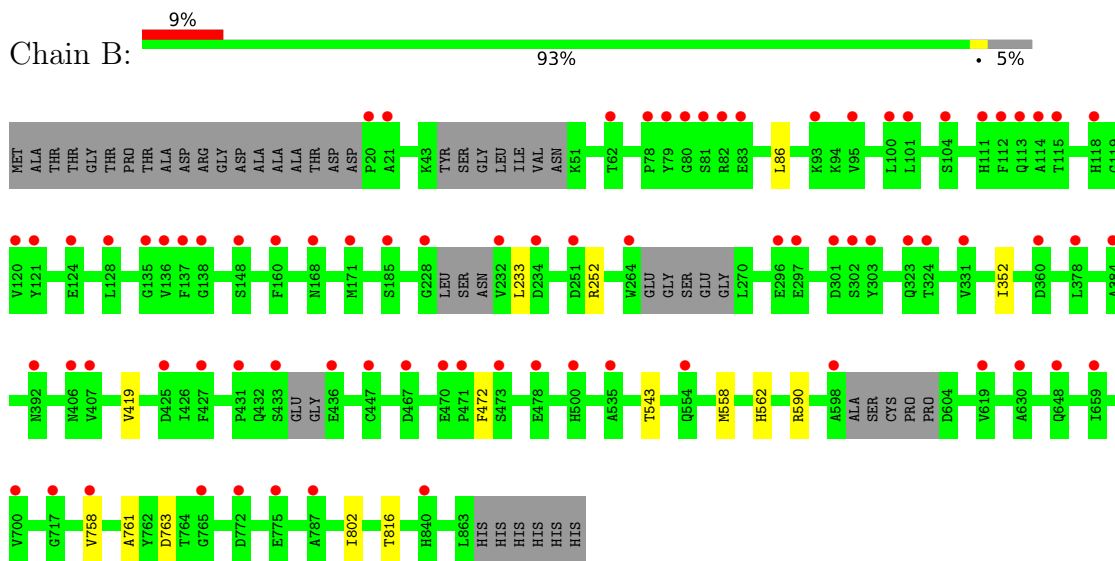
3 Residue-property plots [i](#)

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.

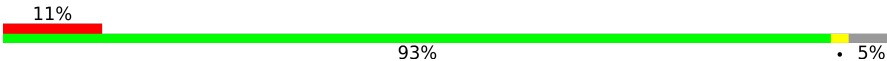
- Molecule 1: Dipeptidyl peptidase 9

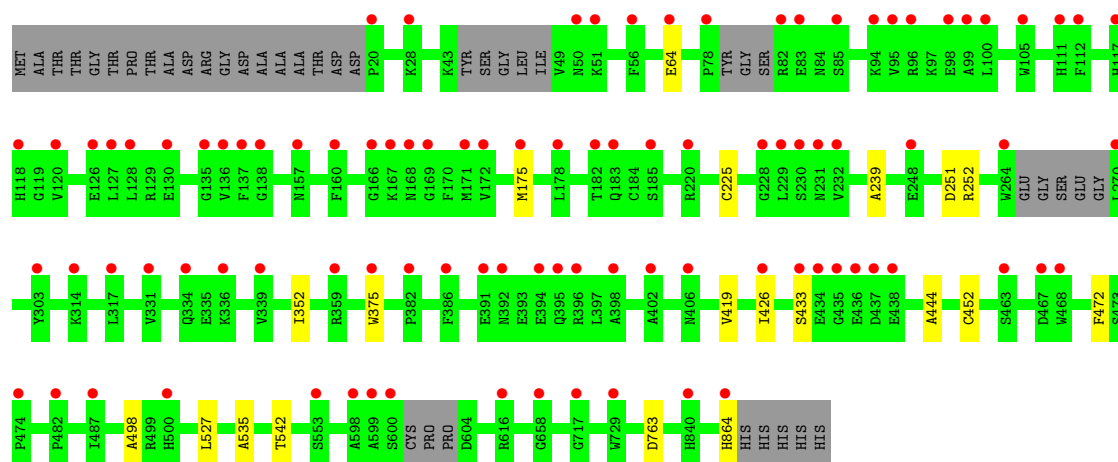


- Molecule 1: Dipeptidyl peptidase 9

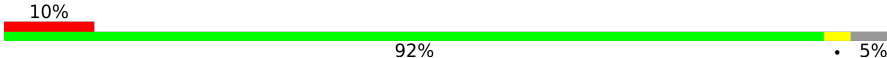


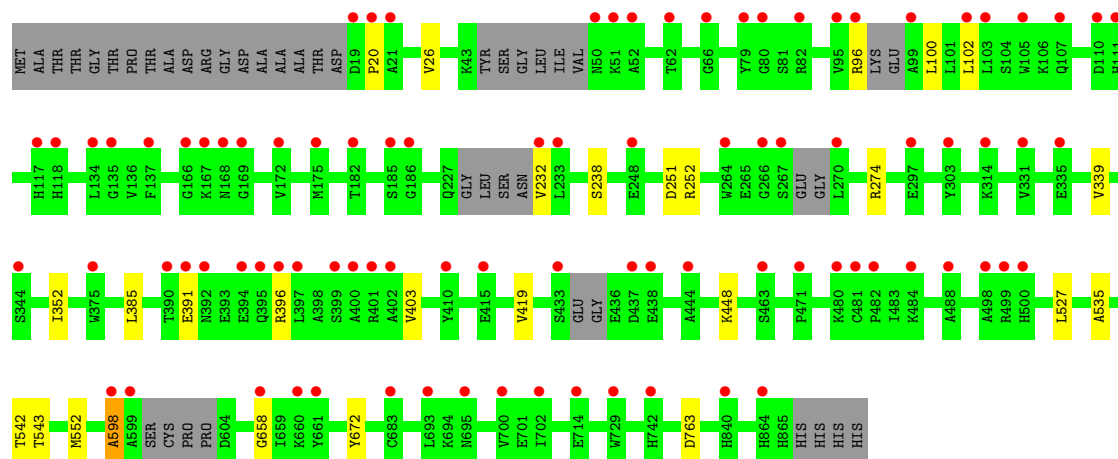
- Molecule 1: Dipeptidyl peptidase 9

Chain C:  11% 93% 5%



• Molecule 1: Dipeptidyl peptidase 9

Chain D:  10% 92% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.79Å 117.44Å 163.46Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	157.52 – 2.78 157.52 – 2.78	Depositor EDS
% Data completeness (in resolution range)	94.4 (157.52-2.78) 94.4 (157.52-2.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.267 , 0.349 0.271 , 0.355	Depositor DCC
R_{free} test set	732 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27476	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2803e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.89	2/6903 (0.0%)	1.01	1/9365 (0.0%)
1	B	0.89	3/6880 (0.0%)	1.01	3/9331 (0.0%)
1	C	0.87	1/6946 (0.0%)	1.02	3/9424 (0.0%)
1	D	0.87	2/6935 (0.0%)	1.02	4/9408 (0.0%)
All	All	0.88	8/27664 (0.0%)	1.01	11/37528 (0.0%)

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	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	LEU	CG-CD1	-8.31	1.25	1.52
1	D	96	ARG	CD-NE	7.47	1.56	1.46
1	B	233	LEU	CG-CD2	6.91	1.75	1.52
1	A	233	LEU	N-CA	6.23	1.54	1.46
1	C	175	MET	SD-CE	5.80	1.94	1.79
1	D	100	LEU	CB-CG	-5.34	1.42	1.53
1	A	825	ARG	NE-CZ	5.22	1.38	1.33
1	B	590	ARG	CD-NE	5.11	1.53	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LEU	CB-CG-CD1	8.37	135.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	ARG	CD-NE-CZ	7.02	134.23	124.40
1	B	763	ASP	N-CA-C	6.60	118.52	110.41
1	A	763	ASP	N-CA-C	6.56	118.47	110.41
1	D	763	ASP	N-CA-C	6.53	118.44	110.41
1	C	64	GLU	CB-CG-CD	6.24	123.21	112.60
1	C	763	ASP	N-CA-C	6.01	117.80	110.41
1	D	658	GLY	N-CA-C	5.42	120.42	114.40
1	D	598	ALA	N-CA-C	5.33	122.16	110.80
1	B	472	PHE	N-CA-C	5.32	117.16	109.07
1	C	472	PHE	N-CA-C	5.25	116.27	108.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	471	PRO	Peptide

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	6702	0	6469	4	0
1	B	6680	0	6470	3	0
1	C	6743	0	6526	7	0
1	D	6732	0	6498	6	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0
3	A	162	0	0	0	0
3	B	125	0	0	0	0
3	C	113	0	0	0	0
3	D	147	0	0	1	0
All	All	27476	0	25963	20	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 0.

All (20) 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:C:375[B]:TRP:HE3	1:C:375[B]:TRP:O	1.53	0.90
1:C:375[B]:TRP:O	1:C:375[B]:TRP:CE3	2.33	0.81
1:D:448:LYS:HB3	3:D:1023:HOH:O	2.03	0.57
1:A:426:ILE:HD12	1:A:498:ALA:HB2	1.89	0.54
1:D:339:VAL:HG21	1:D:403:VAL:HG21	1.91	0.53
1:B:758:VAL:HG13	1:B:761:ALA:HB3	1.91	0.52
1:C:426:ILE:HD12	1:C:498:ALA:HB2	1.94	0.49
1:D:339:VAL:HG23	1:D:385:LEU:O	2.13	0.48
1:A:566:VAL:HG23	1:A:654:ASN:HA	1.97	0.46
1:A:527:LEU:HB3	1:A:542:THR:HG23	2.00	0.44
1:B:802:ILE:HG21	1:B:816:THR:HG23	2.00	0.43
1:B:252:ARG:NH1	1:B:352:ILE:O	2.51	0.43
1:D:252:ARG:NH1	1:D:352:ILE:O	2.52	0.43
1:C:444:ALA:HB1	1:C:452:CYS:SG	2.60	0.42
1:D:26:VAL:HG21	1:D:672:TYR:CZ	2.54	0.42
1:D:527:LEU:HB3	1:D:542:THR:HG23	2.01	0.42
1:C:225:CYS:SG	1:C:239:ALA:HB2	2.59	0.42
1:C:252:ARG:NH1	1:C:352:ILE:O	2.51	0.41
1:A:108:MET:HG2	1:A:171:MET:HE1	2.03	0.41
1:C:527:LEU:HB3	1:C:542:THR:HG23	2.04	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	814/869 (94%)	780 (96%)	32 (4%)	2 (0%)	43	70
1	B	811/869 (93%)	779 (96%)	31 (4%)	1 (0%)	48	75
1	C	821/869 (94%)	783 (95%)	35 (4%)	3 (0%)	30	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	815/869 (94%)	782 (96%)	29 (4%)	4 (0%)	24	52
All	All	3261/3476 (94%)	3124 (96%)	127 (4%)	10 (0%)	36	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	PRO
1	A	20	PRO
1	D	535	ALA
1	D	598	ALA
1	C	535	ALA
1	C	433	SER
1	A	419	VAL
1	B	419	VAL
1	D	419	VAL
1	C	419	VAL

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	728/759 (96%)	725 (100%)	3 (0%)	84	93
1	B	725/759 (96%)	721 (99%)	4 (1%)	78	91
1	C	732/759 (96%)	730 (100%)	2 (0%)	86	94
1	D	730/759 (96%)	722 (99%)	8 (1%)	65	85
All	All	2915/3036 (96%)	2898 (99%)	17 (1%)	78	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	543	THR
1	A	558	MET
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	543	THR
1	B	558	MET
1	B	562	HIS
1	C	251	ASP
1	C	864	HIS
1	D	102	LEU
1	D	232	VAL
1	D	238	SER
1	D	251	ASP
1	D	274	ARG
1	D	391	GLU
1	D	543	THR
1	D	552	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	57	GLN
1	A	60	GLN
1	A	107	GLN
1	A	157	ASN
1	A	323	GLN
1	A	374	GLN
1	A	424	HIS
1	A	500	HIS
1	A	614	HIS
1	A	696	GLN
1	A	705	GLN
1	A	837	ASN
1	B	107	GLN
1	B	226	HIS
1	B	374	GLN
1	B	392	ASN
1	B	395	GLN
1	B	500	HIS
1	B	696	GLN
1	B	798	ASN
1	B	812	HIS
1	B	831	GLN
1	B	837	ASN
1	C	29	HIS

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	161	HIS
1	C	500	HIS
1	C	507	ASN
1	C	573	HIS
1	C	586	HIS
1	C	614	HIS
1	C	684	GLN
1	C	696	GLN
1	C	798	ASN
1	C	812	HIS
1	C	831	GLN
1	C	837	ASN
1	D	25	GLN
1	D	27	GLN
1	D	68	HIS
1	D	107	GLN
1	D	161	HIS
1	D	205	ASN
1	D	392	ASN
1	D	614	HIS
1	D	632	GLN
1	D	684	GLN
1	D	696	GLN
1	D	798	ASN
1	D	812	HIS
1	D	831	GLN
1	D	833	GLN
1	D	837	ASN

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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CW8	D	901	1	18,19,19	1.51	1 (5%)	21,26,26	8.44	6 (28%)
2	CW8	C	901	1	18,19,19	1.59	1 (5%)	21,26,26	8.04	8 (38%)
2	CW8	A	901	1	18,19,19	1.71	2 (11%)	21,26,26	8.07	10 (47%)
2	CW8	B	901	1	18,19,19	1.54	2 (11%)	21,26,26	8.20	9 (42%)

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	D	901	1	-	1/12/34/34	0/2/2/2
2	CW8	C	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	B	901	1	-	0/12/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	CW8	C23-N24	6.24	1.26	1.14
2	C	901	CW8	C23-N24	6.00	1.25	1.14
2	D	901	CW8	C23-N24	5.97	1.25	1.14
2	B	901	CW8	C23-N24	5.92	1.25	1.14
2	A	901	CW8	C21-C23	2.28	1.52	1.48
2	B	901	CW8	C21-C23	2.22	1.52	1.48

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	CW8	C21-C23-N24	-37.92	116.41	177.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	CW8	C21-C23-N24	-36.05	119.41	177.23
2	C	901	CW8	C21-C23-N24	-35.91	119.64	177.23
2	A	901	CW8	C21-C23-N24	-35.83	119.77	177.23
2	B	901	CW8	C20-C17-C16	-4.89	98.55	104.52
2	B	901	CW8	C23-C21-N15	4.61	116.73	110.74
2	C	901	CW8	C13-C5-N1	-4.08	103.23	110.09
2	B	901	CW8	C7-C5-C13	3.93	115.25	110.33
2	A	901	CW8	C23-C21-N15	3.92	115.83	110.74
2	D	901	CW8	C17-C16-N15	3.77	108.64	103.13
2	D	901	CW8	C23-C21-N15	3.75	115.62	110.74
2	A	901	CW8	C13-C5-N1	-3.28	104.57	110.09
2	B	901	CW8	C13-C5-N1	-3.28	104.58	110.09
2	B	901	CW8	F19-C17-C20	3.27	112.68	108.89
2	B	901	CW8	C17-C16-N15	2.91	107.39	103.13
2	A	901	CW8	C8-C7-C5	2.76	115.86	111.80
2	A	901	CW8	F19-C17-C16	2.70	112.30	108.41
2	A	901	CW8	F19-C17-C20	-2.69	105.78	108.89
2	D	901	CW8	C13-C5-N1	-2.56	105.78	110.09
2	A	901	CW8	C7-C5-C13	2.54	113.51	110.33
2	C	901	CW8	C17-C16-N15	2.54	106.85	103.13
2	C	901	CW8	C8-C7-C5	2.49	115.48	111.80
2	C	901	CW8	C7-C5-C13	2.48	113.44	110.33
2	D	901	CW8	C7-C5-C13	2.47	113.42	110.33
2	A	901	CW8	C17-C16-N15	2.45	106.72	103.13
2	C	901	CW8	C23-C21-N15	2.32	113.75	110.74
2	D	901	CW8	C16-N15-C21	-2.29	108.82	111.84
2	C	901	CW8	C20-C17-C16	-2.26	101.76	104.52
2	B	901	CW8	F19-C17-C16	2.21	111.59	108.41
2	A	901	CW8	C10-C9-C8	2.20	115.93	111.42
2	C	901	CW8	C12-C7-C8	-2.15	105.76	109.43
2	A	901	CW8	O14-C13-C5	-2.12	115.95	119.95
2	B	901	CW8	C16-N15-C21	-2.01	109.19	111.84

There are no chirality outliers.

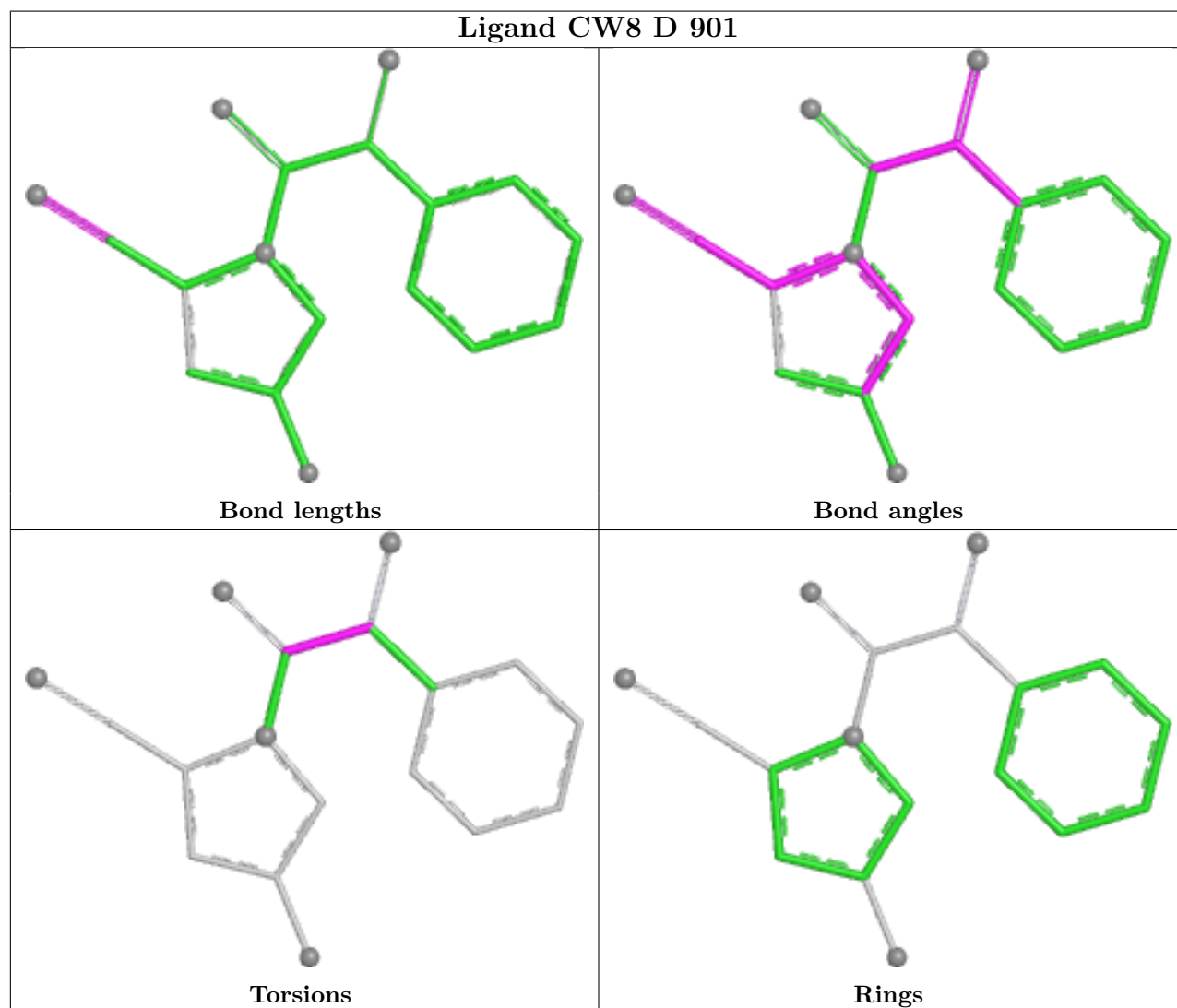
All (1) torsion outliers are listed below:

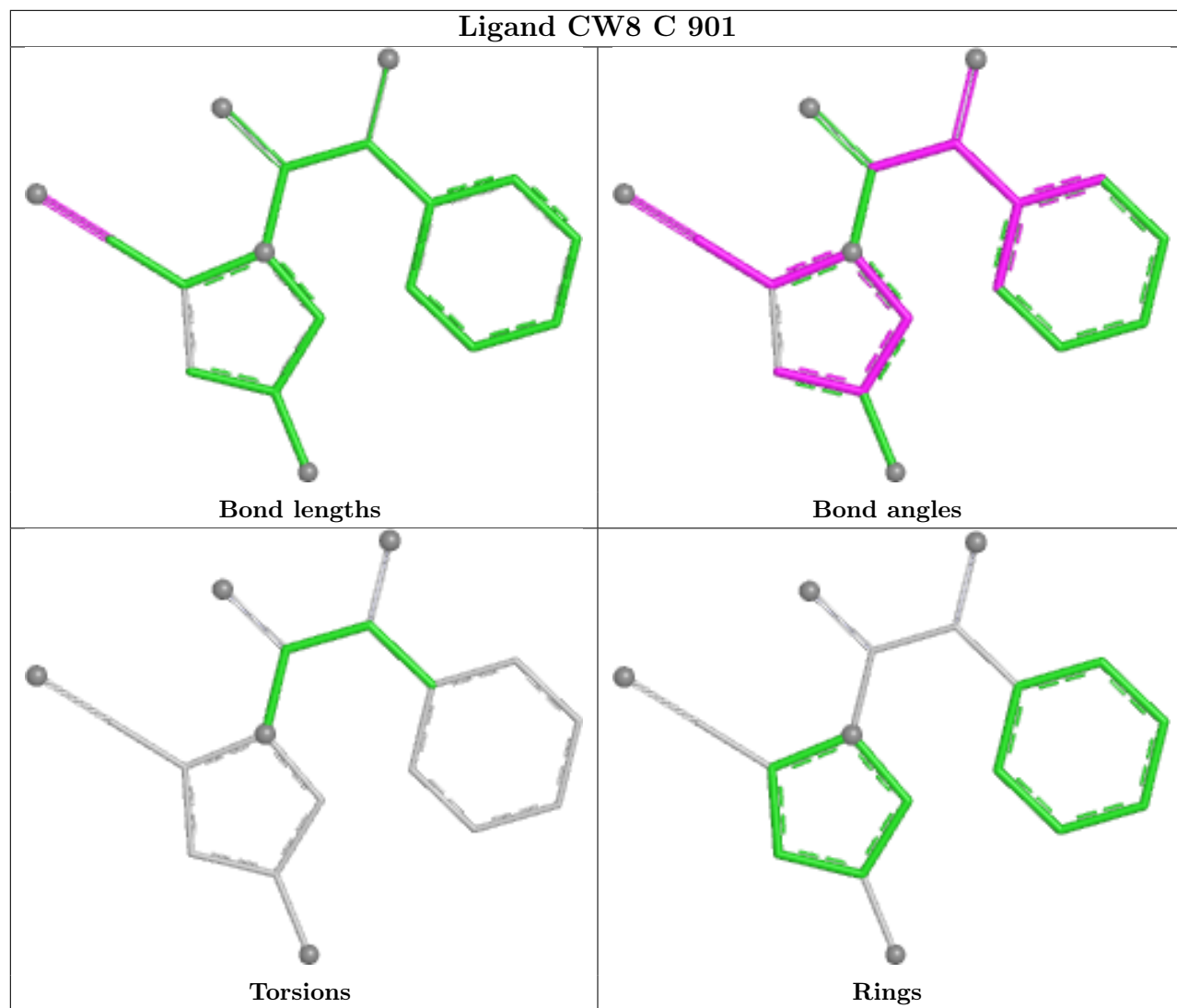
Mol	Chain	Res	Type	Atoms
2	D	901	CW8	N15-C13-C5-N1

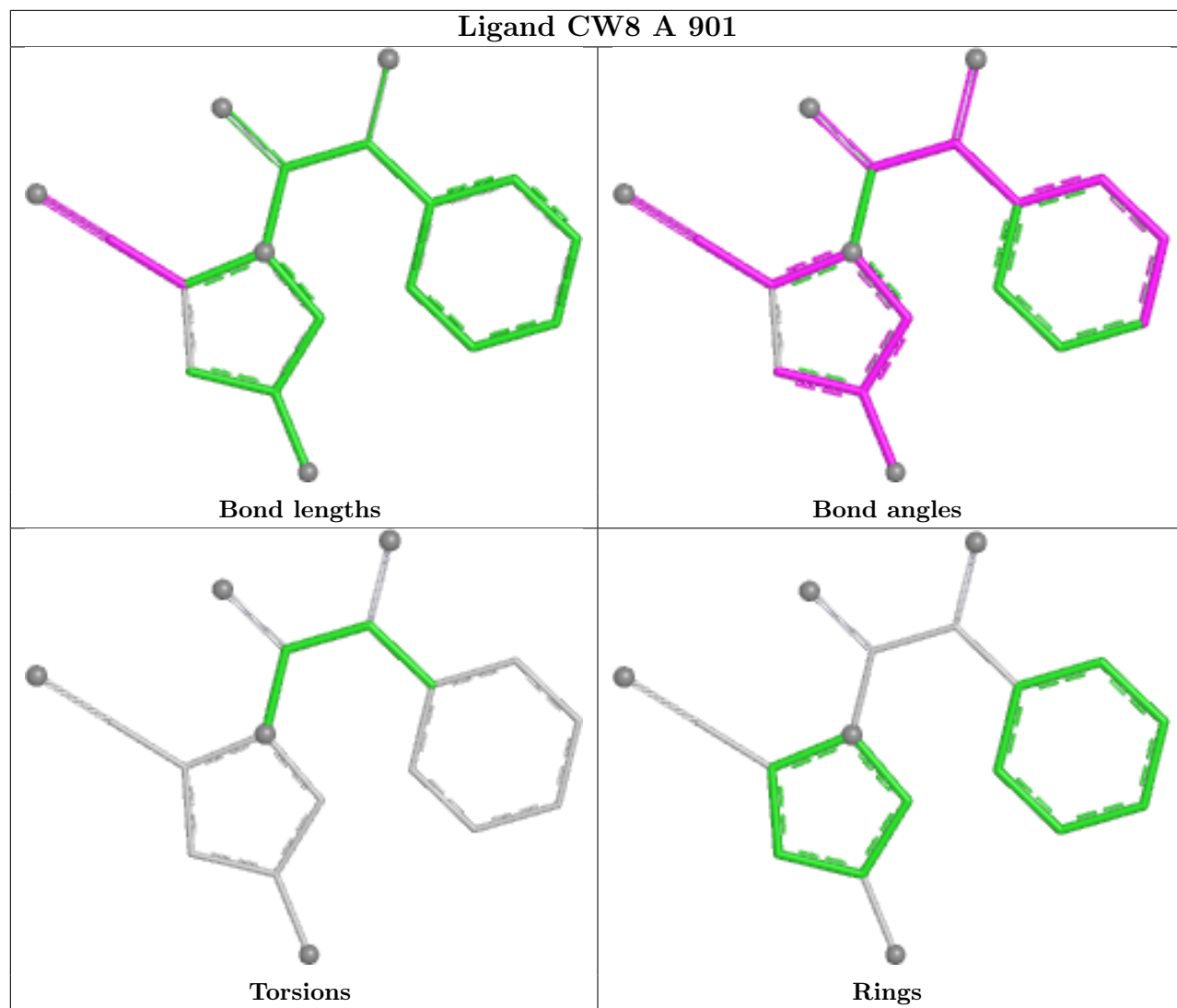
There are no ring outliers.

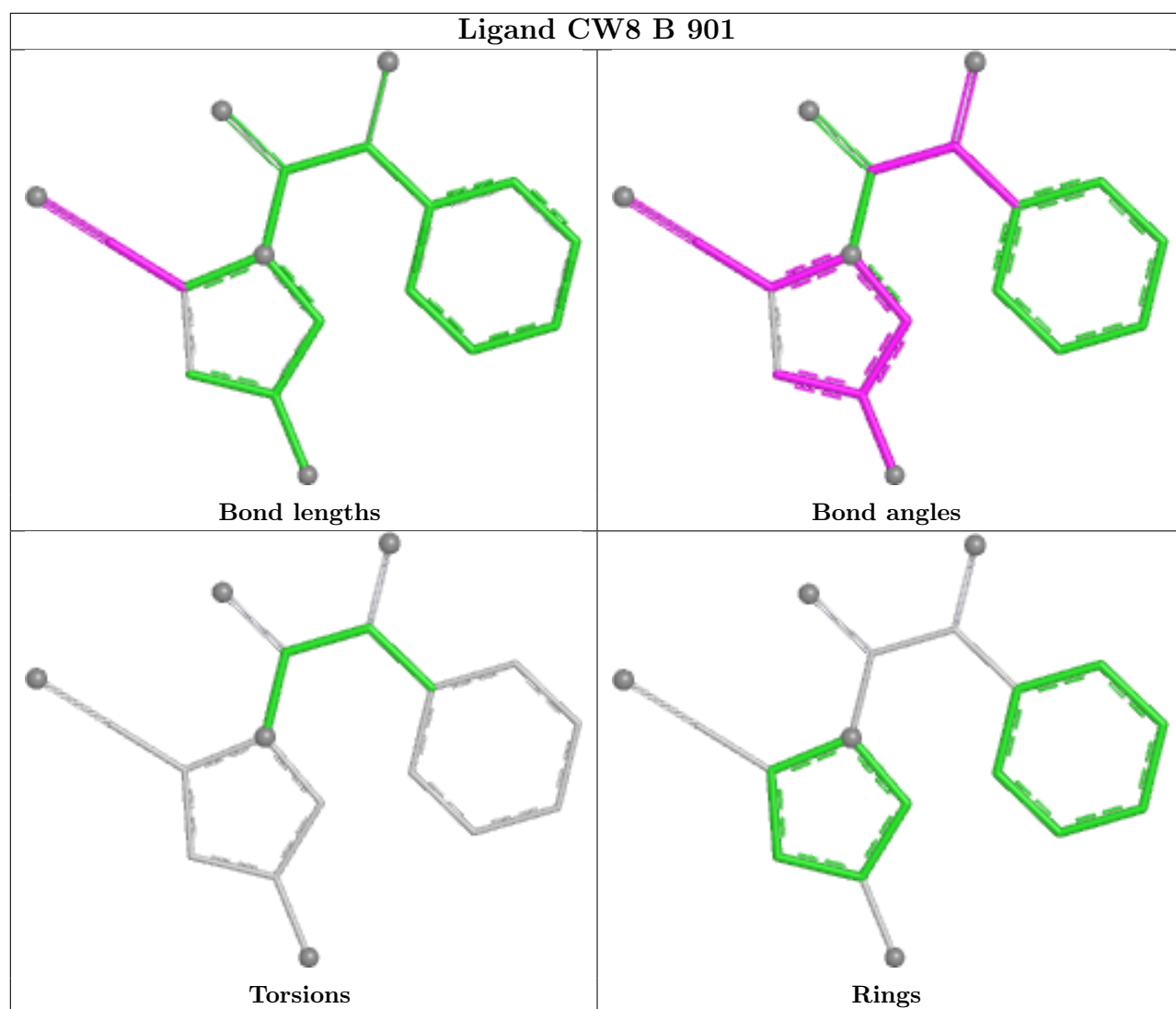
No monomer is involved in short contacts.

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, 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	825/869 (94%)	0.77	76 (9%) 14 11	15, 41, 81, 123	69 (8%)
1	B	822/869 (94%)	0.84	79 (9%) 13 11	14, 42, 77, 137	67 (8%)
1	C	829/869 (95%)	0.82	95 (11%) 9 7	14, 39, 83, 120	61 (7%)
1	D	827/869 (95%)	0.81	90 (10%) 10 8	13, 38, 77, 126	62 (7%)
All	All	3303/3476 (95%)	0.81	340 (10%) 12 9	13, 40, 80, 137	259 (7%)

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	ASN	5.8
1	D	19	ASP	5.7
1	A	433	SER	5.6
1	B	598	ALA	5.1
1	C	20	PRO	5.0
1	A	82	ARG	4.9
1	D	135	GLY	4.8
1	B	20	PRO	4.7
1	A	598	ALA	4.7
1	C	138	GLY	4.7
1	D	79	TYR	4.7
1	D	232	VAL	4.6
1	D	80	GLY	4.6
1	B	392	ASN	4.6
1	C	392	ASN	4.6
1	C	99	ALA	4.5
1	C	434	GLU	4.5
1	C	500	HIS	4.3
1	D	390	THR	4.3
1	C	375[A]	TRP	4.3
1	A	135	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLY	4.2
1	D	599	ALA	4.2
1	D	397	LEU	4.2
1	D	392	ASN	4.1
1	A	232	VAL	4.1
1	A	392	ASN	4.1
1	A	500	HIS	4.0
1	B	228	GLY	3.9
1	D	96	ARG	3.9
1	C	228	GLY	3.9
1	D	303	TYR	3.9
1	D	500	HIS	3.9
1	A	396	ARG	3.9
1	B	82	ARG	3.9
1	C	136	VAL	3.8
1	B	425	ASP	3.8
1	A	393	GLU	3.8
1	D	172	VAL	3.8
1	A	484	LYS	3.8
1	A	63	ASP	3.8
1	D	433	SER	3.8
1	D	169	GLY	3.8
1	A	395	GLN	3.7
1	C	264	TRP	3.7
1	B	232	VAL	3.7
1	D	117	HIS	3.7
1	A	20	PRO	3.7
1	C	168	ASN	3.6
1	D	20	PRO	3.6
1	C	864	HIS	3.6
1	D	51	LYS	3.6
1	D	118	HIS	3.6
1	A	19	ASP	3.6
1	C	83	GLU	3.6
1	B	135	GLY	3.5
1	A	118	HIS	3.5
1	B	21	ALA	3.5
1	C	51	LYS	3.5
1	C	82	ARG	3.5
1	A	231	ASN	3.4
1	C	78	PRO	3.4
1	C	100	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	114	ALA	3.4
1	C	482	PRO	3.4
1	D	134	LEU	3.4
1	D	402	ALA	3.4
1	D	660	LYS	3.4
1	B	433	SER	3.4
1	D	248	GLU	3.4
1	C	598	ALA	3.4
1	C	303	TYR	3.3
1	D	50	ASN	3.3
1	D	95	VAL	3.3
1	D	137	PHE	3.3
1	D	267	SER	3.2
1	C	50	ASN	3.2
1	B	93	LYS	3.2
1	C	98	GLU	3.2
1	A	390	THR	3.2
1	A	133	ARG	3.2
1	B	124	GLU	3.2
1	D	375[A]	TRP	3.2
1	C	463	SER	3.2
1	B	406	ASN	3.1
1	B	128	LEU	3.1
1	B	83	GLU	3.1
1	B	302	SER	3.1
1	D	21	ALA	3.1
1	D	52	ALA	3.1
1	A	403	VAL	3.1
1	B	303	TYR	3.1
1	B	427	PHE	3.1
1	C	231	ASN	3.1
1	C	169	GLY	3.1
1	D	62	THR	3.1
1	B	251	ASP	3.0
1	C	717	GLY	3.0
1	D	395	GLN	3.0
1	A	499	ARG	3.0
1	D	400	ALA	3.0
1	A	127	LEU	3.0
1	A	471	PRO	3.0
1	A	137	PHE	3.0
1	B	264	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	476	GLU	3.0
1	D	314	LYS	3.0
1	D	391	GLU	2.9
1	D	463	SER	2.9
1	B	113	GLN	2.9
1	A	175	MET	2.9
1	D	437	ASP	2.9
1	C	135	GLY	2.9
1	C	166	GLY	2.9
1	A	100	LEU	2.9
1	C	111	HIS	2.9
1	D	331	VAL	2.9
1	D	111	HIS	2.9
1	D	185	SER	2.9
1	A	844	CYS	2.9
1	D	66	GLY	2.9
1	C	599	ALA	2.9
1	C	729[A]	TRP	2.9
1	B	659	ILE	2.9
1	B	121	TYR	2.9
1	A	233	LEU	2.9
1	C	840	HIS	2.9
1	C	126	GLU	2.8
1	A	264	TRP	2.8
1	A	168	ASN	2.8
1	D	186	GLY	2.8
1	B	535	ALA	2.8
1	D	99	ALA	2.8
1	A	117	HIS	2.8
1	B	500	HIS	2.8
1	D	175	MET	2.8
1	B	431	PRO	2.8
1	B	234	ASP	2.8
1	A	397	LEU	2.8
1	B	79	TYR	2.8
1	B	137	PHE	2.8
1	C	230	SER	2.8
1	C	600	SER	2.8
1	C	128	LEU	2.8
1	D	110	ASP	2.8
1	B	384	ALA	2.8
1	D	661	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	864	HIS	2.8
1	D	598	ALA	2.7
1	C	85	SER	2.7
1	C	117	HIS	2.7
1	C	436	GLU	2.7
1	C	438	GLU	2.7
1	B	700	VAL	2.7
1	C	95	VAL	2.7
1	C	395	GLN	2.7
1	D	344	SER	2.7
1	C	232	VAL	2.7
1	D	742	HIS	2.7
1	A	470	GLU	2.7
1	D	335	GLU	2.7
1	B	619	VAL	2.7
1	C	386	PHE	2.7
1	B	100	LEU	2.6
1	D	103	LEU	2.6
1	B	120	VAL	2.6
1	B	787	ALA	2.6
1	A	138	GLY	2.6
1	B	470	GLU	2.6
1	C	167	LYS	2.6
1	A	469	SER	2.6
1	C	229	LEU	2.6
1	C	28	LYS	2.6
1	D	438	GLU	2.6
1	C	56	PHE	2.6
1	C	396	ARG	2.6
1	A	326	SER	2.5
1	B	324	THR	2.5
1	A	659	ILE	2.5
1	C	487	ILE	2.5
1	B	378	LEU	2.5
1	C	616	ARG	2.5
1	D	401	ARG	2.5
1	A	394	GLU	2.5
1	A	269	GLY	2.5
1	B	407	VAL	2.5
1	C	120	VAL	2.5
1	A	113	GLN	2.5
1	A	472	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	840	HIS	2.5
1	D	166	GLY	2.5
1	B	323	GLN	2.5
1	B	331	VAL	2.5
1	C	157	ASN	2.5
1	D	480	LYS	2.5
1	A	283	SER	2.5
1	B	81	SER	2.5
1	C	433	SER	2.5
1	A	438	GLU	2.5
1	C	474	PRO	2.5
1	A	416	VAL	2.5
1	C	402	ALA	2.5
1	B	62	THR	2.4
1	C	185	SER	2.4
1	C	553	SER	2.4
1	B	772	ASP	2.4
1	C	171	MET	2.4
1	C	359	ARG	2.4
1	A	702	ILE	2.4
1	C	175	MET	2.4
1	C	336	LYS	2.4
1	B	758	VAL	2.4
1	C	112	PHE	2.4
1	C	127	LEU	2.4
1	D	471	PRO	2.4
1	D	700	VAL	2.4
1	A	79	TYR	2.4
1	D	182	THR	2.4
1	A	81	SER	2.4
1	B	297	GLU	2.4
1	B	171	MET	2.4
1	D	167	LYS	2.4
1	C	220	ARG	2.4
1	B	112	PHE	2.4
1	C	137	PHE	2.4
1	D	270	LEU	2.3
1	C	426	ILE	2.3
1	A	125	GLU	2.3
1	A	425	ASP	2.3
1	A	583	ASP	2.3
1	B	467	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	264	TRP	2.3
1	A	78	PRO	2.3
1	A	658	GLY	2.3
1	C	96	ARG	2.3
1	C	160	PHE	2.3
1	C	178	LEU	2.3
1	D	410	TYR	2.3
1	B	78	PRO	2.3
1	D	415	GLU	2.3
1	B	185	SER	2.3
1	D	396	ARG	2.3
1	D	481	CYS	2.3
1	D	693	LEU	2.3
1	C	398	ALA	2.3
1	B	111	HIS	2.3
1	C	394	GLU	2.3
1	A	680	ARG	2.3
1	D	233	LEU	2.3
1	B	160	PHE	2.3
1	A	180	ILE	2.2
1	A	124	GLU	2.2
1	B	648	GLN	2.2
1	C	467	ASP	2.2
1	D	399	SER	2.2
1	B	717	GLY	2.2
1	D	105	TRP	2.2
1	C	331	VAL	2.2
1	A	21	ALA	2.2
1	A	289	HIS	2.2
1	C	118	HIS	2.2
1	B	447	CYS	2.2
1	D	683	CYS	2.2
1	B	436	GLU	2.2
1	D	297	GLU	2.2
1	D	107	GLN	2.2
1	B	80	GLY	2.2
1	B	765	GLY	2.2
1	C	658	GLY	2.2
1	B	101	LEU	2.2
1	A	619	VAL	2.2
1	D	498	ALA	2.2
1	B	478	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	303	TYR	2.2
1	A	604	ASP	2.2
1	C	435	GLY	2.2
1	D	484	LYS	2.2
1	A	331	VAL	2.2
1	A	468	TRP	2.2
1	C	468	TRP	2.2
1	B	775	GLU	2.2
1	C	64	GLU	2.2
1	D	82	ARG	2.2
1	B	471	PRO	2.2
1	B	554	GLN	2.2
1	C	314	LYS	2.2
1	D	658	GLY	2.2
1	C	172	VAL	2.2
1	C	105	TRP	2.1
1	D	488	ALA	2.1
1	C	248	GLU	2.1
1	C	391	GLU	2.1
1	D	394	GLU	2.1
1	D	482	PRO	2.1
1	C	183	GLN	2.1
1	D	695	ASN	2.1
1	C	317	LEU	2.1
1	A	66	GLY	2.1
1	B	95	VAL	2.1
1	B	118	HIS	2.1
1	B	301	ASP	2.1
1	C	437	ASP	2.1
1	B	104	SER	2.1
1	C	182	THR	2.1
1	C	382	PRO	2.1
1	B	168	ASN	2.1
1	B	136	VAL	2.1
1	A	298	ARG	2.1
1	D	729[A]	TRP	2.1
1	D	266	GLY	2.1
1	B	360	ASP	2.1
1	A	391	GLU	2.1
1	A	402	ALA	2.1
1	C	130	GLU	2.1
1	C	334	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.1
1	A	406	ASN	2.1
1	A	810	ASN	2.1
1	A	700	VAL	2.1
1	D	499	ARG	2.0
1	D	714	GLU	2.0
1	B	473	SER	2.0
1	C	94	LYS	2.0
1	C	270	LEU	2.0
1	A	717	GLY	2.0
1	C	339	VAL	2.0
1	A	477	ASP	2.0
1	B	296	GLU	2.0
1	A	692	ALA	2.0
1	A	787	ALA	2.0
1	B	630	ALA	2.0
1	D	444	ALA	2.0
1	B	148	SER	2.0
1	A	177	PRO	2.0
1	B	115	THR	2.0
1	A	111	HIS	2.0
1	B	840	HIS	2.0
1	A	40	GLY	2.0
1	C	406	ASN	2.0
1	D	702	ILE	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 ⓘ

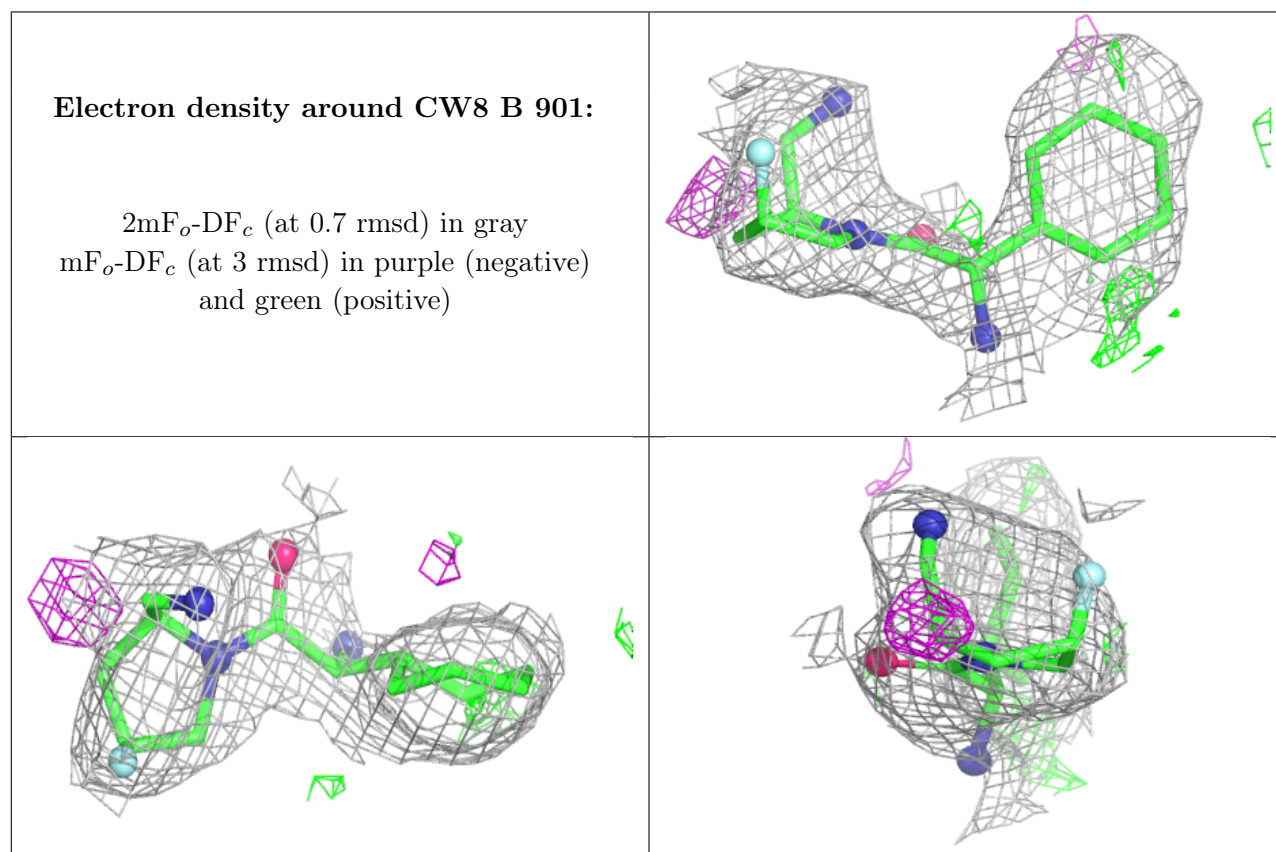
There are no oligosaccharides in this entry.

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.

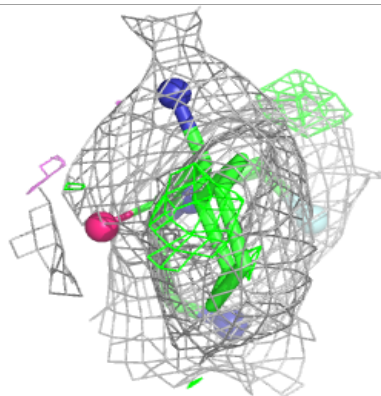
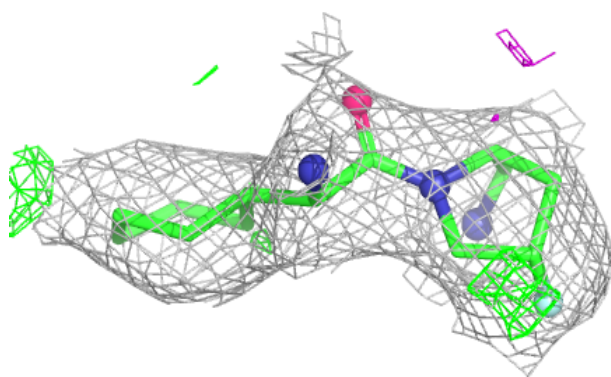
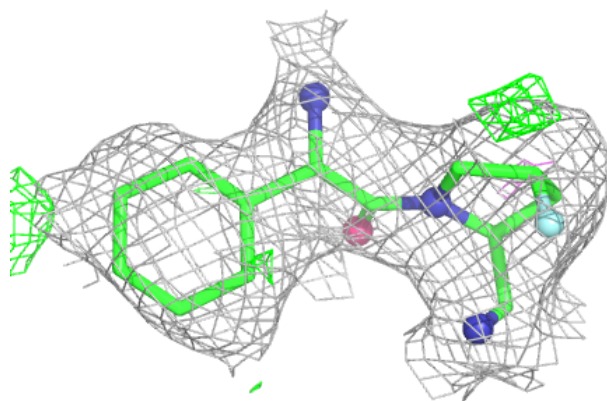
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CW8	B	901	18/18	0.80	0.20	23,51,62,64	0
2	CW8	D	901	18/18	0.88	0.16	22,39,60,63	0
2	CW8	A	901	18/18	0.89	0.17	28,44,59,70	0
2	CW8	C	901	18/18	0.91	0.13	21,40,47,50	0

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.



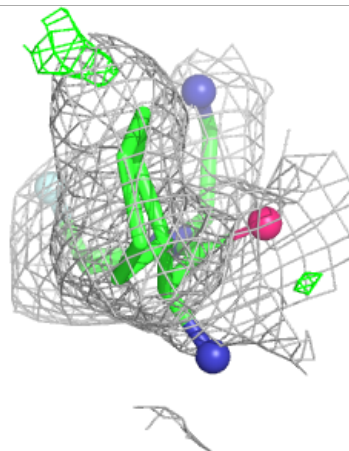
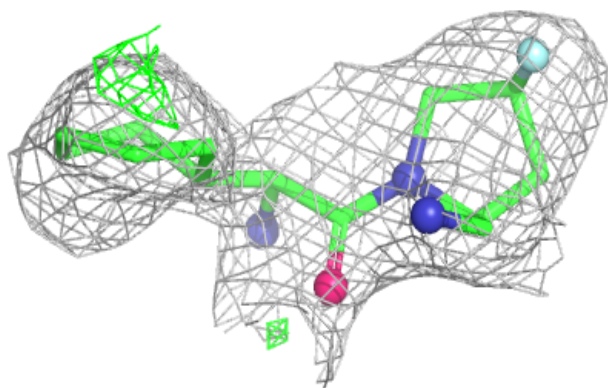
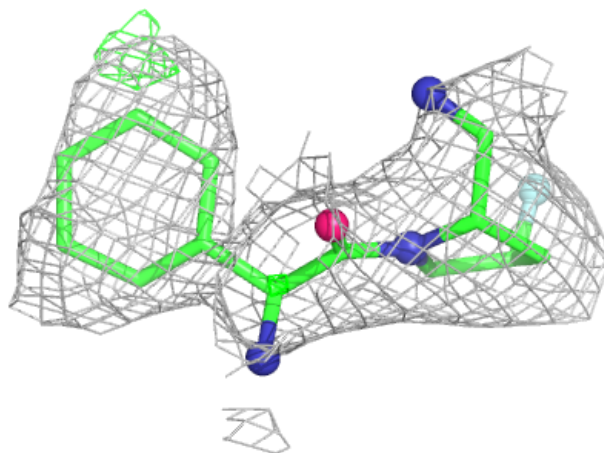
Electron density around CW8 D 901:

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



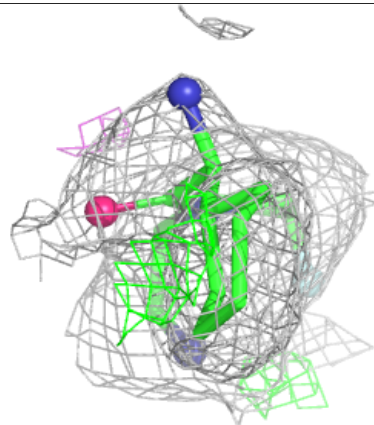
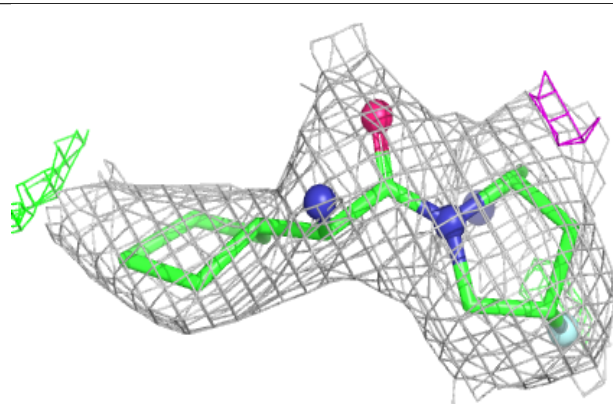
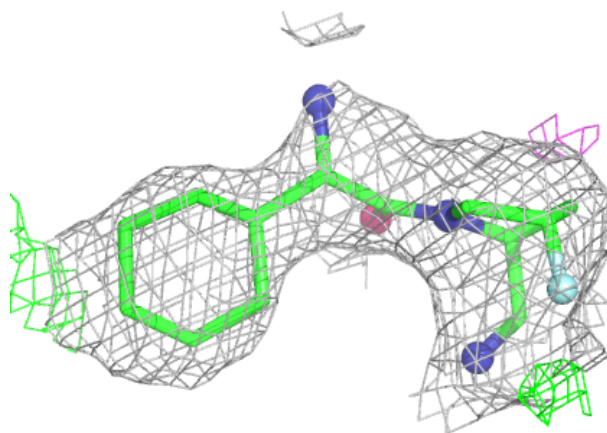
Electron density around CW8 A 901:

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



Electron density around CW8 C 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 ⓘ

There are no such residues in this entry.