Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 06:06 AM EDT

PDB ID	:	7SVN
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 (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:

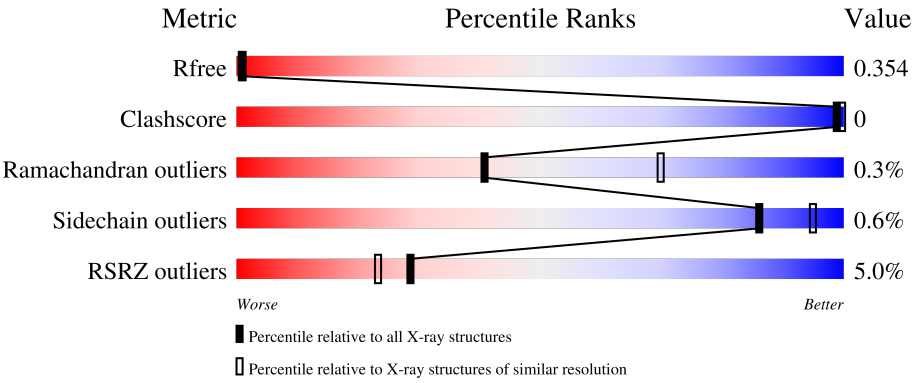
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.78 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 <=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	6% 93% • 5%
1	B	869	4% 92% • 5%
1	C	869	4% 93% • 5%
1	D	869	5% 92% • 5%

2 Entry composition (i)

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:

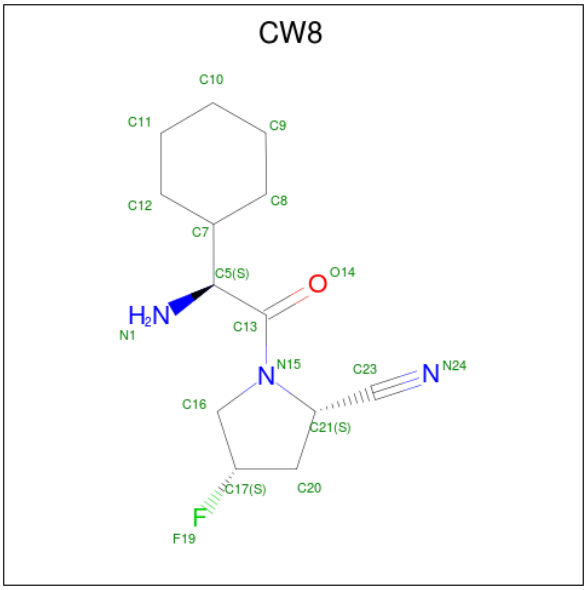
Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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 (three-letter code: CW8) (formula: $C_{13}H_{20}FN_3O$) (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			

Continued on next page...

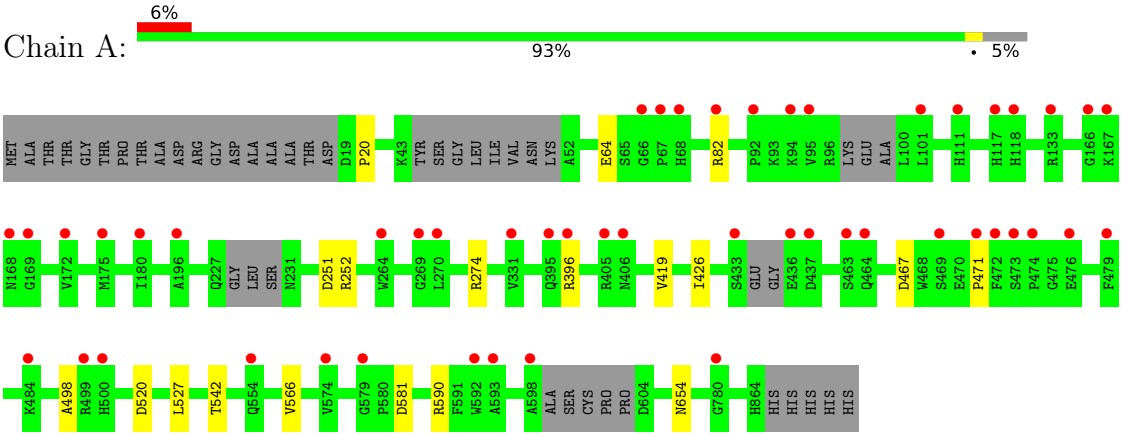
Continued from previous page...

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

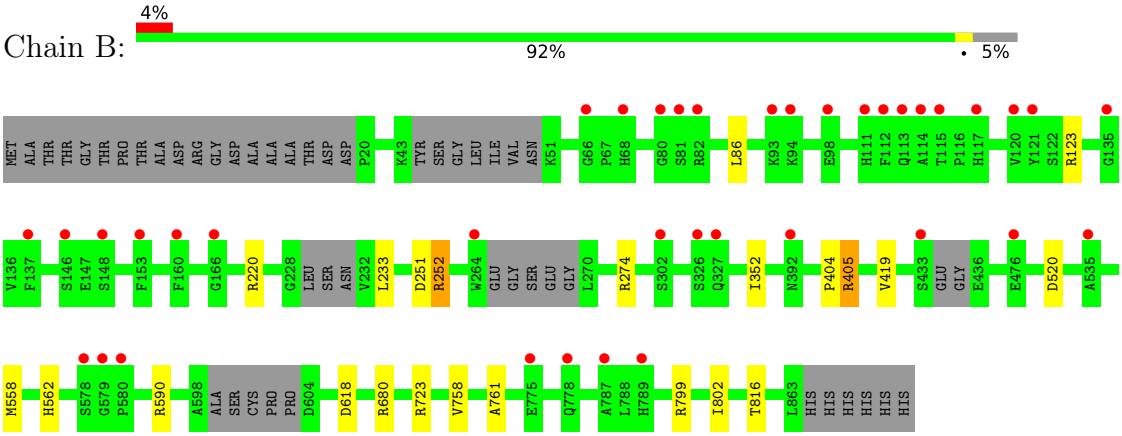
3 Residue-property plots (i)

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.

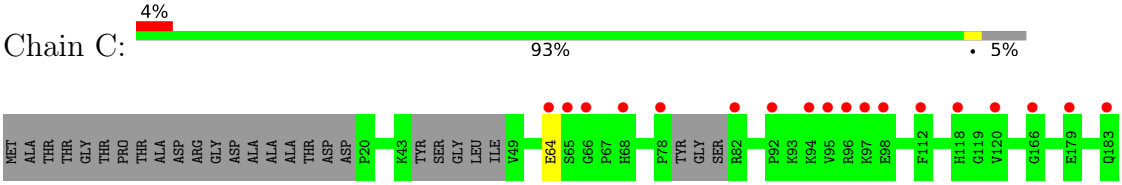
• Molecule 1: Dipeptidyl peptidase 9

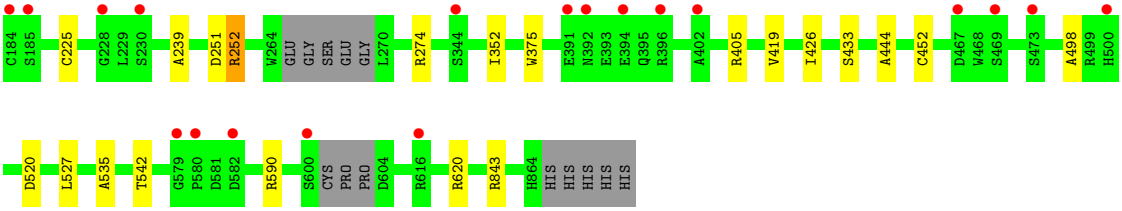


• Molecule 1: Dipeptidyl peptidase 9

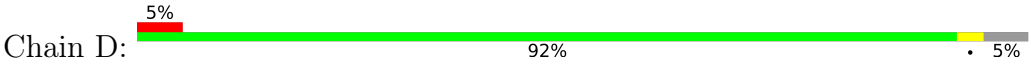


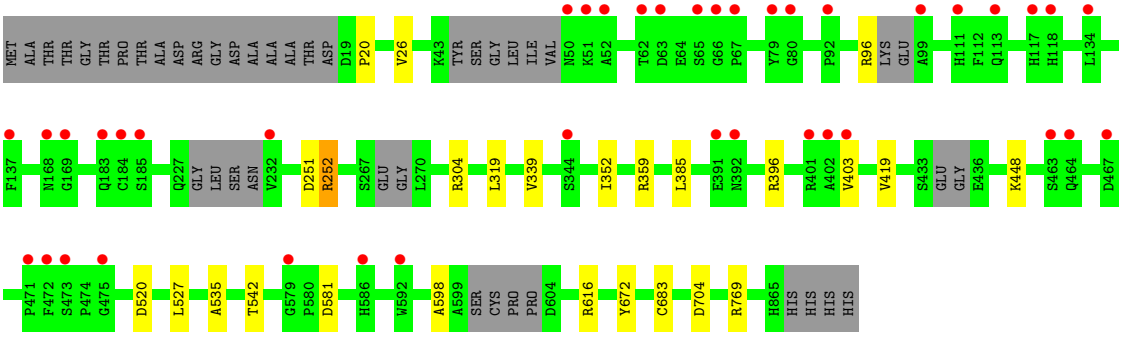
• Molecule 1: Dipeptidyl peptidase 9





• Molecule 1: Dipeptidyl peptidase 9





4 Data and refinement statistics (i)

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 49.01 – 2.78	Depositor EDS
% Data completeness (in resolution range)	94.4 (157.52-2.78) 94.4 (49.01-2.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.267 , 0.349 0.271 , 0.354	Depositor DCC
R_{free} test set	732 reflections (0.71%)	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)	0.32 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	1/6903 (0.0%)	0.82	7/9365 (0.1%)
1	B	0.68	2/6880 (0.0%)	0.83	12/9331 (0.1%)
1	C	0.67	1/6946 (0.0%)	0.82	8/9424 (0.1%)
1	D	0.67	1/6935 (0.0%)	0.84	9/9408 (0.1%)
All	All	0.68	5/27664 (0.0%)	0.83	36/37528 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	LEU	CG-CD1	-7.22	1.25	1.51
1	C	64	GLU	CG-CD	-6.43	1.42	1.51
1	B	233	LEU	CG-CD2	6.35	1.75	1.51
1	D	96	ARG	CD-NE	6.04	1.56	1.46
1	A	64	GLU	CB-CG	5.23	1.62	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	233	LEU	CB-CG-CD1	14.60	135.82	111.00
1	D	396	ARG	CD-NE-CZ	7.59	134.23	123.60
1	C	405	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	405	ARG	NE-CZ-NH1	7.17	123.89	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	252	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	252	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	405	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	252	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	233	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	A	252	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	123	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	252	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	396	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	B	274	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	558	MET	CG-SD-CE	5.55	109.09	100.20
1	D	304	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	590	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	616	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	274	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	274	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	467	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	620	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	252	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	590	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	396	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	590	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	843	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	769	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	799	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	359	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	704	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	680	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	252	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	220	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	82	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	723	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	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	3	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	19	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 (19) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	47	76
1	B	811/869 (93%)	779 (96%)	31 (4%)	1 (0%)	51	80
1	C	821/869 (94%)	783 (95%)	35 (4%)	3 (0%)	34	64
1	D	815/869 (94%)	782 (96%)	29 (4%)	4 (0%)	29	58
All	All	3261/3476 (94%)	3124 (96%)	127 (4%)	10 (0%)	41	70

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 (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	728/759 (96%)	725 (100%)	3 (0%)	91	96
1	B	725/759 (96%)	718 (99%)	7 (1%)	76	91
1	C	732/759 (96%)	730 (100%)	2 (0%)	92	97
1	D	730/759 (96%)	725 (99%)	5 (1%)	84	94
All	All	2915/3036 (96%)	2898 (99%)	17 (1%)	86	95

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

Mol	Chain	Res	Type
1	A	251	ASP
1	A	520	ASP
1	A	581	ASP
1	B	86	LEU
1	B	251	ASP
1	B	404	PRO
1	B	405	ARG
1	B	520	ASP
1	B	562	HIS
1	B	618	ASP
1	C	251	ASP
1	C	520	ASP
1	D	251	ASP
1	D	319	LEU
1	D	520	ASP
1	D	581	ASP
1	D	683	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	B	226	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	424	HIS
1	C	812	HIS
1	D	525	HIS
1	D	695	ASN
1	D	815	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

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	A	901	1	18,19,19	1.65	2 (11%)	18,26,26	8.64	8 (44%)
2	CW8	B	901	1	18,19,19	1.50	2 (11%)	18,26,26	8.66	4 (22%)
2	CW8	C	901	1	18,19,19	1.55	1 (5%)	18,26,26	8.60	5 (27%)
2	CW8	D	901	1	18,19,19	1.47	1 (5%)	18,26,26	9.01	4 (22%)

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	A	901	1	-	0/12/34/34	0/2/2/2
2	CW8	B	901	1	-	0/12/34/34	0/2/2/2
2	CW8	C	901	1	-	0/12/34/34	0/2/2/2
2	CW8	D	901	1	-	1/12/34/34	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	6.05	1.26	1.14
2	C	901	CW8	C23-N24	5.82	1.25	1.14
2	D	901	CW8	C23-N24	5.79	1.25	1.14
2	B	901	CW8	C23-N24	5.74	1.25	1.14
2	A	901	CW8	C21-C23	2.21	1.52	1.48
2	B	901	CW8	C21-C23	2.15	1.52	1.48

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	CW8	C21-C23-N24	-37.76	116.41	177.23
2	B	901	CW8	C21-C23-N24	-35.90	119.41	177.23
2	C	901	CW8	C21-C23-N24	-35.75	119.64	177.23
2	A	901	CW8	C21-C23-N24	-35.68	119.77	177.23
2	C	901	CW8	C13-C5-N1	-4.59	103.23	110.22
2	B	901	CW8	C23-C21-N15	4.41	116.73	110.73
2	A	901	CW8	C23-C21-N15	3.75	115.83	110.73
2	A	901	CW8	C13-C5-N1	-3.71	104.57	110.22
2	B	901	CW8	C13-C5-N1	-3.70	104.58	110.22
2	D	901	CW8	C23-C21-N15	3.59	115.62	110.73
2	B	901	CW8	F19-C17-C20	3.15	112.68	108.98
2	A	901	CW8	C8-C7-C5	3.00	115.86	111.86
2	D	901	CW8	C13-C5-N1	-2.91	105.78	110.22
2	A	901	CW8	F19-C17-C20	-2.73	105.78	108.98
2	C	901	CW8	C8-C7-C5	2.71	115.48	111.86
2	C	901	CW8	C23-C21-N15	2.22	113.75	110.73
2	A	901	CW8	C10-C9-C8	2.22	115.93	111.42
2	A	901	CW8	F19-C17-C16	2.21	112.30	108.62
2	C	901	CW8	C12-C7-C8	-2.09	105.76	109.44
2	A	901	CW8	O14-C13-C5	-2.07	115.95	119.99
2	D	901	CW8	C16-N15-C21	-2.01	108.82	111.71

There are no chirality outliers.

All (1) torsion outliers are listed below:

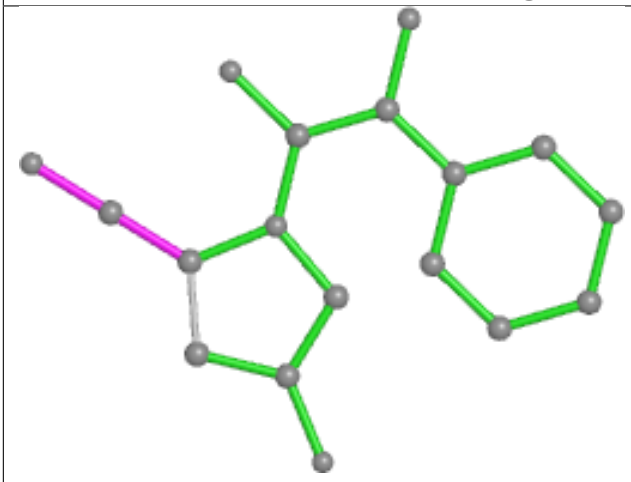
Mol	Chain	Res	Type	Atoms
2	D	901	CW8	O14-C13-C5-N1

There are no ring outliers.

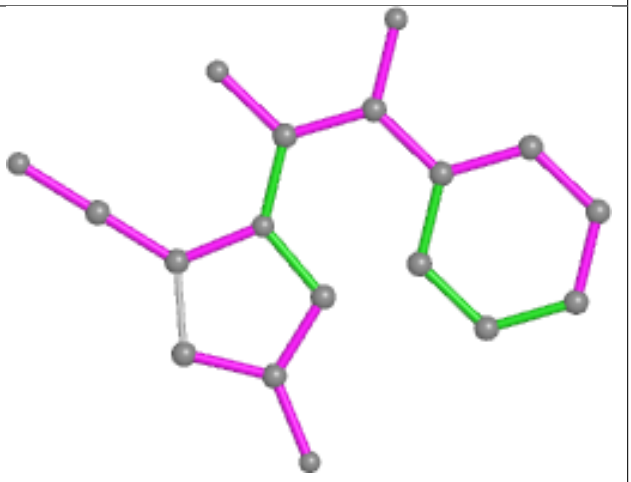
No monomer is involved in short contacts.

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 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.

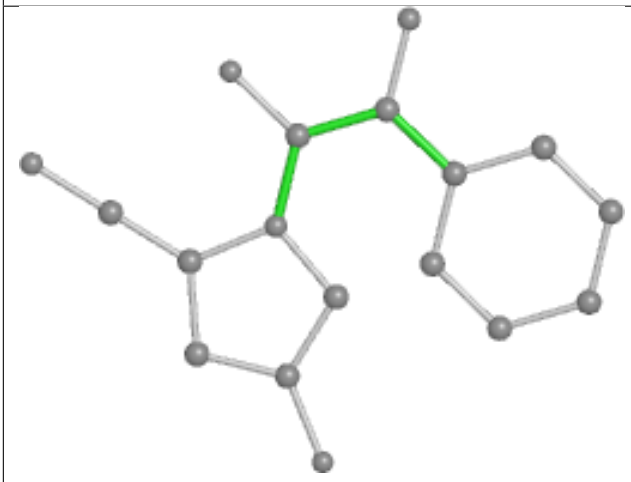
Ligand CW8 A 901



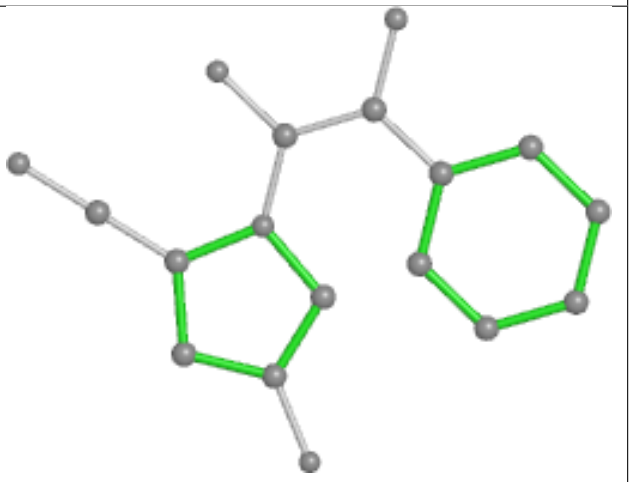
Bond lengths



Bond angles

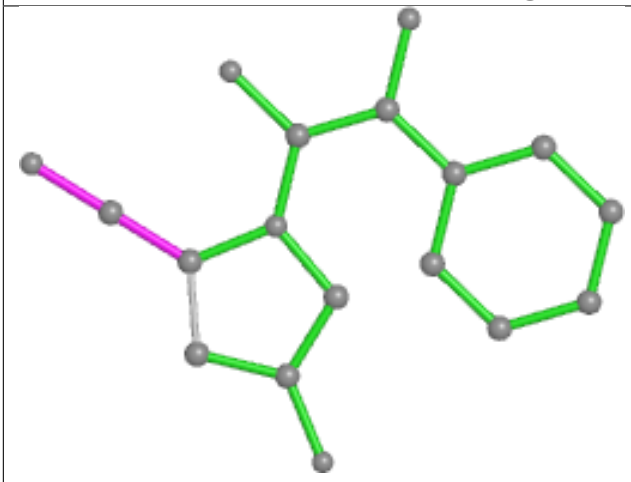


Torsions

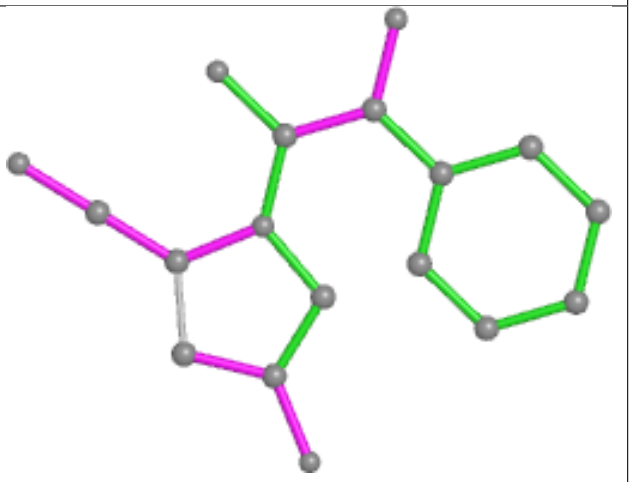


Rings

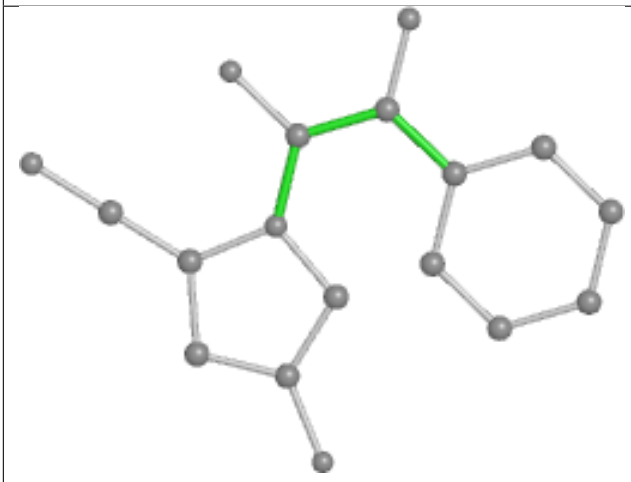
Ligand CW8 B 901



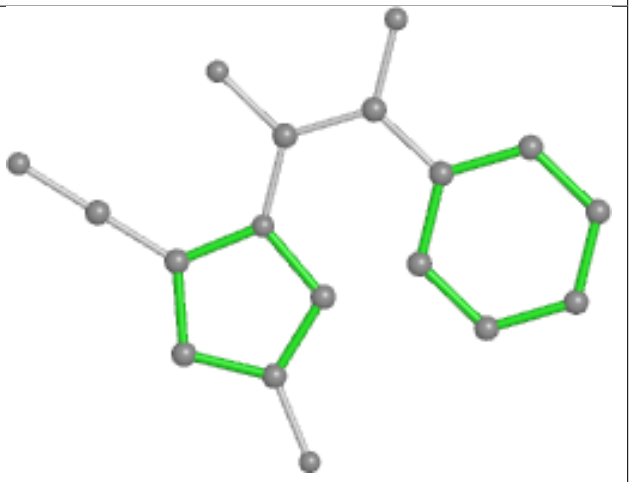
Bond lengths



Bond angles

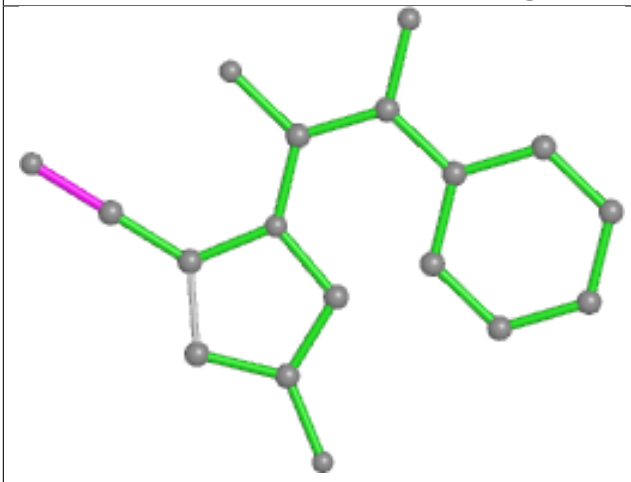


Torsions

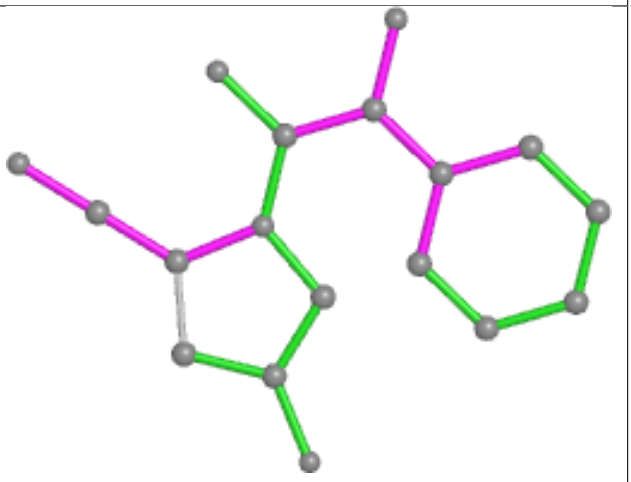


Rings

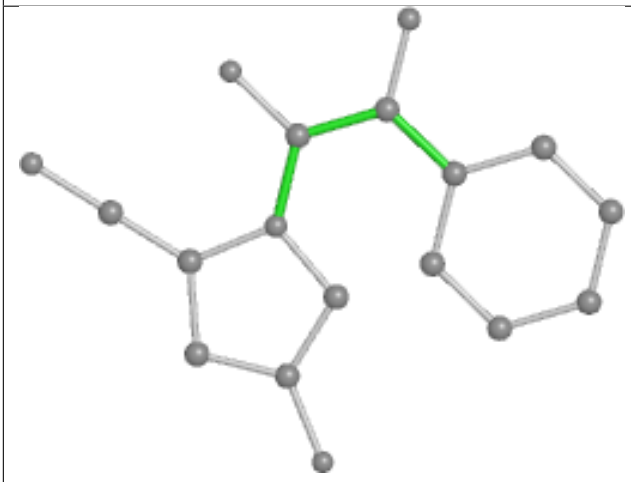
Ligand CW8 C 901



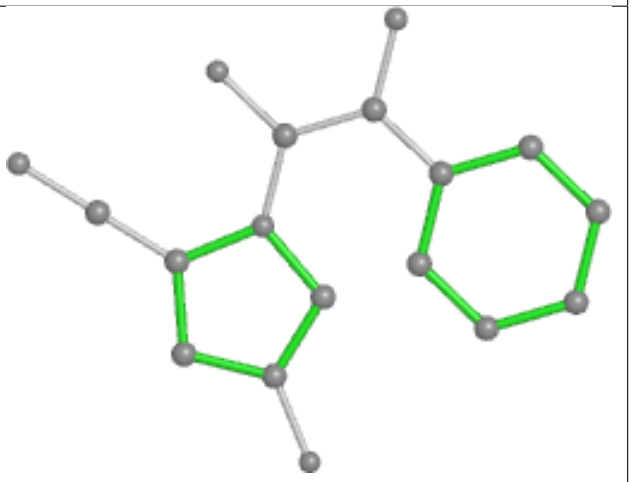
Bond lengths



Bond angles

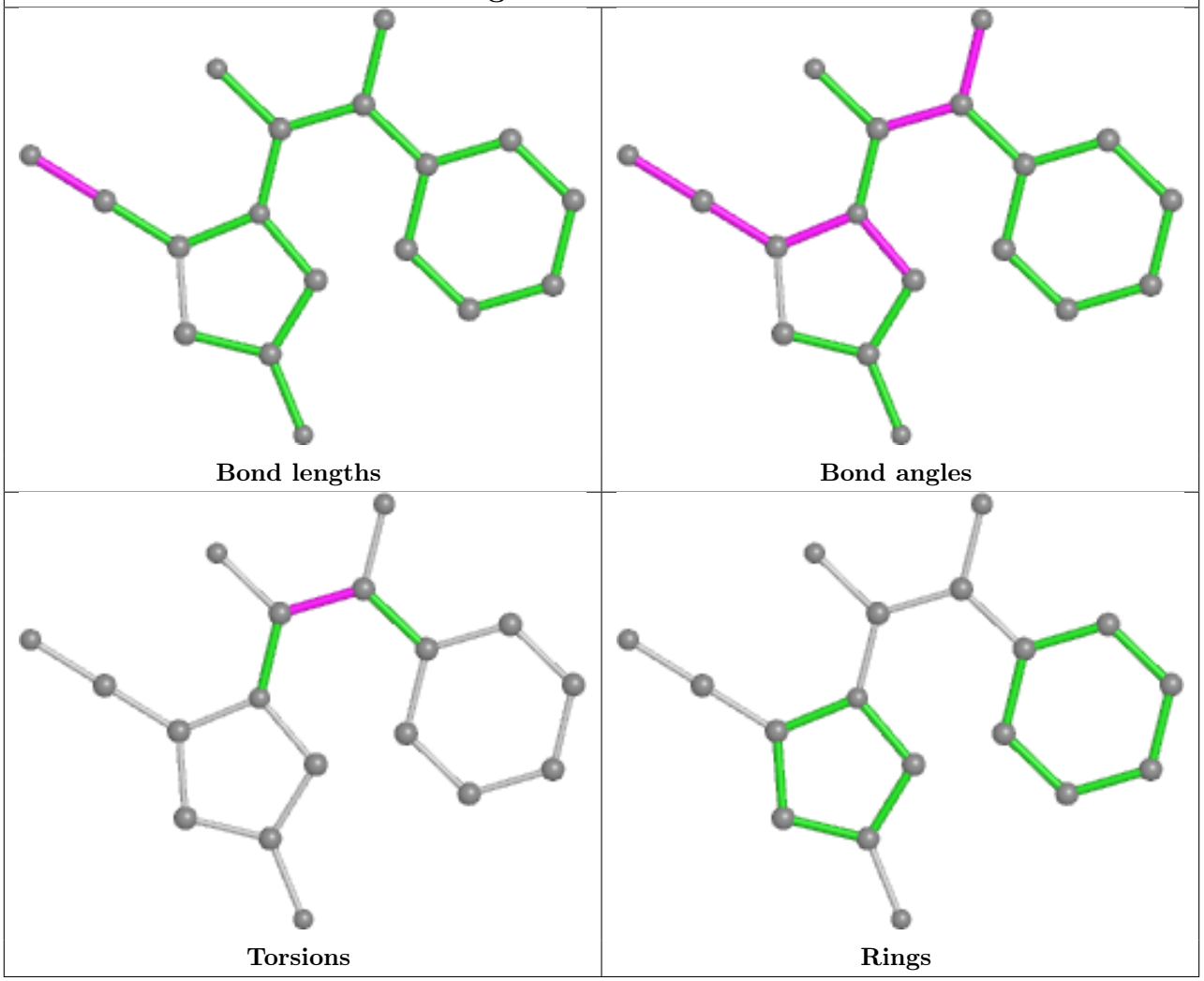


Torsions



Rings

Ligand CW8 D 901



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^{th} 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%)	0.31	50 (6%)	21	16	15, 42, 84, 132	68 (8%)
1	B	822/869 (94%)	0.21	38 (4%)	32	26	16, 42, 85, 137	66 (8%)
1	C	829/869 (95%)	0.15	37 (4%)	33	27	14, 39, 87, 120	59 (7%)
1	D	827/869 (95%)	0.17	40 (4%)	30	24	13, 39, 81, 130	60 (7%)
All	All	3303/3476 (95%)	0.21	165 (4%)	28	23	13, 41, 85, 137	253 (7%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	HIS	7.2
1	A	118	HIS	5.5
1	A	476	GLU	5.1
1	B	112	PHE	5.0
1	D	80	GLY	4.6
1	B	81	SER	4.6
1	C	228	GLY	4.5
1	B	113	GLN	4.4
1	B	578	SER	4.3
1	A	500	HIS	4.2
1	A	269	GLY	4.2
1	A	472	PHE	4.2
1	C	184	CYS	4.2
1	D	51	LYS	4.2
1	A	433	SER	4.2
1	D	66	GLY	4.2
1	C	579	GLY	4.1
1	A	471	PRO	4.1
1	A	264	TRP	4.0
1	D	403	VAL	4.0
1	A	133	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	471	PRO	3.9
1	A	94	LYS	3.9
1	B	66	GLY	3.9
1	C	68	HIS	3.8
1	D	62	THR	3.8
1	A	66	GLY	3.8
1	C	95	VAL	3.7
1	C	98	GLU	3.7
1	D	392	ASN	3.7
1	B	137	PHE	3.7
1	B	114	ALA	3.6
1	B	135	GLY	3.6
1	D	232	VAL	3.6
1	A	92	PRO	3.6
1	B	433	SER	3.6
1	B	120	VAL	3.4
1	A	396	ARG	3.4
1	C	230	SER	3.4
1	C	120	VAL	3.4
1	A	499	ARG	3.3
1	B	82	ARG	3.3
1	D	99	ALA	3.3
1	B	111	HIS	3.1
1	D	65	SER	3.1
1	A	469	SER	3.1
1	B	580	PRO	3.1
1	D	63	ASP	3.1
1	A	169	GLY	3.0
1	D	463	SER	3.0
1	B	121	TYR	2.9
1	A	172	VAL	2.9
1	B	117	HIS	2.9
1	C	78	PRO	2.9
1	D	50	ASN	2.9
1	A	270	LEU	2.9
1	C	616	ARG	2.8
1	A	168	ASN	2.8
1	D	92	PRO	2.8
1	D	472	PHE	2.8
1	B	115	THR	2.8
1	A	473	SER	2.7
1	C	185	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	185	SER	2.7
1	C	600	SER	2.7
1	B	160	PHE	2.7
1	A	574	VAL	2.7
1	A	592	TRP	2.7
1	C	396	ARG	2.7
1	C	94	LYS	2.6
1	C	183	GLN	2.6
1	D	579	GLY	2.6
1	B	392	ASN	2.6
1	C	96	ARG	2.6
1	B	98	GLU	2.6
1	A	593	ALA	2.6
1	C	402	ALA	2.6
1	D	67	PRO	2.6
1	D	464	GLN	2.6
1	A	196	ALA	2.6
1	C	391	GLU	2.6
1	B	80	GLY	2.6
1	D	52	ALA	2.5
1	D	586	HIS	2.5
1	A	405	ARG	2.5
1	B	326	SER	2.5
1	D	401	ARG	2.5
1	B	775	GLU	2.5
1	B	264	TRP	2.5
1	D	473	SER	2.5
1	D	467	ASP	2.5
1	C	473	SER	2.5
1	D	111	HIS	2.5
1	A	598	ALA	2.4
1	B	787	ALA	2.4
1	B	778	GLN	2.4
1	C	500	HIS	2.4
1	D	402	ALA	2.4
1	C	112	PHE	2.4
1	D	79	TYR	2.4
1	C	92	PRO	2.4
1	D	391	GLU	2.4
1	A	117	HIS	2.4
1	B	146	SER	2.4
1	B	153	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	476	GLU	2.4
1	A	463	SER	2.4
1	B	302	SER	2.4
1	C	65	SER	2.4
1	A	95	VAL	2.4
1	D	168	ASN	2.4
1	C	97	LYS	2.3
1	A	406	ASN	2.3
1	D	183	GLN	2.3
1	C	394	GLU	2.3
1	B	535	ALA	2.3
1	A	175	MET	2.3
1	C	582	ASP	2.3
1	A	68	HIS	2.3
1	A	554	GLN	2.3
1	A	474	PRO	2.2
1	A	437	ASP	2.2
1	D	475	GLY	2.2
1	C	469	SER	2.2
1	D	592	TRP	2.2
1	A	101	LEU	2.2
1	C	166	GLY	2.2
1	C	467	ASP	2.2
1	D	137	PHE	2.2
1	A	395	GLN	2.2
1	B	166	GLY	2.2
1	A	82	ARG	2.2
1	A	479	PHE	2.2
1	C	118	HIS	2.2
1	C	66	GLY	2.2
1	C	179	GLU	2.1
1	A	111	HIS	2.1
1	A	579	GLY	2.1
1	D	117	HIS	2.1
1	D	169	GLY	2.1
1	A	484	LYS	2.1
1	B	93	LYS	2.1
1	A	464	GLN	2.1
1	C	344	SER	2.1
1	A	166	GLY	2.1
1	C	580	PRO	2.1
1	B	148	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	579	GLY	2.1
1	B	68	HIS	2.1
1	C	392	ASN	2.1
1	D	344	SER	2.1
1	A	180	ILE	2.1
1	B	327	GLN	2.1
1	B	94	LYS	2.1
1	A	780	GLY	2.1
1	A	167	LYS	2.0
1	C	82	ARG	2.0
1	A	67	PRO	2.0
1	C	64	GLU	2.0
1	D	134	LEU	2.0
1	B	789	HIS	2.0
1	D	113	GLN	2.0
1	D	184	CYS	2.0
1	A	436	GLU	2.0
1	A	331	VAL	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)

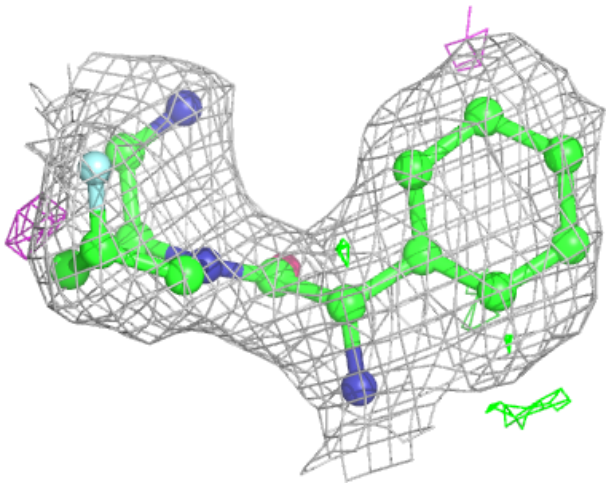
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

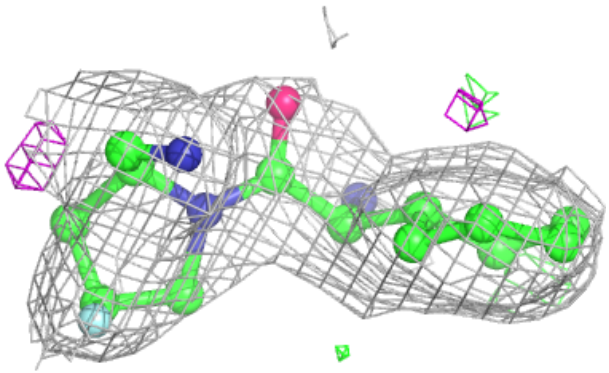
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CW8	B	901	18/18	0.86	0.24	23,51,62,64	0
2	CW8	A	901	18/18	0.88	0.33	28,44,59,70	0
2	CW8	D	901	18/18	0.92	0.32	22,39,60,63	0
2	CW8	C	901	18/18	0.93	0.23	21,40,47,50	0

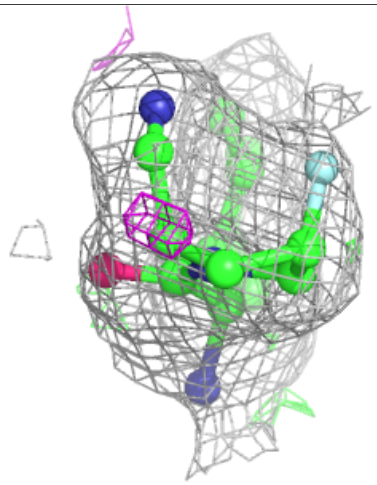
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CW8 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)

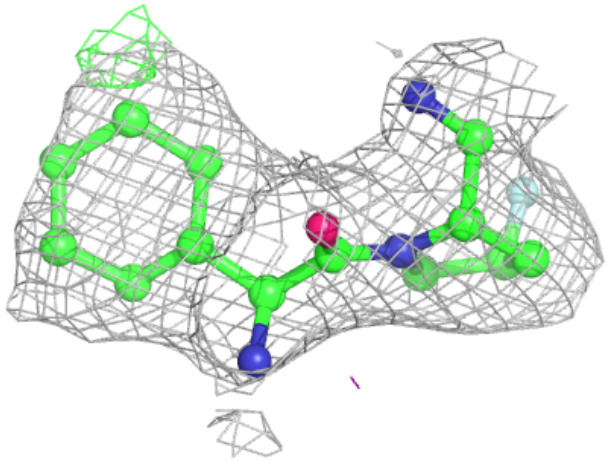


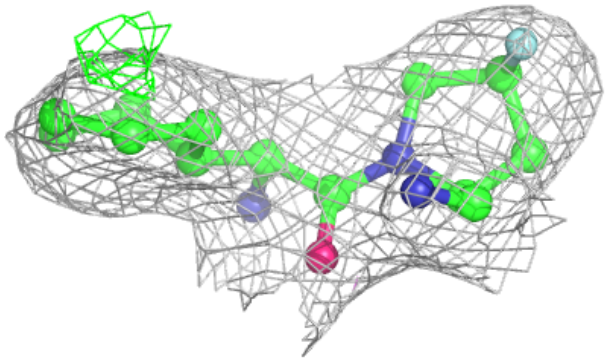


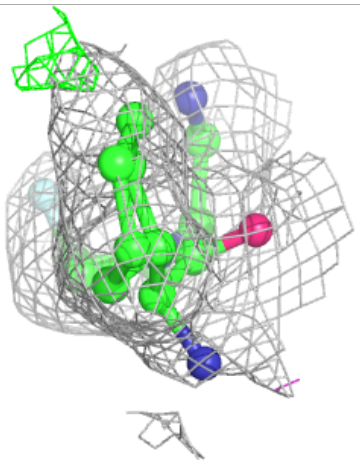


Electron density around CW8 A 901:

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

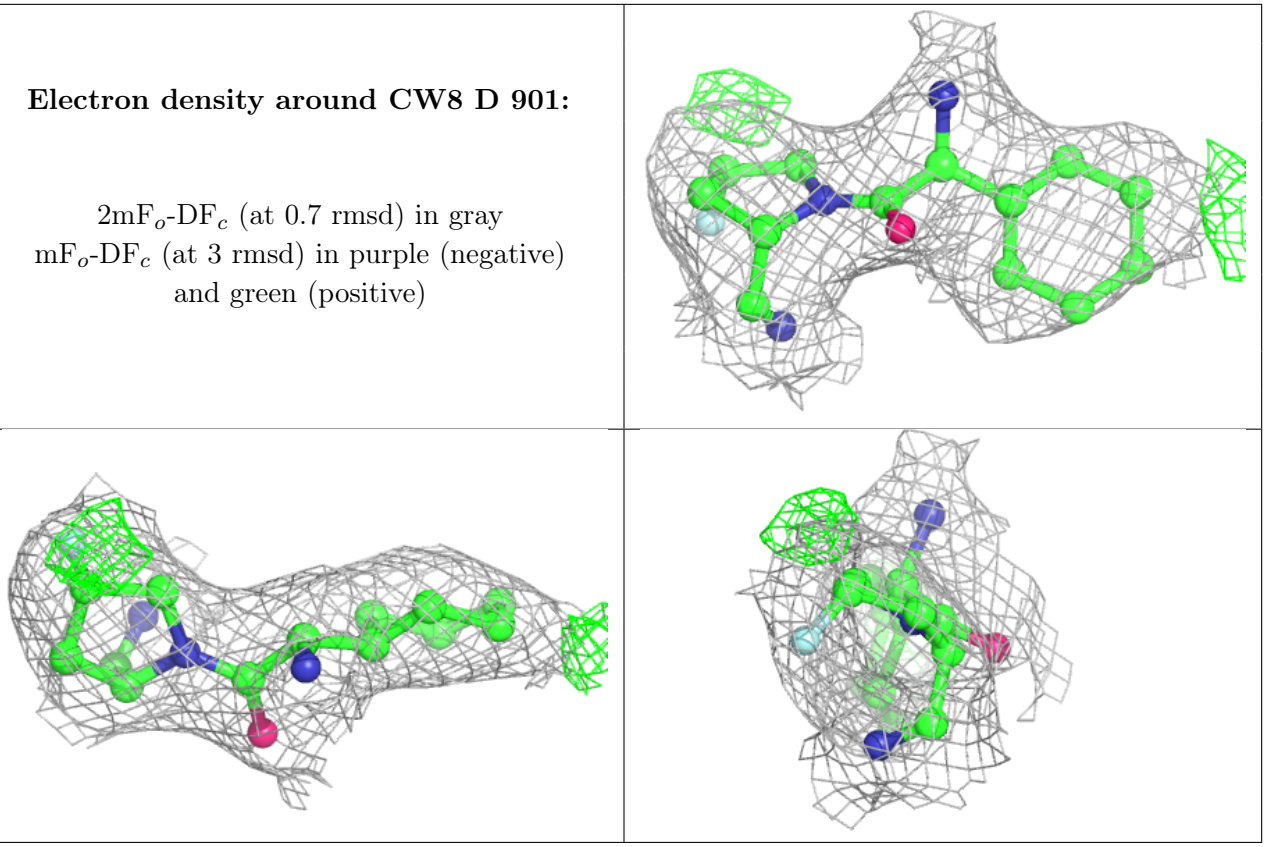






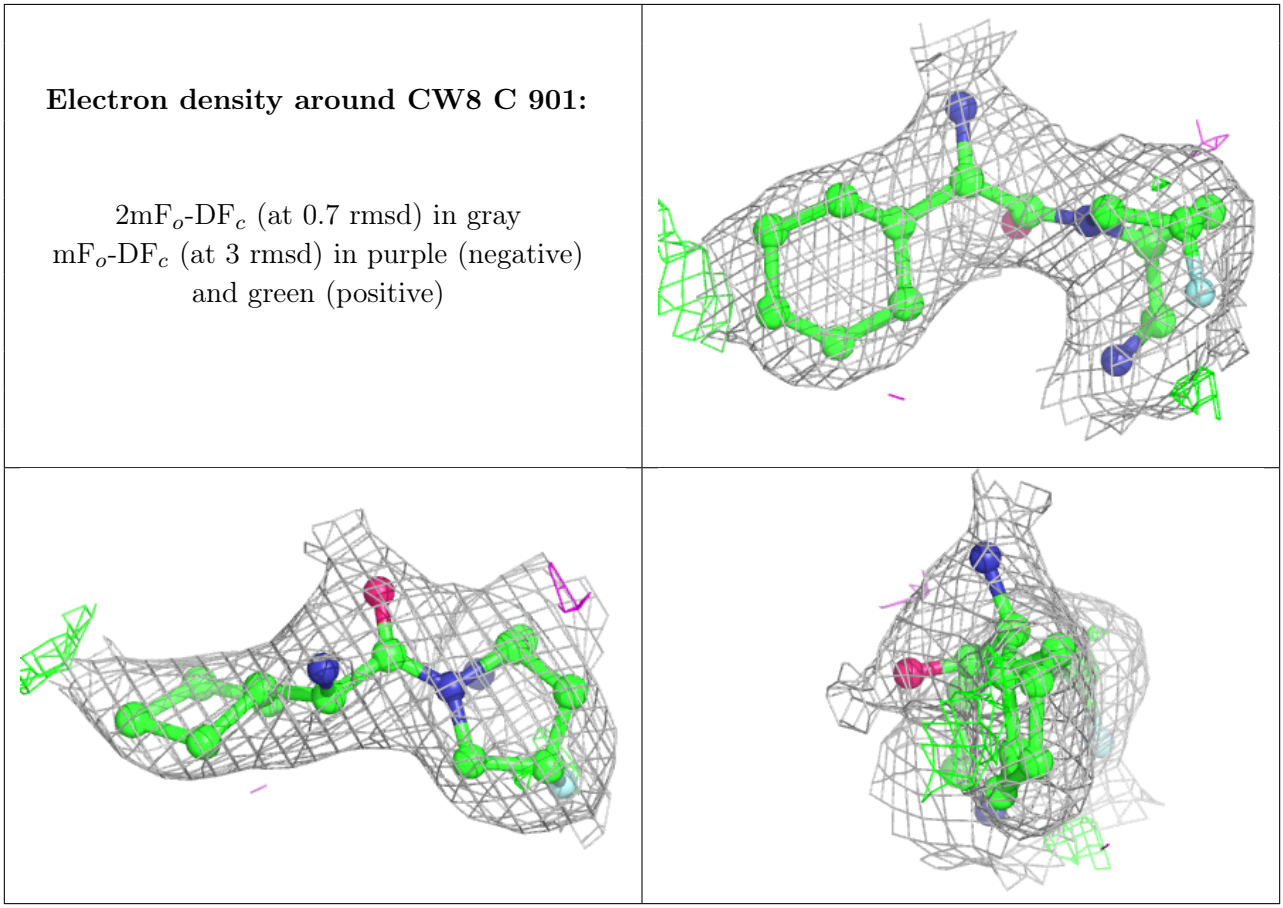
Electron density around CW8 D 901:

$2mF_o$-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 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 (i)

There are no such residues in this entry.