



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:26 AM UTC

PDB ID : 7SVO / pdb_00007svo
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

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

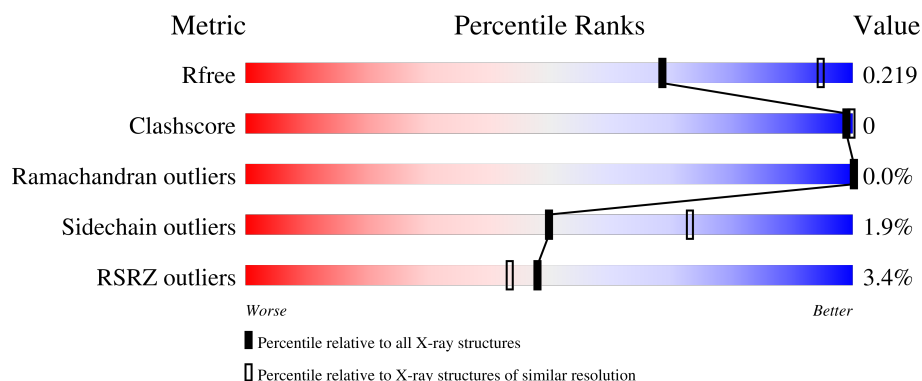
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

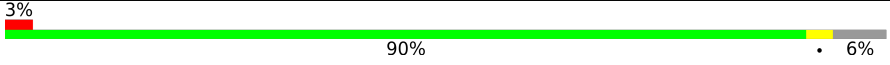
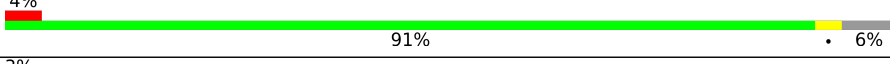
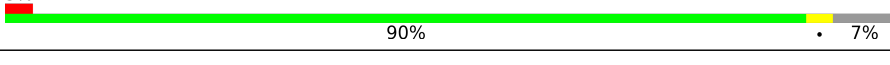
The reported resolution of this entry is 2.58 Å.

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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 ≥ 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	
1	B	903	
1	C	903	

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.

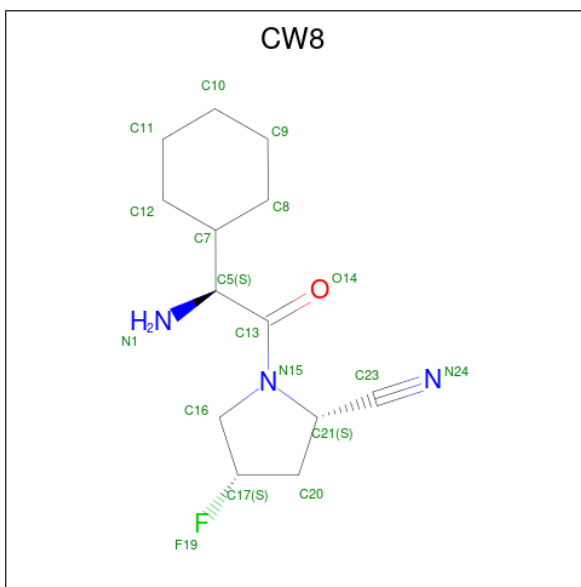
- Molecule 1 is a protein called Dipeptidyl peptidase 8.

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:

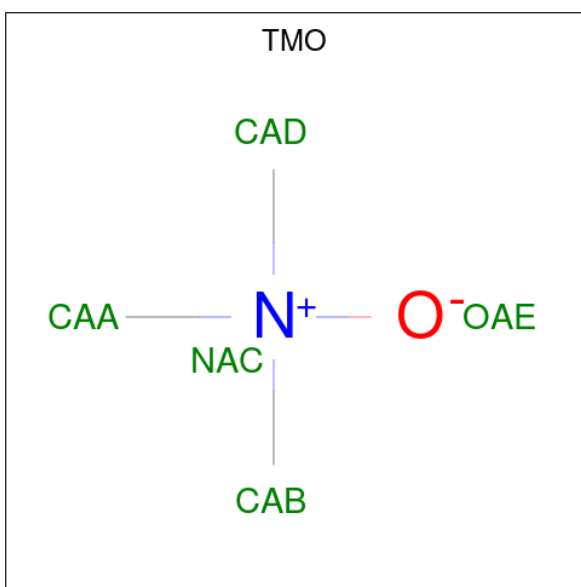
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q6V1X1
A	-3	ALA	-	expression tag	UNP Q6V1X1
A	-2	MET	-	expression tag	UNP Q6V1X1
A	-1	GLY	-	expression tag	UNP Q6V1X1
A	0	SER	-	expression tag	UNP Q6V1X1
B	-4	GLY	-	expression tag	UNP Q6V1X1
B	-3	ALA	-	expression tag	UNP Q6V1X1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

- Molecule 3 is trimethylamine oxide (CCD ID: 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		

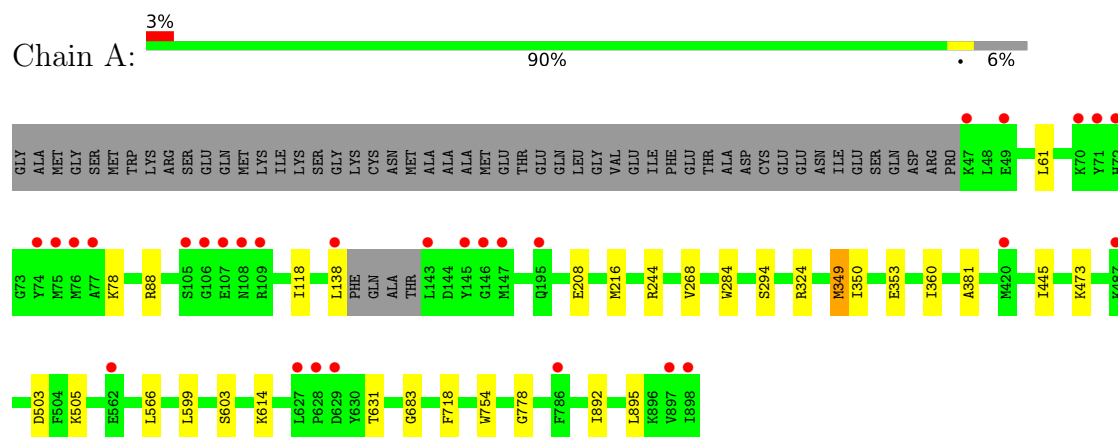
- Molecule 4 is water.

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		

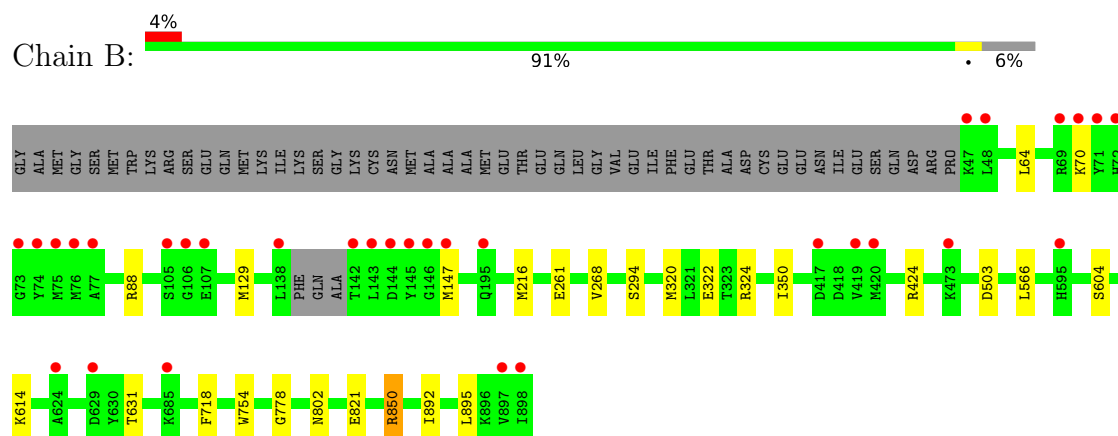
3 Residue-property plots [i](#)

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.

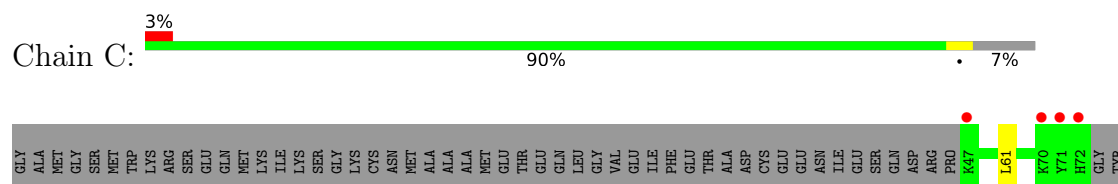
- Molecule 1: Dipeptidyl peptidase 8

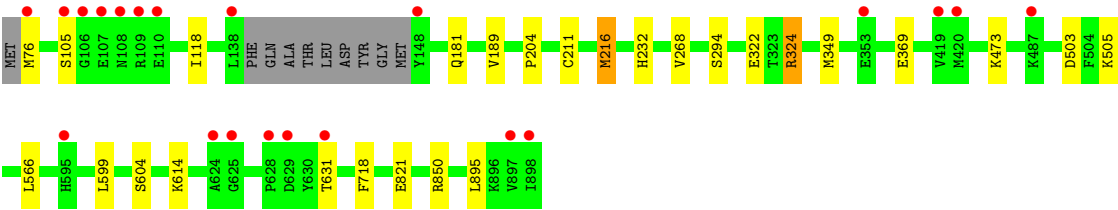


- Molecule 1: Dipeptidyl peptidase 8



- 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, α , β , γ	162.82Å 246.02Å 261.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.77 – 2.58 135.77 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (135.77-2.58) 97.5 (135.77-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.180 , 0.208 0.186 , 0.219	Depositor DCC
R_{free} test set	949 reflections (0.58%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: TMO, 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	0.92	2/7140 (0.0%)	1.04	6/9683 (0.1%)
1	B	0.93	1/7164 (0.0%)	1.04	8/9718 (0.1%)
1	C	0.93	3/7083 (0.0%)	1.04	4/9607 (0.0%)
All	All	0.93	6/21387 (0.0%)	1.04	18/29008 (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	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	9.65	1.72	1.53
1	C	505	LYS	CD-CE	-6.03	1.34	1.52
1	C	850	ARG	NE-CZ	5.57	1.39	1.33
1	B	70	LYS	N-CA	5.50	1.53	1.46
1	C	76	MET	CB-CG	5.47	1.68	1.52
1	A	505	LYS	CD-CE	-5.44	1.36	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	505	LYS	CG-CD-CE	8.00	129.70	111.30
1	A	503	ASP	N-CA-C	7.46	120.28	111.71
1	C	503	ASP	N-CA-C	7.25	120.05	111.71
1	B	850	ARG	NE-CZ-NH2	7.23	125.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	892	ILE	CB-CG1-CD1	6.57	127.59	113.80
1	B	503	ASP	N-CA-C	6.52	119.21	111.71
1	B	850	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	B	892	ILE	CB-CG1-CD1	6.14	126.69	113.80
1	B	850	ARG	CD-NE-CZ	6.01	132.81	124.40
1	B	324	ARG	CG-CD-NE	5.85	124.86	112.00
1	C	324	ARG	CG-CD-NE	5.83	124.83	112.00
1	B	424	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	324	ARG	CB-CG-CD	5.64	124.28	111.30
1	A	324	ARG	CG-CD-NE	5.47	124.04	112.00
1	A	505	LYS	CG-CD-CE	5.38	123.67	111.30
1	C	324	ARG	CB-CG-CD	5.37	123.65	111.30
1	A	683	GLY	N-CA-C	5.29	120.48	114.67
1	B	324	ARG	CB-CG-CD	5.25	123.38	111.30

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 [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	6947	0	6753	7	0
1	B	6970	0	6772	5	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
4	A	200	0	0	1	0
4	B	243	0	0	0	1
4	C	259	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21620	0	20323	18	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 (18) 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:O	1:B:268[A]:VAL:HG23	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:189:VAL:CG1	1:C:204:PRO:HA	2.47	0.45
1:C:181:GLN:HE22	1:C:216:MET:HE3	1.80	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:208:GLU:CD	1:B:802:ASN:HA	2.43	0.42
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
1:A:349:MET:HE2	1:A:360:ILE:HD12	2.03	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%)	48	69
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%)	743 (98%)	14 (2%)	51	74
1	B	760/797 (95%)	747 (98%)	13 (2%)	53	76
1	C	752/797 (94%)	736 (98%)	16 (2%)	47	71
All	All	2269/2391 (95%)	2226 (98%)	43 (2%)	50	73

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	78	LYS
1	A	88	ARG
1	A	216	MET
1	A	268	VAL
1	A	294	SER
1	A	349	MET
1	A	350	ILE

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Mol	Chain	Res	Type
1	A	353	GLU
1	A	473	LYS
1	A	603	SER
1	A	631	THR
1	A	718	PHE
1	A	895	LEU
1	B	64	LEU
1	B	88	ARG
1	B	129	MET
1	B	147	MET
1	B	216	MET
1	B	261	GLU
1	B	294	SER
1	B	350	ILE
1	B	604	SER
1	B	631	THR
1	B	718	PHE
1	B	821	GLU
1	B	895	LEU
1	C	61	LEU
1	C	105	SER
1	C	216	MET
1	C	268	VAL
1	C	294	SER
1	C	322[A]	GLU
1	C	322[B]	GLU
1	C	324	ARG
1	C	349	MET
1	C	369	GLU
1	C	473	LYS
1	C	604	SER
1	C	631	THR
1	C	718	PHE
1	C	821	GLU
1	C	895	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	173	GLN
1	A	188	HIS

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Mol	Chain	Res	Type
1	A	258	ASN
1	A	882	HIS
1	A	887	ASN
1	B	95	HIS
1	B	173	GLN
1	B	258	ASN
1	B	673	GLN
1	B	879	HIS
1	B	882	HIS
1	B	887	ASN
1	C	173	GLN
1	C	181	GLN
1	C	234	ASN
1	C	254	ASN
1	C	423	GLN
1	C	525	HIS
1	C	580	HIS
1	C	673	GLN
1	C	879	HIS
1	C	882	HIS
1	C	887	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	903	-	4,4,4	6.51	1 (25%)	6,6,6	0.16	0
3	TMO	B	907	-	4,4,4	6.07	1 (25%)	6,6,6	0.25	0
3	TMO	A	902	-	4,4,4	6.34	1 (25%)	6,6,6	0.21	0
3	TMO	A	903	-	4,4,4	6.31	1 (25%)	6,6,6	0.16	0
3	TMO	C	902	-	4,4,4	6.39	1 (25%)	6,6,6	0.18	0
3	TMO	B	905	-	4,4,4	6.19	1 (25%)	6,6,6	0.21	0
3	TMO	B	903	-	4,4,4	6.42	1 (25%)	6,6,6	0.19	0
3	TMO	B	904	-	4,4,4	6.24	1 (25%)	6,6,6	0.20	0
2	CW8	C	901	1	18,19,19	1.75	1 (5%)	21,26,26	7.68	3 (14%)
3	TMO	B	902	-	4,4,4	6.13	1 (25%)	6,6,6	0.23	0
2	CW8	A	901	1	18,19,19	1.53	2 (11%)	21,26,26	7.73	3 (14%)
3	TMO	C	904	-	4,4,4	6.26	1 (25%)	6,6,6	0.20	0
2	CW8	B	901	1	18,19,19	1.68	1 (5%)	21,26,26	7.57	2 (9%)
3	TMO	B	906	-	4,4,4	6.12	1 (25%)	6,6,6	0.23	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	C	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	A	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	6.89	1.27	1.14
2	B	901	CW8	C23-N24	6.59	1.27	1.14
2	A	901	CW8	C23-N24	5.57	1.25	1.14
2	A	901	CW8	C5-C13	-2.37	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	CW8	C21-C23-N24	-35.00	121.10	177.23
2	C	901	CW8	C21-C23-N24	-34.82	121.39	177.23
2	B	901	CW8	C21-C23-N24	-34.32	122.19	177.23
2	A	901	CW8	C13-C5-N1	-3.34	104.47	110.09
2	B	901	CW8	C13-C5-N1	-3.22	104.67	110.09
2	C	901	CW8	C13-C5-N1	-2.66	105.61	110.09
2	A	901	CW8	F19-C17-C16	2.53	112.05	108.41
2	C	901	CW8	C23-C21-N15	2.05	113.41	110.74

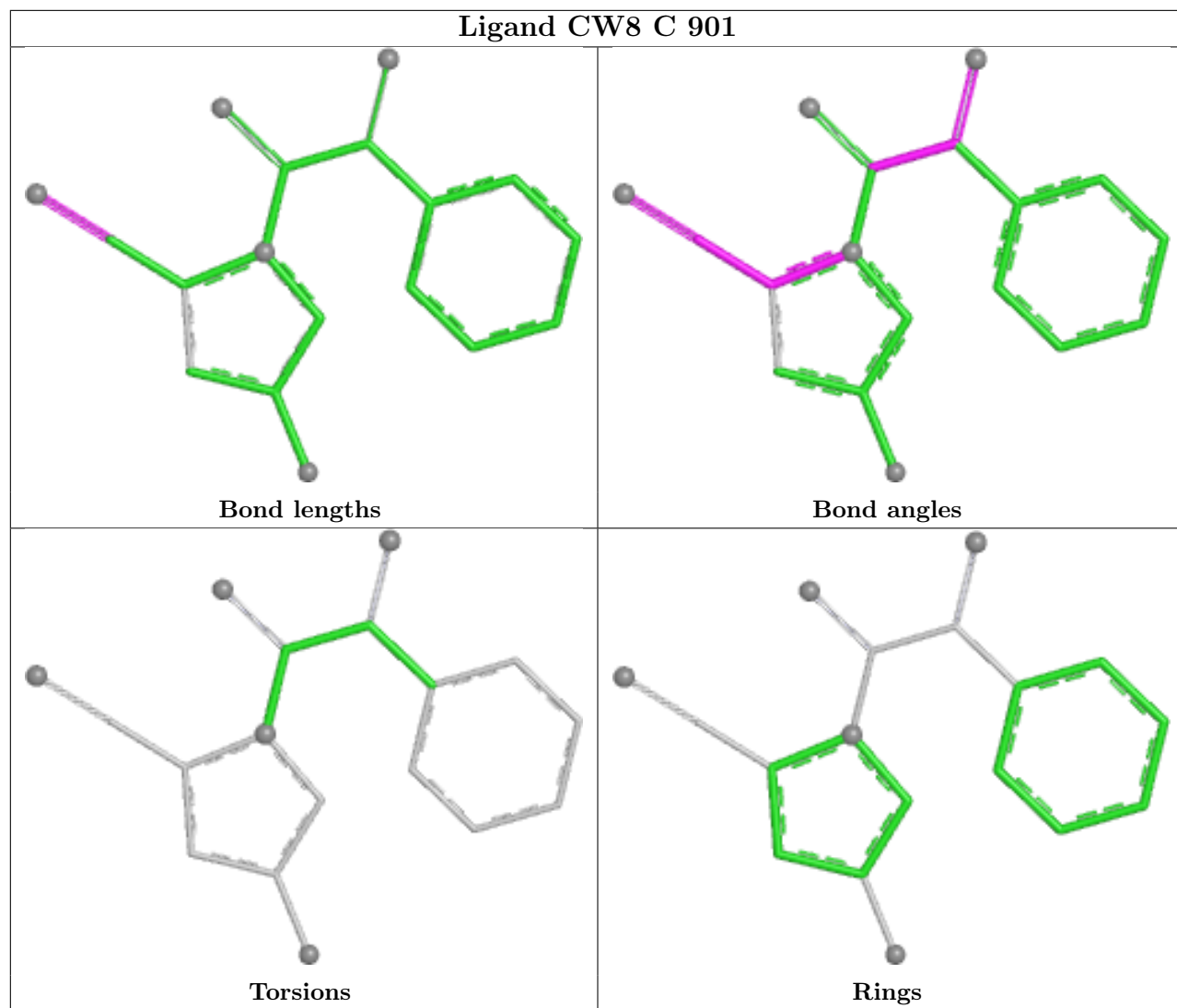
There are no chirality outliers.

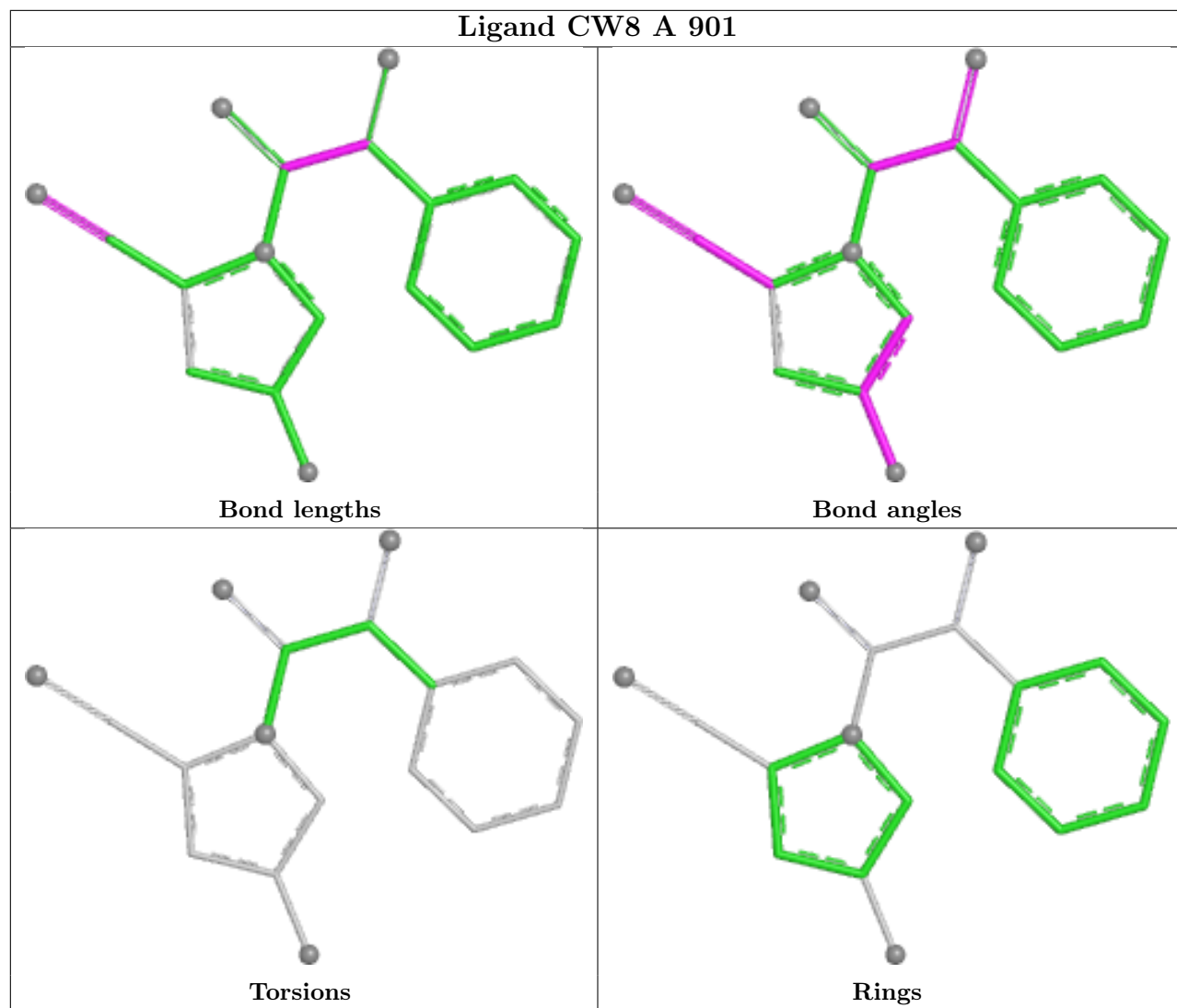
There are no torsion outliers.

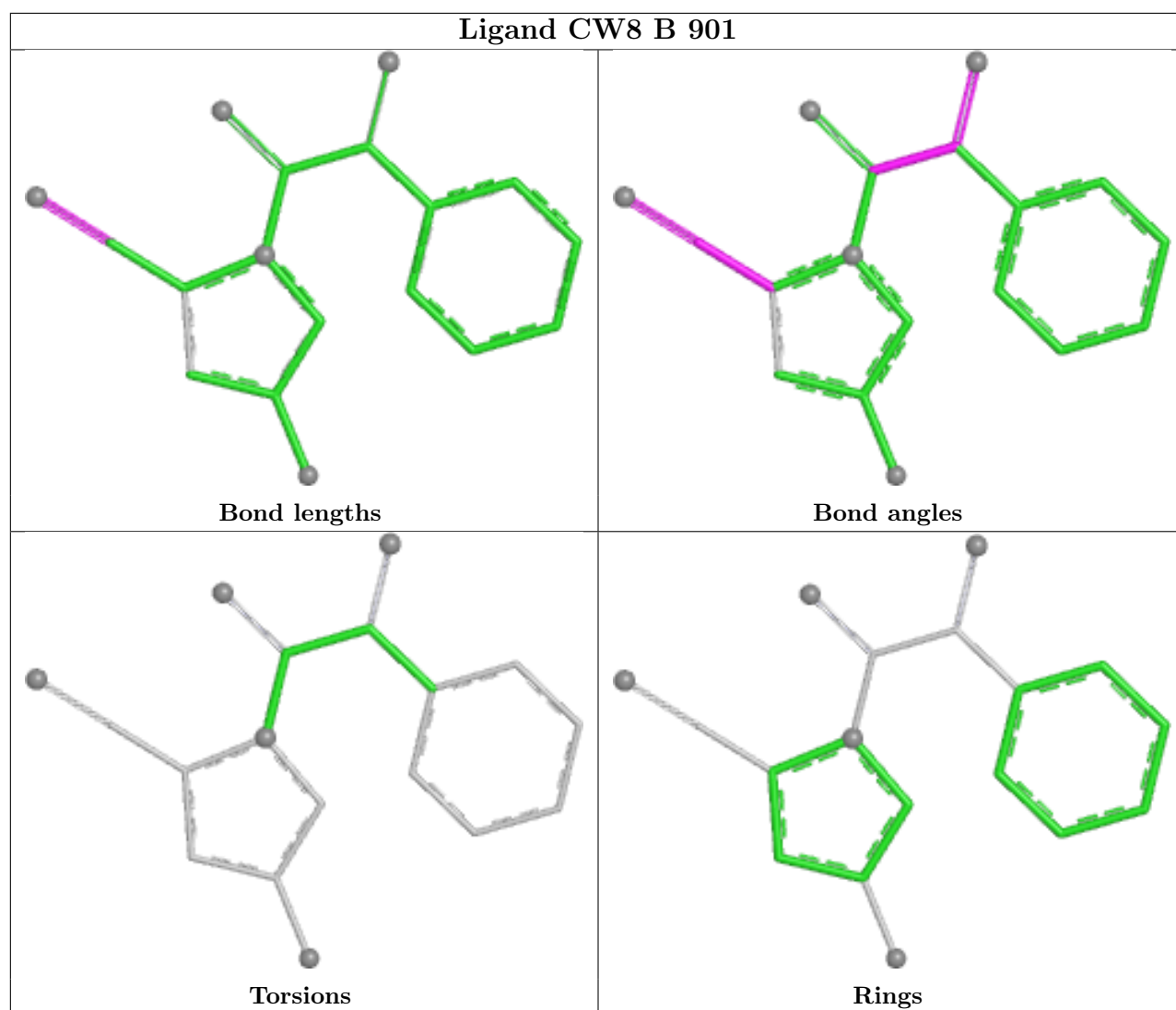
There are no ring outliers.

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, 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	848/903 (93%)	-0.09	29 (3%)	48	43	20, 60, 100, 180	32 (3%)
1	B	849/903 (94%)	-0.13	32 (3%)	44	39	19, 58, 99, 174	40 (4%)
1	C	840/903 (93%)	-0.16	25 (2%)	52	48	18, 56, 95, 157	36 (4%)
All	All	2537/2709 (93%)	-0.12	86 (3%)	48	43	18, 58, 99, 180	108 (4%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	8.0
1	B	72	HIS	5.6
1	A	72	HIS	5.5
1	C	138	LEU	5.4
1	A	75	MET	5.2
1	B	74	TYR	5.2
1	C	72	HIS	4.9
1	B	75	MET	4.8
1	B	898	ILE	4.7
1	C	76	MET	4.5
1	A	76	MET	4.3
1	B	76	MET	4.3
1	A	138	LEU	4.3
1	A	107	GLU	4.2
1	A	105	SER	4.0
1	A	420	MET	4.0
1	A	898	ILE	4.0
1	B	147	MET	3.9
1	C	107	GLU	3.9
1	A	74	TYR	3.8
1	C	47	LYS	3.7
1	A	145	TYR	3.7
1	C	105	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	195	GLN	3.6
1	A	195	GLN	3.6
1	C	420	MET	3.5
1	A	106	GLY	3.5
1	B	146	GLY	3.4
1	C	629	ASP	3.4
1	A	143	LEU	3.3
1	B	47	LYS	3.3
1	A	487	LYS	3.3
1	A	147	MET	3.2
1	A	629	ASP	3.2
1	C	70	LYS	3.2
1	B	144	ASP	3.1
1	C	106	GLY	3.1
1	B	71	TYR	3.1
1	A	71	TYR	3.1
1	A	628	PRO	3.0
1	B	105	SER	3.0
1	B	473	LYS	3.0
1	B	142	THR	3.0
1	B	420	MET	2.9
1	C	897	VAL	2.9
1	C	628	PRO	2.9
1	A	49	GLU	2.9
1	C	108	ASN	2.8
1	B	595[A]	HIS	2.8
1	C	898	ILE	2.8
1	A	108	ASN	2.8
1	C	624	ALA	2.8
1	C	109	ARG	2.8
1	B	629	ASP	2.8
1	B	145	TYR	2.7
1	B	143	LEU	2.6
1	A	897	VAL	2.6
1	C	71	TYR	2.5
1	B	73	GLY	2.5
1	B	897	VAL	2.5
1	C	148	TYR	2.5
1	C	625	GLY	2.5
1	B	69	ARG	2.4
1	B	624	ALA	2.4
1	A	109	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLY	2.4
1	A	70	LYS	2.4
1	B	70	LYS	2.4
1	C	487	LYS	2.4
1	C	110	GLU	2.4
1	C	353	GLU	2.4
1	C	595[A]	HIS	2.3
1	A	786	PHE	2.3
1	C	419	VAL	2.3
1	B	419	VAL	2.2
1	A	47	LYS	2.2
1	A	146	GLY	2.2
1	C	631	THR	2.1
1	B	77	ALA	2.1
1	A	562	GLU	2.1
1	A	77	ALA	2.1
1	B	48	LEU	2.1
1	B	107	GLU	2.1
1	B	685	LYS	2.1
1	B	417	ASP	2.0
1	A	627	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TMO	B	904	5/5	0.75	0.33	108,110,145,156	0
3	TMO	C	903	5/5	0.88	0.28	67,86,96,101	0

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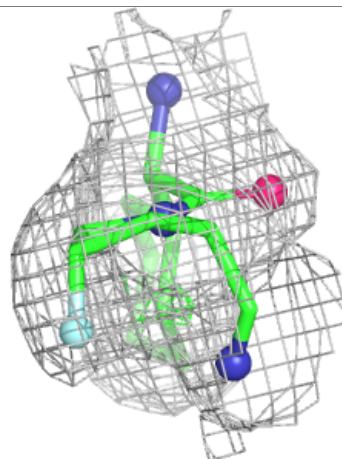
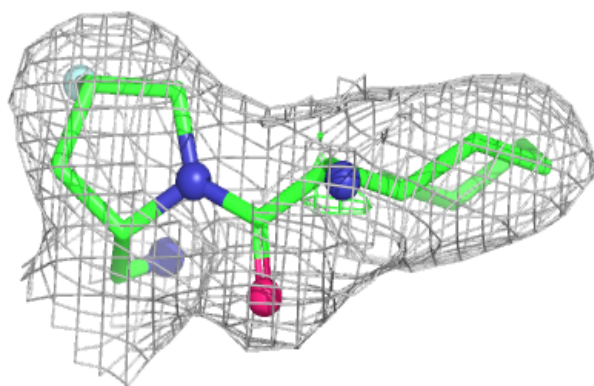
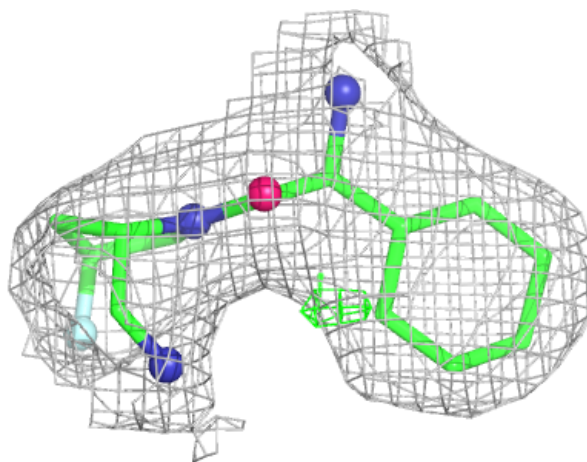
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TMO	C	904	5/5	0.88	0.33	81,108,120,131	0
3	TMO	B	907	5/5	0.90	0.30	94,95,121,129	0
3	TMO	C	902	5/5	0.91	0.18	73,74,91,101	0
3	TMO	A	902	5/5	0.91	0.22	93,97,114,130	0
3	TMO	B	903	5/5	0.91	0.27	89,96,118,121	0
3	TMO	B	902	5/5	0.92	0.23	74,81,91,95	0
3	TMO	B	905	5/5	0.92	0.21	79,122,135,139	0
3	TMO	A	903	5/5	0.92	0.23	86,94,102,116	0
3	TMO	B	906	5/5	0.93	0.21	80,92,117,119	0
2	CW8	C	901	18/18	0.97	0.07	28,40,45,46	0
2	CW8	B	901	18/18	0.97	0.07	38,43,46,50	0
2	CW8	A	901	18/18	0.98	0.07	32,45,52,53	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.

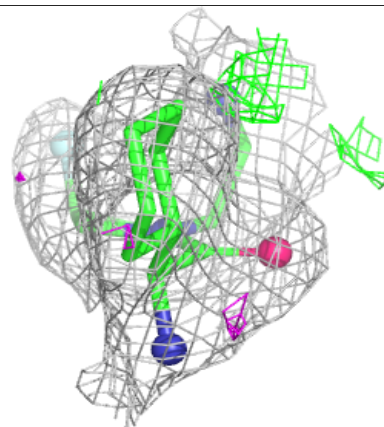
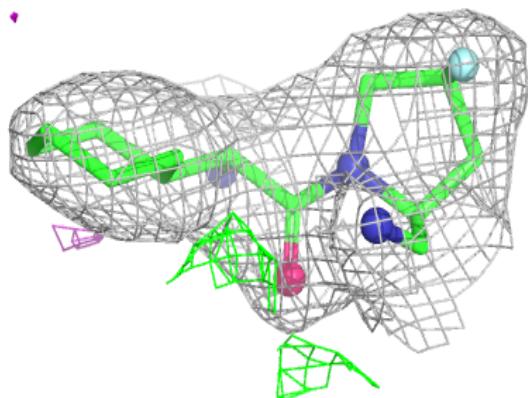
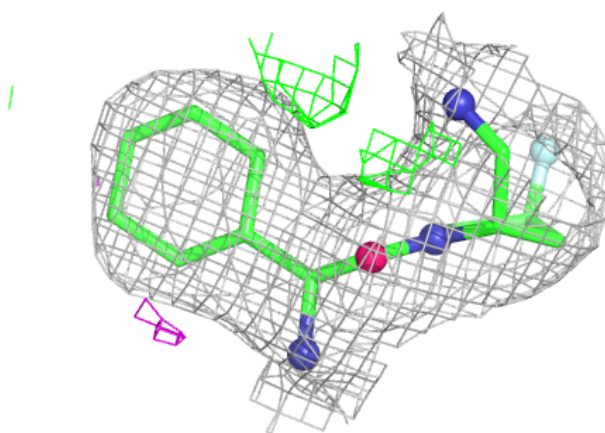
Electron density around CW8 C 901:

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

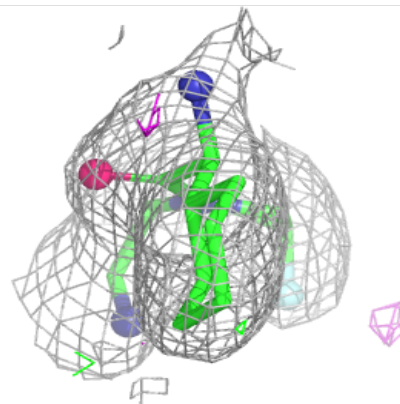
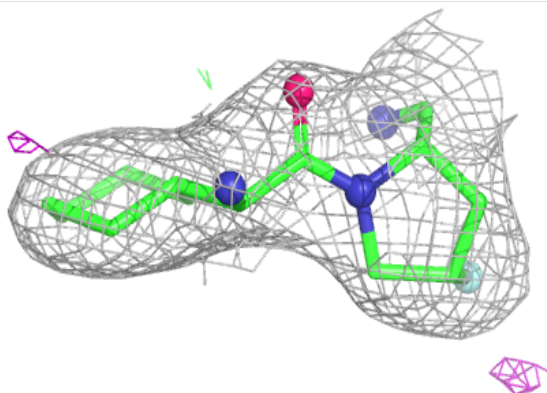
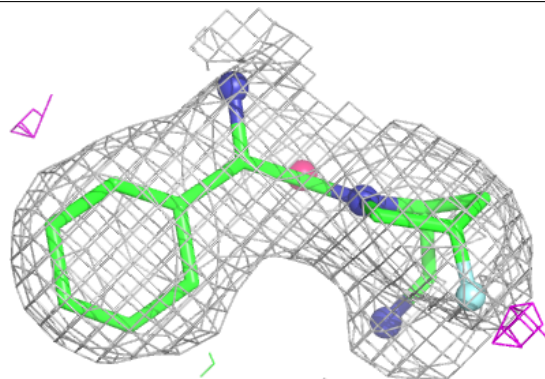


Electron density around CW8 B 901:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.