



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:41 am BST

PDB ID : 5CGV
Title : 2009 H1N1 PA endonuclease in complex with L-742,001
Authors : Kumar, G.; White, S.W.
Deposited on : 2015-07-09
Resolution : 2.17 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

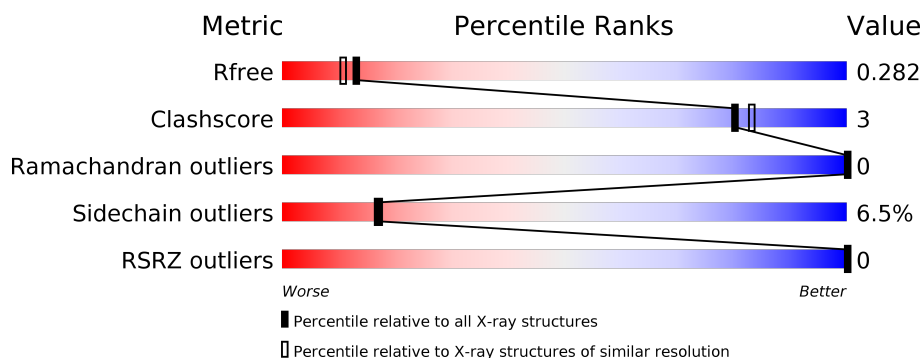
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on 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	187	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 10px;"> 82% 11% •• 5% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1553 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1452	918	249	274	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP C3W5S0
A	?	-	HIS	deletion	UNP C3W5S0
A	?	-	PHE	deletion	UNP C3W5S0
A	?	-	ILE	deletion	UNP C3W5S0
A	?	-	ASP	deletion	UNP C3W5S0
A	?	-	GLU	deletion	UNP C3W5S0
A	?	-	ARG	deletion	UNP C3W5S0
A	?	-	GLY	deletion	UNP C3W5S0
A	?	-	GLU	deletion	UNP C3W5S0
A	?	-	SER	deletion	UNP C3W5S0
A	?	-	ILE	deletion	UNP C3W5S0
A	?	-	ILE	deletion	UNP C3W5S0
A	?	-	VAL	deletion	UNP C3W5S0
A	?	-	GLU	deletion	UNP C3W5S0
A	?	-	SER	deletion	UNP C3W5S0
A	?	-	GLY	deletion	UNP C3W5S0
A	?	-	ASP	deletion	UNP C3W5S0
A	?	-	PRO	deletion	UNP C3W5S0
A	?	-	ASN	deletion	UNP C3W5S0
A	51	GLY	ALA	linker	UNP C3W5S0
A	52	GLY	LEU	linker	UNP C3W5S0
A	53	SER	LEU	linker	UNP C3W5S0
A	197	ALA	-	expression tag	UNP C3W5S0
A	198	ALA	-	expression tag	UNP C3W5S0
A	199	ALA	-	expression tag	UNP C3W5S0
A	200	GLU	-	expression tag	UNP C3W5S0
A	201	LEU	-	expression tag	UNP C3W5S0

Continued on next page...

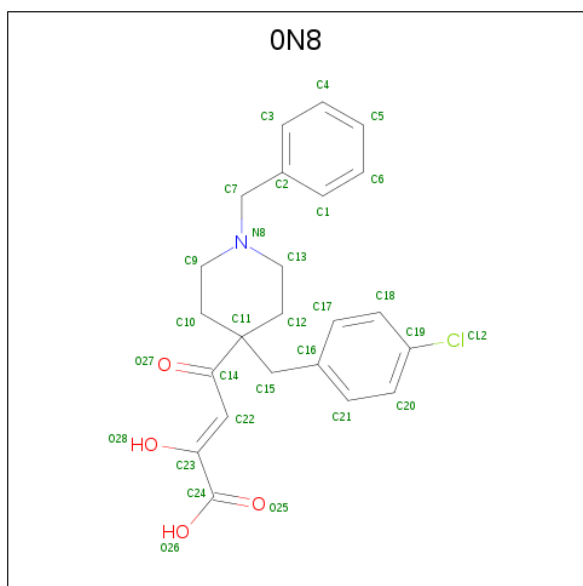
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	-	expression tag	UNP C3W5S0
A	203	LEU	-	expression tag	UNP C3W5S0
A	204	VAL	-	expression tag	UNP C3W5S0
A	205	PRO	-	expression tag	UNP C3W5S0
A	206	ARG	-	expression tag	UNP C3W5S0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0

- Molecule 3 is (2Z)-4-[1-benzyl-4-(4-chlorobenzyl)piperidin-4-yl]-2-hydroxy-4-oxobut-2-enoic acid (three-letter code: ON8) (formula: C₂₃H₂₄ClNO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 29 23 1 1 4	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



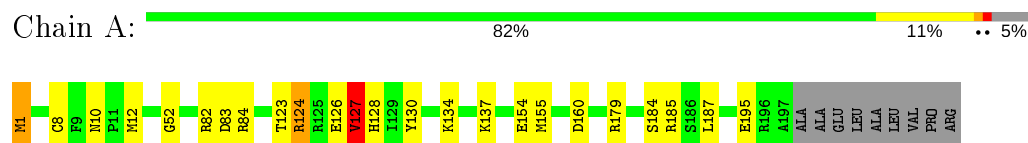
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		

i

- Molecule 1: Polymerase acidic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.90 Å 73.90 Å 127.46 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.17 45.16 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.17) 99.8 (45.16-2.17)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.18 Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.199 , 0.282 0.208 , 0.282	Depositor DCC
R_{free} test set	549 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	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	0.95	EDS
Total number of atoms	1553	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: GOL, MN, ON8

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	1.11	1/1482 (0.1%)	1.13	9/1994 (0.5%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	N-CA	6.56	1.59	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	179	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	83	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	160	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	82	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	82	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	160	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	127	VAL	CG1-CB-CG2	5.09	119.05	110.90
1	A	84	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	GLY	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	1452	0	1403	8	0
2	A	2	0	0	0	0
3	A	29	0	22	0	0
4	A	6	0	8	0	0
5	A	64	0	0	0	0
All	All	1553	0	1433	8	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 3.

All (8) 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:A:127:VAL:HG13	1:A:155:MET:CB	2.38	0.53
1:A:124:ARG:HG2	1:A:195:GLU:OE1	2.11	0.51
1:A:124:ARG:HG3	1:A:195:GLU:HB2	1.95	0.49
1:A:127:VAL:HG13	1:A:155:MET:HB3	1.94	0.48
1:A:127:VAL:HG13	1:A:155:MET:HB2	2.00	0.44
1:A:126:GLU:OE2	1:A:128:HIS:ND1	2.31	0.43
1:A:123:THR:HB	1:A:130:TYR:CD2	2.54	0.43
1:A:1:MET:HB2	1:A:187:LEU:HD22	2.01	0.43

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	176/187 (94%)	171 (97%)	5 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	155/166 (93%)	145 (94%)	10 (6%)	17	17

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	10	ASN
1	A	12	MET
1	A	124	ARG
1	A	127	VAL
1	A	134	LYS
1	A	137	LYS
1	A	154	GLU
1	A	184	SER
1	A	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GOL	A	304	-	5,5,5	0.35	0	5,5,5	0.63	0
3	0N8	A	303	2	28,31,31	1.53	3 (10%)	35,43,43	2.71	13 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	304	-	-	1/4/4/4	-
3	0N8	A	303	2	-	3/19/35/35	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	0N8	C10-C11	4.23	1.61	1.54
3	A	303	0N8	C22-C14	3.08	1.51	1.41
3	A	303	0N8	C19-CL2	2.69	1.80	1.74

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	0N8	C12-C13-N8	7.85	118.98	111.23
3	A	303	0N8	C10-C9-N8	7.08	118.22	111.23
3	A	303	0N8	C23-C22-C14	5.54	126.30	120.80
3	A	303	0N8	C12-C11-C15	-3.93	101.78	109.84
3	A	303	0N8	C10-C11-C15	3.67	117.36	109.84
3	A	303	0N8	C9-C10-C11	3.51	113.30	109.17
3	A	303	0N8	C17-C18-C19	2.92	122.32	119.24
3	A	303	0N8	C13-N8-C9	2.89	115.33	108.83
3	A	303	0N8	C7-N8-C9	2.61	116.88	111.06
3	A	303	0N8	C20-C19-C18	-2.54	117.95	121.24
3	A	303	0N8	C11-C15-C16	-2.39	112.96	116.29
3	A	303	0N8	C12-C11-C10	-2.38	105.00	108.13
3	A	303	0N8	C2-C7-N8	2.27	117.53	113.12

There are no chirality outliers.

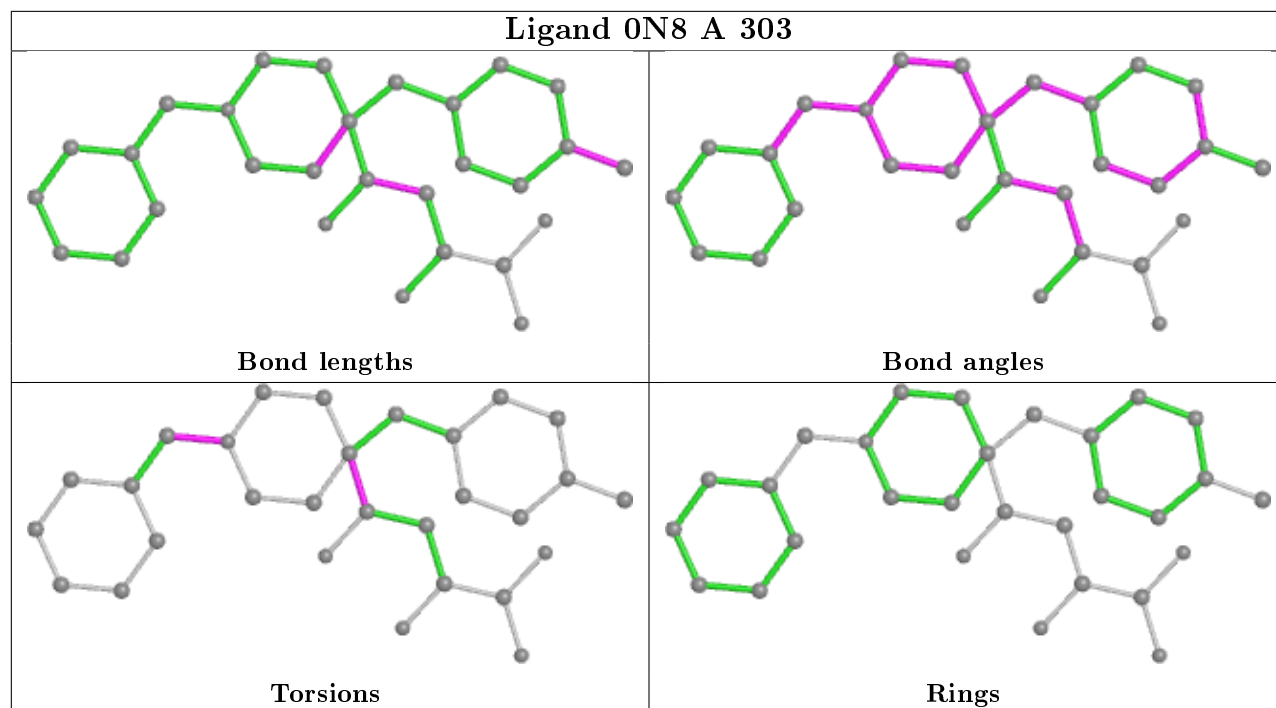
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	0N8	C2-C7-N8-C9
3	A	303	0N8	C15-C11-C14-O27
3	A	303	0N8	C12-C11-C14-O27
4	A	304	GOL	O1-C1-C2-C3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	178/187 (95%)	-0.31	0 100 100	20, 37, 63, 76	0

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands [i](#)

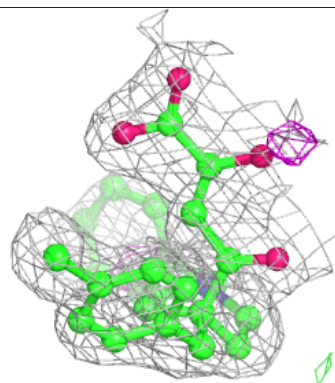
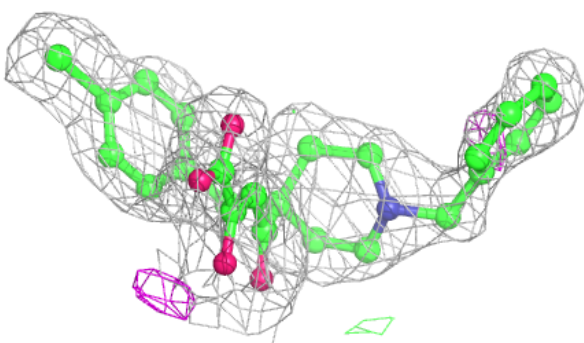
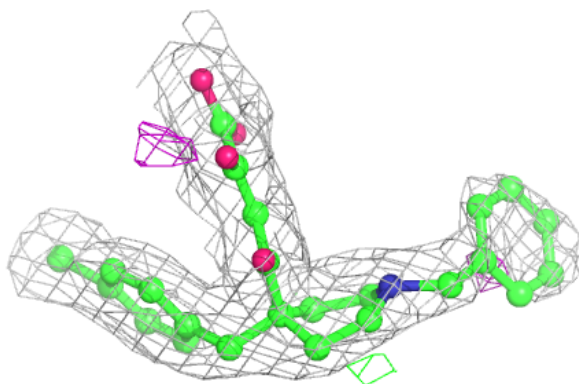
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	301	1/1	0.92	0.06	49,49,49,49	0
3	0N8	A	303	29/29	0.92	0.12	27,39,53,57	0
4	GOL	A	304	6/6	0.93	0.11	38,43,47,51	0
2	MN	A	302	1/1	0.97	0.05	59,59,59,59	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 0N8 A 303:

$2mF_o-DF_c$ (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.