



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 11:37 PM EDT

PDB ID : 5MTK
Title : Crystal structure of human Caspase-1 with (3S,6S,10aS)-N-((2S,3S)-2-hydroxy-5-oxotetrahydrofuran-3-yl)-6-(isoquinoline-1-carboxamido)-5-oxodecahydropyrrolo[1,2-a]azocine-3-carboxamide (PGE-3935199)
Authors : Brethon, A.; Chantalat, L.; Christin, O.; Clary, L.; Fournier, J.F.; Gastreich, M.; Harris, C.; Pascau, J.; Isabet, T.; Rodeschin, V.; Thoreau, E.; Roche, D.
Deposited on : 2017-01-09
Resolution : 2.53 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) 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	:	2.37.1
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)	:	2.37.1

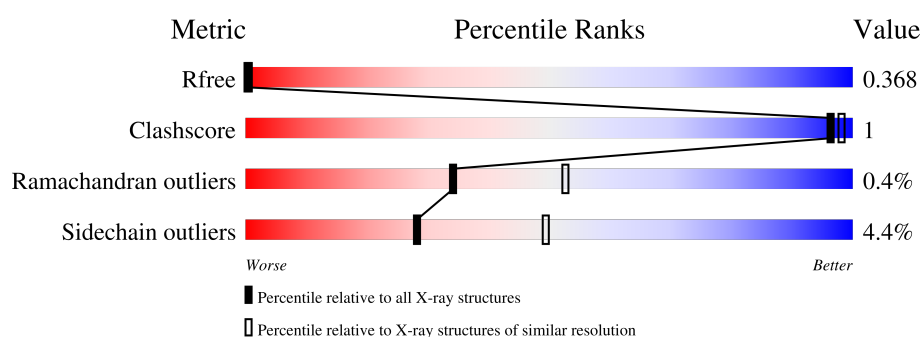
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	179	 84% 8% 7%
2	B	89	 93% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2069 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 Caspase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	1	0
			1304	818	226	248	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP P29466

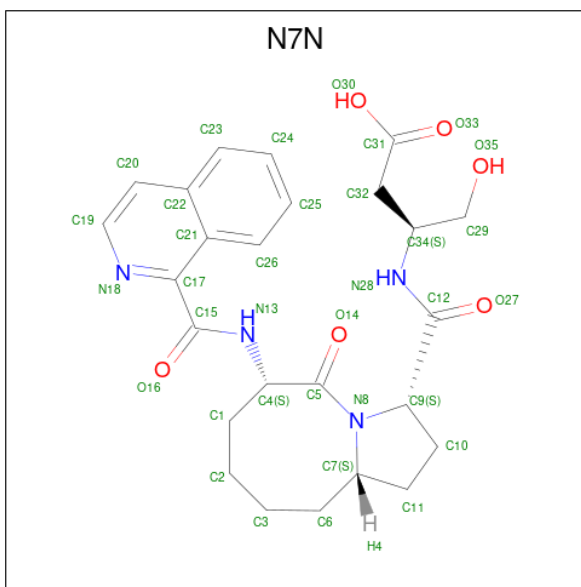
- Molecule 2 is a protein called Caspase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			713	454	125	127	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	316	MET	-	initiating methionine	UNP P29466

- Molecule 3 is (3 {S})-3-[[[(3 {S}),6 {S}),10 {a} {S}]-6-(isoquinolin-1-ylcarbonylamino)-5-oxidanilidene-2,3,6,7,8,9,10,10 {a}-octahydro-1 {H}-pyrrolo[1,2-a]azocin-3-yl]carbonylamino]-4-oxidanyl-butanoic acid (three-letter code: N7N) (formula: C₂₅H₃₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	25	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	8	Total	O	0	0
			8	8		

- Molecule 1: Caspase-1

MET	ASN	PRO	ALA	MET	PRO	THR	SER	SER	G128		I144		W145	GLN	LYS		S149		I152		L164		I186		K204	N205		D210		H220		E223		T267		L273		K276		V292		F295		K296	ASP
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- Molecule 2: Caspase-1

Sequence logo for the 10th position. The y-axis is labeled 'bits' and ranges from 0 to 0.4. The x-axis shows the amino acid sequence: MET, ALA, I318, K319, K320, S332, D365, Q379, H404. The bars for I318, K319, and K320 are colored red, while the others are blue.

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.59Å 64.59Å 161.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.53 50.39 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.53) 98.2 (50.39-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.243 , 0.299 0.298 , 0.368	Depositor DCC
R_{free} test set	563 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2069	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: N7N

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	0.42	0/1325	0.58	0/1784
2	B	0.43	0/733	0.60	0/988
All	All	0.42	0/2058	0.59	0/2772

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1304	0	1313	4	0
2	B	713	0	688	0	0
3	A	35	0	0	0	0
4	A	9	0	0	0	0
4	B	8	0	0	0	0
All	All	2069	0	2001	4	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 1.

All (4) 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:186:ILE:HD13	1:A:204:LYS:HE2	1.87	0.56
1:A:164:LEU:HD11	1:A:223:GLU:HB2	1.90	0.52
1:A:149:SER:HB2	1:A:152:ILE:HD12	2.00	0.42
1:A:273:LEU:HA	1:A:276:LYS:HD2	2.01	0.42

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	163/179 (91%)	154 (94%)	8 (5%)	1 (1%)	25	41
2	B	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
All	All	248/268 (92%)	234 (94%)	13 (5%)	1 (0%)	34	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN

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	148/159 (93%)	142 (96%)	6 (4%)	30	53
2	B	79/80 (99%)	75 (95%)	4 (5%)	24	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	227/239 (95%)	217 (96%)	10 (4%)	28 49

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	332	SER
2	B	365	ASP
2	B	379	GLN
1	A	267	THR
1	A	292	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	195	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	N7N	A	301	1	36,38,38	1.61	11 (30%)	40,53,53	1.15	4 (10%)

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
3	N7N	A	301	1	-	5/22/50/50	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	N7N	C17-C21	3.06	1.46	1.43
3	A	301	N7N	C29-C34	2.63	1.56	1.52
3	A	301	N7N	C15-N13	2.60	1.39	1.34
3	A	301	N7N	C7-N8	2.57	1.51	1.47
3	A	301	N7N	C19-N18	2.53	1.39	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	N7N	C10-C9-N8	3.37	106.32	103.09
3	A	301	N7N	C11-C7-N8	3.21	105.29	101.70
3	A	301	N7N	C10-C11-C7	2.71	108.10	104.05
3	A	301	N7N	C11-C10-C9	2.22	106.90	103.84

There are no chirality outliers.

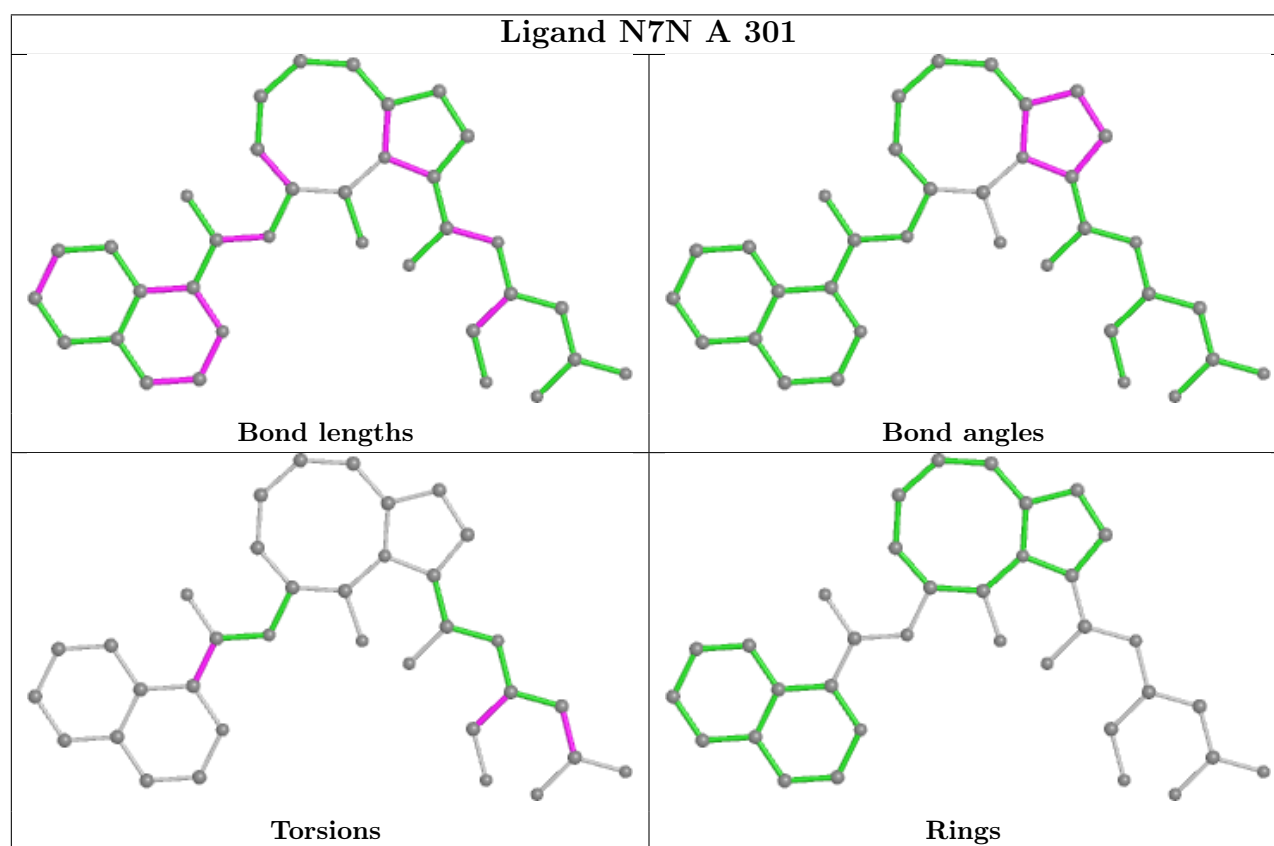
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	N7N	O35-C29-C34-C32
3	A	301	N7N	O35-C29-C34-N28
3	A	301	N7N	O33-C31-C32-C34
3	A	301	N7N	O30-C31-C32-C34
3	A	301	N7N	O16-C15-C17-N18

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

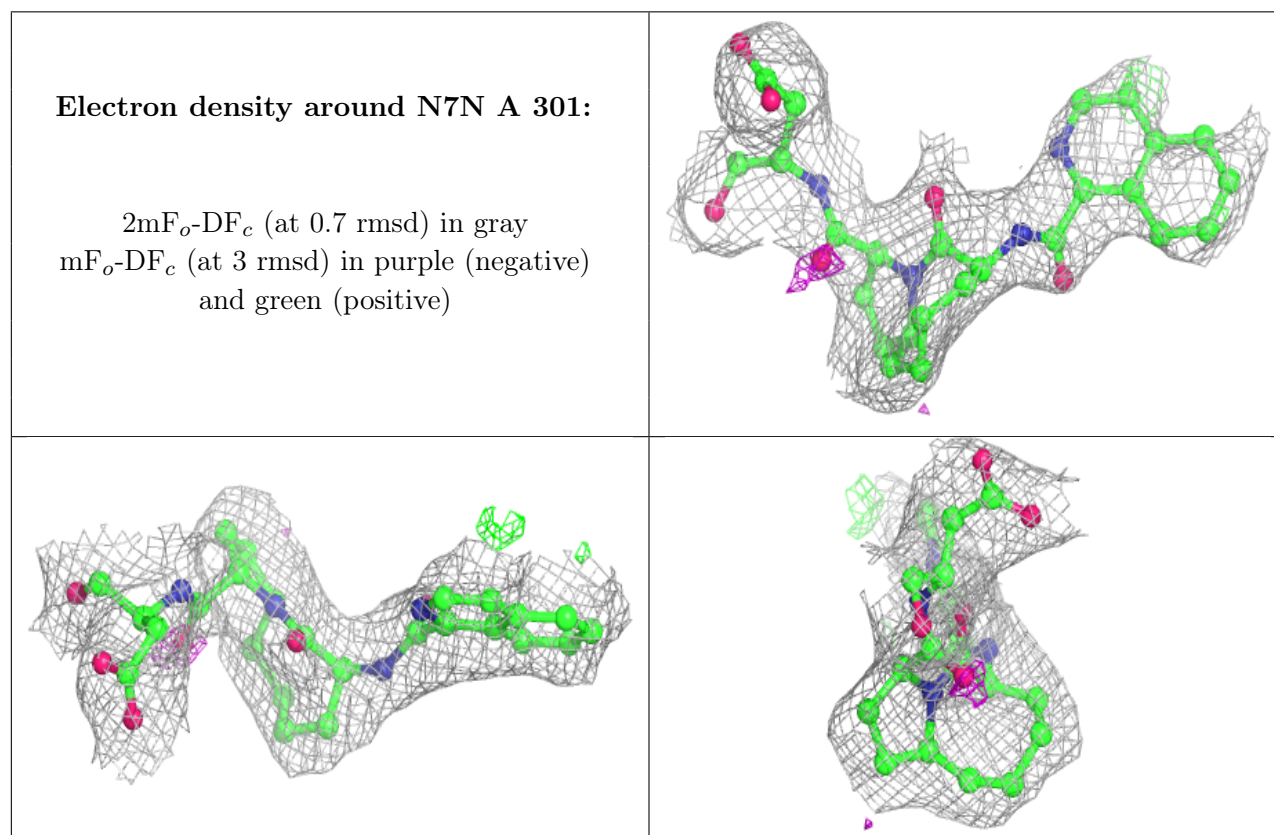
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.