



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:36 am BST

PDB ID : 3BPR
Title : Crystal structure of catalytic domain of the proto-oncogene tyrosine-protein kinase MER in complex with inhibitor C52
Authors : Walker, J.R.; Huang, X.; Finerty Jr, P.J.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-12-19
Resolution : 2.80 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

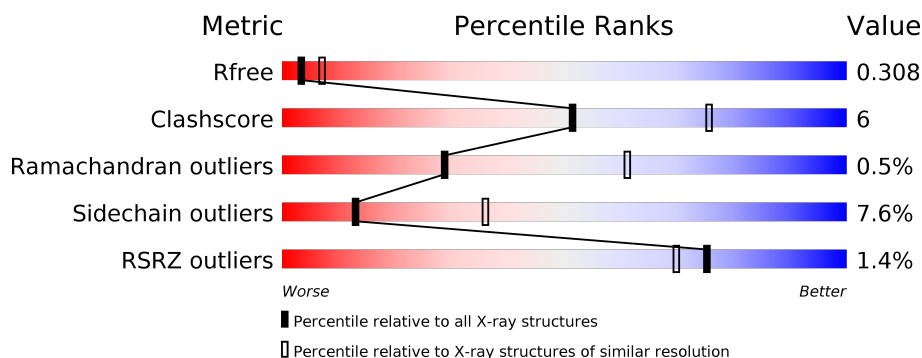
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	313	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>11%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	313	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	313	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	313	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8399 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 Proto-oncogene tyrosine-protein kinase MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	2	0
			2027	1299	332	375	21			
1	B	256	Total	C	N	O	S	0	2	0
			2012	1289	336	368	19			
1	C	259	Total	C	N	O	S	0	4	0
			2073	1326	348	379	20			
1	D	259	Total	C	N	O	S	0	3	0
			2057	1316	345	376	20			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	MET	-	EXPRESSION TAG	UNP Q12866
A	553	GLY	-	EXPRESSION TAG	UNP Q12866
A	554	SER	-	EXPRESSION TAG	UNP Q12866
A	555	SER	-	EXPRESSION TAG	UNP Q12866
A	556	HIS	-	EXPRESSION TAG	UNP Q12866
A	557	HIS	-	EXPRESSION TAG	UNP Q12866
A	558	HIS	-	EXPRESSION TAG	UNP Q12866
A	559	HIS	-	EXPRESSION TAG	UNP Q12866
A	560	HIS	-	EXPRESSION TAG	UNP Q12866
A	561	HIS	-	EXPRESSION TAG	UNP Q12866
A	562	SER	-	EXPRESSION TAG	UNP Q12866
A	563	SER	-	EXPRESSION TAG	UNP Q12866
A	564	GLY	-	EXPRESSION TAG	UNP Q12866
A	565	LEU	-	EXPRESSION TAG	UNP Q12866
A	566	VAL	-	EXPRESSION TAG	UNP Q12866
A	567	PRO	-	EXPRESSION TAG	UNP Q12866
A	568	ARG	-	EXPRESSION TAG	UNP Q12866
A	569	GLY	-	EXPRESSION TAG	UNP Q12866
B	552	MET	-	EXPRESSION TAG	UNP Q12866
B	553	GLY	-	EXPRESSION TAG	UNP Q12866
B	554	SER	-	EXPRESSION TAG	UNP Q12866

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Chain	Residue	Modelled	Actual	Comment	Reference
B	555	SER	-	EXPRESSION TAG	UNP Q12866
B	556	HIS	-	EXPRESSION TAG	UNP Q12866
B	557	HIS	-	EXPRESSION TAG	UNP Q12866
B	558	HIS	-	EXPRESSION TAG	UNP Q12866
B	559	HIS	-	EXPRESSION TAG	UNP Q12866
B	560	HIS	-	EXPRESSION TAG	UNP Q12866
B	561	HIS	-	EXPRESSION TAG	UNP Q12866
B	562	SER	-	EXPRESSION TAG	UNP Q12866
B	563	SER	-	EXPRESSION TAG	UNP Q12866
B	564	GLY	-	EXPRESSION TAG	UNP Q12866
B	565	LEU	-	EXPRESSION TAG	UNP Q12866
B	566	VAL	-	EXPRESSION TAG	UNP Q12866
B	567	PRO	-	EXPRESSION TAG	UNP Q12866
B	568	ARG	-	EXPRESSION TAG	UNP Q12866
B	569	GLY	-	EXPRESSION TAG	UNP Q12866
C	552	MET	-	EXPRESSION TAG	UNP Q12866
C	553	GLY	-	EXPRESSION TAG	UNP Q12866
C	554	SER	-	EXPRESSION TAG	UNP Q12866
C	555	SER	-	EXPRESSION TAG	UNP Q12866
C	556	HIS	-	EXPRESSION TAG	UNP Q12866
C	557	HIS	-	EXPRESSION TAG	UNP Q12866
C	558	HIS	-	EXPRESSION TAG	UNP Q12866
C	559	HIS	-	EXPRESSION TAG	UNP Q12866
C	560	HIS	-	EXPRESSION TAG	UNP Q12866
C	561	HIS	-	EXPRESSION TAG	UNP Q12866
C	562	SER	-	EXPRESSION TAG	UNP Q12866
C	563	SER	-	EXPRESSION TAG	UNP Q12866
C	564	GLY	-	EXPRESSION TAG	UNP Q12866
C	565	LEU	-	EXPRESSION TAG	UNP Q12866
C	566	VAL	-	EXPRESSION TAG	UNP Q12866
C	567	PRO	-	EXPRESSION TAG	UNP Q12866
C	568	ARG	-	EXPRESSION TAG	UNP Q12866
C	569	GLY	-	EXPRESSION TAG	UNP Q12866
D	552	MET	-	EXPRESSION TAG	UNP Q12866
D	553	GLY	-	EXPRESSION TAG	UNP Q12866
D	554	SER	-	EXPRESSION TAG	UNP Q12866
D	555	SER	-	EXPRESSION TAG	UNP Q12866
D	556	HIS	-	EXPRESSION TAG	UNP Q12866
D	557	HIS	-	EXPRESSION TAG	UNP Q12866
D	558	HIS	-	EXPRESSION TAG	UNP Q12866
D	559	HIS	-	EXPRESSION TAG	UNP Q12866
D	560	HIS	-	EXPRESSION TAG	UNP Q12866

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Chain	Residue	Modelled	Actual	Comment	Reference
D	561	HIS	-	EXPRESSION TAG	UNP Q12866
D	562	SER	-	EXPRESSION TAG	UNP Q12866
D	563	SER	-	EXPRESSION TAG	UNP Q12866
D	564	GLY	-	EXPRESSION TAG	UNP Q12866
D	565	LEU	-	EXPRESSION TAG	UNP Q12866
D	566	VAL	-	EXPRESSION TAG	UNP Q12866
D	567	PRO	-	EXPRESSION TAG	UNP Q12866
D	568	ARG	-	EXPRESSION TAG	UNP Q12866
D	569	GLY	-	EXPRESSION TAG	UNP Q12866

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- The chemical structure of OLP (Oxalyl-L-phenylalanine) is shown with the following atom labels:
- Phenylalanine side chain:** CAJ (CH₂), OAC (OH), CAK (CH), N2 (NH), C2 (C), N1 (N), N3 (NH), C4 (C), C5 (C), C6 (C), N6 (N), N7 (N), C8 (CH), N9 (N), CAA (CH₂), CAW (CH), CAB (CH₃).
 - Oxalyl group:** CL (Cl), CAQ (C=O), CAH (C=O), CAR (C=O).

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

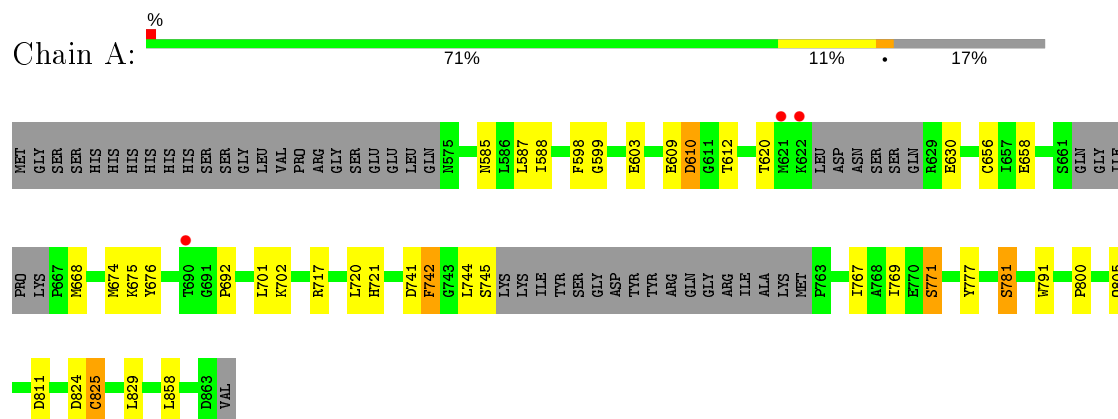
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	31	Total O 31 31	0	0
5	C	32	Total O 32 32	0	0
5	D	29	Total O 29 29	0	0

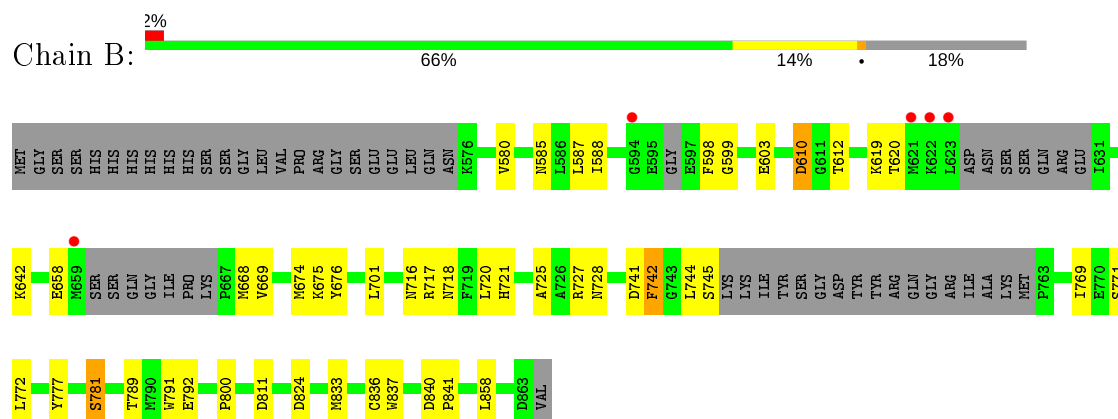
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

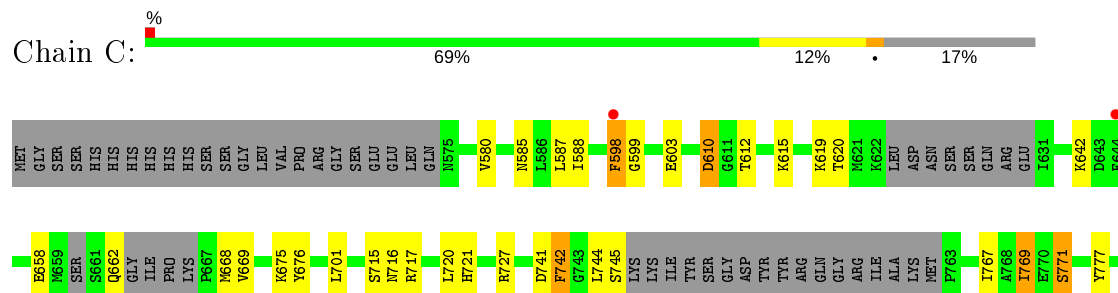
- Molecule 1: Proto-oncogene tyrosine-protein kinase MER



- Molecule 1: Proto-oncogene tyrosine-protein kinase MER

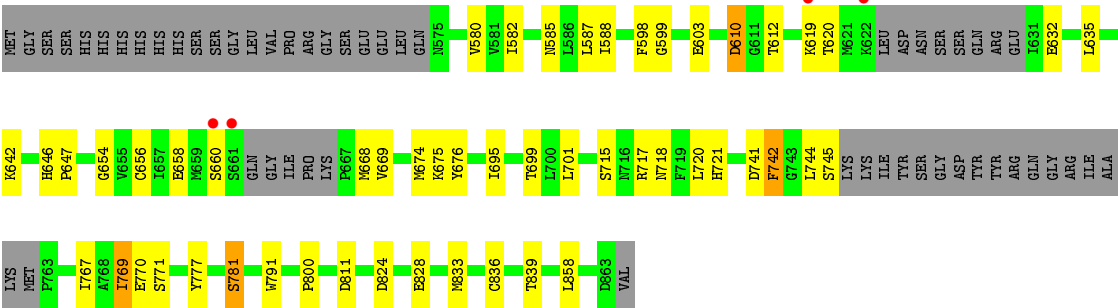


- Molecule 1: Proto-oncogene tyrosine-protein kinase MER





● Molecule 1: Proto-oncogene tyrosine-protein kinase MER



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.00 Å 91.70 Å 120.75 Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	47.30 – 2.80 47.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.30-2.80) 98.7 (47.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.274 , 0.301 0.279 , 0.308	Depositor DCC
R_{free} test set	1889 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 45.20 % 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 1.3674e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLP, NA, CL

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	0.52	0/2068	0.62	0/2803
1	B	0.53	0/2052	0.63	0/2778
1	C	0.53	0/2114	0.62	0/2857
1	D	0.53	0/2098	0.63	0/2836
All	All	0.53	0/8332	0.62	0/11274

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 [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	2027	0	1952	19	0
1	B	2012	0	1961	20	0
1	C	2073	0	2032	19	0
1	D	2057	0	2029	27	0
2	A	24	0	19	4	0
2	B	24	0	19	2	0
2	C	24	0	19	2	0
2	D	24	0	19	4	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	39	0	0	1	0
5	B	31	0	0	1	0
5	C	32	0	0	0	0
5	D	29	0	0	1	0
All	All	8399	0	8050	91	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 6.

All (91) 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:674:MET:O	2:A:900:OLP:HAG	1.78	0.84
1:D:674:MET:O	2:D:900:OLP:HAG	1.86	0.76
1:A:675:LYS:O	2:A:900:OLP:HAE	1.90	0.71
1:B:658:GLU:HG3	1:B:668:MET:HE1	1.73	0.71
1:A:658:GLU:HG3	1:A:668:MET:HE1	1.73	0.70
1:C:580:VAL:HG23	1:C:642:LYS:HD2	1.74	0.70
1:A:825[A]:CYS:SG	1:A:829:LEU:HD23	2.34	0.67
1:B:728:ASN:ND2	5:B:128:HOH:O	2.20	0.67
1:D:675:LYS:O	2:D:900:OLP:HAE	1.95	0.66
1:C:658:GLU:HG3	1:C:668:MET:HE1	1.80	0.63
1:D:620:THR:HG22	1:D:668:MET:HG2	1.81	0.62
1:D:658:GLU:HG3	1:D:668:MET:HE1	1.82	0.61
1:B:580:VAL:HG23	1:B:642:LYS:HD2	1.82	0.60
1:B:620:THR:HG22	1:B:668:MET:HG2	1.84	0.59
1:C:620:THR:HG22	1:C:668:MET:HG2	1.86	0.58
1:A:620:THR:HG22	1:A:668:MET:HG2	1.86	0.57
1:B:674:MET:O	2:B:900:OLP:HAG	2.04	0.56
2:D:900:OLP:N1	2:D:900:OLP:HAH	2.21	0.55
1:C:675:LYS:HE3	1:C:676:TYR:CZ	2.41	0.55
1:D:675:LYS:HE3	1:D:676:TYR:CZ	2.41	0.55
1:A:675:LYS:HE3	1:A:676:TYR:CZ	2.42	0.55
1:B:675:LYS:HE3	1:B:676:TYR:CZ	2.43	0.54
1:D:721:HIS:CE1	1:D:742:PHE:HA	2.42	0.54
1:D:587:LEU:O	1:D:588:ILE:HD13	2.09	0.53
1:A:777:TYR:CZ	1:A:781:SER:HB2	2.44	0.52
1:C:777:TYR:CZ	1:C:781:SER:HB2	2.43	0.52
1:C:587:LEU:O	1:C:588:ILE:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:777:TYR:CZ	1:D:781:SER:HB2	2.44	0.52
1:D:632:GLU:HA	1:D:635:LEU:HD12	1.92	0.51
1:C:610:ASP:HB3	1:C:612:THR:H	1.76	0.51
1:C:721:HIS:CE1	1:C:742:PHE:HA	2.45	0.51
1:C:599:GLY:HA3	1:C:620:THR:O	2.11	0.51
2:D:900:OLP:N1	2:D:900:OLP:CAH	2.74	0.50
1:B:777:TYR:CZ	1:B:781:SER:HB2	2.46	0.49
1:B:599:GLY:HA3	1:B:620:THR:O	2.12	0.49
1:D:660:SER:HB2	5:D:28:HOH:O	2.13	0.49
1:B:587:LEU:O	1:B:588:ILE:HD13	2.13	0.48
1:D:701:LEU:HB2	1:D:858:LEU:HD13	1.96	0.48
2:C:900:OLP:HAH	2:C:900:OLP:N1	2.29	0.48
1:A:599:GLY:HA3	1:A:620:THR:O	2.14	0.47
1:A:610:ASP:HB3	1:A:612:THR:H	1.79	0.47
1:D:791:TRP:CZ3	1:D:800:PRO:HA	2.50	0.47
1:B:791:TRP:CZ3	1:B:800:PRO:HA	2.50	0.47
1:A:587:LEU:O	1:A:588:ILE:HD13	2.15	0.47
1:D:582:ILE:HD11	1:D:654:GLY:HA3	1.97	0.47
1:B:701:LEU:HB2	1:B:858:LEU:HD13	1.97	0.46
1:D:656:CYS:HB3	1:D:668:MET:CE	2.45	0.46
1:D:828:GLU:CD	1:D:828:GLU:H	2.19	0.46
1:B:725:ALA:HB1	1:B:727[A]:ARG:NH1	2.31	0.46
2:A:900:OLP:HAH	2:A:900:OLP:N1	2.31	0.46
1:C:580:VAL:HA	1:C:642:LYS:NZ	2.30	0.45
1:A:805:GLN:NE2	5:A:64:HOH:O	2.49	0.45
1:B:610:ASP:HB3	1:B:612:THR:H	1.81	0.45
1:D:599:GLY:HA3	1:D:620:THR:O	2.16	0.45
1:C:619:LYS:HB2	1:C:669:VAL:CG2	2.47	0.45
1:B:789:THR:O	1:B:792:GLU:HB2	2.17	0.45
1:A:777:TYR:CE2	1:A:781:SER:HB2	2.52	0.44
1:B:840:ASP:OD1	1:B:841:PRO:HD2	2.17	0.44
1:D:619:LYS:HB2	1:D:669:VAL:CG2	2.47	0.44
1:C:619:LYS:HB2	1:C:669:VAL:HG22	1.99	0.44
1:D:610:ASP:HB3	1:D:612:THR:H	1.83	0.43
1:A:702:LYS:HD2	1:A:702:LYS:HA	1.87	0.43
1:C:833:MET:O	1:C:836:CYS:HB2	2.18	0.43
1:A:701:LEU:HB2	1:A:858:LEU:HD13	2.00	0.43
1:A:791:TRP:CZ3	1:A:800:PRO:HA	2.54	0.42
2:A:900:OLP:N1	2:A:900:OLP:CAH	2.80	0.42
1:C:767:ILE:CG2	1:C:771:SER:HB2	2.49	0.42
1:C:769:ILE:H	1:C:769:ILE:HG13	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:TRP:CZ3	1:C:800:PRO:HA	2.55	0.42
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.84	0.42
1:B:619:LYS:HB2	1:B:669:VAL:CG2	2.49	0.42
1:B:721:HIS:CE1	1:B:742:PHE:HA	2.54	0.42
1:D:695:ILE:CG2	1:D:699:THR:HB	2.50	0.42
1:A:656:CYS:HB3	1:A:668:MET:CE	2.50	0.42
1:C:615:LYS:HA	1:C:615:LYS:HD2	1.86	0.42
1:D:646:HIS:ND1	1:D:647:PRO:HD2	2.35	0.42
1:D:769:ILE:HD12	1:D:770:GLU:OE1	2.20	0.41
1:D:619:LYS:HB2	1:D:669:VAL:HG22	2.02	0.41
1:C:701:LEU:HB2	1:C:858:LEU:HD13	2.02	0.41
1:A:767:ILE:CG2	1:A:771:SER:HB2	2.50	0.41
1:A:721:HIS:CE1	1:A:742:PHE:HA	2.56	0.41
1:D:767:ILE:CG2	1:D:771:SER:HB2	2.51	0.41
2:C:900:OLP:N1	2:C:900:OLP:CAH	2.84	0.41
1:B:833:MET:O	1:B:836:CYS:HB2	2.21	0.41
1:D:580:VAL:HG23	1:D:642:LYS:HD2	2.02	0.41
1:D:769:ILE:HD11	1:D:839:THR:O	2.21	0.40
1:B:675:LYS:O	2:B:900:OLP:HAE	2.21	0.40
1:D:777:TYR:CE2	1:D:781:SER:HB2	2.56	0.40
1:D:833:MET:O	1:D:836:CYS:HB2	2.21	0.40
1:B:716:ASN:C	1:B:718:ASN:H	2.25	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	255/313 (82%)	239 (94%)	14 (6%)	2 (1%)	19	49
1	B	248/313 (79%)	234 (94%)	13 (5%)	1 (0%)	34	66
1	C	253/313 (81%)	234 (92%)	18 (7%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	254/313 (81%)	236 (93%)	17 (7%)	1 (0%)	34	66
All	All	1010/1252 (81%)	943 (93%)	62 (6%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	PHE
1	B	598	PHE
1	D	598	PHE
1	C	598	PHE
1	A	692	PRO

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	214/280 (76%)	196 (92%)	18 (8%)	11	31
1	B	215/280 (77%)	199 (93%)	16 (7%)	13	37
1	C	224/280 (80%)	204 (91%)	20 (9%)	9	28
1	D	223/280 (80%)	208 (93%)	15 (7%)	16	43
All	All	876/1120 (78%)	807 (92%)	69 (8%)	13	34

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	ASN
1	A	603	GLU
1	A	609	GLU
1	A	610	ASP
1	A	630	GLU
1	A	717	ARG
1	A	720	LEU
1	A	741	ASP
1	A	742	PHE

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Mol	Chain	Res	Type
1	A	744	LEU
1	A	745	SER
1	A	769	ILE
1	A	771	SER
1	A	781	SER
1	A	811	ASP
1	A	824	ASP
1	A	825[A]	CYS
1	A	825[B]	CYS
1	B	585	ASN
1	B	603	GLU
1	B	610	ASP
1	B	717	ARG
1	B	720	LEU
1	B	741	ASP
1	B	742	PHE
1	B	744	LEU
1	B	745	SER
1	B	769	ILE
1	B	771	SER
1	B	772	LEU
1	B	781	SER
1	B	811	ASP
1	B	824	ASP
1	B	837	TRP
1	C	585	ASN
1	C	598	PHE
1	C	603	GLU
1	C	610	ASP
1	C	662	GLN
1	C	715	SER
1	C	717[A]	ARG
1	C	717[B]	ARG
1	C	720	LEU
1	C	727[A]	ARG
1	C	727[B]	ARG
1	C	741	ASP
1	C	742	PHE
1	C	744	LEU
1	C	745	SER
1	C	769	ILE
1	C	771	SER

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Mol	Chain	Res	Type
1	C	781	SER
1	C	811	ASP
1	C	824	ASP
1	D	585	ASN
1	D	603	GLU
1	D	610	ASP
1	D	715	SER
1	D	717	ARG
1	D	718	ASN
1	D	720	LEU
1	D	741	ASP
1	D	742	PHE
1	D	744	LEU
1	D	745	SER
1	D	769	ILE
1	D	781	SER
1	D	811	ASP
1	D	824	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	608	GLN
1	A	728	ASN
1	B	608	GLN
1	B	728	ASN
1	C	608	GLN
1	C	662	GLN
1	C	728	ASN
1	D	608	GLN
1	D	728	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
2	OLP	B	900	-	18,26,26	3.04	4 (22%)	19,36,36	1.71	3 (15%)
2	OLP	A	900	-	18,26,26	3.10	5 (27%)	19,36,36	1.79	3 (15%)
2	OLP	D	900	-	18,26,26	3.09	6 (33%)	19,36,36	1.87	3 (15%)
2	OLP	C	900	-	18,26,26	2.87	4 (22%)	19,36,36	1.90	5 (26%)

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	OLP	B	900	-	-	4/9/12/12	0/2/3/3
2	OLP	A	900	-	-	5/9/12/12	0/2/3/3
2	OLP	D	900	-	-	4/9/12/12	0/2/3/3
2	OLP	C	900	-	-	5/9/12/12	0/2/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	OLP	C4-N9	-11.34	1.32	1.47
2	D	900	OLP	C4-N9	-11.01	1.33	1.47
2	B	900	OLP	C4-N9	-10.77	1.33	1.47
2	C	900	OLP	C4-N9	-10.43	1.33	1.47
2	D	900	OLP	CAR-N6	-4.53	1.34	1.42
2	B	900	OLP	CAR-N6	-4.13	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	OLP	CAR-N6	-3.87	1.35	1.42
2	B	900	OLP	C8-N9	-3.54	1.33	1.45
2	C	900	OLP	CAR-N6	-3.41	1.36	1.42
2	C	900	OLP	C8-N9	-3.41	1.33	1.45
2	A	900	OLP	C8-N9	-3.40	1.33	1.45
2	D	900	OLP	C8-N9	-3.26	1.34	1.45
2	B	900	OLP	C5-C4	-2.27	1.39	1.53
2	C	900	OLP	C5-C4	-2.20	1.39	1.53
2	D	900	OLP	C5-C4	-2.19	1.39	1.53
2	D	900	OLP	CAQ-CL	-2.15	1.69	1.74
2	D	900	OLP	C2-N1	-2.08	1.35	1.44
2	A	900	OLP	C5-C4	-2.04	1.40	1.53
2	A	900	OLP	C2-N1	-2.01	1.36	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	OLP	C4-C5-N7	4.87	108.92	102.46
2	C	900	OLP	CAK-N2-C2	4.78	127.58	114.79
2	A	900	OLP	C4-C5-N7	4.60	108.56	102.46
2	B	900	OLP	C4-C5-N7	4.42	108.32	102.46
2	A	900	OLP	C8-N9-CAW	4.18	122.61	114.09
2	D	900	OLP	C8-N9-CAW	3.95	122.16	114.09
2	C	900	OLP	C8-N9-CAW	3.94	122.13	114.09
2	B	900	OLP	C8-N9-CAW	3.78	121.81	114.09
2	C	900	OLP	C4-C5-N7	3.51	107.11	102.46
2	A	900	OLP	CAK-N2-C2	3.11	123.10	114.79
2	B	900	OLP	CAK-N2-C2	3.03	122.90	114.79
2	D	900	OLP	CAK-N2-C2	2.94	122.66	114.79
2	C	900	OLP	CAR-CAH-CAQ	2.59	120.91	119.06
2	C	900	OLP	C4-N9-CAW	2.06	128.53	117.52

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	OLP	CAB-CAW-N9-C8
2	A	900	OLP	CAA-CAW-N9-C8
2	B	900	OLP	CAB-CAW-N9-C8
2	B	900	OLP	CAA-CAW-N9-C8
2	D	900	OLP	CAB-CAW-N9-C8
2	C	900	OLP	CAB-CAW-N9-C8

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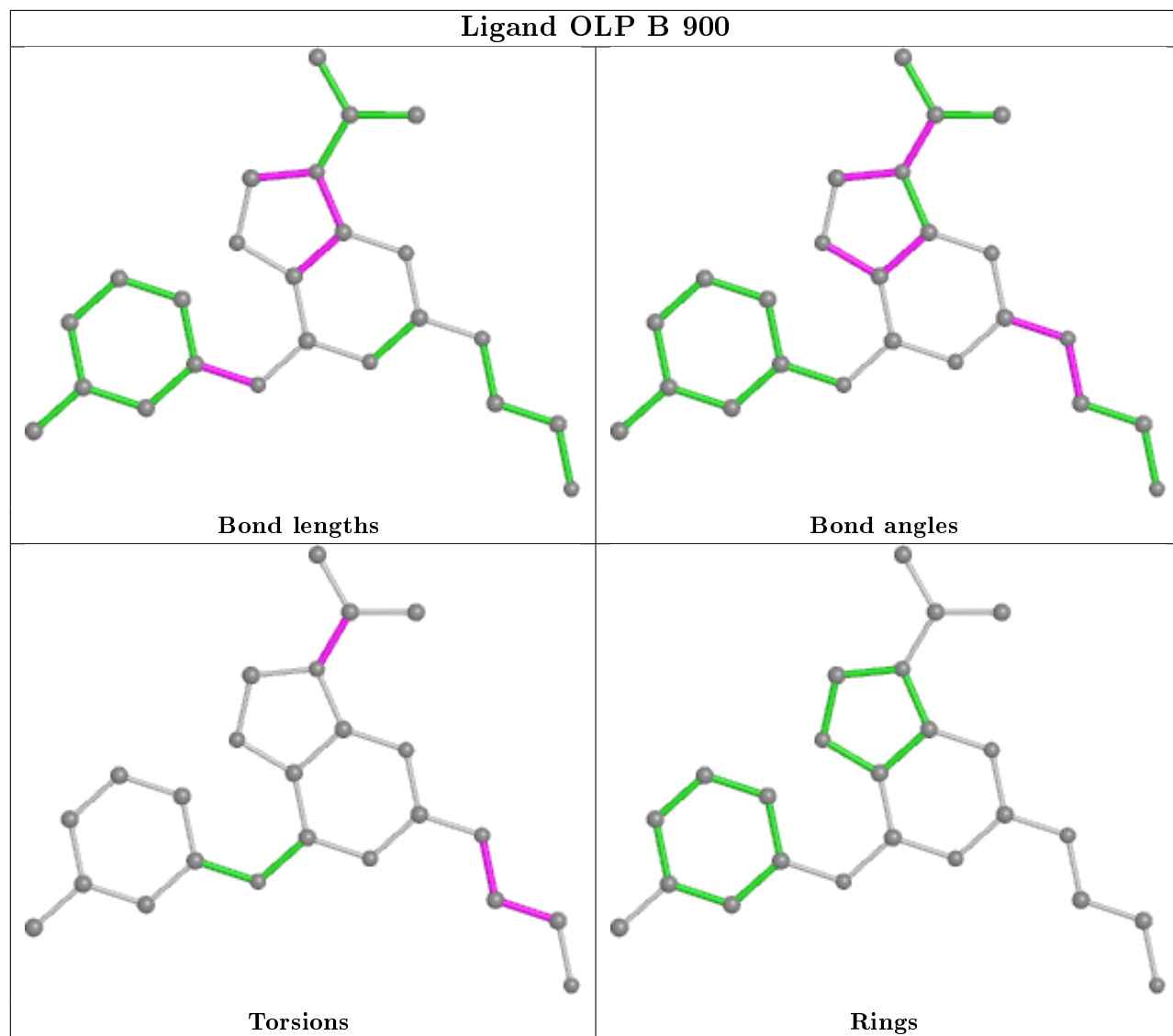
Mol	Chain	Res	Type	Atoms
2	C	900	OLP	CAA-CAW-N9-C8
2	A	900	OLP	OAC-CAJ-CAK-N2
2	B	900	OLP	CAJ-CAK-N2-C2
2	C	900	OLP	CAJ-CAK-N2-C2
2	A	900	OLP	CAJ-CAK-N2-C2
2	C	900	OLP	CAH-CAR-N6-C6
2	B	900	OLP	OAC-CAJ-CAK-N2
2	D	900	OLP	CAH-CAR-N6-C6
2	C	900	OLP	CAG-CAR-N6-C6
2	A	900	OLP	CAH-CAR-N6-C6
2	D	900	OLP	CAJ-CAK-N2-C2
2	D	900	OLP	CAA-CAW-N9-C8

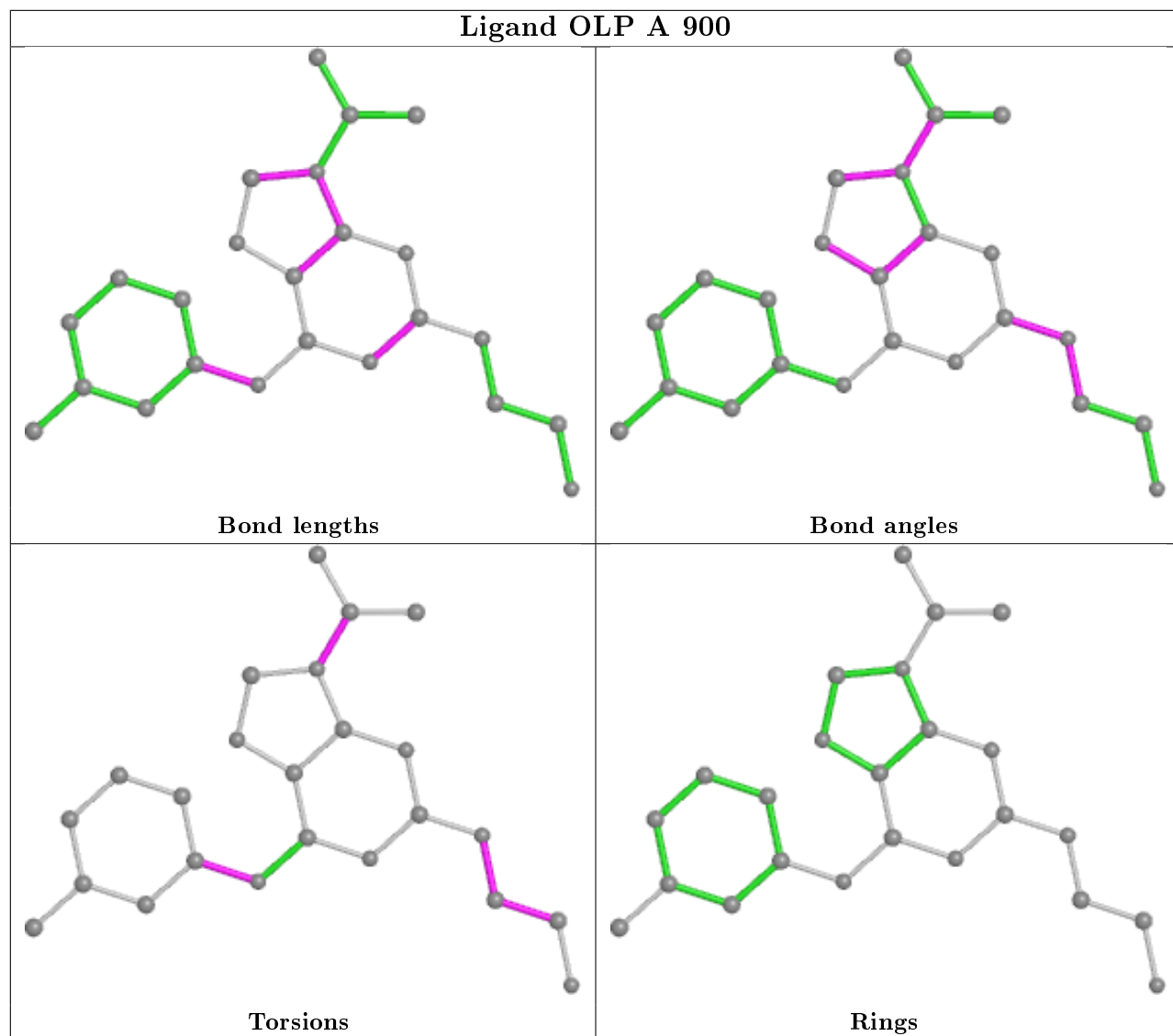
There are no ring outliers.

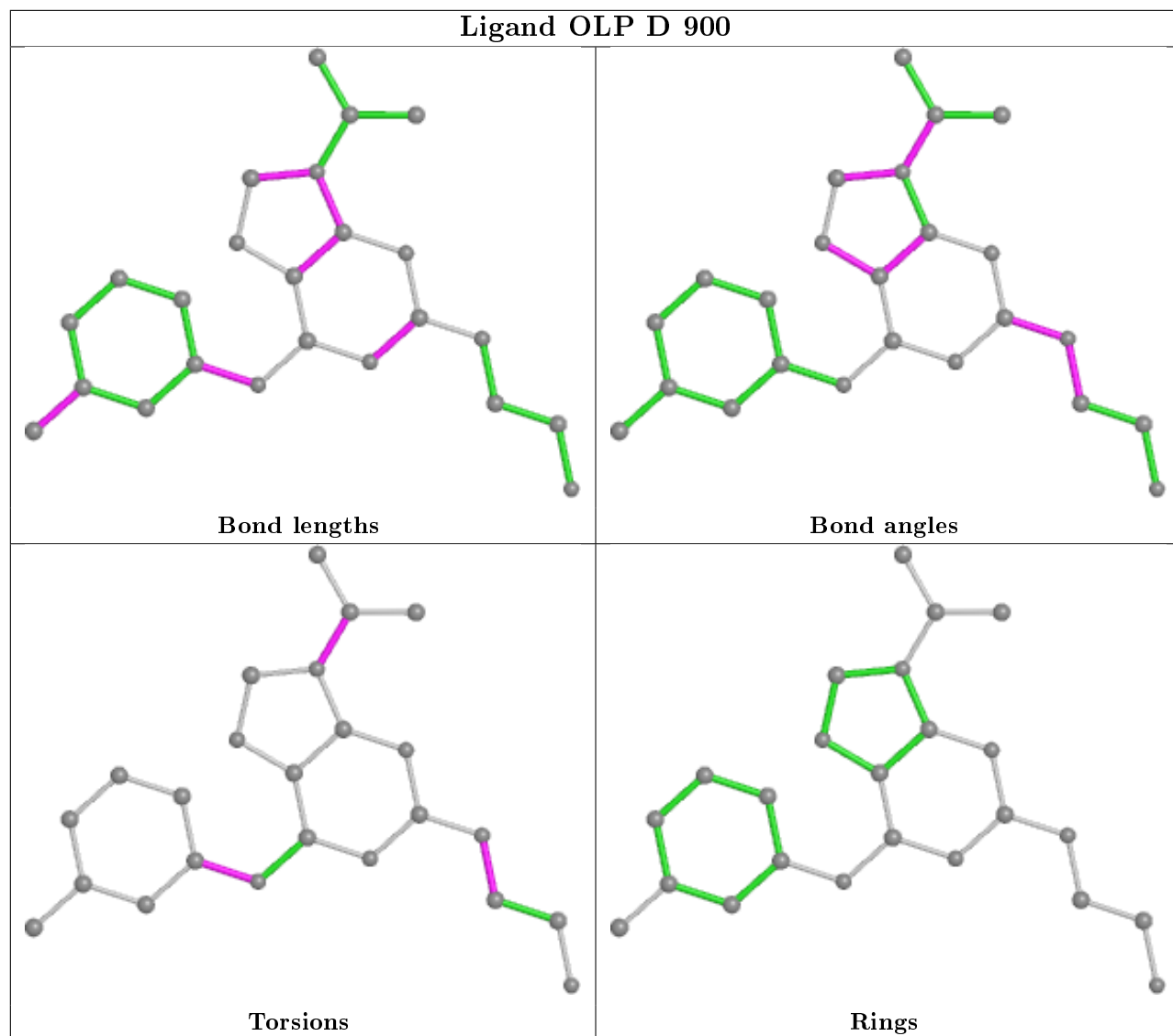
4 monomers are involved in 12 short contacts:

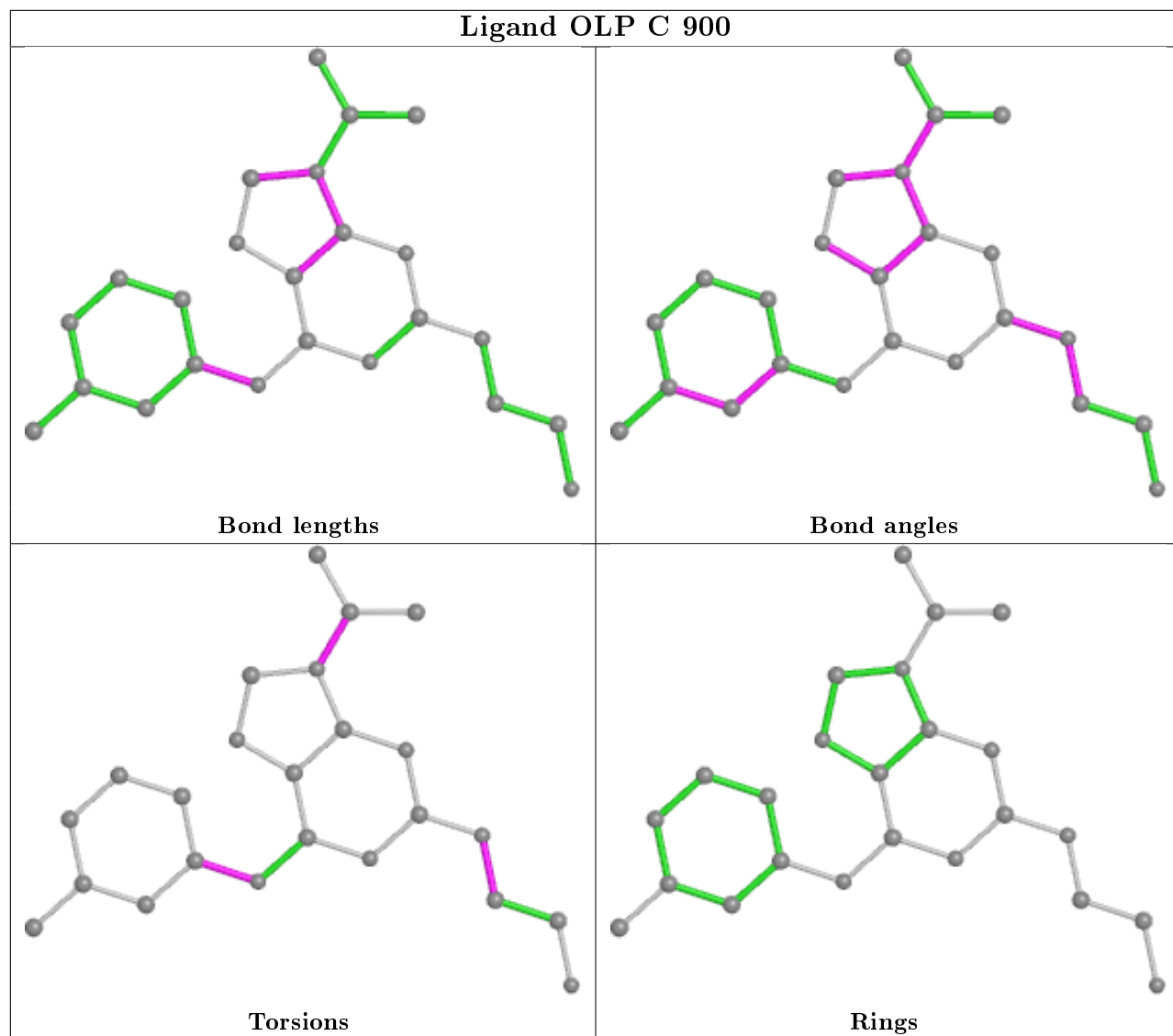
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	OLP	2	0
2	A	900	OLP	4	0
2	D	900	OLP	4	0
2	C	900	OLP	2	0

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	261/313 (83%)	-0.02	3 (1%) 80 75	41, 58, 90, 117	0
1	B	256/313 (81%)	-0.01	5 (1%) 65 56	38, 56, 86, 109	0
1	C	259/313 (82%)	0.03	2 (0%) 86 81	35, 55, 83, 106	0
1	D	259/313 (82%)	0.05	4 (1%) 73 68	38, 56, 89, 133	0
All	All	1035/1252 (82%)	0.01	14 (1%) 75 70	35, 57, 88, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	622	LYS	3.3
1	A	621	MET	3.0
1	B	659	MET	3.0
1	B	622	LYS	2.8
1	A	690	THR	2.7
1	B	621	MET	2.6
1	D	661	SER	2.6
1	C	644	PHE	2.4
1	D	660	SER	2.4
1	A	622	LYS	2.3
1	C	598	PHE	2.1
1	D	619	LYS	2.1
1	B	623	LEU	2.1
1	B	594	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

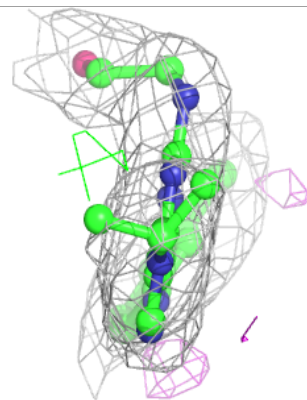
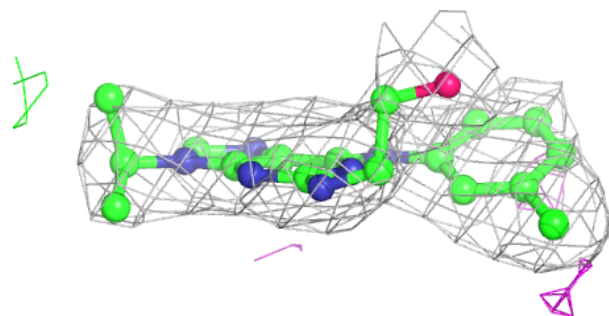
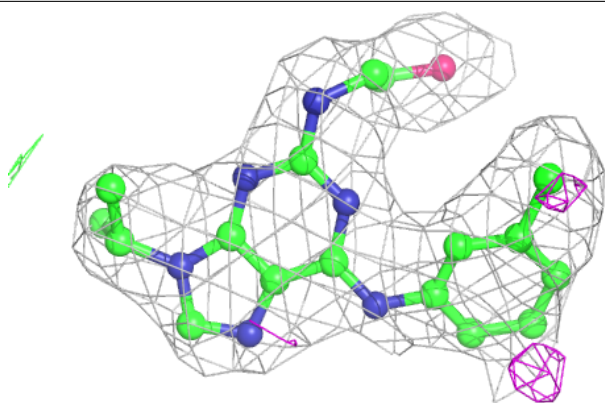
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLP	D	900	24/24	0.93	0.21	44,52,58,62	0
2	OLP	B	900	24/24	0.94	0.22	49,53,57,59	0
2	OLP	C	900	24/24	0.94	0.21	47,52,56,59	0
2	OLP	A	900	24/24	0.96	0.19	46,49,53,57	0
3	NA	B	1	1/1	0.96	0.10	35,35,35,35	0
4	CL	D	134	1/1	0.98	0.14	32,32,32,32	0
4	CL	C	133	1/1	0.99	0.18	43,43,43,43	0

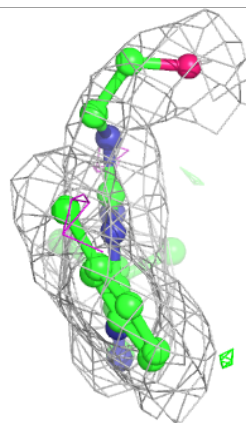
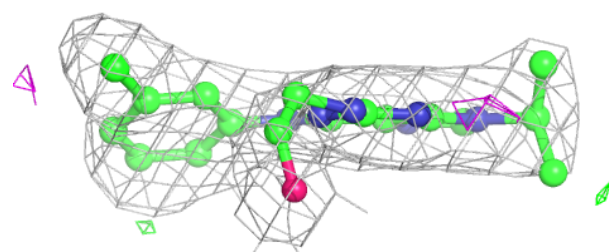
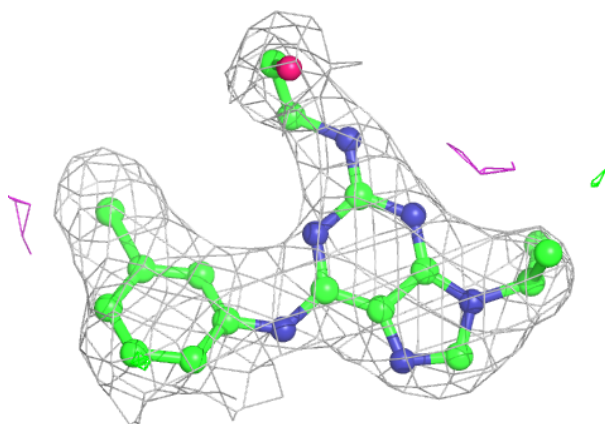
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLP D 900:

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

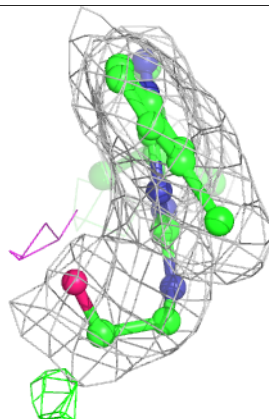
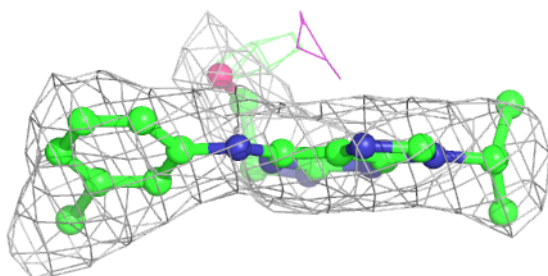
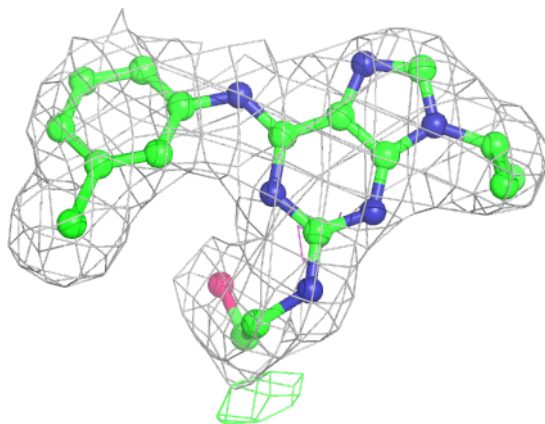
**Electron density around OLP B 900:**

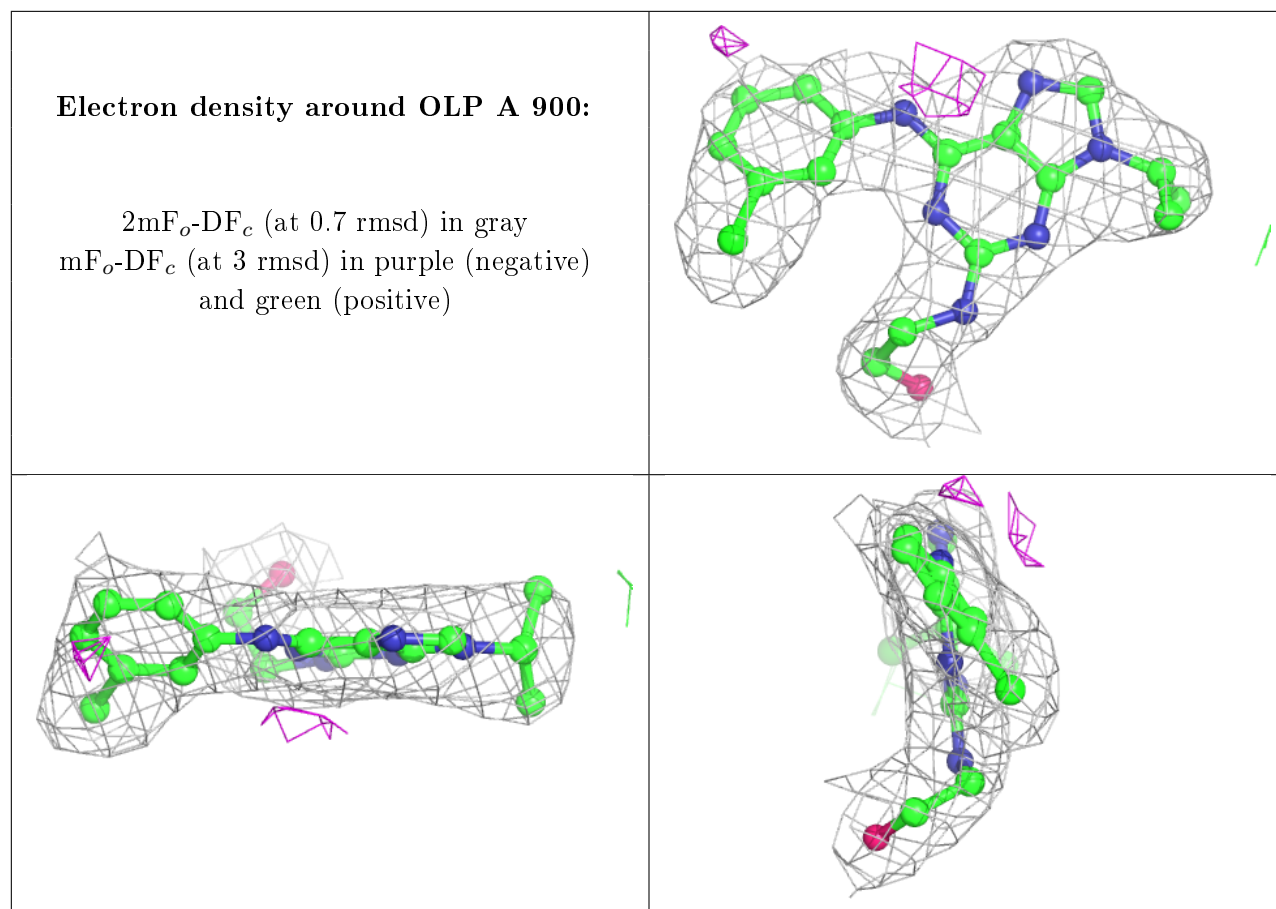
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLP C 900:

$2mF_o-DF_c$ (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.