WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 09:36 PM EDT

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)

The following versions of software and data (see references ①) were used in the production of this report:

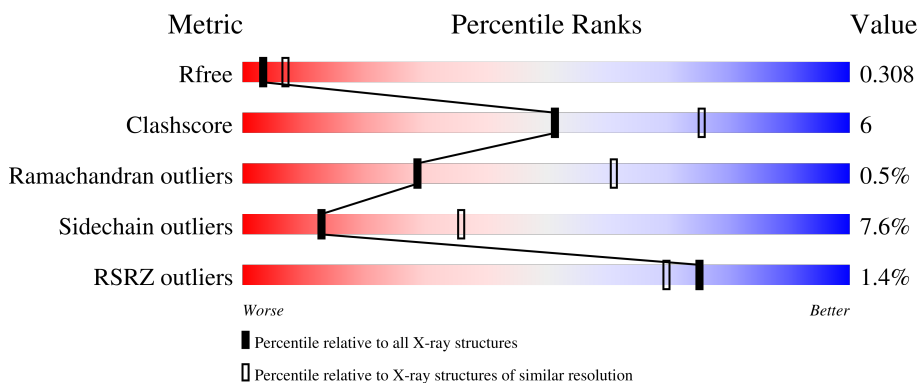|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1   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	Percentile Ranks	Value
Rfree		0.308
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		7.6%
RSRZ outliers		1.4%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	71% 11% · 17%
1	B	313	66% 14% · 18%
1	C	313	69% 12% · 17%
1	D	313	66% 16% · 17%

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 2027	C 1299	N 332	O 375	S 21	0	2	0
1	B	256	Total 2012	C 1289	N 336	O 368	S 19	0	2	0
1	C	259	Total 2073	C 1326	N 348	O 379	S 20	0	4	0
1	D	259	Total 2057	C 1316	N 345	O 376	S 20	0	3	0

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

W O R L D W I D E
PDB
PROTEIN DATA BANK

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is 2-(2-HYDROXYETHYLAMINO)-6-(3-CHLOROANILINO)-9-ISOPROPYL PURINE (three-letter code: OLP) (formula: $C_{16}H_{19}ClN_6O$).
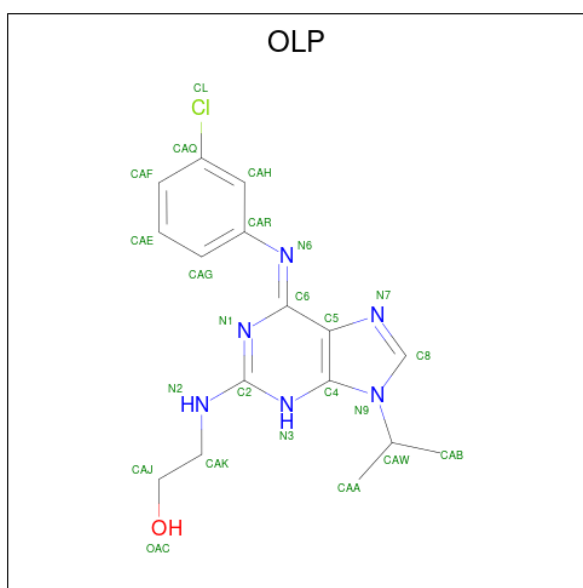
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
2	B	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
2	C	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
2	D	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		

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

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

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

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

- Molecule 5 is water.

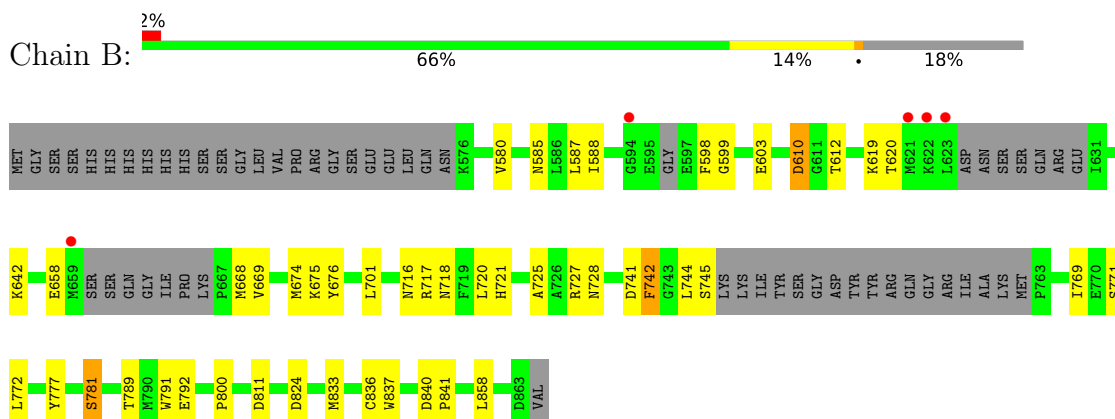| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	31	Total 31	O 31	0	0
5	C	32	Total 32	O 32	0	0
5	D	29	Total 29	O 29	0	0

3 Residue-property plots ⓘ

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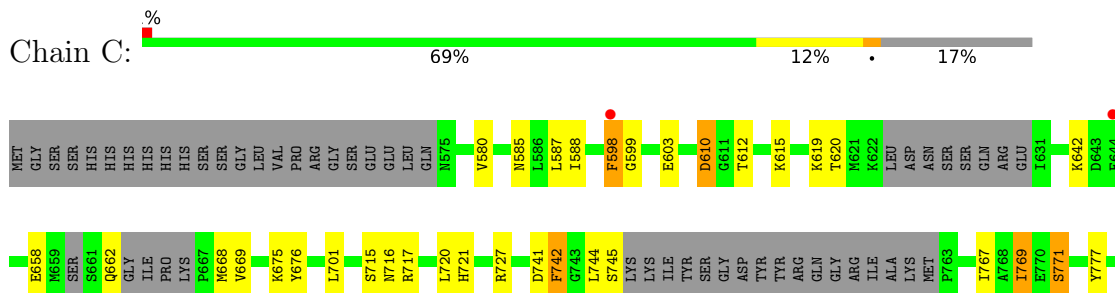
• Molecule 1: Proto-oncogene tyrosine-protein kinase MER

Chain A:

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

Chain B:

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

Chain C:

S781 W791 P800 D811 D824 M833 C336 L858 D863 VAL

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

Chain D:

%

66% 16% • 17%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER GLU GLU LEU GLN N575 V580 V581 I582 N585 L586 L587 I588 F598 G599 E603 D610 G611 T612 K619 T620 M621 K622 LEU ASP ASN SER SER GLN ARG GLU I631 E632 L635

K642 H646 P647 G654 V655 C656 I657 E658 M659 S660 S661 GLN GLY ILE PRO LYS P667 M668 V669 M674 K675 Y676 I695 T699 L700 L701 S715 N716 R717 N718 F719 L720 H721 D741 F742 G743 L744 S745 LYS LYS ILE TYR SER GLY ASP TYR TYR ARG GLN GLY ARG ILE ALA

LYS MET P763 I767 A768 I769 E770 S771 Y777 S781 W791 P800 D811 D824 E828 M833 C836 T839 L858 D863 VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.00Å 91.70Å 120.75Å 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
$< I/\sigma(I) >$ [1]	2.90 (at 2.81Å)	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]	$< |L| > = 0.51$, $< L^2 > = 0.34$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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 ⓘ

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

Continued on next page...

Continued from previous page...

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.

The worst 5 of 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

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
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

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	715	SER
1	D	718	ASN
1	D	769	ILE
1	B	742	PHE
1	B	741	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	608	GLN
1	D	728	ASN
1	B	728	ASN
1	C	608	GLN
1	C	662	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 monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

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	D	900	-	23,26,26	1.28	2 (8%)	27,36,36	2.26	8 (29%)
2	OLP	A	900	-	23,26,26	1.18	1 (4%)	27,36,36	2.10	6 (22%)
2	OLP	C	900	-	23,26,26	1.19	2 (8%)	27,36,36	2.34	10 (37%)
2	OLP	B	900	-	23,26,26	1.31	1 (4%)	27,36,36	2.23	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLP	D	900	-	-	5/10/12/12	0/3/3/3
2	OLP	A	900	-	-	5/10/12/12	0/3/3/3
2	OLP	C	900	-	-	5/10/12/12	0/3/3/3
2	OLP	B	900	-	-	5/10/12/12	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	OLP	CAR-N6	-4.47	1.34	1.42
2	B	900	OLP	CAR-N6	-4.08	1.35	1.42
2	A	900	OLP	CAR-N6	-3.81	1.35	1.42
2	C	900	OLP	CAR-N6	-3.36	1.36	1.42
2	C	900	OLP	C6-N6	2.25	1.37	1.31

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	OLP	C2-N1-C6	6.63	123.06	115.17
2	C	900	OLP	C2-N3-C4	6.16	122.27	115.28
2	B	900	OLP	C2-N1-C6	5.84	122.12	115.17
2	D	900	OLP	C2-N1-C6	5.67	121.91	115.17
2	D	900	OLP	C2-N3-C4	5.60	121.63	115.28

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	OLP	CAB-CAW-N9-C8
2	A	900	OLP	CAB-CAW-N9-C4
2	B	900	OLP	CAB-CAW-N9-C8
2	B	900	OLP	CAB-CAW-N9-C4
2	C	900	OLP	CAB-CAW-N9-C8

There are no ring outliers.

4 monomers are involved in 12 short contacts:

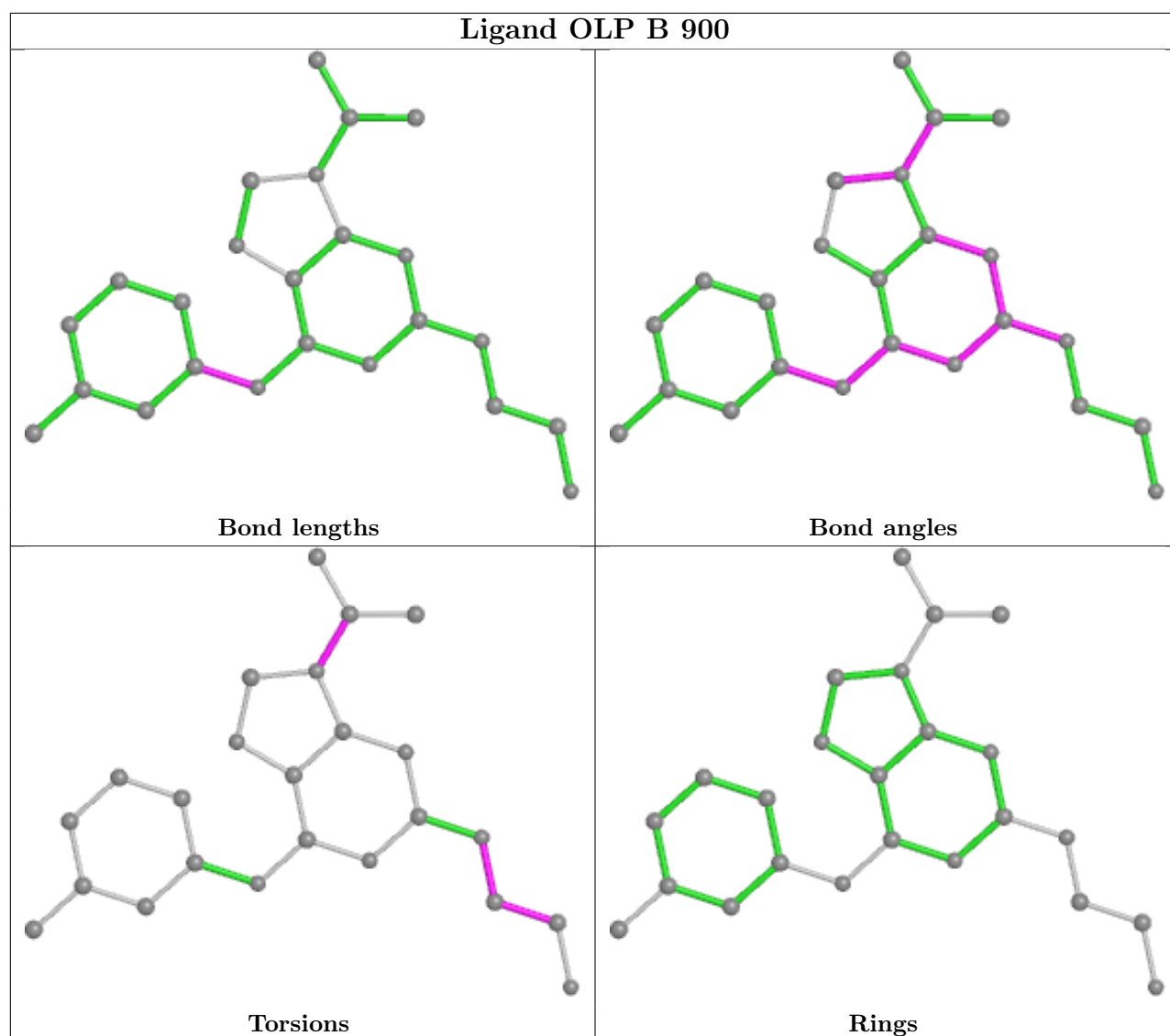| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	OLP	4	0
2	A	900	OLP	4	0
2	C	900	OLP	2	0
2	B	900	OLP	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OLP D 900

Bond lengths

Bond angles

Torsions

Rings

Ligand OLP A 900

Bond lengths

Bond angles

Torsions

Rings

Ligand OLP C 900

Bond lengths

Bond angles

Torsions

Rings

Ligand OLP B 900

Bond lengths

Bond angles

Torsions

Rings
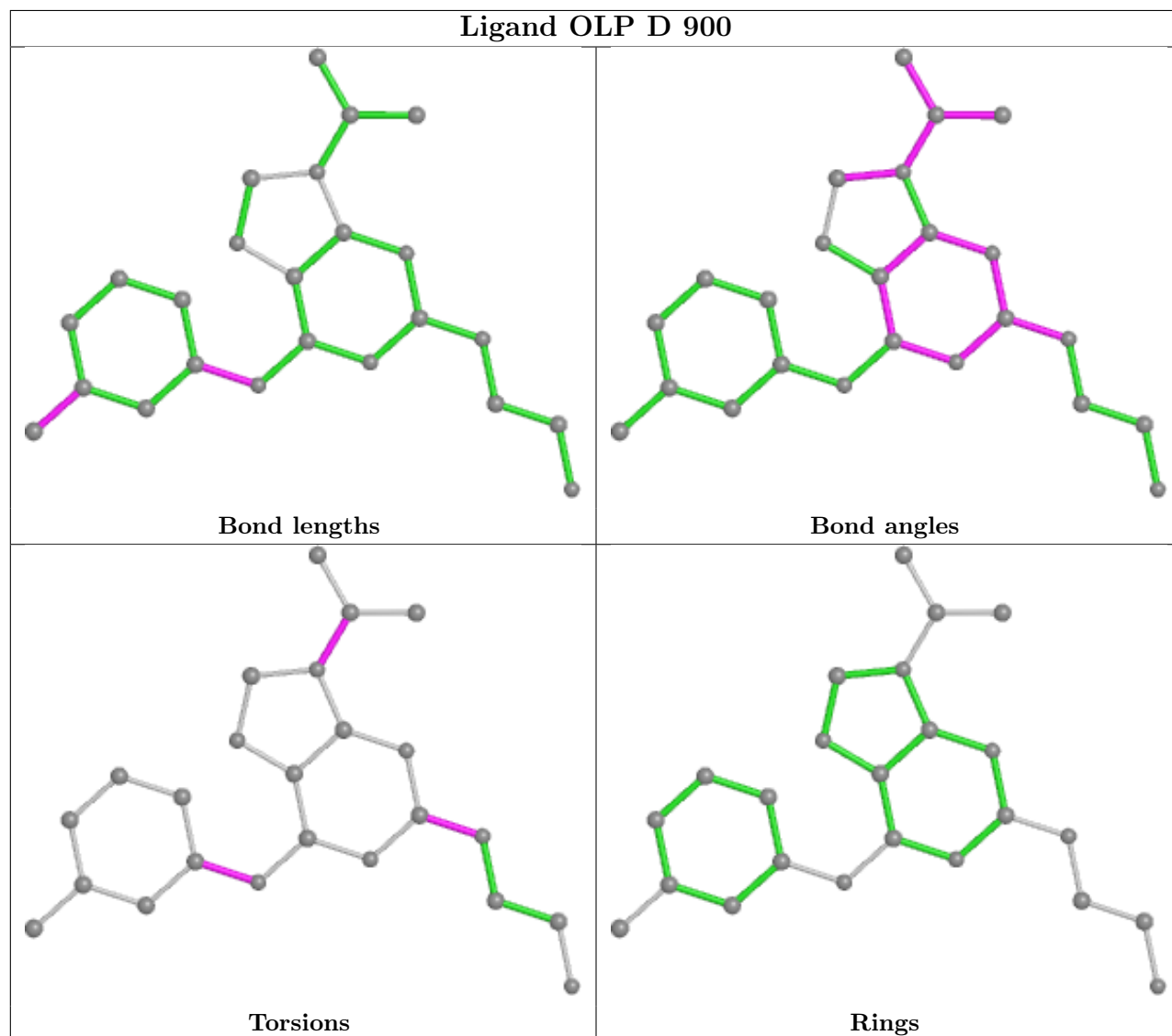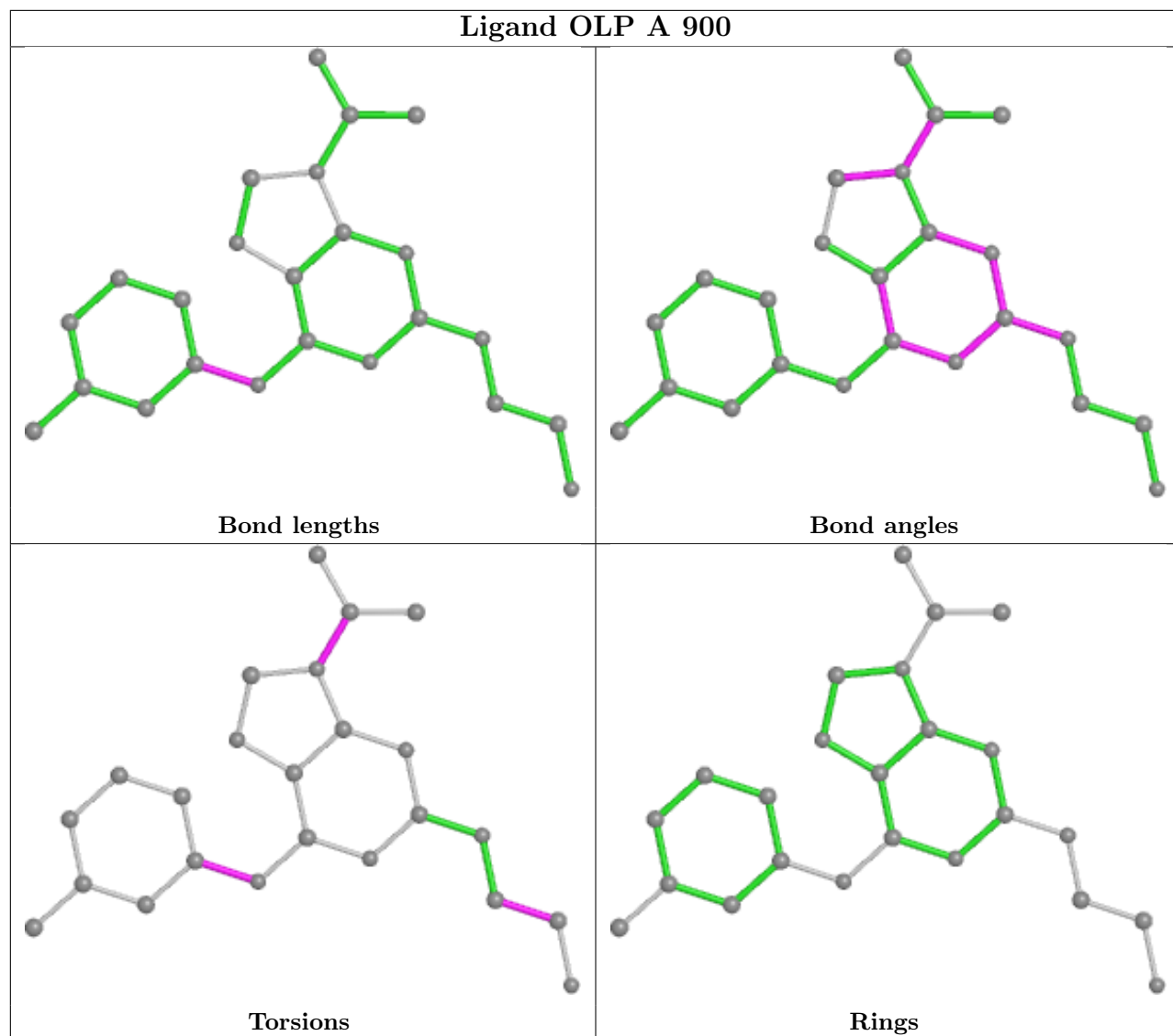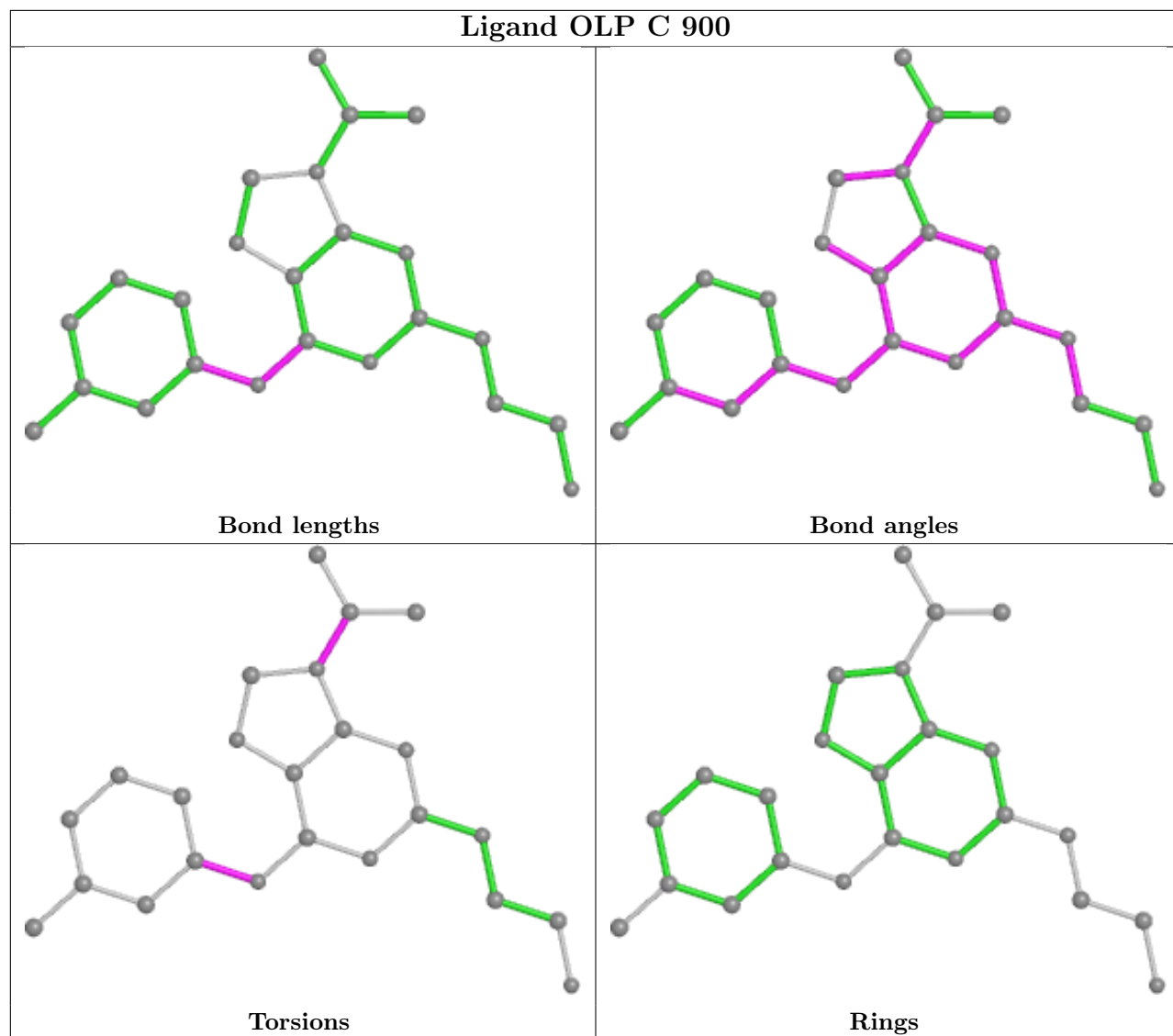
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	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

The worst 5 of 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

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

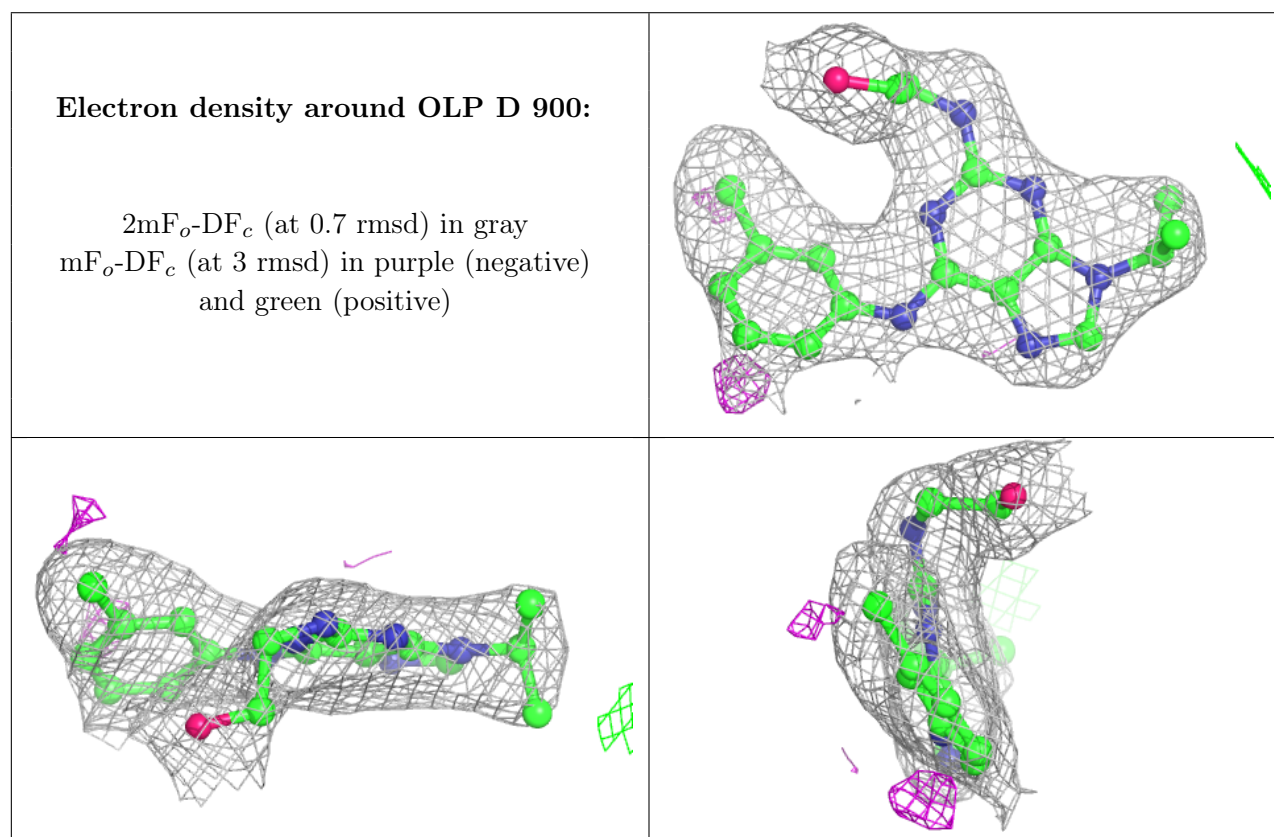There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	OLP	D	900	24/24	0.93	0.21	44,52,58,62	0
2	OLP	C	900	24/24	0.94	0.21	47,52,56,59	0
2	OLP	B	900	24/24	0.94	0.22	49,53,57,59	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.
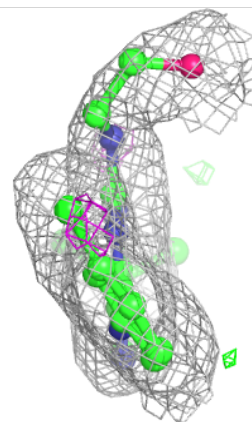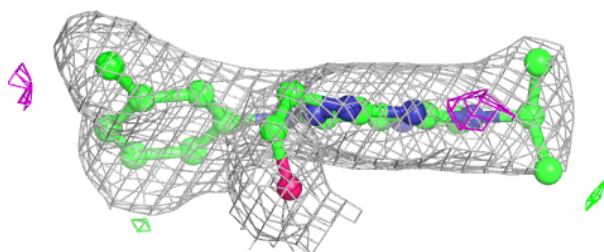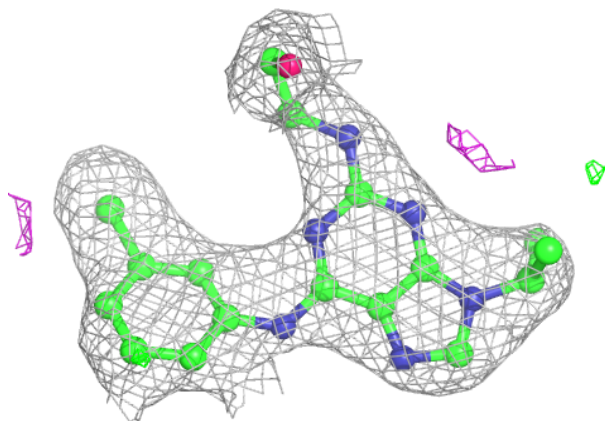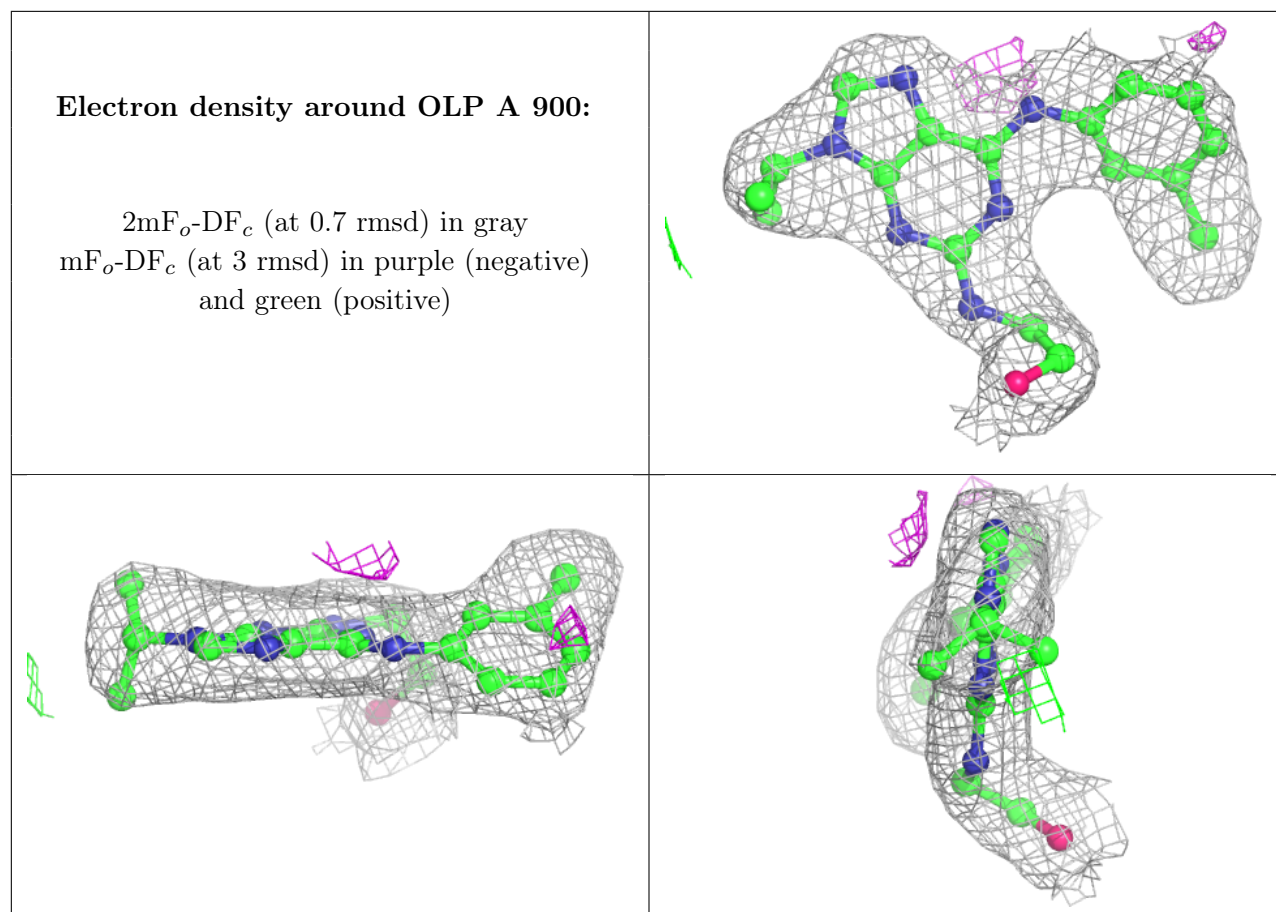

Electron density around OLP D 900:

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

Electron density around OLP C 900:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
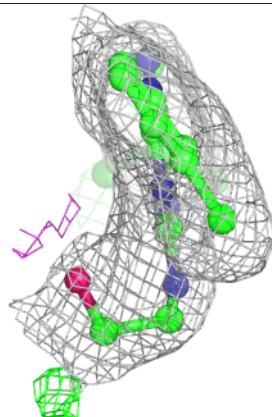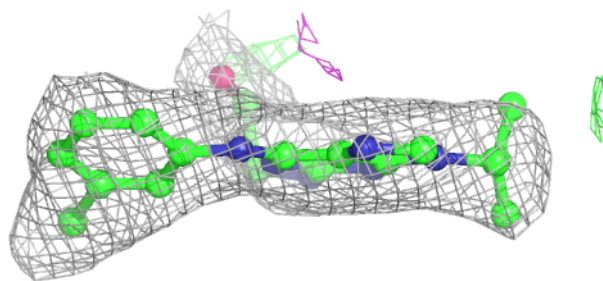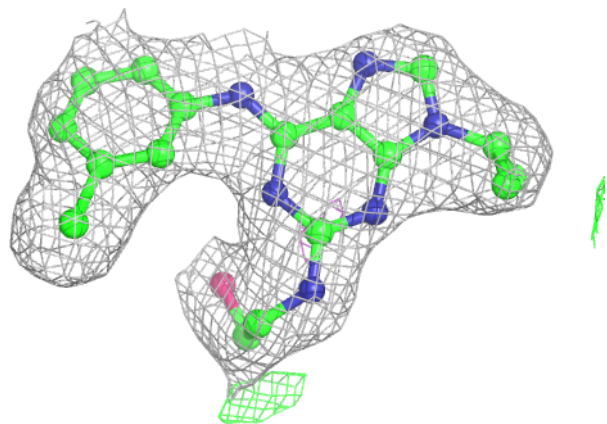
Electron density around OLP B 900:

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

Electron density around OLP A 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.