



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:30 AM UTC

PDB ID : 3BPR / pdb_00003bpr
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 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	:	4-5-2 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

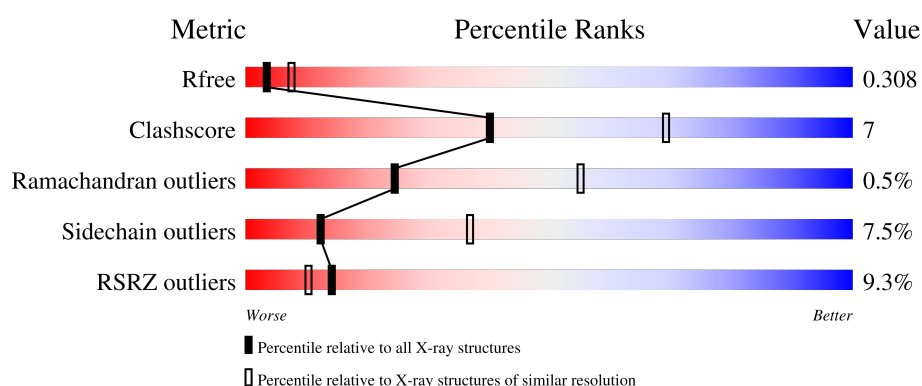
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	 7% 69% 13% • 17%
1	B	313	 7% 66% 15% • 18%
1	C	313	 8% 67% 13% • 17%
1	D	313	 9% 64% 17% • 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	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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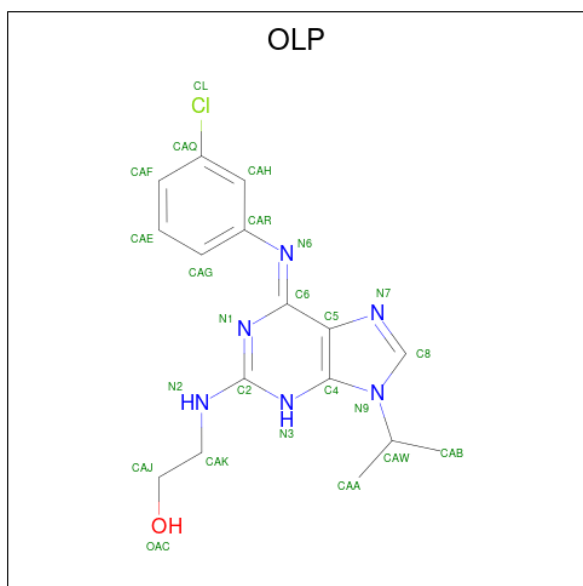
Chain	Residue	Modelled	Actual	Comment	Reference
B	555	SER	-	expression tag	UNP Q12866
B	556	HIS	-	expression tag	UNP Q12866
B	557	HIS	-	expression tag	UNP Q12866
B	558	HIS	-	expression tag	UNP Q12866
B	559	HIS	-	expression tag	UNP Q12866
B	560	HIS	-	expression tag	UNP Q12866
B	561	HIS	-	expression tag	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

- Molecule 2 is 2-(2-HYDROXYETHYLAMINO)-6-(3-CHLOROANILINO)-9-ISOPROPYL PURINE (CCD ID: OLP) (formula: C₁₆H₁₉ClN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 24	C 16	Cl 1	N 6	O 1	0	0
2	B	1	Total 24	C 16	Cl 1	N 6	O 1	0	0
2	C	1	Total 24	C 16	Cl 1	N 6	O 1	0	0
2	D	1	Total 24	C 16	Cl 1	N 6	O 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

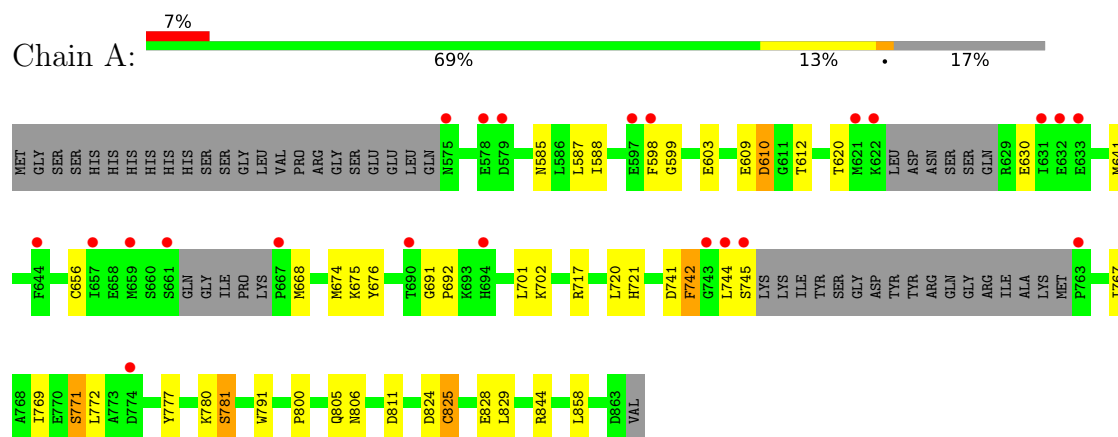
- Molecule 5 is water.

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

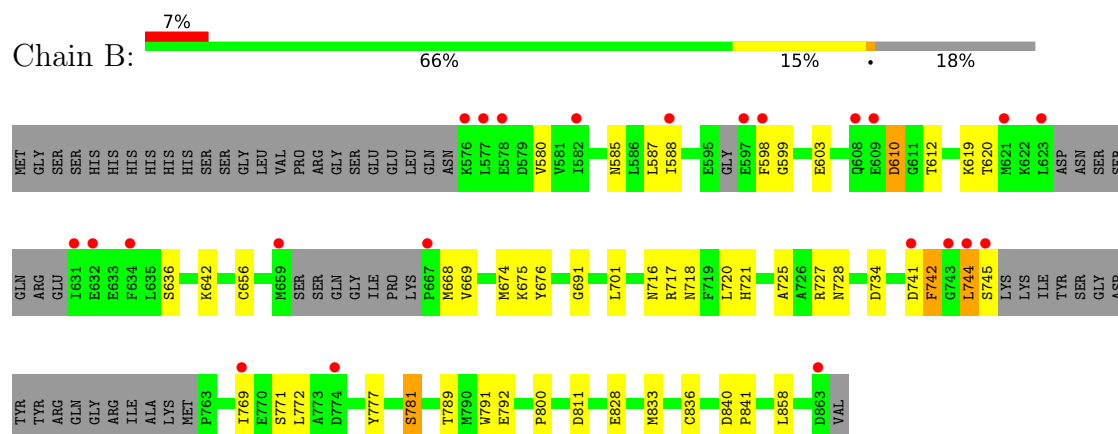
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

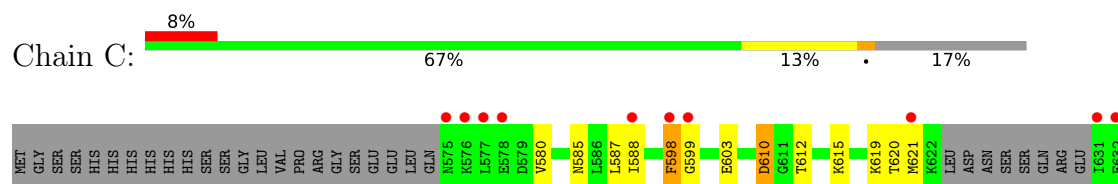
- Molecule 1: Proto-oncogene tyrosine-protein kinase MER

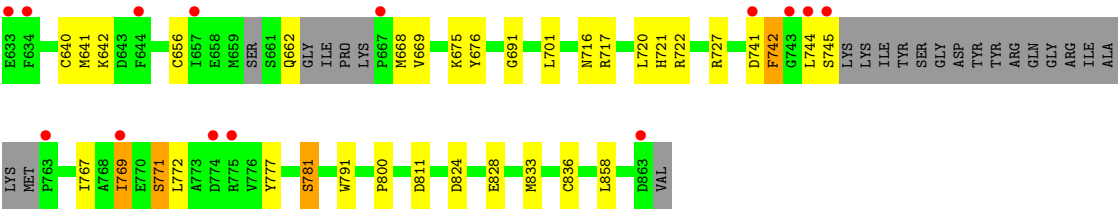


- Molecule 1: Proto-oncogene tyrosine-protein kinase MER

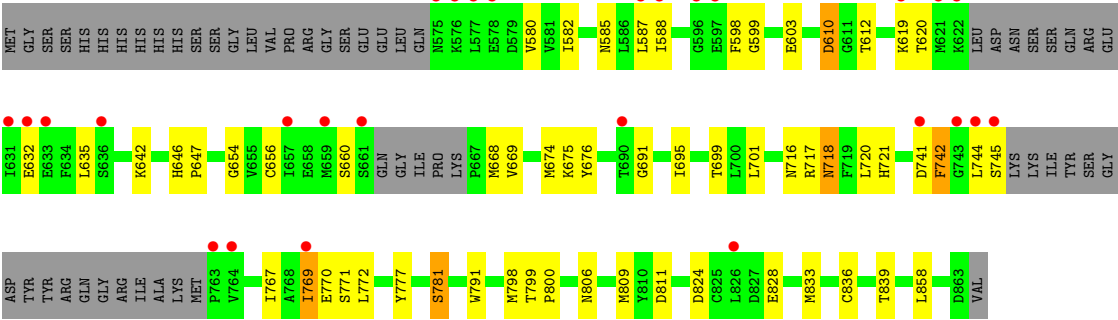


- Molecule 1: Proto-oncogene tyrosine-protein kinase MER





● 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	70.00Å 91.70Å 120.75Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	47.30 – 2.80 47.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.30-2.80) 98.7 (47.30-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.01%)	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 , 69.5	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.*

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: NA, CL, OLP

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	0.63	0/2068	0.88	3/2803 (0.1%)
1	B	0.64	0/2052	0.92	2/2778 (0.1%)
1	C	0.65	0/2114	0.89	2/2857 (0.1%)
1	D	0.66	0/2098	0.90	5/2836 (0.2%)
All	All	0.64	0/8332	0.90	12/11274 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	691	GLY	CA-C-N	6.33	127.75	119.84
1	B	691	GLY	C-N-CA	6.33	127.75	119.84
1	C	691	GLY	CA-C-N	6.32	127.74	119.84
1	C	691	GLY	C-N-CA	6.32	127.74	119.84
1	D	691	GLY	CA-C-N	6.26	127.67	119.84
1	D	691	GLY	C-N-CA	6.26	127.67	119.84
1	A	806	ASN	N-CA-C	5.68	117.92	111.11
1	A	691	GLY	CA-C-N	5.57	126.80	119.84
1	A	691	GLY	C-N-CA	5.57	126.80	119.84
1	D	799	THR	N-CA-C	-5.36	103.02	109.83
1	D	809	MET	N-CA-C	5.22	116.66	111.07
1	D	806	ASN	N-CA-C	5.17	117.31	111.11

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	22	0
1	B	2012	0	1961	24	0
1	C	2073	0	2032	26	0
1	D	2057	0	2029	29	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
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	107	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 7.

All (107) 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:656:CYS:HB3	1:D:668:MET:HE3	1.64	0.78
1:D:674:MET:O	2:D:900:OLP:HAG	1.86	0.76
1:A:656:CYS:HB3	1:A:668:MET:HE3	1.71	0.73
1:A:675:LYS:O	2:A:900:OLP:HAE	1.90	0.71
1:C:580:VAL:HG23	1:C:642:LYS:HD2	1.74	0.70
1:C:656:CYS:HB3	1:C:668:MET:HE3	1.73	0.69
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:B:656:CYS:HB3	1:B:668:MET:HE3	1.79	0.64
1:D:620:THR:HG22	1:D:668:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:656:CYS:CB	1:A:668:MET:HE3	2.34	0.58
1:C:620:THR:HG22	1:C:668:MET:HG2	1.86	0.58
1:D:656:CYS:CB	1:D:668:MET:HE3	2.31	0.58
1:A:620:THR:HG22	1:A:668:MET:HG2	1.86	0.57
1:C:656:CYS:CB	1:C:668:MET:HE3	2.34	0.57
1:B:674:MET:O	2:B:900:OLP:HAG	2.04	0.56
2:D:900:OLP:HAH	2:D:900:OLP:N1	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:B:656:CYS:CB	1:B:668:MET:HE3	2.37	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
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
1:D:828:GLU:H	1:D:828:GLU:CD	2.19	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:C:598:PHE:HE2	1:C:621:MET:HE3	1.76	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:828:GLU:H	1:B:828:GLU:CD	2.23	0.46
1:B:701:LEU:HB2	1:B:858:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:716:ASN:C	1:B:718:ASN:H	2.25	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:C:828:GLU:H	1:C:828:GLU:CD	2.25	0.44
1:D:619:LYS:HB2	1:D:669:VAL:CG2	2.47	0.44
1:D:716:ASN:C	1:D:718:ASN:H	2.26	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:828:GLU:H	1:A:828:GLU:CD	2.26	0.43
1:A:702:LYS:HA	1:A:702:LYS:HD2	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:B:734:ASP:OD1	1:B:734:ASP:C	2.61	0.42
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:641:MET:HE3	1:C:742:PHE:CE1	2.54	0.42
1:C:769:ILE:H	1:C:769:ILE:HG13	1.69	0.42
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:C:615:LYS:HD2	1:C:615:LYS:HA	1.86	0.42
1:D:646:HIS:ND1	1:D:647:PRO:HD2	2.35	0.42
1:C:721:HIS:C	1:C:722:ARG:HG3	2.44	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:B:619:LYS:HZ3	1:B:744:LEU:HD23	1.86	0.41
1:D:798:MET:HE2	1:D:798:MET:HB3	2.00	0.41
1:A:721:HIS:CE1	1:A:742:PHE:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:ILE:CG2	1:D:771:SER:HB2	2.51	0.41
1:A:641:MET:HE3	1:A:742:PHE:CE1	2.55	0.41
1:A:780:LYS:NZ	1:A:844:ARG:O	2.49	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:C:640:CYS:O	1:C:641:MET:C	2.64	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

There are no symmetry-related clashes.

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	255/313 (82%)	239 (94%)	14 (6%)	2 (1%)	16	44
1	B	248/313 (79%)	234 (94%)	13 (5%)	1 (0%)	30	60
1	C	253/313 (81%)	234 (92%)	18 (7%)	1 (0%)	30	60
1	D	254/313 (81%)	236 (93%)	17 (7%)	1 (0%)	30	60
All	All	1010/1252 (81%)	943 (93%)	62 (6%)	5 (0%)	24	55

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

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Mol	Chain	Res	Type
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%)	195 (91%)	19 (9%)	9	29
1	B	215/280 (77%)	200 (93%)	15 (7%)	14	40
1	C	224/280 (80%)	205 (92%)	19 (8%)	10	31
1	D	223/280 (80%)	208 (93%)	15 (7%)	15	42
All	All	876/1120 (78%)	808 (92%)	68 (8%)	12	35

All (68) 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
1	A	744	LEU
1	A	745	SER
1	A	769	ILE
1	A	771	SER
1	A	772	LEU
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

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Mol	Chain	Res	Type
1	B	603	GLU
1	B	610	ASP
1	B	636	SER
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	C	585	ASN
1	C	603	GLU
1	C	610	ASP
1	C	662	GLN
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
1	C	772	LEU
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	717	ARG
1	D	718	ASN
1	D	720	LEU
1	D	741	ASP
1	D	742	PHE
1	D	744	LEU

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Mol	Chain	Res	Type
1	D	745	SER
1	D	769	ILE
1	D	772	LEU
1	D	781	SER
1	D	811	ASP
1	D	824	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	608	GLN
1	A	728	ASN
1	A	817	HIS
1	B	585	ASN
1	B	608	GLN
1	B	728	ASN
1	C	608	GLN
1	C	662	GLN
1	C	728	ASN
1	D	585	ASN
1	D	608	GLN
1	D	728	ASN
1	D	817	HIS

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](#)

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	C	900	-	25,26,26	1.49	4 (16%)	26,36,36	1.57	7 (26%)
2	OLP	A	900	-	25,26,26	1.66	4 (16%)	26,36,36	1.32	4 (15%)
2	OLP	B	900	-	25,26,26	1.67	4 (16%)	26,36,36	1.53	5 (19%)
2	OLP	D	900	-	25,26,26	1.64	4 (16%)	26,36,36	1.64	6 (23%)

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	C	900	-	-	4/11/12/12	0/3/3/3
2	OLP	A	900	-	-	4/11/12/12	0/3/3/3
2	OLP	B	900	-	-	4/11/12/12	0/3/3/3
2	OLP	D	900	-	-	4/11/12/12	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	OLP	CAR-N6	-4.49	1.34	1.42
2	A	900	OLP	C4-N9	-4.48	1.32	1.37
2	B	900	OLP	CAR-N6	-4.10	1.35	1.42
2	D	900	OLP	C4-N9	-4.06	1.33	1.37
2	A	900	OLP	CAR-N6	-3.84	1.35	1.42
2	B	900	OLP	C4-N9	-3.75	1.33	1.37
2	C	900	OLP	CAR-N6	-3.38	1.36	1.42
2	C	900	OLP	C4-N9	-3.31	1.33	1.37
2	B	900	OLP	C5-N7	-2.88	1.33	1.39
2	A	900	OLP	C5-N7	-2.79	1.33	1.39
2	D	900	OLP	C5-N7	-2.73	1.33	1.39
2	C	900	OLP	C5-N7	-2.61	1.33	1.39
2	C	900	OLP	C2-N1	2.59	1.36	1.32
2	B	900	OLP	C2-N1	2.45	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	OLP	C2-N1	2.18	1.36	1.32
2	D	900	OLP	C2-N1	2.03	1.35	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	OLP	C8-N9-C4	4.49	110.46	106.67
2	D	900	OLP	CAB-CAW-N9	3.93	114.96	110.14
2	A	900	OLP	C8-N9-C4	3.79	109.86	106.67
2	D	900	OLP	C8-N9-C4	3.56	109.67	106.67
2	C	900	OLP	C8-N9-C4	3.16	109.34	106.67
2	B	900	OLP	N9-C8-N7	-3.01	107.81	113.40
2	B	900	OLP	N3-C2-N1	-2.95	118.71	123.68
2	C	900	OLP	N9-C8-N7	-2.83	108.15	113.40
2	D	900	OLP	CAA-CAW-N9	-2.79	106.72	110.14
2	D	900	OLP	N3-C2-N1	-2.75	119.05	123.68
2	C	900	OLP	N3-C2-N1	-2.71	119.11	123.68
2	B	900	OLP	C5-C4-N9	-2.63	105.03	106.25
2	C	900	OLP	N2-C2-N1	2.60	123.78	120.19
2	C	900	OLP	C8-N7-C5	2.60	108.89	104.26
2	A	900	OLP	N3-C2-N1	-2.58	119.33	123.68
2	C	900	OLP	CAR-CAH-CAQ	2.49	120.91	119.06
2	D	900	OLP	N9-C8-N7	-2.46	108.84	113.40
2	A	900	OLP	N9-C8-N7	-2.40	108.96	113.40
2	B	900	OLP	C8-N7-C5	2.31	108.37	104.26
2	C	900	OLP	CAK-N2-C2	2.24	127.58	123.36
2	D	900	OLP	C5-C4-N9	-2.18	105.24	106.25
2	A	900	OLP	C5-C4-N9	-2.06	105.29	106.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	900	OLP	CAB-CAW-N9-C8
2	D	900	OLP	CAB-CAW-N9-C4
2	A	900	OLP	OAC-CAJ-CAK-N2
2	A	900	OLP	CAB-CAW-N9-C4
2	C	900	OLP	CAB-CAW-N9-C4
2	B	900	OLP	CAB-CAW-N9-C4
2	A	900	OLP	CAB-CAW-N9-C8
2	C	900	OLP	CAB-CAW-N9-C8
2	C	900	OLP	CAH-CAR-N6-C6

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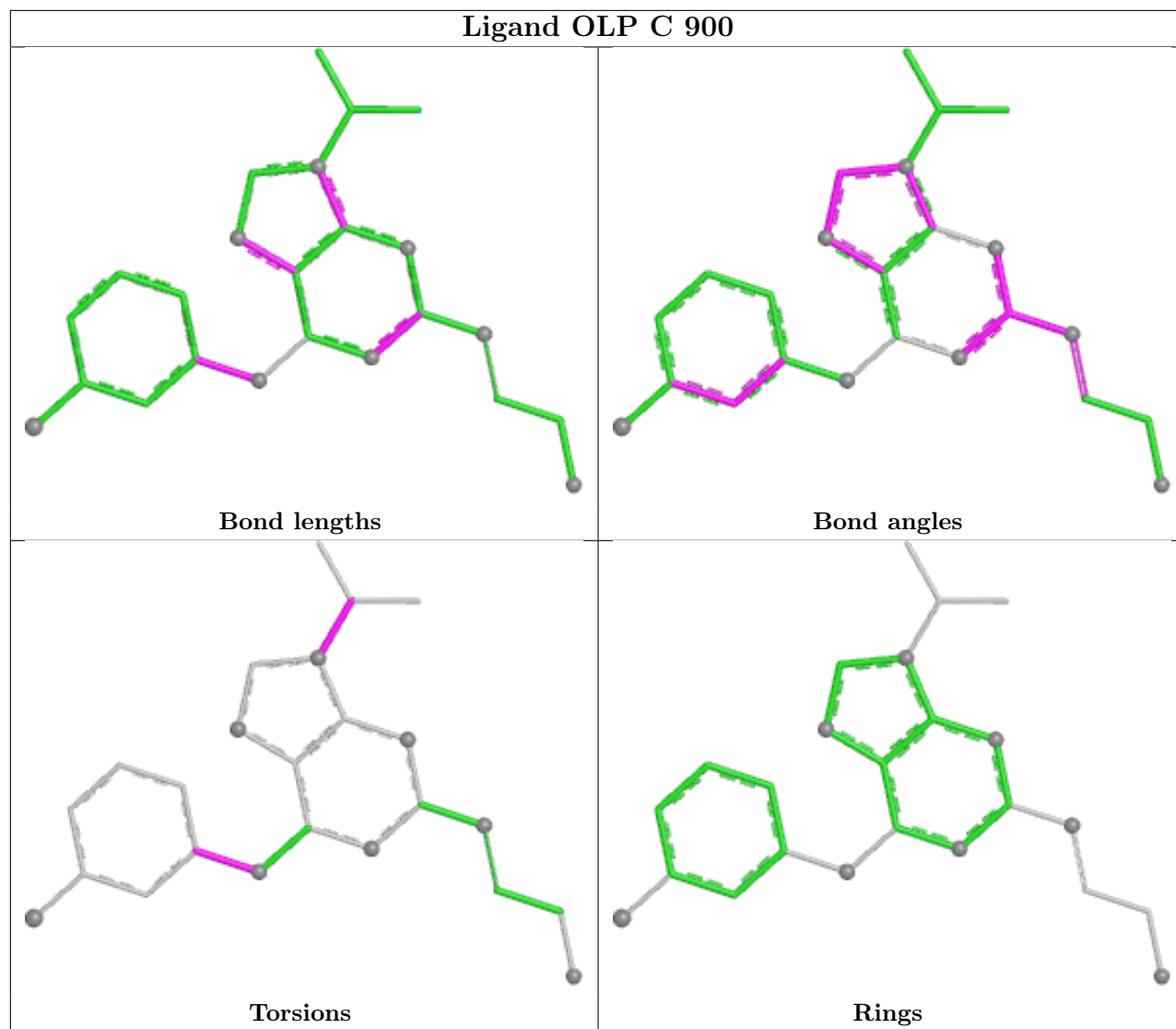
Mol	Chain	Res	Type	Atoms
2	D	900	OLP	CAH-CAR-N6-C6
2	B	900	OLP	OAC-CAJ-CAK-N2
2	C	900	OLP	CAG-CAR-N6-C6
2	B	900	OLP	CAB-CAW-N9-C8
2	A	900	OLP	CAH-CAR-N6-C6
2	D	900	OLP	OAC-CAJ-CAK-N2
2	B	900	OLP	CAH-CAR-N6-C6

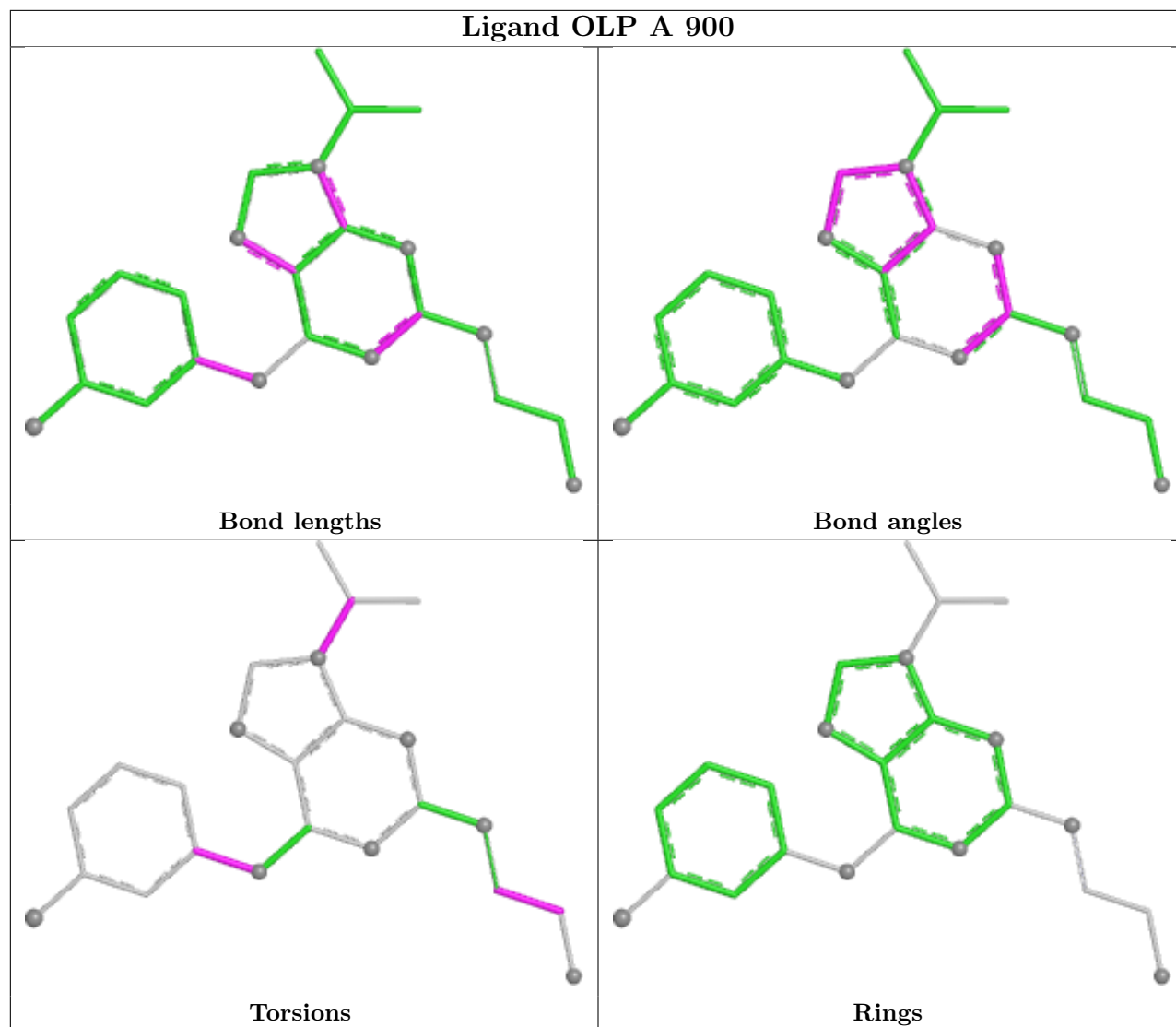
There are no ring outliers.

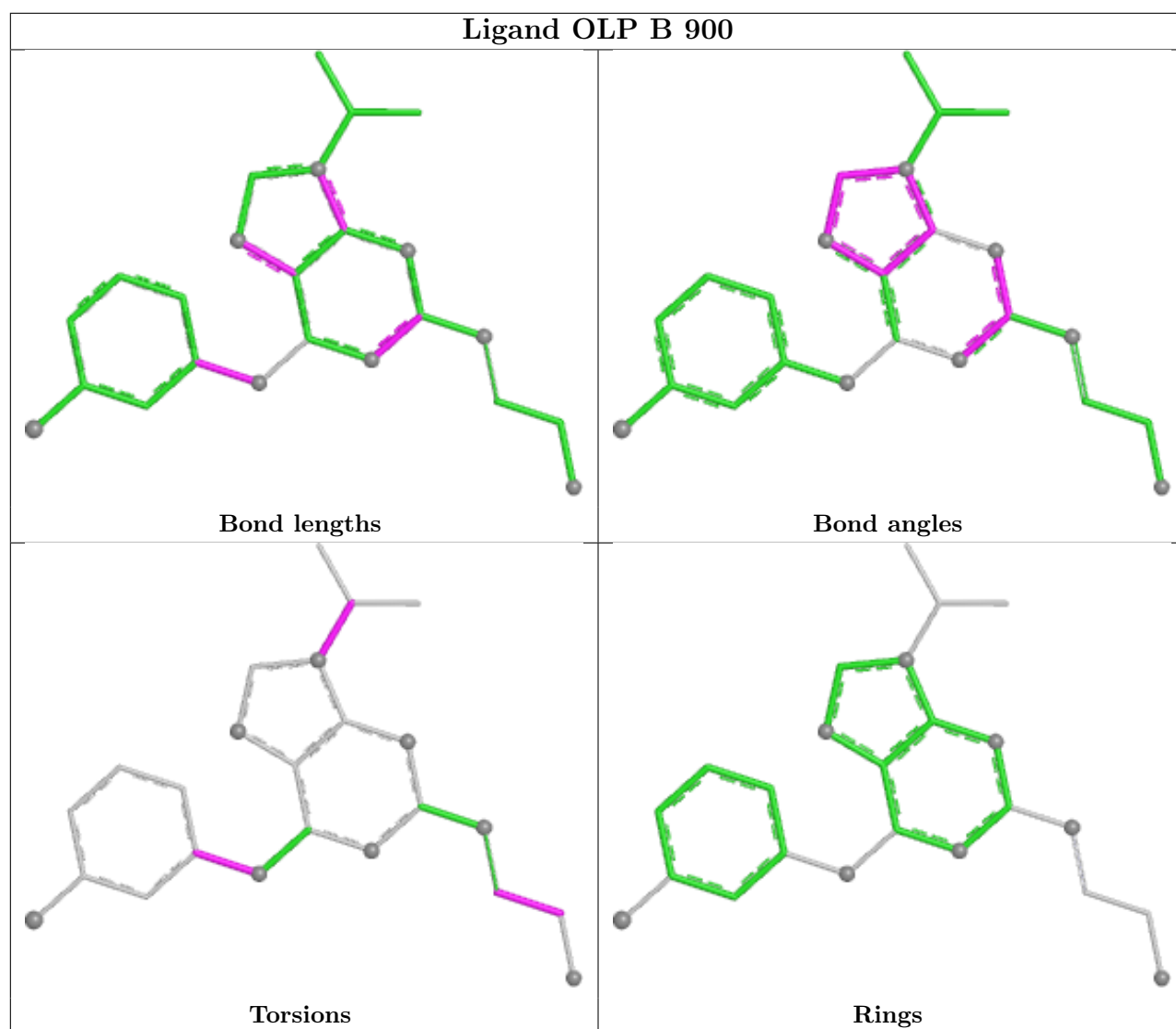
4 monomers are involved in 12 short contacts:

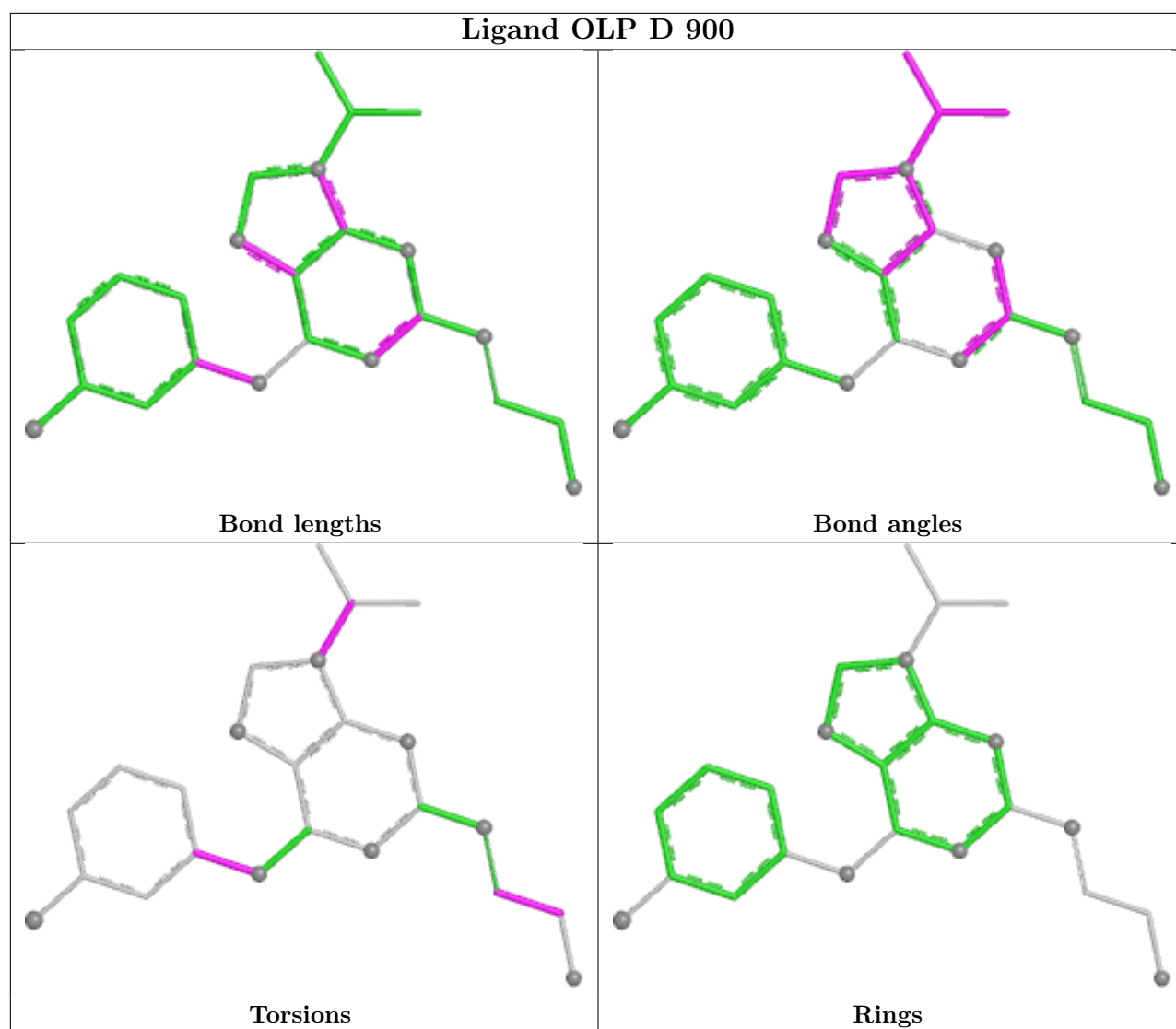
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	OLP	2	0
2	A	900	OLP	4	0
2	B	900	OLP	2	0
2	D	900	OLP	4	0

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%)	0.79	22 (8%)	17 12	25, 58, 90, 117	2 (0%)
1	B	256/313 (81%)	0.73	23 (8%)	15 11	19, 56, 86, 109	2 (0%)
1	C	259/313 (82%)	0.81	24 (9%)	14 10	18, 55, 83, 106	4 (1%)
1	D	259/313 (82%)	0.82	27 (10%)	11 8	22, 56, 89, 133	3 (1%)
All	All	1035/1252 (82%)	0.79	96 (9%)	14 10	18, 56, 88, 133	11 (1%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	ASN	6.1
1	D	575	ASN	6.1
1	D	745	SER	5.5
1	A	661	SER	4.9
1	B	631	ILE	4.5
1	B	745	SER	4.3
1	C	575	ASN	4.2
1	C	744	LEU	4.1
1	B	659	MET	4.0
1	C	743	GLY	4.0
1	C	745	SER	3.9
1	B	623	LEU	3.8
1	C	598	PHE	3.8
1	A	632	GLU	3.7
1	C	633	GLU	3.6
1	C	631	ILE	3.6
1	A	745	SER	3.6
1	B	598	PHE	3.6
1	C	667	PRO	3.4
1	B	621	MET	3.4
1	C	576	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	578	GLU	3.3
1	A	744	LEU	3.3
1	D	744	LEU	3.3
1	A	690	THR	3.2
1	D	622	LYS	3.2
1	A	622	LYS	3.1
1	B	578	GLU	3.1
1	D	632	GLU	3.1
1	D	657	ILE	3.1
1	D	763	PRO	3.0
1	B	667	PRO	3.0
1	A	578	GLU	3.0
1	D	633	GLU	3.0
1	B	744	LEU	2.9
1	C	632	GLU	2.9
1	A	621	MET	2.9
1	C	599	GLY	2.9
1	C	588	ILE	2.9
1	A	597	GLU	2.9
1	B	576	LYS	2.9
1	C	774	ASP	2.9
1	C	763	PRO	2.8
1	A	657	ILE	2.8
1	D	576	LYS	2.8
1	C	578	GLU	2.8
1	D	661	SER	2.8
1	D	636	SER	2.7
1	C	741	ASP	2.7
1	D	631	ILE	2.7
1	A	633	GLU	2.7
1	B	597	GLU	2.7
1	D	619	LYS	2.7
1	B	632	GLU	2.7
1	D	577	LEU	2.6
1	A	579	ASP	2.6
1	C	644	PHE	2.6
1	A	694	HIS	2.6
1	A	659	MET	2.6
1	B	863	ASP	2.6
1	A	743	GLY	2.5
1	A	598	PHE	2.5
1	B	741	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	621	MET	2.5
1	B	634	PHE	2.5
1	D	597	GLU	2.5
1	D	741	ASP	2.4
1	B	769	ILE	2.4
1	A	644	PHE	2.4
1	C	577	LEU	2.4
1	C	657	ILE	2.4
1	D	743	GLY	2.4
1	B	577	LEU	2.4
1	A	631	ILE	2.3
1	B	588	ILE	2.3
1	D	769	ILE	2.3
1	A	763	PRO	2.3
1	A	667	PRO	2.2
1	C	621	MET	2.2
1	C	775	ARG	2.2
1	B	609	GLU	2.2
1	C	769	ILE	2.2
1	C	634	PHE	2.2
1	B	582	ILE	2.1
1	D	587	LEU	2.1
1	D	826	LEU	2.1
1	D	690	THR	2.1
1	D	764	VAL	2.1
1	B	743	GLY	2.1
1	D	596	GLY	2.0
1	B	774	ASP	2.0
1	C	863	ASP	2.0
1	D	588	ILE	2.0
1	B	608	GLN	2.0
1	A	774	ASP	2.0
1	D	659	MET	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](#)

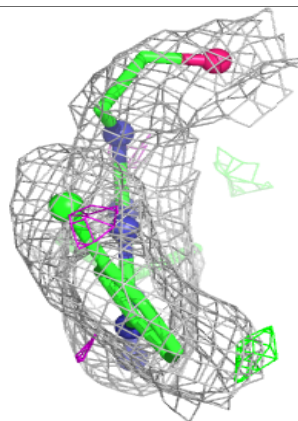
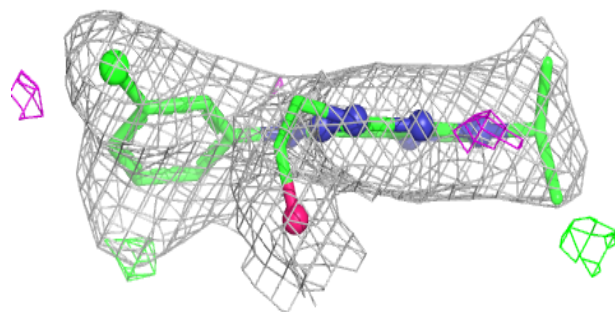
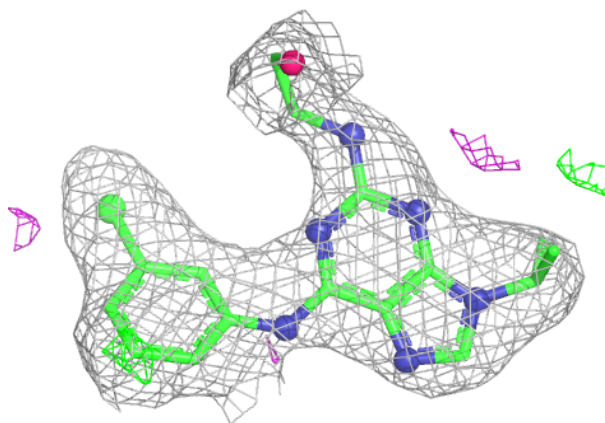
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
2	OLP	B	900	24/24	0.85	0.15	49,53,57,59	0
2	OLP	C	900	24/24	0.85	0.15	47,52,56,59	0
2	OLP	D	900	24/24	0.87	0.14	44,52,58,62	0
2	OLP	A	900	24/24	0.90	0.12	46,49,53,57	0
3	NA	B	1	1/1	0.95	0.12	35,35,35,35	0
4	CL	C	133	1/1	0.98	0.07	43,43,43,43	0
4	CL	D	134	1/1	0.99	0.03	32,32,32,32	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.

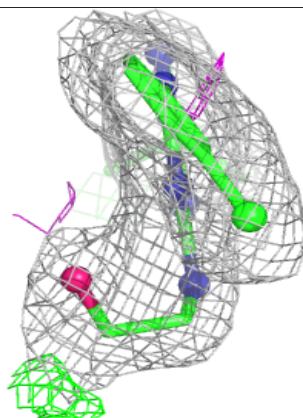
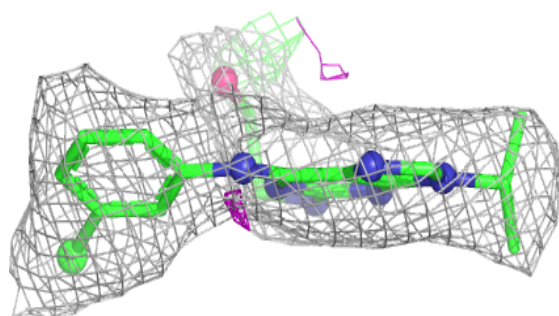
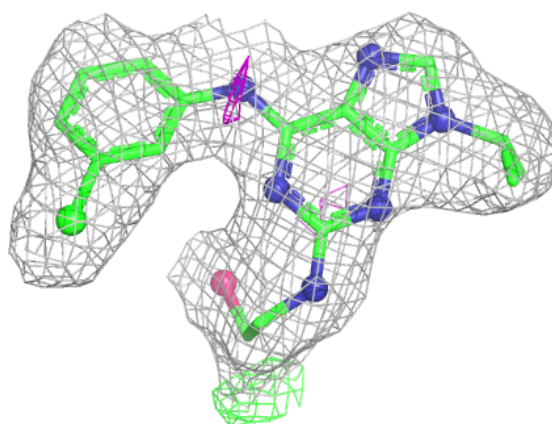
Electron density around OLP B 900:

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

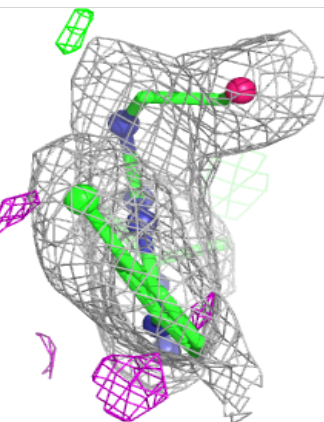
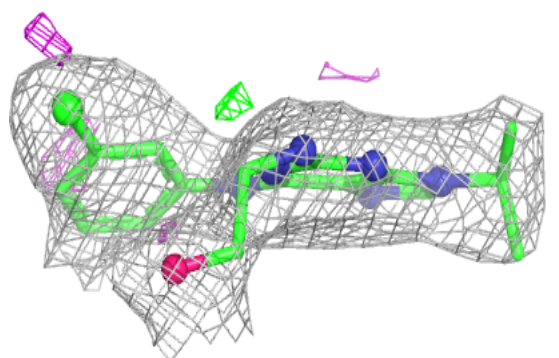
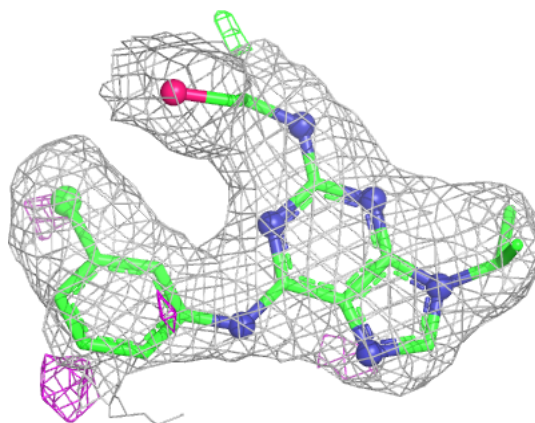


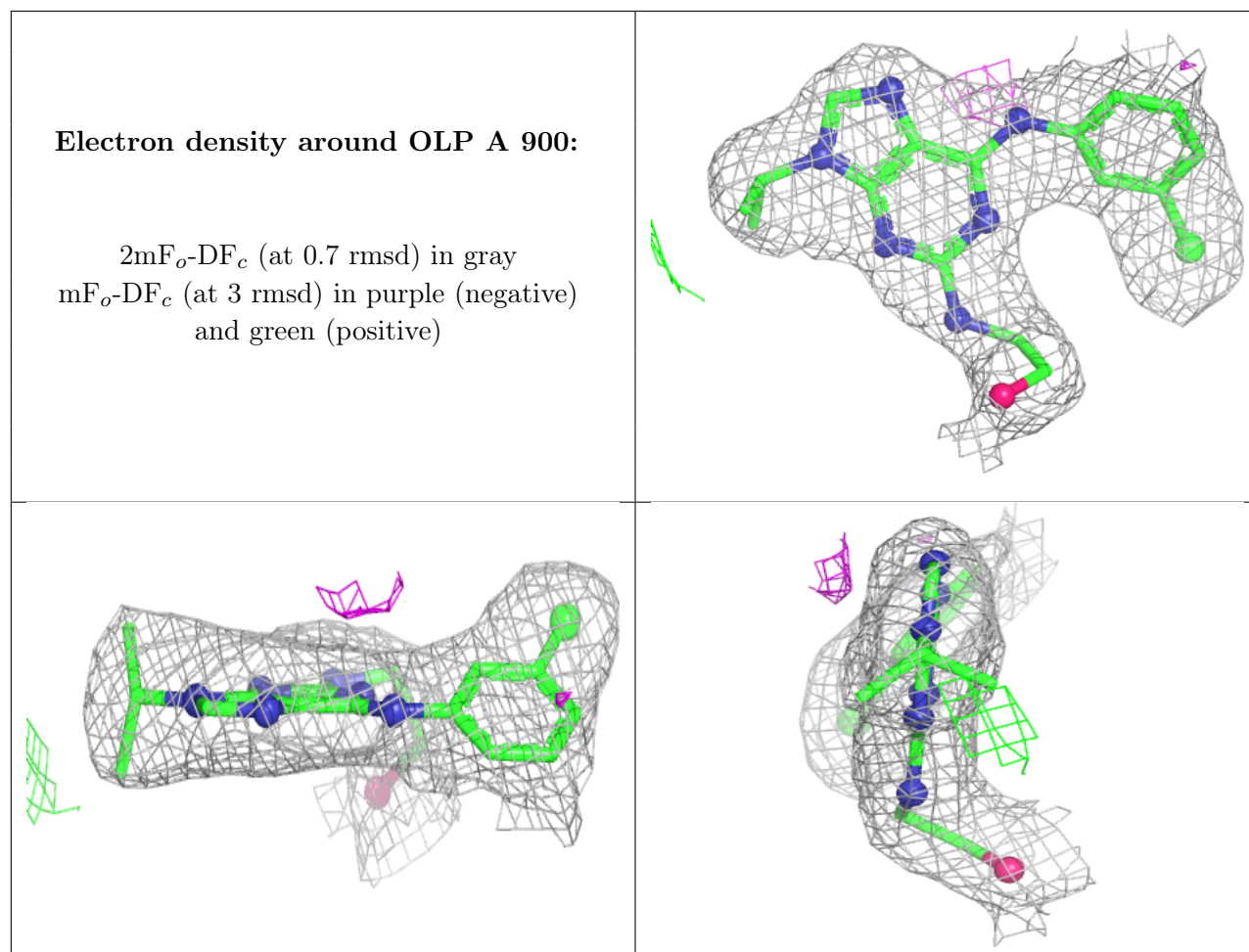
Electron density around OLP C 900:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.