



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 3G6O / pdb_00003g6o
Title : Crystal structure of P. aeruginosa bacteriophytochrome PaBphP photosensory core domain mutant Q188L
Authors : Yang, X.; Kuk, J.; Moffat, K.
Deposited on : 2009-02-07
Resolution : 2.85 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 ⓘ](#)) 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

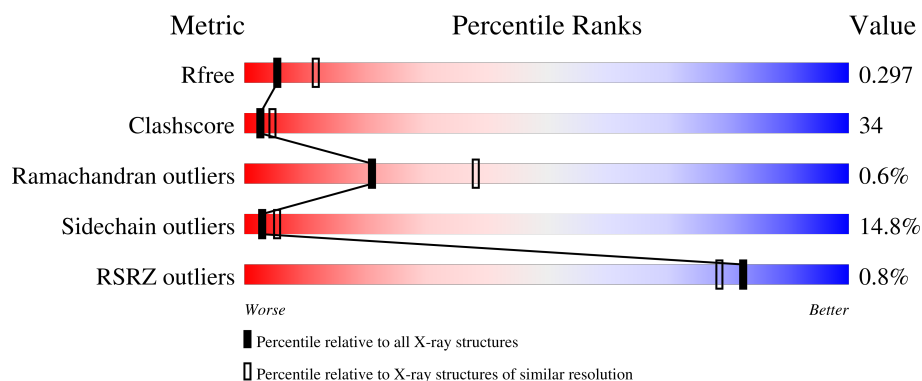
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	505	% 41% 39% 10% 10%
1	B	505	% 44% 39% 7% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7512 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.

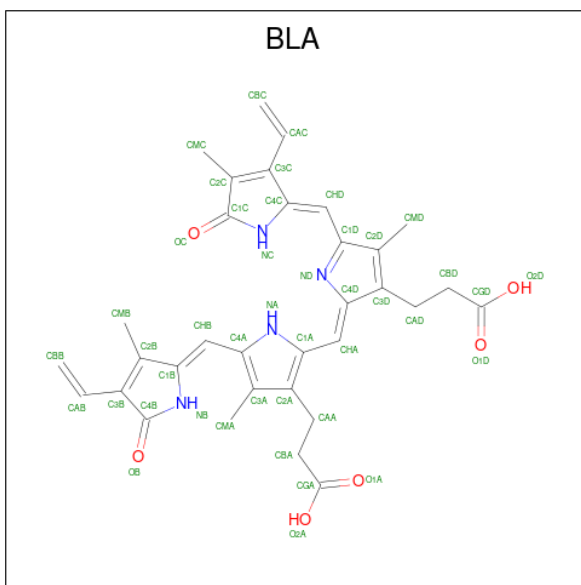
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	6	0
			3666	2313	653	680	20			
1	B	457	Total	C	N	O	S	0	7	0
			3672	2316	654	682	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	GLN	engineered mutation	UNP Q9HWR3
A	498	LEU	-	expression tag	UNP Q9HWR3
A	499	GLU	-	expression tag	UNP Q9HWR3
A	500	HIS	-	expression tag	UNP Q9HWR3
A	501	HIS	-	expression tag	UNP Q9HWR3
A	502	HIS	-	expression tag	UNP Q9HWR3
A	503	HIS	-	expression tag	UNP Q9HWR3
A	504	HIS	-	expression tag	UNP Q9HWR3
A	505	HIS	-	expression tag	UNP Q9HWR3
B	188	LEU	GLN	engineered mutation	UNP Q9HWR3
B	498	LEU	-	expression tag	UNP Q9HWR3
B	499	GLU	-	expression tag	UNP Q9HWR3
B	500	HIS	-	expression tag	UNP Q9HWR3
B	501	HIS	-	expression tag	UNP Q9HWR3
B	502	HIS	-	expression tag	UNP Q9HWR3
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 86	C 66	N 8	O 12	0	1
2	B	1	Total 86	C 66	N 8	O 12	0	1

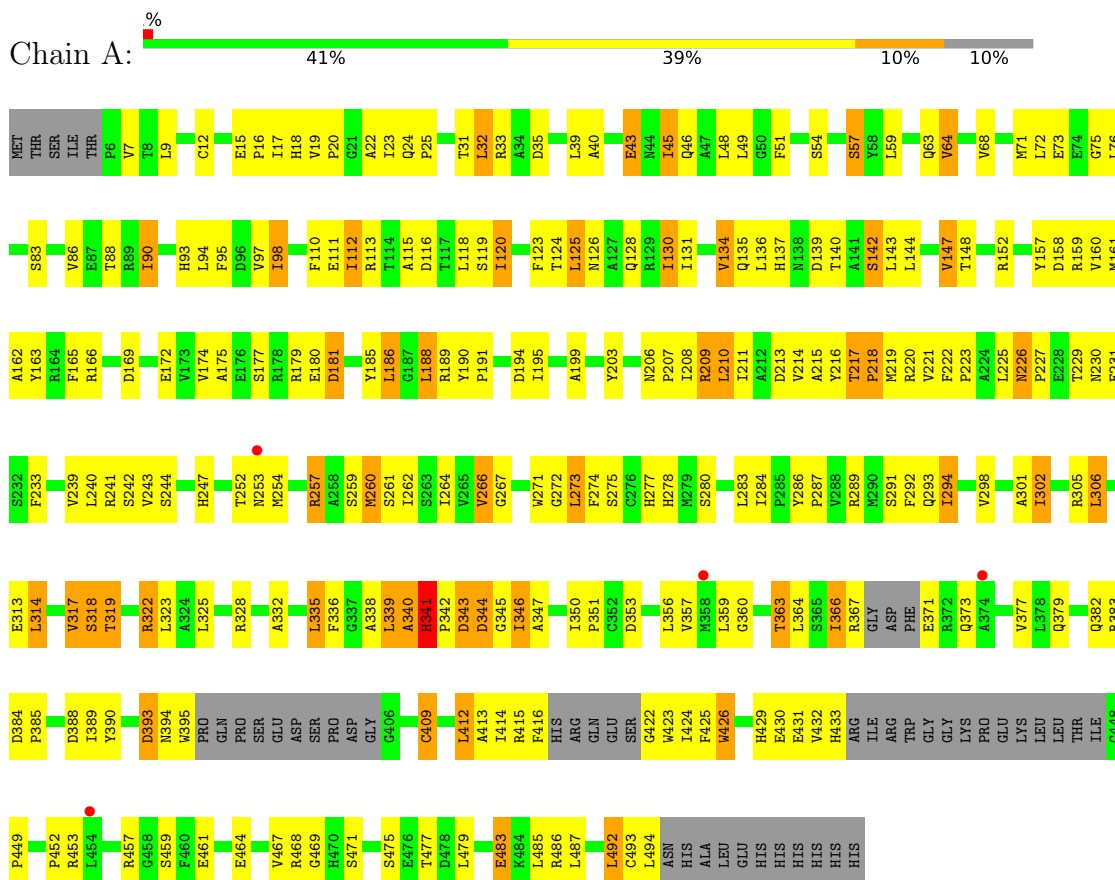
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

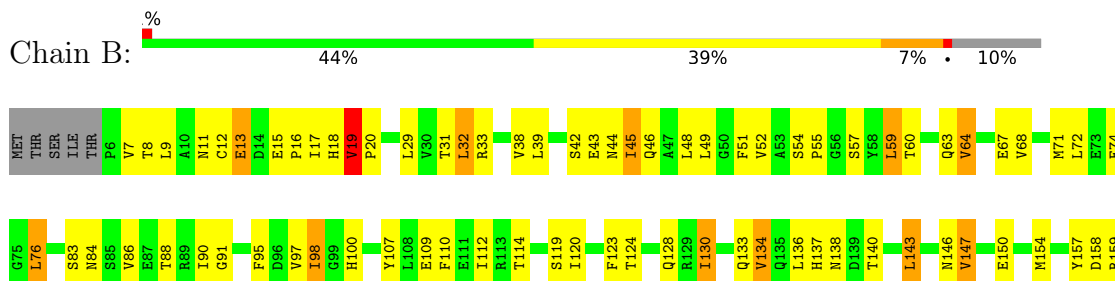
3 Residue-property plots

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: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome



V160	M161	A162	Y163	R164	E172	V173	V174	A175	S177	R178	R179	E180	D181	L182	Y185	L186	G187	L188	R189	Y190	D194	I195	Q198	A199	R200	R201	L202	Y203	N206	P207	I208	R209	L210	I211	A212	D213	V214	A215	Y216	T217	P218	M219	R220	V221	F222	P223	N226	T229	N230	E231	S232					
F233	D234	L235	S236	Y237	S238	V239	L240	R241	N253	M254	G255	V256	R257	S259	M260	S261	I262	S263	I264	V265	V266	W271	G272	L273	F274	S275	C276	H277	H278	M279	S280	P281	I284	P285	Y286	P287	V288	R289	M290	S291	F292	Q293	F294	F295	S296	Q297	V298	I302	R305	L306	E313					
V317	S318	T319	E320	R321	R322	L323	A324	R328	A329	R330	L339	A340	H341	P342	D343	D344	G345	I346	G354	A355	L356	V357	M358	L359	G360	I366	R367	GLY	ASP	PHE	E371	R372	Q373	N376	V377	L378	Q379	R380	L381	Q382	D388	I389	Y390	H391	T392	D393	N394	W395	PRO	GLN	PRO	SER	GLU			
ASP	SER	PRO	ASP	GLY	G406	C409	G410	V411	L412	A413	T414	R415	F416	HIS	ARG	GLN	GLU	SER	G422	W423	I424	HIS	F425	W426	E430	E431	W432	W433	ARG	ILE	ARG	TRP	GLY	GLY	LYS	PRO	PRO	GLU	LYS	LEU	LEU	THR	ILE	G448	P449	L454	T455	W463	V466	V467	R468	C469	H470	S471	T472	P473
W474	E483	K484	L485	R486	L487	D488	L489	W490	E491	L492	C493	L494	ASN	HIS	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	E430	E431	W432	W433	ARG	ILE	ARG	TRP	GLY	GLY	LYS	PRO	PRO	GLU	LYS	LEU	LEU	THR	ILE	G448	P449	L454	T455	W463	V466	V467	R468	C469	H470	S471	T472	P473

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	109.79Å 109.79Å 189.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.47 – 2.85 42.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	82.8 (42.47-2.85) 82.8 (42.47-2.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.229 , 0.298 0.224 , 0.297	Depositor DCC
R_{free} test set	1331 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: BLA

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	0/3746	0.92	9/5083 (0.2%)
1	B	0.41	0/3752	0.90	10/5091 (0.2%)
All	All	0.42	0/7498	0.91	19/10174 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	THR	CA-C-N	8.87	130.93	119.84
1	B	217	THR	C-N-CA	8.87	130.93	119.84
1	B	226	ASN	CA-C-N	7.90	128.33	119.32
1	B	226	ASN	C-N-CA	7.90	128.33	119.32
1	B	236	SER	N-CA-C	-7.31	100.41	110.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	LEU	Peptide
1	A	341	HIS	Peptide
1	A	90	ILE	Peptide

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	3666	0	3592	254	0
1	B	3672	0	3596	245	0
2	A	86	0	62	17	0
2	B	86	0	62	20	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
All	All	7512	0	7312	505	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 34.

The worst 5 of 505 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:209[A]:ARG:HH11	1:A:209[A]:ARG:HG2	1.21	1.04
1:A:194:ASP:HB3	2:A:900[A]:BLA:HHB	1.45	0.97
2:A:900[A]:BLA:HMA2	2:A:900[A]:BLA:HMB2	1.47	0.96
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.48	0.95
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.34	0.93

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	453/505 (90%)	415 (92%)	35 (8%)	3 (1%)	18 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	454/505 (90%)	411 (90%)	41 (9%)	2 (0%)	30	48
All	All	907/1010 (90%)	826 (91%)	76 (8%)	5 (1%)	21	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	LEU
1	A	341	HIS
1	A	218	PRO
1	A	452	PRO
1	B	342	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	394/431 (91%)	327 (83%)	67 (17%)	2	3
1	B	395/431 (92%)	346 (88%)	49 (12%)	4	8
All	All	789/862 (92%)	673 (85%)	116 (15%)	3	5

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	CYS
1	B	468	ARG
1	B	59	LEU
1	B	455	THR
1	B	319	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	HIS

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	433	HIS
1	B	308	GLN
1	A	138	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	$\# Z > 2$
2	BLA	A	900[B]	1	46,46,46	2.55	19 (41%)	66,67,67	1.54	12 (18%)
2	BLA	A	900[A]	1	46,46,46	2.60	18 (39%)	66,67,67	1.44	12 (18%)
2	BLA	B	900[B]	1	46,46,46	2.63	18 (39%)	66,67,67	1.35	7 (10%)
2	BLA	B	900[A]	1	46,46,46	2.60	19 (41%)	66,67,67	1.54	13 (19%)

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	BLA	A	900[B]	1	-	6/26/74/74	0/4/4/4
2	BLA	A	900[A]	1	-	9/26/74/74	0/4/4/4
2	BLA	B	900[B]	1	-	6/26/74/74	0/4/4/4
2	BLA	B	900[A]	1	-	9/26/74/74	0/4/4/4

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900[A]	BLA	CHD-C4C	6.57	1.53	1.37
2	B	900[B]	BLA	CHD-C4C	6.51	1.53	1.37
2	A	900[A]	BLA	CHD-C4C	6.50	1.53	1.37
2	A	900[A]	BLA	CHB-C1B	6.48	1.53	1.37
2	A	900[B]	BLA	CHD-C4C	6.36	1.53	1.37

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[B]	BLA	C4C-CHD-C1D	-5.08	115.57	128.06
2	A	900[B]	BLA	CHA-C4D-ND	3.73	132.43	124.60
2	B	900[B]	BLA	CHA-C4D-ND	3.70	132.36	124.60
2	A	900[A]	BLA	CMB-C2B-C1B	3.57	128.51	124.16
2	B	900[A]	BLA	C4C-CHD-C1D	-3.38	119.75	128.06

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

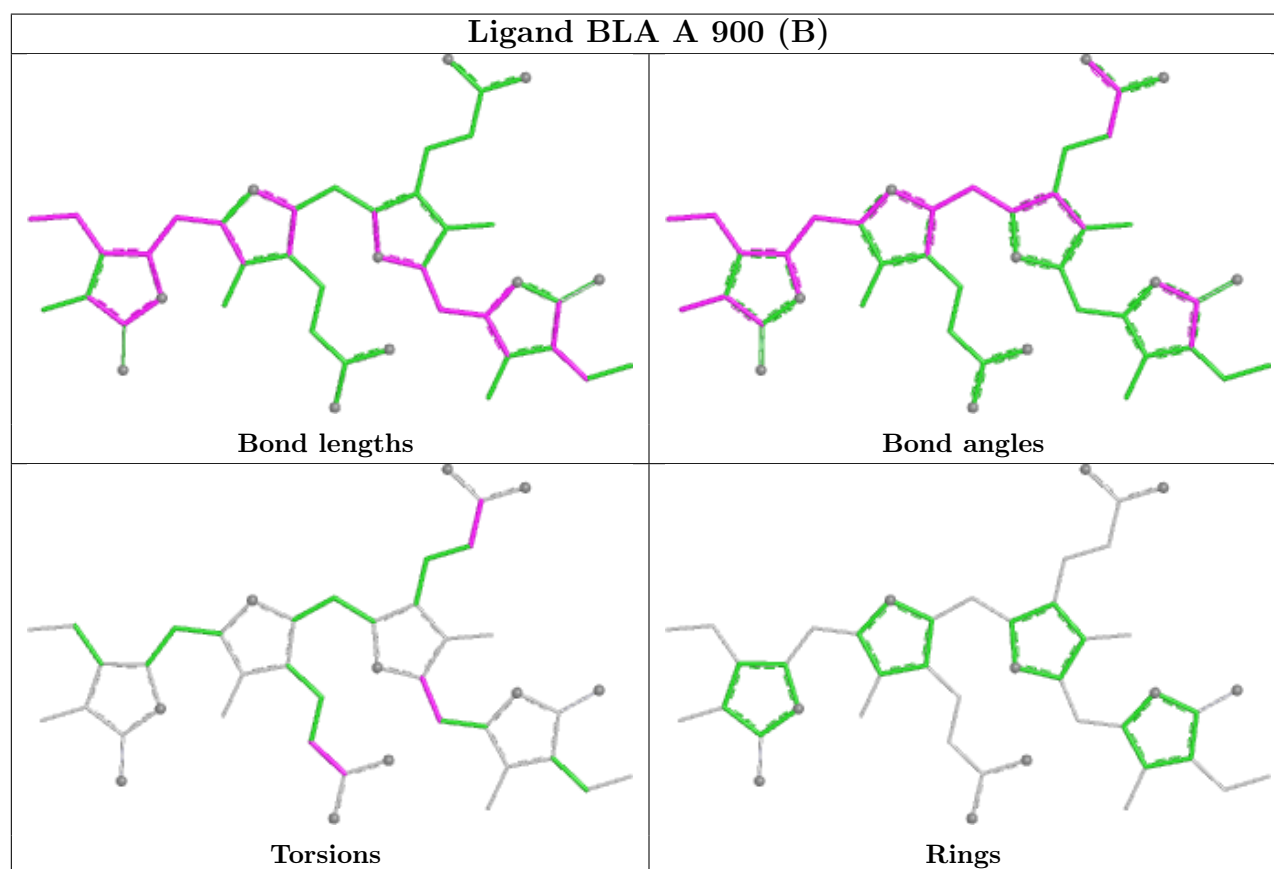
Mol	Chain	Res	Type	Atoms
2	B	900[A]	BLA	NB-C1B-CHB-C4A
2	B	900[A]	BLA	C2B-C1B-CHB-C4A
2	B	900[A]	BLA	NA-C4A-CHB-C1B
2	B	900[B]	BLA	NA-C4A-CHB-C1B
2	A	900[A]	BLA	C3A-C4A-CHB-C1B

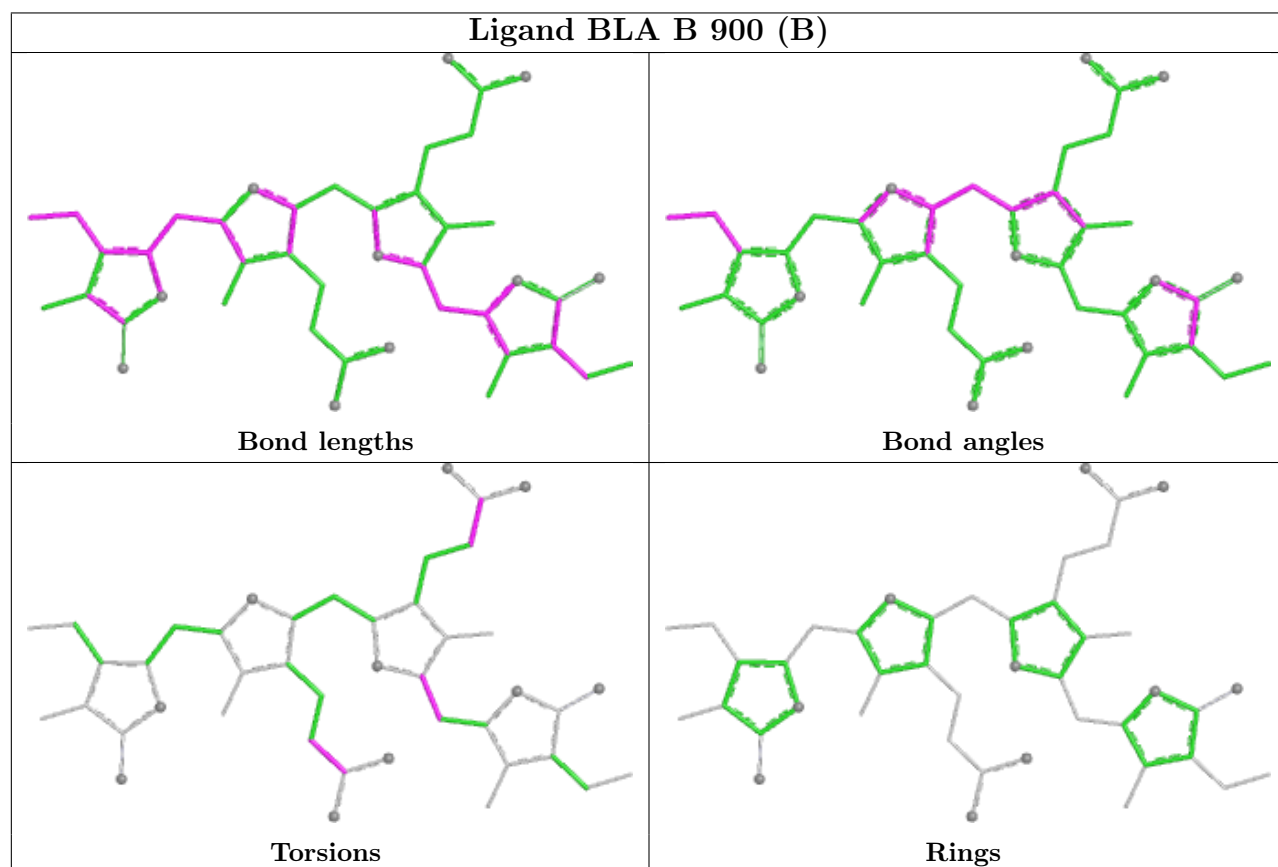
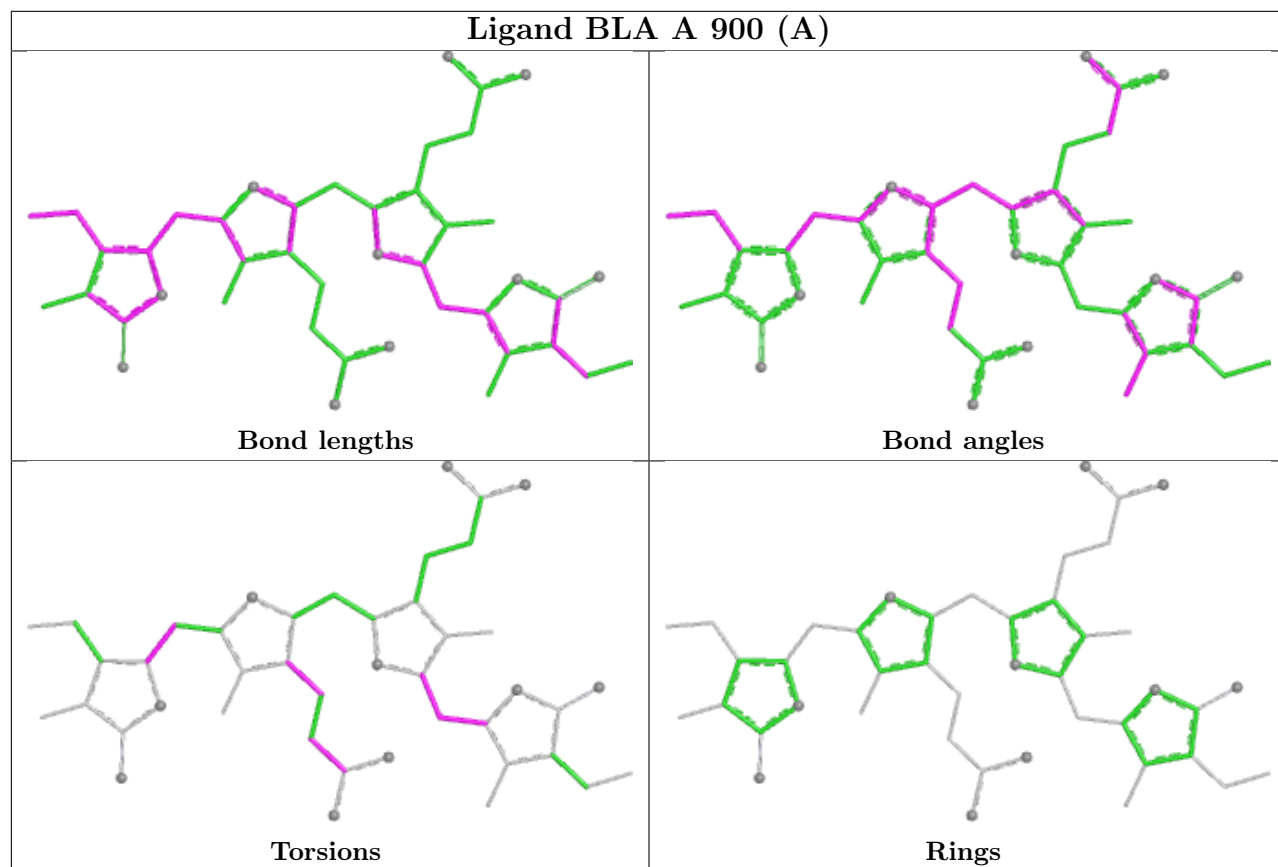
There are no ring outliers.

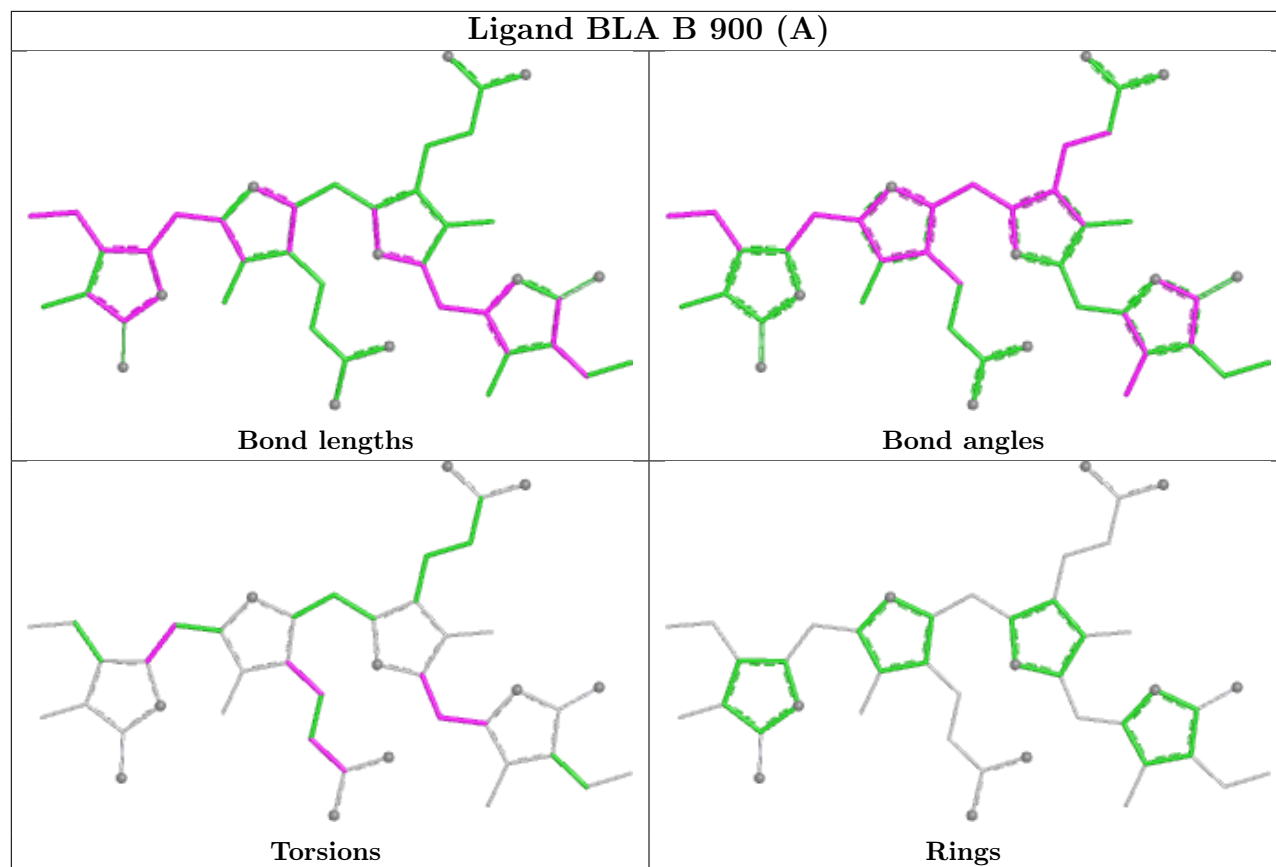
4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900[B]	BLA	8	0
2	A	900[A]	BLA	9	0
2	B	900[B]	BLA	13	0
2	B	900[A]	BLA	7	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/505 (90%)	-0.47	4 (0%) 81 76	44, 119, 216, 317	6 (1%)
1	B	457/505 (90%)	-0.49	3 (0%) 84 80	43, 118, 230, 373	7 (1%)
All	All	914/1010 (90%)	-0.48	7 (0%) 82 78	43, 119, 222, 373	13 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	ALA	5.2
1	B	425	PHE	3.0
1	B	356	LEU	2.9
1	A	358	MET	2.8
1	A	253	ASN	2.7

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](#)

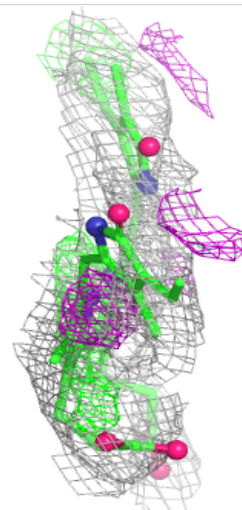
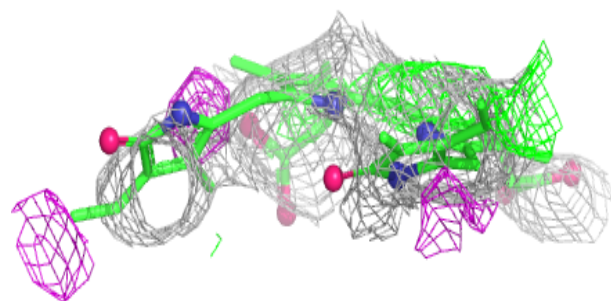
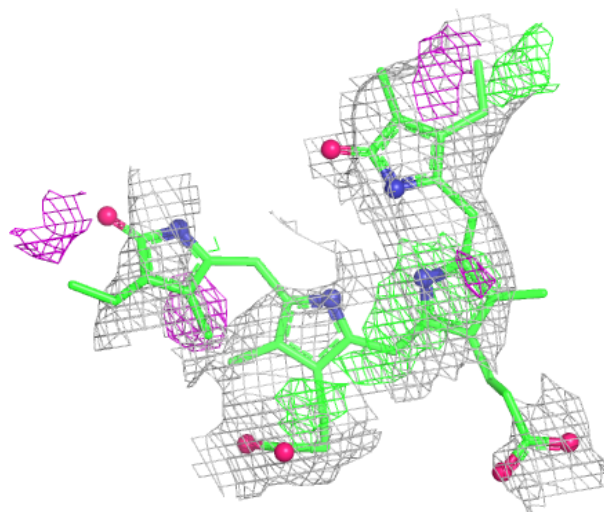
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	BLA	A	900[A]	43/43	0.97	0.12	92,130,170,177	43
2	BLA	A	900[B]	43/43	0.97	0.12	85,127,170,173	43
2	BLA	B	900[A]	43/43	0.98	0.12	85,123,149,164	43
2	BLA	B	900[B]	43/43	0.98	0.12	79,114,146,176	43

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.

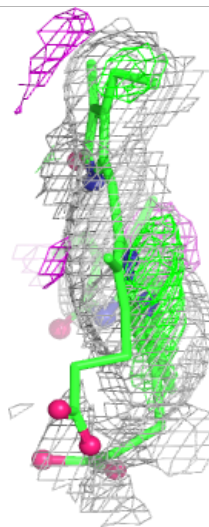
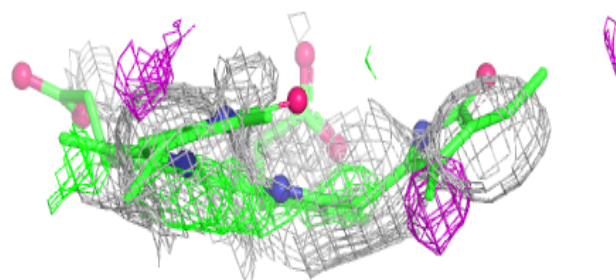
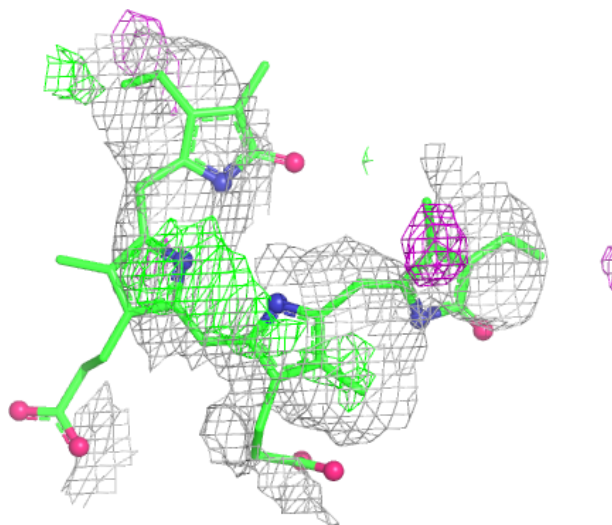
Electron density around BLA A 900 (A):

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



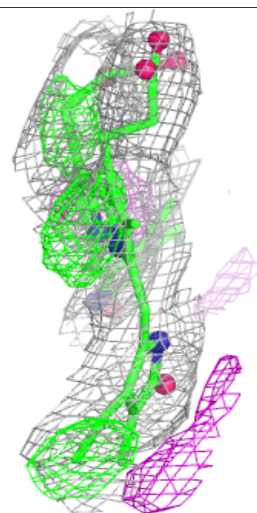
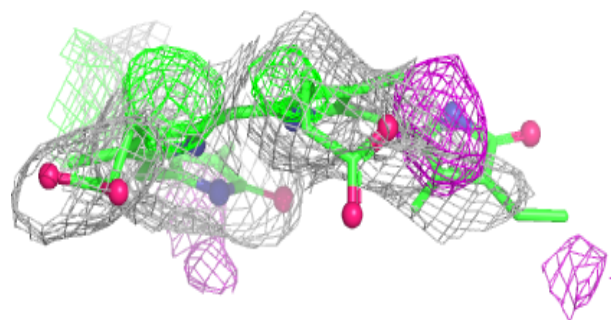
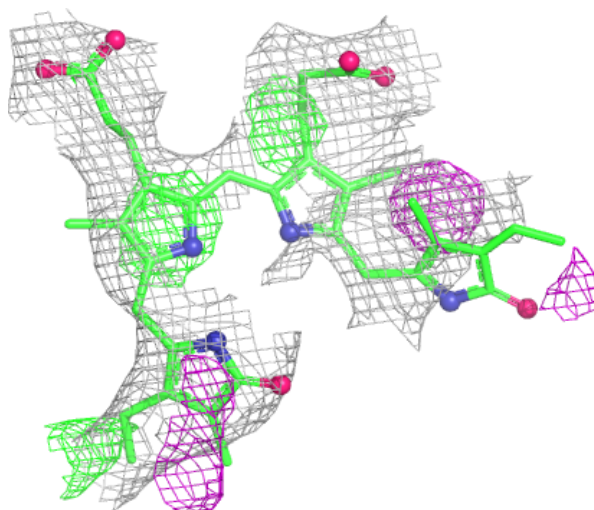
Electron density around BLA A 900 (B):

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



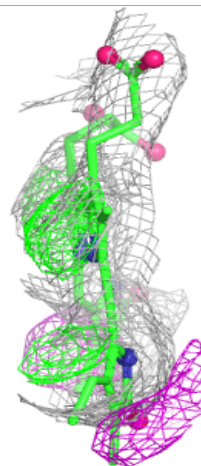
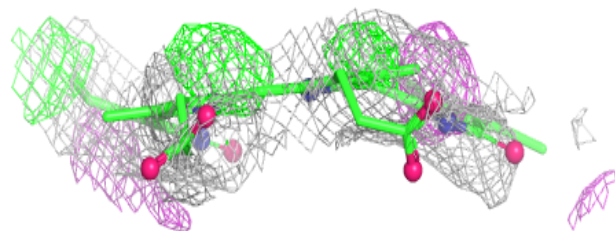
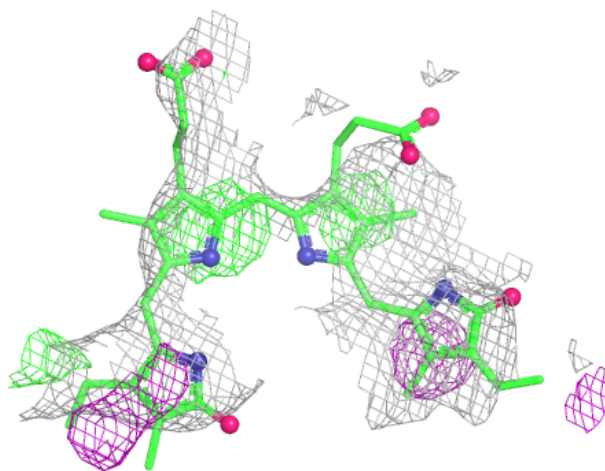
Electron density around BLA B 900 (A):

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



Electron density around BLA B 900 (B):

$2mF_o-DF_c$ (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.