



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:28 PM UTC

PDB ID : 6HRK / pdb_00006hrk
Title : Structure of a far-red fluorescent biliprotein derived from a far-red induced allophycocyanin F subunit from a thermophilic cyanobacterium *Chroococcidiopsis thermalis*
Authors : Hou, Y.-N.; Hoepfner, A.; Ding, W.-L.; Gaertner, W.; Zhao, K.-H.
Deposited on : 2018-09-27
Resolution : 2.52 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 ⓘ](#)) 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

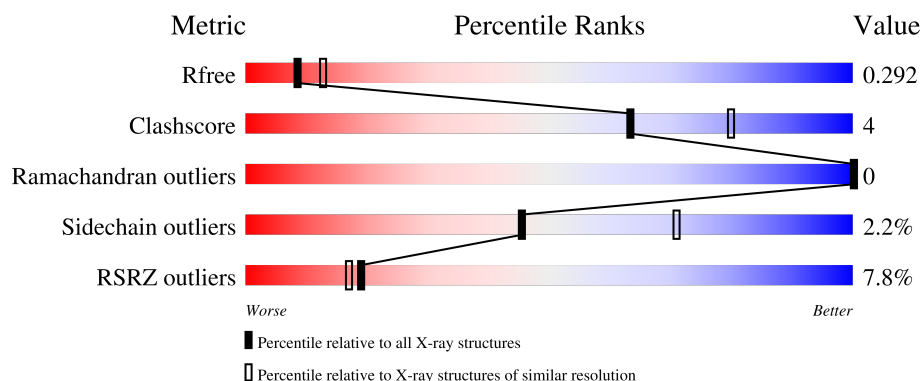
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

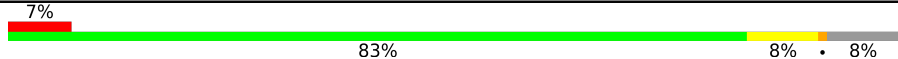
The reported resolution of this entry is 2.52 Å.

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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	147	
1	B	147	
1	C	147	
1	D	147	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4251 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 Allophycocyanin beta-18 subunit apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1005	641	169	185	10			
1	B	135	Total	C	N	O	S	0	0	0
			1019	648	174	187	10			
1	C	135	Total	C	N	O	S	0	0	0
			1023	648	177	188	10			
1	D	135	Total	C	N	O	S	0	0	0
			1032	654	177	191	10			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	LEU	engineered mutation	UNP K9TY40
A	46	THR	SER	engineered mutation	UNP K9TY40
A	51	VAL	ILE	engineered mutation	UNP K9TY40
A	58	GLN	LEU	engineered mutation	UNP K9TY40
A	68	ARG	SER	engineered mutation	UNP K9TY40
A	72	CYS	ASN	engineered mutation	UNP K9TY40
A	82	CYS	TYR	engineered mutation	UNP K9TY40
A	92	MET	TYR	engineered mutation	UNP K9TY40
A	101	GLY	ASP	engineered mutation	UNP K9TY40
A	109	MET	LEU	engineered mutation	UNP K9TY40
A	113	PHE	LEU	engineered mutation	UNP K9TY40
A	125	CYS	GLY	engineered mutation	UNP K9TY40
A	136	LYS	ASN	engineered mutation	UNP K9TY40
A	143	ALA	VAL	engineered mutation	UNP K9TY40
A	151	ALA	THR	engineered mutation	UNP K9TY40
A	160	ILE	VAL	engineered mutation	UNP K9TY40
A	161	ALA	VAL	engineered mutation	UNP K9TY40
A	163	VAL	GLU	engineered mutation	UNP K9TY40
A	170	LEU	-	expression tag	UNP K9TY40
A	171	GLU	-	expression tag	UNP K9TY40
A	172	HIS	-	expression tag	UNP K9TY40

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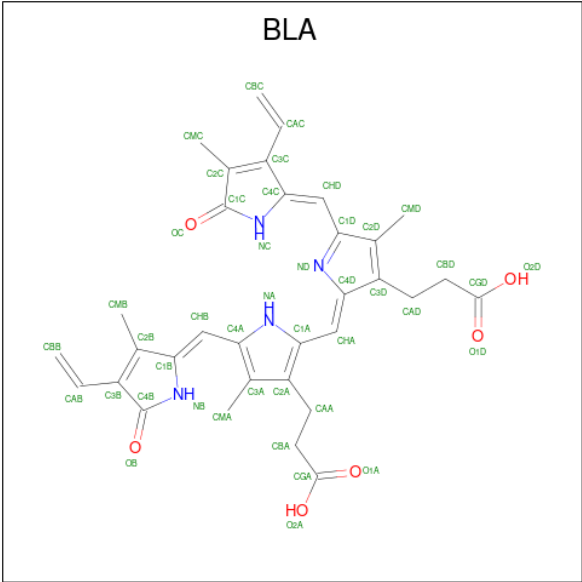
Chain	Residue	Modelled	Actual	Comment	Reference
A	173	HIS	-	expression tag	UNP K9TY40
A	174	HIS	-	expression tag	UNP K9TY40
A	175	HIS	-	expression tag	UNP K9TY40
A	176	HIS	-	expression tag	UNP K9TY40
A	177	HIS	-	expression tag	UNP K9TY40
B	31	MET	LEU	engineered mutation	UNP K9TY40
B	46	THR	SER	engineered mutation	UNP K9TY40
B	51	VAL	ILE	engineered mutation	UNP K9TY40
B	58	GLN	LEU	engineered mutation	UNP K9TY40
B	68	ARG	SER	engineered mutation	UNP K9TY40
B	72	CYS	ASN	engineered mutation	UNP K9TY40
B	82	CYS	TYR	engineered mutation	UNP K9TY40
B	92	MET	TYR	engineered mutation	UNP K9TY40
B	101	GLY	ASP	engineered mutation	UNP K9TY40
B	109	MET	LEU	engineered mutation	UNP K9TY40
B	113	PHE	LEU	engineered mutation	UNP K9TY40
B	125	CYS	GLY	engineered mutation	UNP K9TY40
B	136	LYS	ASN	engineered mutation	UNP K9TY40
B	143	ALA	VAL	engineered mutation	UNP K9TY40
B	151	ALA	THR	engineered mutation	UNP K9TY40
B	160	ILE	VAL	engineered mutation	UNP K9TY40
B	161	ALA	VAL	engineered mutation	UNP K9TY40
B	163	VAL	GLU	engineered mutation	UNP K9TY40
B	170	LEU	-	expression tag	UNP K9TY40
B	171	GLU	-	expression tag	UNP K9TY40
B	172	HIS	-	expression tag	UNP K9TY40
B	173	HIS	-	expression tag	UNP K9TY40
B	174	HIS	-	expression tag	UNP K9TY40
B	175	HIS	-	expression tag	UNP K9TY40
B	176	HIS	-	expression tag	UNP K9TY40
B	177	HIS	-	expression tag	UNP K9TY40
C	31	MET	LEU	engineered mutation	UNP K9TY40
C	46	THR	SER	engineered mutation	UNP K9TY40
C	51	VAL	ILE	engineered mutation	UNP K9TY40
C	58	GLN	LEU	engineered mutation	UNP K9TY40
C	68	ARG	SER	engineered mutation	UNP K9TY40
C	72	CYS	ASN	engineered mutation	UNP K9TY40
C	82	CYS	TYR	engineered mutation	UNP K9TY40
C	92	MET	TYR	engineered mutation	UNP K9TY40
C	101	GLY	ASP	engineered mutation	UNP K9TY40
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C	113	PHE	LEU	engineered mutation	UNP K9TY40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	125	CYS	GLY	engineered mutation	UNP K9TY40
C	136	LYS	ASN	engineered mutation	UNP K9TY40
C	143	ALA	VAL	engineered mutation	UNP K9TY40
C	151	ALA	THR	engineered mutation	UNP K9TY40
C	160	ILE	VAL	engineered mutation	UNP K9TY40
C	161	ALA	VAL	engineered mutation	UNP K9TY40
C	163	VAL	GLU	engineered mutation	UNP K9TY40
C	170	LEU	-	expression tag	UNP K9TY40
C	171	GLU	-	expression tag	UNP K9TY40
C	172	HIS	-	expression tag	UNP K9TY40
C	173	HIS	-	expression tag	UNP K9TY40
C	174	HIS	-	expression tag	UNP K9TY40
C	175	HIS	-	expression tag	UNP K9TY40
C	176	HIS	-	expression tag	UNP K9TY40
C	177	HIS	-	expression tag	UNP K9TY40
D	31	MET	LEU	engineered mutation	UNP K9TY40
D	46	THR	SER	engineered mutation	UNP K9TY40
D	51	VAL	ILE	engineered mutation	UNP K9TY40
D	58	GLN	LEU	engineered mutation	UNP K9TY40
D	68	ARG	SER	engineered mutation	UNP K9TY40
D	72	CYS	ASN	engineered mutation	UNP K9TY40
D	82	CYS	TYR	engineered mutation	UNP K9TY40
D	92	MET	TYR	engineered mutation	UNP K9TY40
D	101	GLY	ASP	engineered mutation	UNP K9TY40
D	109	MET	LEU	engineered mutation	UNP K9TY40
D	113	PHE	LEU	engineered mutation	UNP K9TY40
D	125	CYS	GLY	engineered mutation	UNP K9TY40
D	136	LYS	ASN	engineered mutation	UNP K9TY40
D	143	ALA	VAL	engineered mutation	UNP K9TY40
D	151	ALA	THR	engineered mutation	UNP K9TY40
D	160	ILE	VAL	engineered mutation	UNP K9TY40
D	161	ALA	VAL	engineered mutation	UNP K9TY40
D	163	VAL	GLU	engineered mutation	UNP K9TY40
D	170	LEU	-	expression tag	UNP K9TY40
D	171	GLU	-	expression tag	UNP K9TY40
D	172	HIS	-	expression tag	UNP K9TY40
D	173	HIS	-	expression tag	UNP K9TY40
D	174	HIS	-	expression tag	UNP K9TY40
D	175	HIS	-	expression tag	UNP K9TY40
D	176	HIS	-	expression tag	UNP K9TY40
D	177	HIS	-	expression tag	UNP K9TY40

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

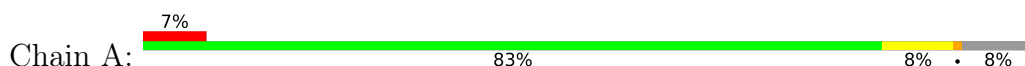


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		

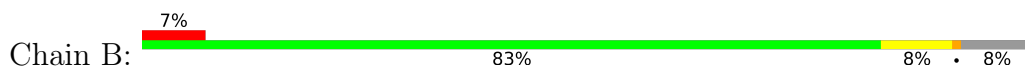
3 Residue-property plots [i](#)

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.

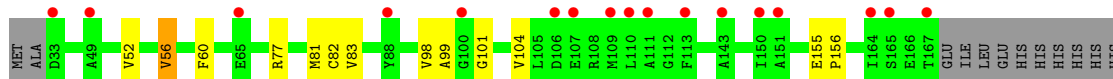
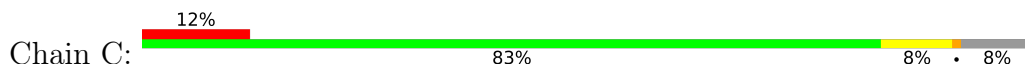
- Molecule 1: Allophycocyanin beta-18 subunit apoprotein



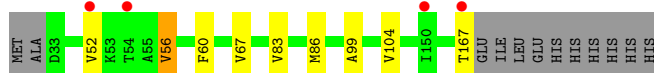
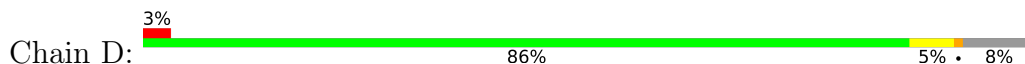
- Molecule 1: Allophycocyanin beta-18 subunit apoprotein



- Molecule 1: Allophycocyanin beta-18 subunit apoprotein



- Molecule 1: Allophycocyanin beta-18 subunit apoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.25Å 74.82Å 61.03Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	47.39 – 2.52 47.39 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.5 (47.39-2.52) 92.6 (47.39-2.52)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.274 , 0.332 0.240 , 0.292	Depositor DCC
R_{free} test set	870 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 18.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.024 for -h,-k,l 0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4251	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/1021	0.92	0/1383
1	B	0.60	0/1035	0.94	1/1400 (0.1%)
1	C	0.63	0/1039	0.89	0/1404
1	D	0.59	0/1048	0.93	0/1416
All	All	0.60	0/4143	0.92	1/5603 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	GLU	N-CA-C	7.30	119.20	110.44

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	1005	0	990	10	0
1	B	1019	0	1013	10	0
1	C	1023	0	1018	10	0
1	D	1032	0	1036	5	0
2	A	43	0	29	2	0
2	B	43	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	29	3	0
2	D	43	0	29	0	0
All	All	4251	0	4173	34	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 4.

All (34) 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:C:82:CYS:HA	2:C:201:BLA:HHD	1.76	0.66
1:D:52:VAL:O	1:D:56:VAL:HG23	1.97	0.65
1:B:56:VAL:HG22	1:B:86:MET:SD	2.39	0.62
1:B:52:VAL:O	1:B:56:VAL:HG23	1.99	0.62
1:D:56:VAL:HG21	1:D:83:VAL:HG12	1.81	0.61
1:A:56:VAL:HG21	1:A:83:VAL:HG12	1.84	0.60
1:A:82:CYS:HA	2:A:201:BLA:HHD	1.85	0.58
1:D:56:VAL:HG22	1:D:86:MET:SD	2.45	0.57
1:B:56:VAL:HG21	1:B:83:VAL:HG12	1.88	0.56
1:C:99:ALA:HB3	1:C:104:VAL:HG21	1.89	0.55
1:C:77:ARG:HG2	1:C:81:MET:HE2	1.87	0.55
1:B:82:CYS:HA	2:B:201:BLA:HHD	1.87	0.54
1:A:52:VAL:O	1:A:56:VAL:HG23	2.08	0.54
1:C:101:GLY:O	1:C:104:VAL:HG22	2.10	0.52
1:B:147:MET:HB3	1:B:150:ILE:HD11	1.92	0.52
1:B:150:ILE:HG22	1:B:153:VAL:HG23	1.92	0.51
1:C:56:VAL:HG12	1:C:60:PHE:CZ	2.47	0.49
1:B:150:ILE:CG2	1:B:153:VAL:HG23	2.42	0.49
1:C:56:VAL:HG21	1:C:83:VAL:HG12	1.96	0.48
1:A:104:VAL:HB	2:C:201:BLA:HBB2	1.96	0.47
1:A:56:VAL:HG22	1:A:86:MET:SD	2.54	0.47
1:B:92:MET:HE3	2:B:201:BLA:HAB	1.96	0.46
1:B:82:CYS:CA	2:B:201:BLA:HHD	2.45	0.46
1:A:82:CYS:CA	2:A:201:BLA:HHD	2.48	0.43
1:A:99:ALA:HB1	1:A:104:VAL:HG11	2.02	0.42
1:D:99:ALA:HB1	1:D:104:VAL:HG11	2.01	0.42
1:B:99:ALA:HB1	1:B:104:VAL:HG11	2.03	0.41
1:A:38:VAL:HG13	1:C:98:VAL:HG21	2.02	0.41
1:A:56:VAL:HG12	1:A:60:PHE:CZ	2.55	0.41
1:C:82:CYS:CA	2:C:201:BLA:HHD	2.48	0.41
1:C:155:GLU:HB3	1:C:156:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:VAL:O	1:C:56:VAL:HG23	2.20	0.41
1:D:56:VAL:HG12	1:D:60:PHE:CE2	2.56	0.41
1:A:125:CYS:HB3	1:A:126:PRO:HD3	2.03	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	133/147 (90%)	127 (96%)	6 (4%)	0	100	100
1	B	133/147 (90%)	130 (98%)	3 (2%)	0	100	100
1	C	133/147 (90%)	127 (96%)	6 (4%)	0	100	100
1	D	133/147 (90%)	130 (98%)	3 (2%)	0	100	100
All	All	532/588 (90%)	514 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/122 (83%)	98 (97%)	3 (3%)	36	62
1	B	104/122 (85%)	102 (98%)	2 (2%)	50	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	105/122 (86%)	104 (99%)	1 (1%)	68	85
1	D	108/122 (88%)	105 (97%)	3 (3%)	38	64
All	All	418/488 (86%)	409 (98%)	9 (2%)	45	71

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	65	GLU
1	A	129	ARG
1	B	68	ARG
1	B	150	ILE
1	C	56	VAL
1	D	56	VAL
1	D	67	VAL
1	D	167	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	B	47	ASN
1	B	61	GLN
1	C	47	ASN
1	C	132	GLN
1	D	132	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	B	201	1	46,46,46	3.63	17 (36%)	66,67,67	2.37	23 (34%)
2	BLA	C	201	1	46,46,46	3.63	16 (34%)	66,67,67	2.46	23 (34%)
2	BLA	D	201	1	46,46,46	3.63	17 (36%)	66,67,67	2.38	25 (37%)
2	BLA	A	201	1	46,46,46	3.59	17 (36%)	66,67,67	2.44	24 (36%)

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	B	201	1	-	12/26/74/74	0/4/4/4
2	BLA	C	201	1	-	11/26/74/74	0/4/4/4
2	BLA	D	201	1	-	8/26/74/74	0/4/4/4
2	BLA	A	201	1	-	11/26/74/74	0/4/4/4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	BLA	OB-C4B	13.18	1.48	1.23
2	A	201	BLA	OB-C4B	13.11	1.48	1.23
2	C	201	BLA	OB-C4B	13.09	1.48	1.23
2	D	201	BLA	OB-C4B	12.94	1.48	1.23
2	D	201	BLA	C3C-C2C	7.67	1.52	1.37
2	C	201	BLA	C3C-C2C	7.66	1.52	1.37
2	A	201	BLA	C3C-C2C	7.52	1.52	1.37
2	B	201	BLA	C3C-C2C	7.49	1.52	1.37
2	C	201	BLA	CHA-C4D	7.12	1.52	1.38
2	D	201	BLA	CHA-C4D	7.09	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	BLA	CHA-C4D	7.00	1.51	1.38
2	A	201	BLA	CHA-C4D	6.90	1.51	1.38
2	C	201	BLA	CHD-C4C	6.44	1.53	1.37
2	D	201	BLA	CHD-C4C	6.23	1.52	1.37
2	A	201	BLA	CHD-C4C	6.16	1.52	1.37
2	B	201	BLA	CHB-C1B	6.14	1.52	1.37
2	B	201	BLA	CHD-C4C	6.13	1.52	1.37
2	A	201	BLA	CHB-C1B	6.03	1.52	1.37
2	D	201	BLA	CHB-C1B	5.91	1.52	1.37
2	C	201	BLA	CHB-C1B	5.68	1.51	1.37
2	B	201	BLA	CHB-C4A	5.58	1.53	1.40
2	D	201	BLA	CHB-C4A	5.54	1.52	1.40
2	D	201	BLA	CHA-C1A	5.52	1.52	1.40
2	B	201	BLA	C3D-C2D	5.43	1.48	1.36
2	A	201	BLA	CHB-C4A	5.34	1.52	1.40
2	C	201	BLA	C3D-C2D	5.25	1.48	1.36
2	A	201	BLA	C3D-C2D	5.21	1.48	1.36
2	C	201	BLA	CHD-C1D	5.20	1.52	1.40
2	C	201	BLA	CHA-C1A	5.18	1.52	1.40
2	C	201	BLA	CHB-C4A	5.15	1.52	1.40
2	B	201	BLA	CHA-C1A	5.14	1.52	1.40
2	D	201	BLA	C3D-C2D	5.12	1.47	1.36
2	A	201	BLA	CHA-C1A	5.07	1.51	1.40
2	D	201	BLA	CHD-C1D	4.98	1.52	1.40
2	B	201	BLA	CHD-C1D	4.98	1.52	1.40
2	A	201	BLA	CHD-C1D	4.73	1.51	1.40
2	C	201	BLA	C4C-NC	4.72	1.45	1.37
2	B	201	BLA	C3C-C4C	4.65	1.54	1.45
2	D	201	BLA	C3C-C4C	4.63	1.54	1.45
2	A	201	BLA	C3C-C4C	4.59	1.54	1.45
2	C	201	BLA	C3C-C4C	4.59	1.54	1.45
2	C	201	BLA	CBC-CAC	4.50	1.52	1.30
2	B	201	BLA	CBB-CAB	4.48	1.51	1.30
2	D	201	BLA	CBB-CAB	4.48	1.51	1.30
2	A	201	BLA	CBB-CAB	4.46	1.51	1.30
2	C	201	BLA	CBB-CAB	4.44	1.51	1.30
2	D	201	BLA	CBC-CAC	4.40	1.51	1.30
2	B	201	BLA	CBC-CAC	4.39	1.51	1.30
2	A	201	BLA	CBC-CAC	4.38	1.51	1.30
2	D	201	BLA	C4C-NC	4.38	1.45	1.37
2	B	201	BLA	C4C-NC	4.36	1.45	1.37
2	A	201	BLA	C4C-NC	4.32	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	BLA	C4A-C3A	3.50	1.49	1.41
2	A	201	BLA	C4A-C3A	3.43	1.49	1.41
2	C	201	BLA	C4A-C3A	3.33	1.49	1.41
2	B	201	BLA	C4A-C3A	3.31	1.49	1.41
2	D	201	BLA	C1A-C2A	2.98	1.49	1.42
2	C	201	BLA	C1A-C2A	2.88	1.49	1.42
2	B	201	BLA	C1A-C2A	2.84	1.49	1.42
2	A	201	BLA	C1A-C2A	2.82	1.49	1.42
2	D	201	BLA	CAC-C3C	2.72	1.54	1.47
2	B	201	BLA	CAC-C3C	2.68	1.54	1.47
2	C	201	BLA	CAC-C3C	2.64	1.54	1.47
2	A	201	BLA	CAC-C3C	2.52	1.54	1.47
2	D	201	BLA	C4D-C3D	2.43	1.49	1.45
2	B	201	BLA	C4D-C3D	2.25	1.49	1.45
2	A	201	BLA	C4D-C3D	2.00	1.48	1.45

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	BLA	CHD-C4C-NC	-6.64	111.89	126.06
2	A	201	BLA	CHD-C4C-NC	-6.49	112.22	126.06
2	C	201	BLA	CHD-C4C-NC	-6.06	113.13	126.06
2	A	201	BLA	CMC-C2C-C3C	-5.81	114.38	128.43
2	C	201	BLA	C3C-C4C-NC	-5.75	97.26	106.64
2	D	201	BLA	CMC-C2C-C3C	-5.69	114.67	128.43
2	A	201	BLA	CHD-C4C-C3C	-5.64	111.84	127.94
2	B	201	BLA	CMC-C2C-C3C	-5.64	114.79	128.43
2	C	201	BLA	CMC-C2C-C3C	-5.61	114.86	128.43
2	D	201	BLA	CHD-C4C-NC	-5.58	114.17	126.06
2	D	201	BLA	CHD-C4C-C3C	-5.52	112.18	127.94
2	D	201	BLA	C3B-C4B-NB	5.52	113.06	106.13
2	B	201	BLA	C3C-C4C-NC	-5.47	97.71	106.64
2	A	201	BLA	C3B-C4B-NB	5.46	112.99	106.13
2	B	201	BLA	C3B-C4B-NB	5.36	112.87	106.13
2	C	201	BLA	C3B-C4B-NB	5.34	112.84	106.13
2	D	201	BLA	C3C-C4C-NC	-5.33	97.94	106.64
2	A	201	BLA	C4B-C3B-C2B	-5.14	101.33	107.92
2	B	201	BLA	CHD-C4C-C3C	-5.13	113.28	127.94
2	C	201	BLA	C4A-CHB-C1B	-5.10	116.14	130.82
2	B	201	BLA	C4B-C3B-C2B	-5.09	101.39	107.92
2	D	201	BLA	C4B-C3B-C2B	-4.99	101.52	107.92
2	A	201	BLA	C3C-C4C-NC	-4.93	98.59	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	BLA	CHD-C4C-C3C	-4.82	114.17	127.94
2	A	201	BLA	C4A-CHB-C1B	-4.71	117.27	130.82
2	C	201	BLA	C4B-C3B-C2B	-4.69	101.90	107.92
2	C	201	BLA	C1A-CHA-C4D	-4.49	118.42	128.22
2	C	201	BLA	C1B-NB-C4B	-4.18	105.53	110.66
2	B	201	BLA	C1A-CHA-C4D	-4.13	119.21	128.22
2	B	201	BLA	C4A-CHB-C1B	-4.05	119.18	130.82
2	A	201	BLA	C1B-NB-C4B	-4.01	105.74	110.66
2	D	201	BLA	C1B-NB-C4B	-3.95	105.82	110.66
2	C	201	BLA	CMC-C2C-C1C	-3.92	113.02	121.21
2	A	201	BLA	CAC-C3C-C2C	-3.87	115.85	128.43
2	C	201	BLA	C4D-ND-C1D	3.81	113.51	106.52
2	D	201	BLA	C4A-CHB-C1B	-3.81	119.86	130.82
2	C	201	BLA	CAC-C3C-C2C	-3.70	116.41	128.43
2	B	201	BLA	CMC-C2C-C1C	-3.62	113.64	121.21
2	A	201	BLA	CMC-C2C-C1C	-3.61	113.67	121.21
2	B	201	BLA	CAC-C3C-C2C	-3.58	116.81	128.43
2	B	201	BLA	C1B-NB-C4B	-3.57	106.28	110.66
2	A	201	BLA	C1A-CHA-C4D	-3.54	120.50	128.22
2	D	201	BLA	CAC-C3C-C2C	-3.42	117.30	128.43
2	D	201	BLA	C4D-ND-C1D	3.26	112.50	106.52
2	D	201	BLA	C1A-CHA-C4D	-3.22	121.19	128.22
2	D	201	BLA	CBB-CAB-C3B	-3.19	111.56	127.53
2	B	201	BLA	C4D-ND-C1D	3.17	112.33	106.52
2	A	201	BLA	C4D-ND-C1D	3.16	112.32	106.52
2	C	201	BLA	CBB-CAB-C3B	-3.14	111.83	127.53
2	D	201	BLA	CMC-C2C-C1C	-3.05	114.83	121.21
2	A	201	BLA	CHA-C4D-ND	2.98	130.85	124.60
2	D	201	BLA	CBC-CAC-C3C	-2.93	112.86	127.53
2	A	201	BLA	CBB-CAB-C3B	-2.91	113.00	127.53
2	C	201	BLA	C4C-NC-C1C	2.89	114.21	110.66
2	D	201	BLA	CHA-C4D-ND	2.83	130.54	124.60
2	A	201	BLA	CBC-CAC-C3C	-2.81	113.48	127.53
2	C	201	BLA	C4C-CHD-C1D	-2.80	121.19	128.06
2	A	201	BLA	C4C-NC-C1C	2.79	114.09	110.66
2	B	201	BLA	CBC-CAC-C3C	-2.77	113.67	127.53
2	B	201	BLA	CBB-CAB-C3B	-2.76	113.76	127.53
2	D	201	BLA	C4C-CHD-C1D	-2.74	121.34	128.06
2	C	201	BLA	C2B-C1B-NB	2.72	110.93	106.97
2	B	201	BLA	C4C-CHD-C1D	-2.65	121.55	128.06
2	C	201	BLA	CBC-CAC-C3C	-2.65	114.30	127.53
2	A	201	BLA	C4C-CHD-C1D	-2.62	121.61	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	BLA	CHA-C1A-C2A	-2.62	121.58	127.22
2	C	201	BLA	CMD-C2D-C1D	2.52	129.01	125.10
2	B	201	BLA	CHA-C1A-C2A	-2.47	121.91	127.22
2	C	201	BLA	CHA-C4D-ND	2.46	129.76	124.60
2	D	201	BLA	OB-C4B-C3B	-2.45	123.80	129.71
2	D	201	BLA	CHB-C1B-C2B	-2.44	122.11	126.97
2	B	201	BLA	CHA-C4D-ND	2.43	129.69	124.60
2	A	201	BLA	C2B-C1B-NB	2.39	110.45	106.97
2	B	201	BLA	OB-C4B-C3B	-2.37	124.00	129.71
2	A	201	BLA	CHA-C1A-NA	2.35	130.61	125.29
2	D	201	BLA	O2A-CGA-CBA	2.34	121.39	114.00
2	A	201	BLA	CAD-CBD-CGD	-2.34	107.47	113.67
2	B	201	BLA	C4C-NC-C1C	2.32	113.51	110.66
2	A	201	BLA	CHB-C1B-C2B	-2.31	122.35	126.97
2	D	201	BLA	C4C-NC-C1C	2.31	113.50	110.66
2	D	201	BLA	C2B-C1B-NB	2.30	110.32	106.97
2	B	201	BLA	CHA-C1A-NA	2.30	130.48	125.29
2	D	201	BLA	CHA-C1A-NA	2.26	130.39	125.29
2	B	201	BLA	C3C-C2C-C1C	-2.21	96.83	108.92
2	B	201	BLA	CHB-C1B-C2B	-2.21	122.57	126.97
2	C	201	BLA	OB-C4B-C3B	-2.18	124.44	129.71
2	D	201	BLA	CHA-C1A-C2A	-2.18	122.53	127.22
2	C	201	BLA	CMB-C2B-C1B	2.17	126.80	124.16
2	D	201	BLA	C3C-C2C-C1C	-2.12	97.29	108.92
2	A	201	BLA	OB-C4B-C3B	-2.11	124.62	129.71
2	B	201	BLA	C2B-C1B-NB	2.05	109.96	106.97
2	C	201	BLA	C3C-C2C-C1C	-2.02	97.84	108.92
2	C	201	BLA	CHB-C1B-C2B	-2.02	122.94	126.97
2	A	201	BLA	CMD-C2D-C1D	2.02	128.23	125.10
2	D	201	BLA	O2D-CGD-CBD	2.00	120.33	114.00

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	BLA	C2C-C3C-CAC-CBC
2	A	201	BLA	NC-C4C-CHD-C1D
2	A	201	BLA	ND-C1D-CHD-C4C
2	A	201	BLA	C2D-C1D-CHD-C4C
2	B	201	BLA	NC-C4C-CHD-C1D
2	B	201	BLA	ND-C1D-CHD-C4C
2	B	201	BLA	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
2	C	201	BLA	NC-C4C-CHD-C1D
2	C	201	BLA	ND-C1D-CHD-C4C
2	C	201	BLA	C2D-C1D-CHD-C4C
2	D	201	BLA	C2C-C3C-CAC-CBC
2	D	201	BLA	NC-C4C-CHD-C1D
2	D	201	BLA	ND-C1D-CHD-C4C
2	B	201	BLA	C3A-C4A-CHB-C1B
2	D	201	BLA	C3A-C4A-CHB-C1B
2	D	201	BLA	C2D-C1D-CHD-C4C
2	A	201	BLA	NA-C4A-CHB-C1B
2	B	201	BLA	NA-C4A-CHB-C1B
2	C	201	BLA	NA-C4A-CHB-C1B
2	D	201	BLA	NA-C4A-CHB-C1B
2	A	201	BLA	C3A-C4A-CHB-C1B
2	C	201	BLA	C3A-C4A-CHB-C1B
2	B	201	BLA	C2C-C3C-CAC-CBC
2	C	201	BLA	C4C-C3C-CAC-CBC
2	C	201	BLA	C2C-C3C-CAC-CBC
2	A	201	BLA	C4C-C3C-CAC-CBC
2	B	201	BLA	C4C-C3C-CAC-CBC
2	B	201	BLA	C3D-CAD-CBD-CGD
2	A	201	BLA	CAA-CBA-CGA-O2A
2	A	201	BLA	CAD-CBD-CGD-O2D
2	A	201	BLA	CAD-CBD-CGD-O1D
2	B	201	BLA	CAD-CBD-CGD-O1D
2	C	201	BLA	CAD-CBD-CGD-O1D
2	B	201	BLA	CAD-CBD-CGD-O2D
2	A	201	BLA	CAA-CBA-CGA-O1A
2	C	201	BLA	CAD-CBD-CGD-O2D
2	B	201	BLA	CAA-CBA-CGA-O1A
2	B	201	BLA	CAA-CBA-CGA-O2A
2	C	201	BLA	CAA-CBA-CGA-O2A
2	C	201	BLA	CAA-CBA-CGA-O1A
2	D	201	BLA	CAA-CBA-CGA-O2A
2	D	201	BLA	CAA-CBA-CGA-O1A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

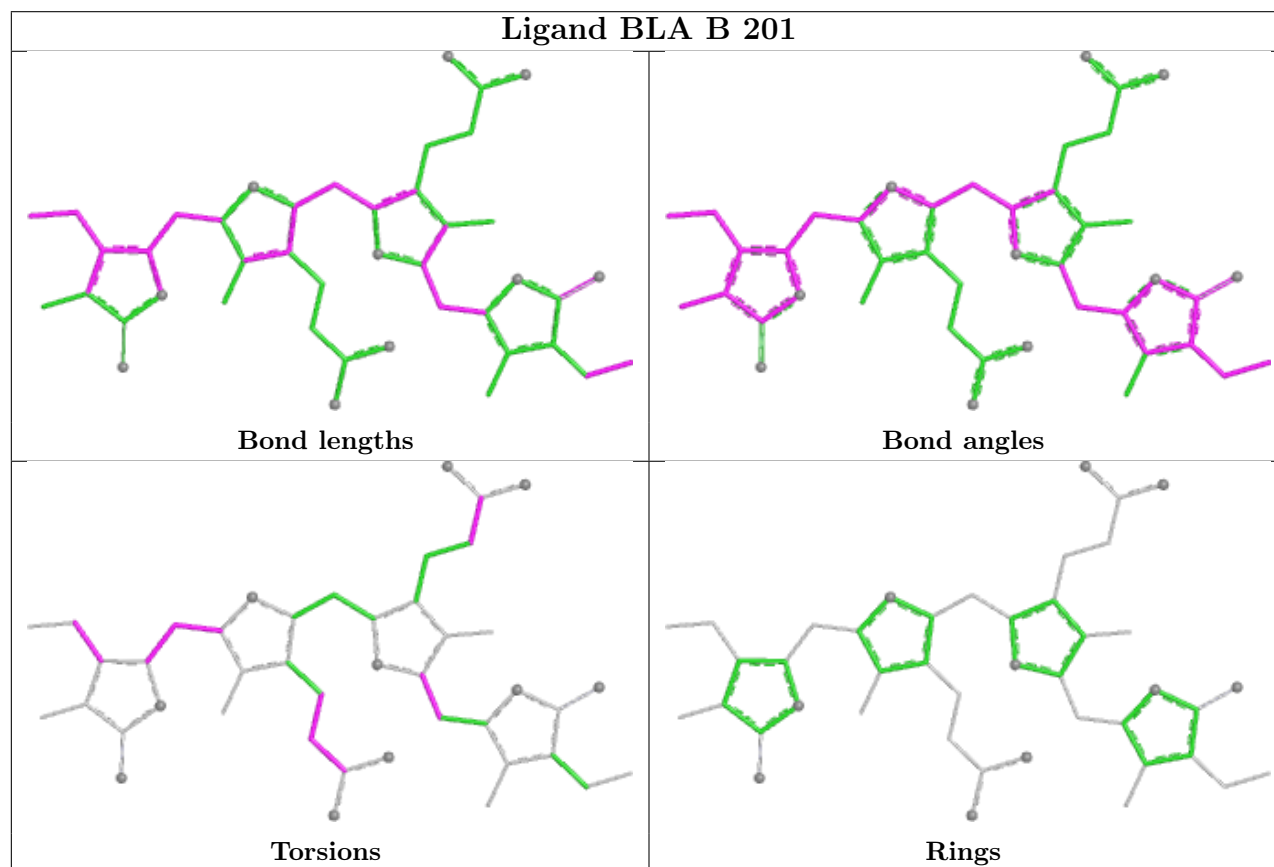
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	BLA	3	0
2	C	201	BLA	3	0

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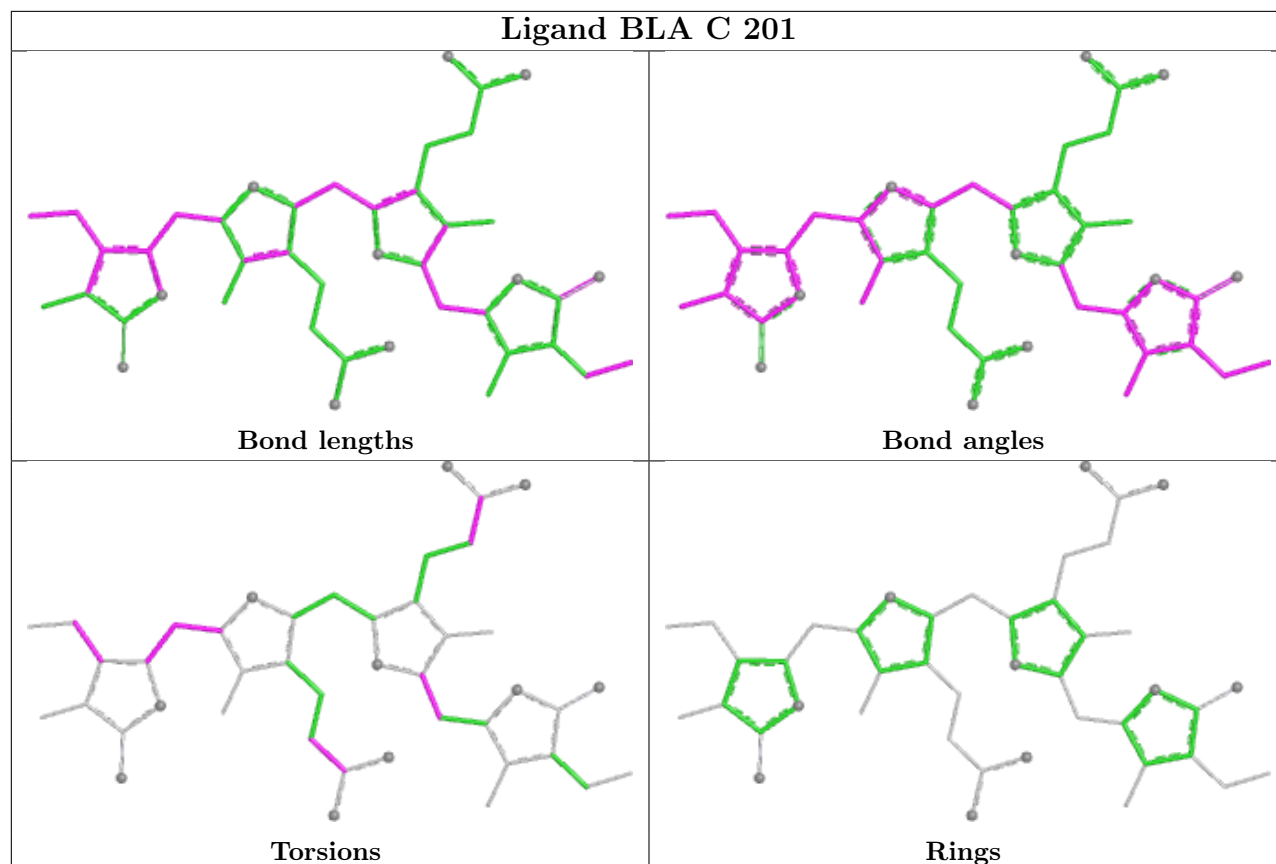
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	BLA	2	0

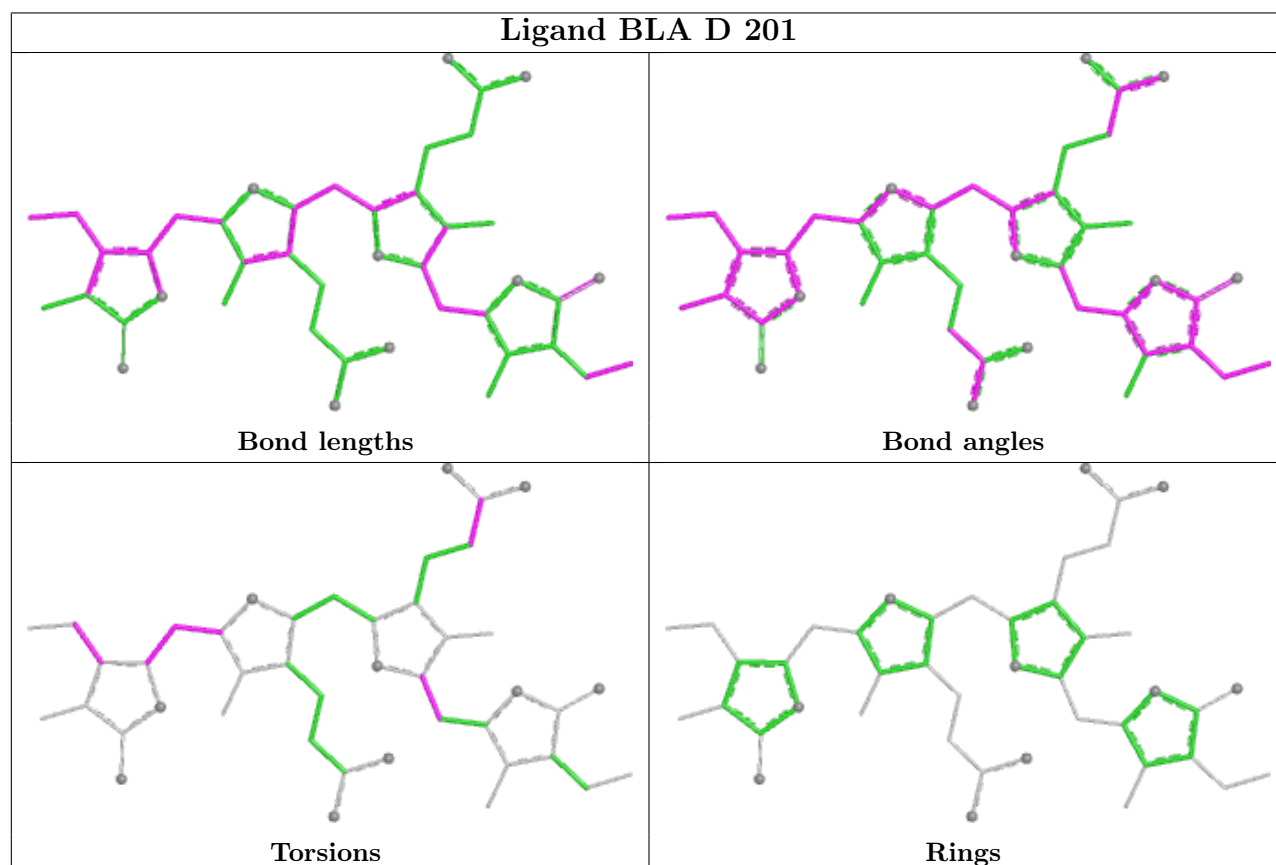
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

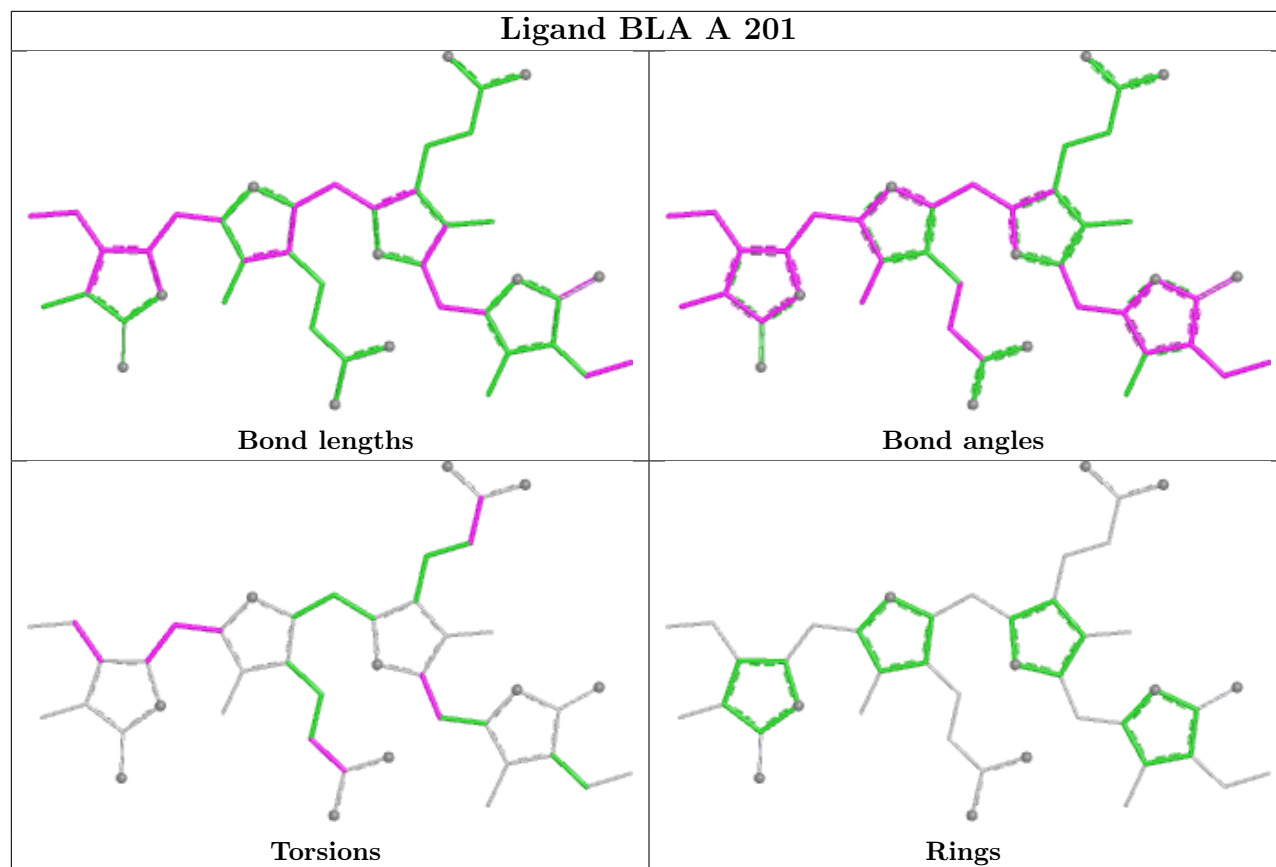


Ligand BLA C 201



Ligand BLA D 201





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	135/147 (91%)	1.08	11 (8%) 18 16	27, 36, 57, 65	0
1	B	135/147 (91%)	0.96	10 (7%) 20 18	27, 35, 54, 67	0
1	C	135/147 (91%)	1.12	17 (12%) 8 6	29, 38, 54, 66	0
1	D	135/147 (91%)	0.61	4 (2%) 52 49	25, 30, 38, 45	0
All	All	540/588 (91%)	0.94	42 (7%) 19 17	25, 35, 52, 67	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ILE	4.4
1	B	149	ASN	4.3
1	A	149	ASN	4.1
1	C	33	ASP	3.6
1	C	111	ALA	3.4
1	C	151	ALA	3.3
1	C	109	MET	3.3
1	C	106	ASP	3.0
1	C	107	GLU	3.0
1	C	110	LEU	3.0
1	B	106	ASP	2.9
1	A	144	THR	2.9
1	A	132	GLN	2.9
1	C	150	ILE	2.9
1	A	33	ASP	2.7
1	B	99	ALA	2.7
1	C	164	ILE	2.6
1	D	150	ILE	2.6
1	A	46	THR	2.6
1	D	167	THR	2.6
1	B	61	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	165	SER	2.5
1	B	163	VAL	2.4
1	C	143	ALA	2.4
1	A	166	GLU	2.4
1	C	167	THR	2.4
1	B	148	THR	2.3
1	A	165	SER	2.3
1	C	49	ALA	2.2
1	C	165	SER	2.2
1	C	88	TYR	2.2
1	C	65	GLU	2.2
1	C	113	PHE	2.2
1	C	100	GLY	2.1
1	B	77	ARG	2.1
1	A	74	TYR	2.1
1	B	119	SER	2.1
1	D	52	VAL	2.1
1	A	44	ILE	2.1
1	B	57	SER	2.1
1	D	54	THR	2.0
1	A	167	THR	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	BLA	B	201	43/43	0.82	0.14	31,35,37,38	0
2	BLA	A	201	43/43	0.85	0.14	31,34,35,36	0

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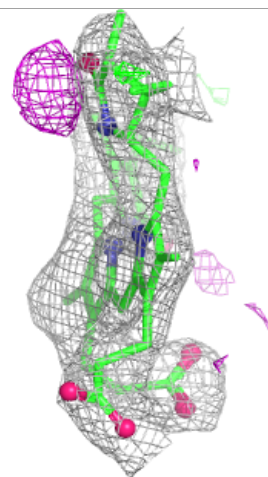
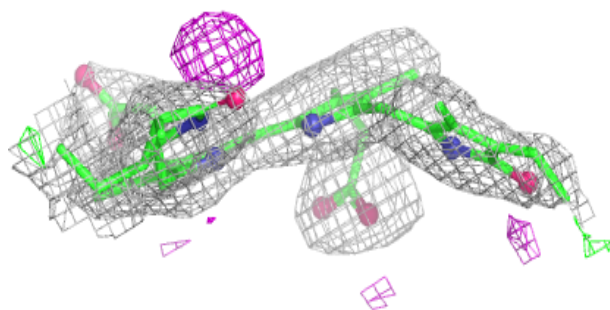
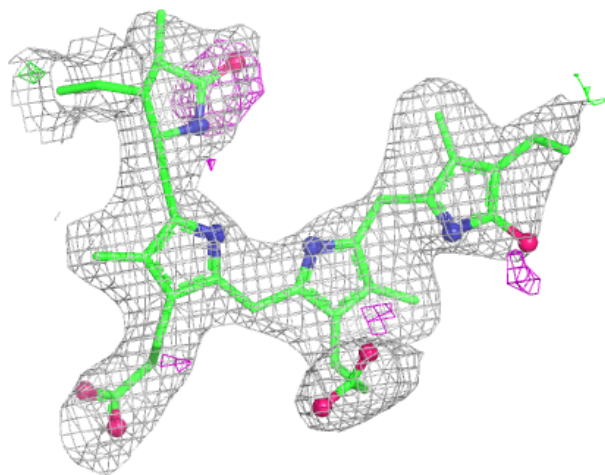
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BLA	D	201	43/43	0.86	0.13	30,33,34,35	0
2	BLA	C	201	43/43	0.87	0.13	29,31,34,35	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.

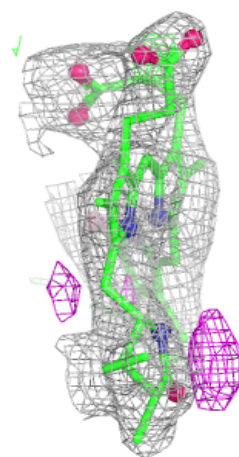
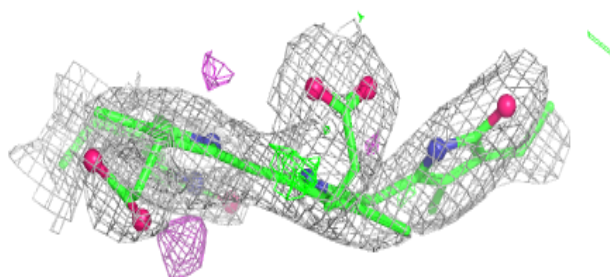
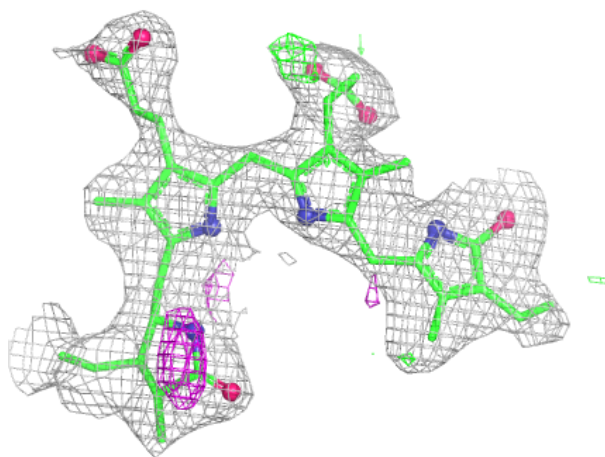
Electron density around BLA B 201:

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



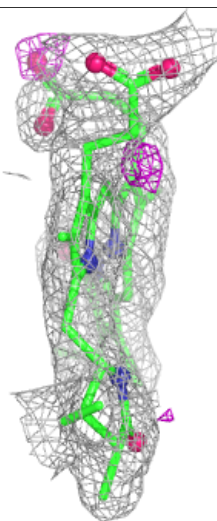
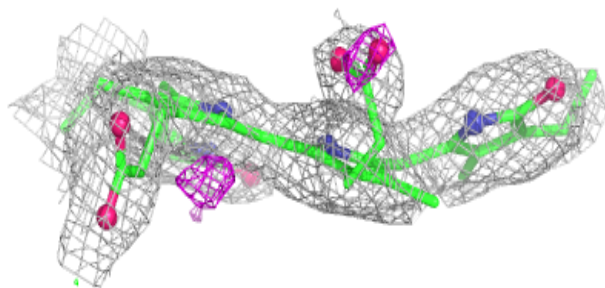
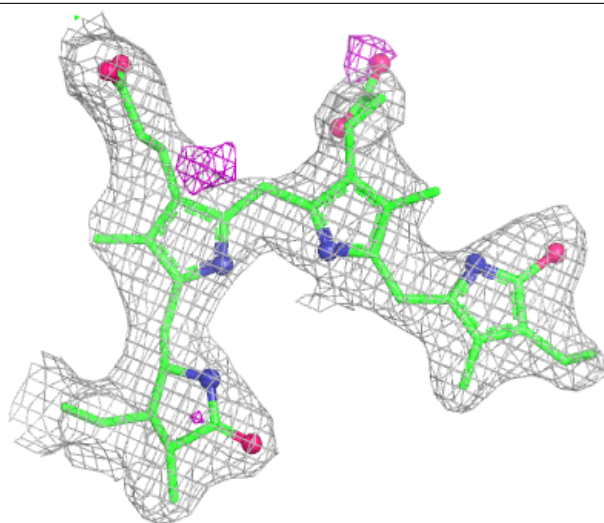
Electron density around BLA A 201:

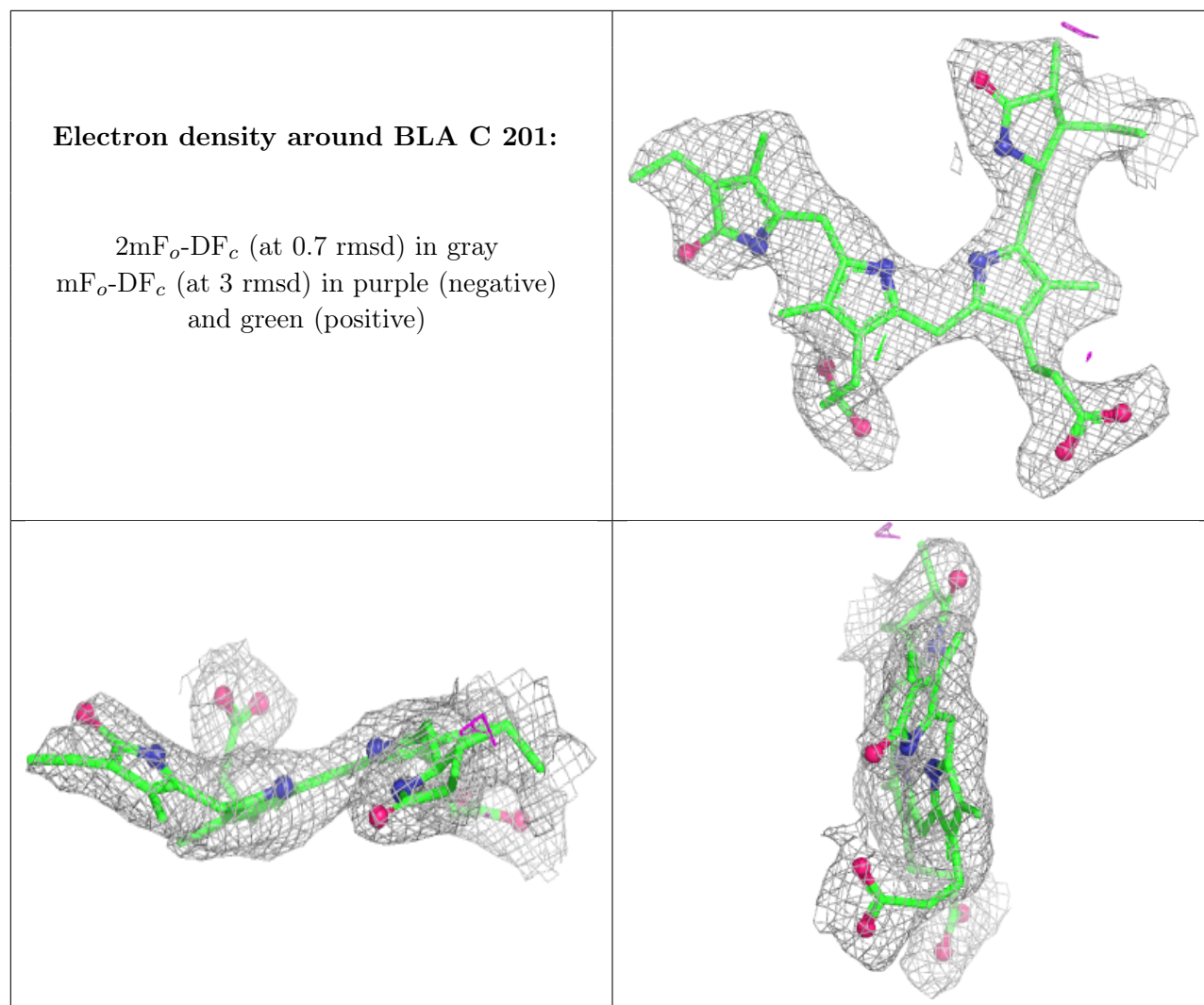
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA D 201:

$2mF_o-DF_c$ (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.