



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:09 am BST

PDB ID : 4BCL  
Title : FMO protein from Prosthecochloris aestuarii 2K at Room Temperature  
Authors : Tronrud, D.E.; Matthews, B.W.  
Deposited on : 1998-04-17  
Resolution : 1.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

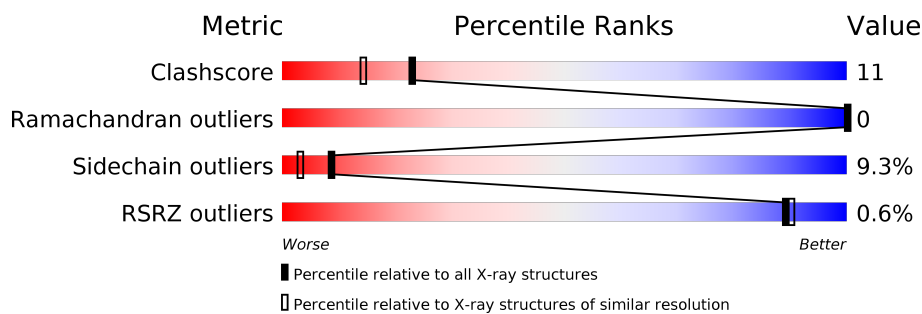
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	366	<div> <div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>61%</span> <span>29%</span> <span>5% . .</span> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3304 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.

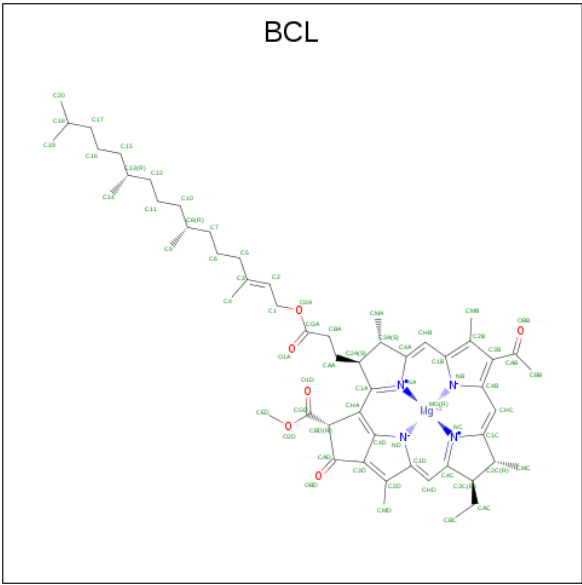
- Molecule 1 is a protein called BACTERIOCHLOROPHYLL A PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2720	1722	481	511	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	GLN	CONFLICT	UNP P11741

- Molecule 2 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
2	A	1	66	55	1	4	6	0	0
2	A	1	66	55	1	4	6	0	0
2	A	1	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

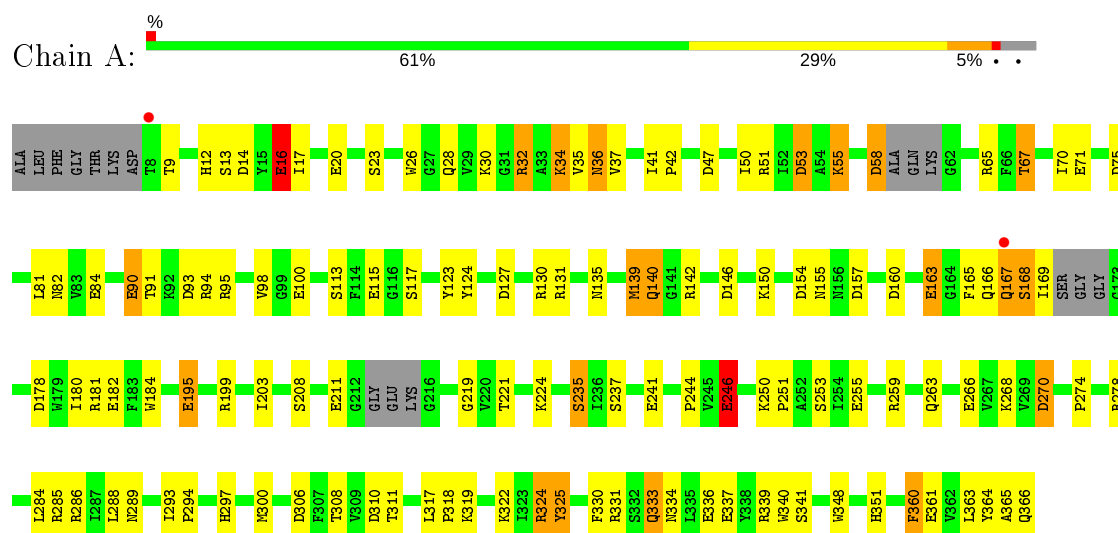
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: BACTERIOCHLOROPHYLL A PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.90 Å 111.90 Å 98.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 22.23 – 1.84	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-1.90) 76.1 (22.23-1.84)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.84 Å)	Xtriage
Refinement program	TNT 4C	Depositor
R, $R_{free}$	0.178 , (Not available) 0.171 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.26	18/2783 (0.6%)	1.80	66/3771 (1.8%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	GLU	CD-OE1	9.45	1.36	1.25
1	A	211	GLU	CD-OE1	9.06	1.35	1.25
1	A	163	GLU	CD-OE1	7.86	1.34	1.25
1	A	241	GLU	CD-OE1	7.77	1.34	1.25
1	A	266	GLU	CD-OE2	7.48	1.33	1.25
1	A	337	GLU	CD-OE1	6.95	1.33	1.25
1	A	246	GLU	CD-OE1	6.60	1.32	1.25
1	A	195	GLU	CD-OE2	-6.58	1.18	1.25
1	A	90	GLU	CD-OE2	6.05	1.32	1.25
1	A	182	GLU	CD-OE2	5.96	1.32	1.25
1	A	361	GLU	CD-OE2	5.95	1.32	1.25
1	A	71	GLU	CD-OE1	5.94	1.32	1.25
1	A	84	GLU	CD-OE2	5.88	1.32	1.25
1	A	100	GLU	CD-OE1	5.68	1.31	1.25
1	A	336	GLU	CD-OE2	5.64	1.31	1.25
1	A	16	GLU	CD-OE1	5.19	1.31	1.25
1	A	20	GLU	CD-OE1	5.14	1.31	1.25
1	A	255	GLU	CD-OE1	5.01	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	TYR	O-C-N	9.47	137.85	122.70
1	A	93	ASP	CB-CG-OD1	-9.31	109.92	118.30
1	A	139	MET	CA-CB-CG	-9.19	97.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ASP	CB-CG-OD1	-8.94	110.25	118.30
1	A	270	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	A	181	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	A	364	TYR	CB-CG-CD2	-8.69	115.78	121.00
1	A	124	TYR	CB-CA-C	-8.60	93.19	110.40
1	A	14	ASP	CB-CG-OD1	-8.32	110.81	118.30
1	A	53	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	95	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	154	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	259	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	306	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	A	199	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	53	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	364	TYR	CB-CG-CD1	6.91	125.15	121.00
1	A	95	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	A	123	TYR	C-N-CA	-6.74	104.86	121.70
1	A	341	SER	N-CA-CB	6.70	120.55	110.50
1	A	155	ASN	N-CA-CB	6.62	122.51	110.60
1	A	142	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	32	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	146	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	259	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	93	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	221	THR	CA-CB-CG2	-6.40	103.44	112.40
1	A	278	ARG	N-CA-CB	-6.31	99.24	110.60
1	A	324	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	90	GLU	CB-CA-C	-6.18	98.04	110.40
1	A	285	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	324	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	47	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	A	93	ASP	CB-CA-C	-6.11	98.18	110.40
1	A	157	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	113	SER	N-CA-CB	6.10	119.65	110.50
1	A	310	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	131	ARG	CG-CD-NE	-5.97	99.26	111.80
1	A	42	PRO	N-CA-CB	5.92	110.40	103.30
1	A	184	TRP	N-CA-CB	-5.90	99.99	110.60
1	A	124	TYR	CA-C-O	-5.86	107.79	120.10
1	A	75	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	331	ARG	N-CA-CB	-5.73	100.28	110.60
1	A	146	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	360	PHE	CB-CG-CD2	-5.68	116.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	286	ARG	CD-NE-CZ	-5.58	115.78	123.60
1	A	65	ARG	CA-CB-CG	-5.46	101.38	113.40
1	A	12	HIS	CB-CA-C	-5.44	99.52	110.40
1	A	160	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	75	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	67	THR	N-CA-CB	-5.40	100.04	110.30
1	A	339	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	91	THR	CA-CB-CG2	-5.28	105.00	112.40
1	A	178	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	235	SER	CB-CA-C	-5.26	100.11	110.10
1	A	34	LYS	CB-CA-C	5.25	120.91	110.40
1	A	157	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	270	ASP	CB-CA-C	-5.19	100.03	110.40
1	A	117	SER	N-CA-CB	-5.14	102.80	110.50
1	A	306	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	115	GLU	C-N-CA	-5.09	111.62	122.30
1	A	308	THR	CA-CB-CG2	-5.08	105.28	112.40
1	A	16	GLU	N-CA-CB	5.03	119.65	110.60
1	A	325	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	195	GLU	CB-CA-C	-5.01	100.38	110.40

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	2720	0	2644	49	0
2	A	462	0	518	28	0
3	A	122	0	0	1	0
All	All	3304	0	3162	72	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 11.

All (72) 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:140:GLN:H	1:A:140:GLN:HE21	1.02	0.93
1:A:36:ASN:H	1:A:36:ASN:HD22	0.95	0.92
1:A:36:ASN:ND2	1:A:36:ASN:H	1.70	0.90
2:A:370:BCL:HBB2	2:A:370:BCL:HMB1	1.63	0.79
1:A:36:ASN:N	1:A:36:ASN:HD22	1.78	0.78
2:A:368:BCL:HMB1	2:A:368:BCL:HBB2	1.68	0.74
1:A:140:GLN:N	1:A:140:GLN:HE21	1.84	0.71
1:A:140:GLN:NE2	1:A:140:GLN:H	1.83	0.70
2:A:369:BCL:HMB1	2:A:369:BCL:CBB	2.23	0.69
2:A:368:BCL:CBB	2:A:368:BCL:HMB1	2.22	0.69
2:A:369:BCL:C4A	2:A:369:BCL:HBA2	2.21	0.69
2:A:370:BCL:CBB	2:A:370:BCL:HMB1	2.23	0.69
1:A:139:MET:HB2	1:A:237:SER:HB2	1.75	0.68
1:A:195:GLU:HG3	1:A:300:MET:SD	2.36	0.65
1:A:55:LYS:HG2	1:A:55:LYS:O	1.96	0.65
1:A:67:THR:HG22	3:A:446:HOH:O	1.97	0.64
2:A:372:BCL:HBB3	2:A:372:BCL:HMB1	1.80	0.64
2:A:373:BCL:HMB1	2:A:373:BCL:HBB2	1.81	0.63
1:A:135:ASN:HD21	1:A:289:ASN:HD21	1.47	0.62
1:A:26:TRP:HA	1:A:274:PRO:HA	1.81	0.62
1:A:246:GLU:CD	1:A:246:GLU:H	2.02	0.62
1:A:333:GLN:HG2	1:A:334:ASN:N	2.18	0.58
1:A:250:LYS:HB2	1:A:251:PRO:HD2	1.87	0.57
1:A:17:ILE:HD11	2:A:369:BCL:HAA1	1.86	0.56
2:A:369:BCL:HBB2	2:A:369:BCL:HMB1	1.88	0.56
1:A:250:LYS:HB2	1:A:251:PRO:CD	2.36	0.56
2:A:372:BCL:HMB1	2:A:372:BCL:CBB	2.38	0.54
1:A:36:ASN:ND2	1:A:36:ASN:N	2.44	0.54
1:A:90:GLU:HG3	1:A:94:ARG:NH1	2.24	0.53
1:A:317:LEU:HB3	1:A:318:PRO:HD2	1.89	0.53
1:A:41:ILE:HD13	1:A:41:ILE:N	2.26	0.51
1:A:348:TRP:O	1:A:351:HIS:HB3	2.11	0.51
1:A:244:PRO:HG2	2:A:373:BCL:HMB3	1.93	0.50
2:A:367:BCL:HBB2	2:A:367:BCL:HMB1	1.93	0.49
1:A:70:ILE:HD12	1:A:81:LEU:HD23	1.95	0.49
1:A:284:LEU:HD23	1:A:365:ALA:HB2	1.94	0.49
1:A:53:ASP:OD1	1:A:253:SER:HB3	2.13	0.49
1:A:246:GLU:OE1	1:A:246:GLU:N	2.38	0.48
1:A:293:ILE:N	1:A:294:PRO:HD2	2.28	0.48
1:A:9:THR:HG21	1:A:37:VAL:CG1	2.43	0.48
2:A:371:BCL:OBB	2:A:371:BCL:HMB1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TYR:HB3	1:A:363:LEU:HD12	1.98	0.46
1:A:166:GLN:O	1:A:167:GLN:C	2.50	0.46
2:A:371:BCL:H42	2:A:373:BCL:H171	1.98	0.45
2:A:371:BCL:HHC	2:A:371:BCL:HBB3	1.97	0.45
1:A:81:LEU:HG	1:A:82:ASN:N	2.30	0.45
2:A:370:BCL:H2A	2:A:370:BCL:O2A	2.16	0.45
1:A:13:SER:O	1:A:311:THR:HA	2.17	0.44
1:A:35:VAL:HG22	1:A:37:VAL:HG13	2.00	0.44
1:A:330:PHE:HA	1:A:340:TRP:CD1	2.52	0.44
1:A:9:THR:HG21	1:A:37:VAL:HG12	1.99	0.44
2:A:369:BCL:HBB3	2:A:369:BCL:HMB1	1.98	0.44
1:A:293:ILE:N	1:A:294:PRO:CD	2.81	0.44
1:A:297:HIS:HB3	2:A:370:BCL:C4D	2.48	0.44
2:A:372:BCL:H111	2:A:372:BCL:H142	1.77	0.43
2:A:367:BCL:HAA1	2:A:367:BCL:CB D	2.49	0.43
1:A:180:ILE:HG21	1:A:203:ILE:HD12	2.02	0.42
2:A:371:BCL:CGD	2:A:371:BCL:H2A	2.48	0.42
1:A:58:ASP:O	1:A:58:ASP:OD1	2.37	0.42
1:A:244:PRO:CG	2:A:373:BCL:HMB3	2.50	0.41
1:A:50:ILE:HD12	1:A:70:ILE:HG12	2.02	0.41
1:A:127:ASP:HA	1:A:130:ARG:HB3	2.02	0.41
1:A:150:LYS:HA	1:A:219:GLY:O	2.20	0.41
2:A:371:BCL:H62	2:A:371:BCL:H102	1.98	0.41
1:A:98:VAL:O	1:A:98:VAL:HG13	2.21	0.41
1:A:16:GLU:OE2	1:A:30:LYS:HD3	2.20	0.41
2:A:371:BCL:H142	2:A:371:BCL:H112	1.30	0.41
1:A:168:SER:O	1:A:169:ILE:C	2.58	0.41
1:A:317:LEU:HB3	1:A:318:PRO:CD	2.49	0.41
1:A:165:PHE:CD2	2:A:367:BCL:H8	2.56	0.40
2:A:367:BCL:HAA1	2:A:367:BCL:CGD	2.52	0.40
2:A:370:BCL:H152	2:A:370:BCL:H111	1.68	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	342/366 (93%)	334 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	291/303 (96%)	264 (91%)	27 (9%)	9	3

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	23	SER
1	A	28	GLN
1	A	32	ARG
1	A	34	LYS
1	A	36	ASN
1	A	51	ARG
1	A	55	LYS
1	A	58	ASP
1	A	140	GLN
1	A	163	GLU
1	A	167	GLN
1	A	168	SER
1	A	208	SER
1	A	224	LYS
1	A	235	SER
1	A	246	GLU
1	A	263	GLN
1	A	268	LYS
1	A	270	ASP
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	319	LYS
1	A	322	LYS
1	A	324	ARG
1	A	333	GLN
1	A	360	PHE
1	A	366	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	79	ASN
1	A	82	ASN
1	A	132	ASN
1	A	140	GLN
1	A	198	GLN
1	A	272	ASN
1	A	289	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	BCL	A	367	1	58,74,74	1.38	6 (10%)	69,115,115	2.32	23 (33%)
2	BCL	A	370	1	58,74,74	1.70	14 (24%)	69,115,115	2.11	21 (30%)
2	BCL	A	371	1	58,74,74	1.71	10 (17%)	69,115,115	2.09	23 (33%)
2	BCL	A	372	3	58,74,74	1.80	14 (24%)	69,115,115	1.86	19 (27%)
2	BCL	A	369	1	58,74,74	1.52	6 (10%)	69,115,115	1.79	17 (24%)
2	BCL	A	373	1	58,74,74	1.74	17 (29%)	69,115,115	1.88	21 (30%)
2	BCL	A	368	1	58,74,74	1.65	10 (17%)	69,115,115	2.07	25 (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	BCL	A	367	1	-	5/37/137/137	-
2	BCL	A	370	1	-	8/37/137/137	-
2	BCL	A	371	1	-	11/37/137/137	-
2	BCL	A	372	3	-	11/37/137/137	-
2	BCL	A	369	1	-	6/37/137/137	-
2	BCL	A	373	1	-	13/37/137/137	-
2	BCL	A	368	1	-	12/37/137/137	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	371	BCL	C4B-NB	7.76	1.42	1.35
2	A	372	BCL	C1B-NB	7.01	1.41	1.35
2	A	369	BCL	C1B-NB	6.42	1.40	1.35
2	A	368	BCL	OBD-CAD	6.01	1.30	1.22
2	A	372	BCL	C4B-NB	4.90	1.39	1.35
2	A	370	BCL	O1D-CGD	-4.48	1.10	1.21
2	A	371	BCL	C1B-NB	4.40	1.39	1.35
2	A	367	BCL	C1B-NB	4.11	1.38	1.35
2	A	372	BCL	C3C-C4C	-4.01	1.46	1.51
2	A	368	BCL	O1D-CGD	-3.98	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	373	BCL	CAC-C3C	3.97	1.61	1.54
2	A	370	BCL	C1D-C2D	3.90	1.51	1.42
2	A	367	BCL	MG-NA	3.81	2.15	2.06
2	A	372	BCL	MG-NA	3.76	2.15	2.06
2	A	373	BCL	MG-NA	3.75	2.15	2.06
2	A	370	BCL	OBD-CAD	3.52	1.27	1.22
2	A	369	BCL	MG-NA	3.50	2.14	2.06
2	A	370	BCL	C1B-NB	3.49	1.38	1.35
2	A	373	BCL	C3B-C2B	-3.44	1.33	1.39
2	A	368	BCL	O2D-CED	3.38	1.53	1.45
2	A	370	BCL	MG-NC	3.25	2.14	2.06
2	A	370	BCL	MG-NA	3.12	2.13	2.06
2	A	368	BCL	C3D-C2D	-3.11	1.33	1.39
2	A	369	BCL	C2A-C1A	-3.07	1.45	1.52
2	A	373	BCL	O2D-CED	3.06	1.52	1.45
2	A	368	BCL	O2D-CGD	-2.99	1.25	1.33
2	A	368	BCL	O2A-CGA	-2.95	1.24	1.33
2	A	373	BCL	CMB-C2B	-2.95	1.45	1.51
2	A	367	BCL	C3C-C4C	-2.94	1.47	1.51
2	A	373	BCL	C4B-NB	2.93	1.37	1.35
2	A	370	BCL	O1A-CGA	-2.92	1.13	1.22
2	A	370	BCL	C1A-CHA	-2.89	1.31	1.43
2	A	373	BCL	C1-C2	2.77	1.57	1.49
2	A	368	BCL	O1A-CGA	-2.77	1.14	1.22
2	A	368	BCL	C3B-C2B	-2.73	1.34	1.39
2	A	372	BCL	C3D-C2D	2.70	1.44	1.39
2	A	373	BCL	C1B-NB	2.70	1.37	1.35
2	A	373	BCL	O1A-CGA	-2.67	1.14	1.22
2	A	368	BCL	C4B-NB	2.64	1.37	1.35
2	A	371	BCL	CAA-C2A	2.60	1.58	1.54
2	A	369	BCL	C1-C2	2.59	1.56	1.49
2	A	372	BCL	MG-NC	2.58	2.12	2.06
2	A	373	BCL	C3B-CAB	-2.56	1.42	1.49
2	A	371	BCL	C6-C7	2.55	1.63	1.52
2	A	373	BCL	C4B-CHC	-2.51	1.34	1.41
2	A	372	BCL	CBD-CGD	-2.51	1.44	1.52
2	A	372	BCL	CMB-C2B	2.48	1.56	1.51
2	A	370	BCL	C1-C2	2.46	1.56	1.49
2	A	373	BCL	C2-C3	2.44	1.38	1.33
2	A	373	BCL	CMD-C2D	-2.44	1.45	1.51
2	A	371	BCL	C1A-CHA	-2.44	1.33	1.43
2	A	372	BCL	CAA-CBA	2.40	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	372	BCL	CMA-C3A	-2.39	1.48	1.53
2	A	370	BCL	OBB-CAB	-2.39	1.15	1.22
2	A	373	BCL	C3D-CAD	-2.37	1.40	1.46
2	A	371	BCL	C4B-CHC	-2.36	1.34	1.41
2	A	373	BCL	O2D-CGD	2.33	1.38	1.33
2	A	369	BCL	CAC-C3C	2.32	1.58	1.54
2	A	368	BCL	C1B-NB	2.28	1.37	1.35
2	A	373	BCL	CAA-CBA	2.26	1.59	1.52
2	A	370	BCL	C3B-C2B	-2.21	1.35	1.39
2	A	370	BCL	C6-C5	2.20	1.60	1.52
2	A	372	BCL	C3D-CAD	-2.19	1.40	1.46
2	A	370	BCL	O2A-CGA	-2.17	1.27	1.33
2	A	372	BCL	C3B-C2B	-2.16	1.35	1.39
2	A	371	BCL	C9-C8	2.15	1.59	1.52
2	A	367	BCL	CBB-CAB	2.15	1.56	1.49
2	A	367	BCL	OBD-CAD	-2.12	1.19	1.22
2	A	372	BCL	C1A-CHA	-2.12	1.34	1.43
2	A	367	BCL	C1A-CHA	-2.09	1.34	1.43
2	A	370	BCL	C3A-C2A	2.08	1.60	1.54
2	A	373	BCL	C4-C3	2.08	1.56	1.50
2	A	369	BCL	CMA-C3A	-2.07	1.48	1.53
2	A	371	BCL	C3D-C2D	2.05	1.43	1.39
2	A	372	BCL	O1D-CGD	-2.03	1.16	1.21
2	A	371	BCL	C2-C3	2.02	1.37	1.33
2	A	371	BCL	C1-C2	2.01	1.55	1.49

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	367	BCL	C4A-NA-C1A	-8.62	102.83	106.71
2	A	371	BCL	C4A-NA-C1A	-7.59	103.30	106.71
2	A	367	BCL	C4D-C3D-CAD	-7.46	104.31	108.47
2	A	370	BCL	C4A-NA-C1A	-7.34	103.40	106.71
2	A	372	BCL	C1-C2-C3	-5.49	116.55	126.04
2	A	370	BCL	CHA-C1A-NA	-5.31	114.23	126.40
2	A	368	BCL	C1C-NC-C4C	-5.15	104.39	106.71
2	A	368	BCL	O2D-CGD-CBD	5.10	120.33	111.27
2	A	370	BCL	CMD-C2D-C3D	5.04	134.11	124.68
2	A	369	BCL	C1B-CHB-C4A	-4.96	120.29	130.12
2	A	373	BCL	CBA-CAA-C2A	-4.90	99.39	113.86
2	A	368	BCL	O2D-CGD-O1D	-4.83	114.40	123.84
2	A	368	BCL	CAC-C3C-C2C	-4.69	102.55	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	367	BCL	OBD-CAD-CBD	-4.52	119.44	125.89
2	A	372	BCL	C2C-C3C-C4C	4.39	107.92	101.34
2	A	372	BCL	C4B-CHC-C1C	-4.32	121.55	130.12
2	A	370	BCL	C1C-NC-C4C	4.27	108.63	106.71
2	A	367	BCL	CMD-C2D-C3D	4.24	132.60	124.68
2	A	369	BCL	C4-C3-C5	4.15	122.25	115.27
2	A	367	BCL	C11-C12-C13	-4.14	102.53	115.92
2	A	368	BCL	CMB-C2B-C1B	-4.09	122.17	128.46
2	A	370	BCL	O2D-CGD-CBD	4.08	118.53	111.27
2	A	371	BCL	CBA-CAA-C2A	-4.07	101.83	113.86
2	A	369	BCL	C2A-C3A-C4A	4.05	108.41	101.87
2	A	370	BCL	CMC-C2C-C1C	-4.02	100.97	111.77
2	A	371	BCL	CED-O2D-CGD	-4.01	106.87	115.94
2	A	371	BCL	O2D-CGD-O1D	-3.99	116.04	123.84
2	A	373	BCL	C1C-NC-C4C	-3.94	104.94	106.71
2	A	371	BCL	C1-C2-C3	-3.81	119.45	126.04
2	A	372	BCL	C4-C3-C5	3.77	121.61	115.27
2	A	373	BCL	C4A-NA-C1A	-3.77	105.01	106.71
2	A	371	BCL	C11-C12-C13	-3.74	103.84	115.92
2	A	373	BCL	CMB-C2B-C1B	-3.70	122.78	128.46
2	A	373	BCL	C11-C10-C8	-3.68	104.03	115.92
2	A	369	BCL	C3A-C2A-C1A	-3.63	95.90	101.34
2	A	371	BCL	CHA-C1A-NA	-3.56	118.24	126.40
2	A	369	BCL	C6-C7-C8	-3.53	104.52	115.92
2	A	373	BCL	C9-C8-C7	-3.49	98.65	111.29
2	A	369	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
2	A	373	BCL	CHA-C1A-NA	-3.41	118.59	126.40
2	A	367	BCL	CBC-CAC-C3C	-3.37	105.96	113.47
2	A	368	BCL	C16-C15-C13	-3.34	105.12	115.92
2	A	373	BCL	C1-C2-C3	-3.33	120.28	126.04
2	A	372	BCL	C4B-C3B-CAB	-3.30	120.75	127.13
2	A	368	BCL	C4B-CHC-C1C	-3.25	123.69	130.12
2	A	372	BCL	C14-C13-C15	-3.24	99.57	111.29
2	A	372	BCL	CHD-C4C-NC	3.23	128.66	125.08
2	A	370	BCL	C16-C17-C18	-3.14	101.16	115.98
2	A	367	BCL	C16-C15-C13	-3.13	105.81	115.92
2	A	367	BCL	C7-C6-C5	-3.12	104.89	113.36
2	A	369	BCL	CAA-C2A-C3A	-3.11	104.26	112.78
2	A	367	BCL	OBB-CAB-CBB	-3.09	113.22	120.17
2	A	373	BCL	CMD-C2D-C3D	3.07	130.42	124.68
2	A	367	BCL	C1-C2-C3	-3.07	120.74	126.04
2	A	370	BCL	CAA-C2A-C1A	-3.05	101.99	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	368	BCL	C11-C10-C8	-2.99	106.25	115.92
2	A	370	BCL	C15-C13-C12	-2.97	96.49	112.13
2	A	371	BCL	CMB-C2B-C1B	-2.97	123.91	128.46
2	A	373	BCL	CHB-C4A-NA	-2.96	120.42	124.51
2	A	372	BCL	C16-C17-C18	-2.95	102.09	115.98
2	A	372	BCL	CAA-C2A-C3A	-2.94	104.73	112.78
2	A	368	BCL	CHA-C1A-NA	-2.91	119.74	126.40
2	A	370	BCL	C4B-CHC-C1C	-2.89	124.39	130.12
2	A	373	BCL	O2A-CGA-O1A	-2.89	116.29	123.59
2	A	368	BCL	C7-C6-C5	-2.89	105.50	113.36
2	A	368	BCL	OBD-CAD-CBD	-2.88	121.79	125.89
2	A	371	BCL	C14-C13-C15	-2.84	101.00	111.29
2	A	371	BCL	CAC-C3C-C2C	-2.81	107.24	114.26
2	A	369	BCL	C7-C6-C5	-2.79	105.78	113.36
2	A	367	BCL	CHA-C1A-NA	-2.78	120.03	126.40
2	A	367	BCL	C1C-NC-C4C	-2.74	105.47	106.71
2	A	372	BCL	C4A-NA-C1A	2.74	107.94	106.71
2	A	370	BCL	CMB-C2B-C1B	-2.74	124.25	128.46
2	A	368	BCL	C4A-NA-C1A	-2.74	105.47	106.71
2	A	373	BCL	C7-C6-C5	-2.73	105.94	113.36
2	A	372	BCL	C4D-C3D-CAD	2.72	109.99	108.47
2	A	373	BCL	OBD-CAD-CBD	-2.72	122.01	125.89
2	A	368	BCL	O2A-CGA-O1A	-2.72	116.74	123.59
2	A	371	BCL	OBD-CAD-CBD	-2.67	122.08	125.89
2	A	370	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
2	A	367	BCL	CGD-CBD-CAD	-2.66	102.12	110.73
2	A	371	BCL	CMD-C2D-C3D	2.65	129.65	124.68
2	A	369	BCL	OBB-CAB-CBB	-2.65	114.20	120.17
2	A	371	BCL	O1D-CGD-CBD	2.65	129.91	124.48
2	A	367	BCL	CAC-C3C-C4C	-2.64	106.73	112.58
2	A	368	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
2	A	371	BCL	O2A-C1-C2	-2.62	101.74	108.64
2	A	368	BCL	C11-C12-C13	-2.62	107.44	115.92
2	A	369	BCL	C1D-CHD-C4C	-2.59	122.05	125.88
2	A	368	BCL	OBB-CAB-CBB	-2.59	114.35	120.17
2	A	370	BCL	C17-C16-C15	-2.57	101.42	113.24
2	A	369	BCL	C9-C8-C10	-2.57	101.97	111.29
2	A	370	BCL	CHC-C1C-NC	-2.57	120.96	124.51
2	A	373	BCL	O2A-CGA-CBA	2.54	119.87	111.91
2	A	371	BCL	C1B-CHB-C4A	-2.53	125.10	130.12
2	A	371	BCL	C7-C6-C5	-2.53	106.49	113.36
2	A	372	BCL	OBD-CAD-CBD	-2.52	122.29	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	368	BCL	CMA-C3A-C4A	-2.51	105.02	111.77
2	A	369	BCL	CMD-C2D-C3D	2.50	129.36	124.68
2	A	370	BCL	C11-C12-C13	-2.50	107.83	115.92
2	A	371	BCL	CAA-CBA-CGA	-2.50	105.95	113.25
2	A	367	BCL	O1D-CGD-CBD	2.49	129.57	124.48
2	A	367	BCL	CMB-C2B-C1B	-2.44	124.72	128.46
2	A	372	BCL	OB B-CAB-CBB	-2.44	114.69	120.17
2	A	372	BCL	C11-C10-C8	-2.43	108.05	115.92
2	A	373	BCL	C2A-C1A-CHA	2.43	128.10	123.86
2	A	372	BCL	C11-C12-C13	-2.41	108.14	115.92
2	A	373	BCL	C12-C11-C10	-2.40	102.20	113.24
2	A	371	BCL	C9-C8-C7	-2.40	102.61	111.29
2	A	371	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
2	A	370	BCL	CMC-C2C-C3C	-2.39	104.20	113.83
2	A	371	BCL	OB B-CAB-CBB	-2.37	114.84	120.17
2	A	370	BCL	O2A-CGA-CBA	2.36	119.33	111.91
2	A	373	BCL	C16-C15-C13	-2.35	108.34	115.92
2	A	370	BCL	O2A-CGA-O1A	-2.34	117.69	123.59
2	A	367	BCL	C3D-CAD-CBD	2.34	110.68	107.61
2	A	367	BCL	CMB-C2B-C3B	2.31	129.00	124.68
2	A	371	BCL	C17-C16-C15	-2.31	102.63	113.24
2	A	373	BCL	C4B-C3B-CAB	-2.28	122.72	127.13
2	A	371	BCL	C1D-CHD-C4C	-2.28	122.51	125.88
2	A	372	BCL	C7-C6-C5	-2.27	107.19	113.36
2	A	370	BCL	C12-C11-C10	-2.26	102.86	113.24
2	A	372	BCL	CHA-C1A-NA	-2.25	121.24	126.40
2	A	369	BCL	CHA-C1A-NA	-2.25	121.24	126.40
2	A	368	BCL	C1D-CHD-C4C	-2.24	122.58	125.88
2	A	373	BCL	C20-C18-C19	-2.21	100.32	110.51
2	A	370	BCL	C11-C10-C8	-2.21	108.79	115.92
2	A	368	BCL	C2A-C3A-C4A	-2.20	98.31	101.87
2	A	369	BCL	CMC-C2C-C3C	-2.20	104.95	113.83
2	A	368	BCL	CHC-C1C-NC	2.19	127.54	124.51
2	A	371	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
2	A	367	BCL	C2C-C3C-C4C	2.15	104.56	101.34
2	A	369	BCL	CAA-C2A-C1A	2.14	119.00	111.97
2	A	368	BCL	C12-C11-C10	-2.14	103.41	113.24
2	A	369	BCL	C1-C2-C3	-2.13	122.36	126.04
2	A	372	BCL	C4-C3-C2	-2.12	118.23	123.68
2	A	368	BCL	CED-O2D-CGD	-2.11	111.16	115.94
2	A	373	BCL	CMA-C3A-C4A	-2.11	106.10	111.77
2	A	372	BCL	CBC-CAC-C3C	-2.11	108.77	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	BCL	CMB-C2B-C3B	2.09	128.59	124.68
2	A	368	BCL	C1B-CHB-C4A	-2.08	126.00	130.12
2	A	369	BCL	CBA-CAA-C2A	-2.08	107.73	113.86
2	A	373	BCL	CMB-C2B-C3B	2.07	128.55	124.68
2	A	367	BCL	C2A-C3A-C4A	-2.06	98.55	101.87
2	A	367	BCL	CHB-C4A-NA	-2.05	121.67	124.51
2	A	367	BCL	C4-C3-C5	2.04	118.71	115.27
2	A	367	BCL	CBB-CAB-C3B	2.04	126.39	120.34
2	A	368	BCL	CMB-C2B-C3B	2.04	128.49	124.68
2	A	368	BCL	C2C-C3C-C4C	-2.01	98.32	101.34

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	371	BCL	C2C-C3C-CAC-CBC
2	A	371	BCL	C4C-C3C-CAC-CBC
2	A	371	BCL	C11-C12-C13-C14
2	A	368	BCL	C4C-C3C-CAC-CBC
2	A	368	BCL	CHA-CBD-CGD-O1D
2	A	368	BCL	CHA-CBD-CGD-O2D
2	A	368	BCL	CBD-CGD-O2D-CED
2	A	371	BCL	C10-C11-C12-C13
2	A	368	BCL	C6-C7-C8-C9
2	A	372	BCL	C13-C15-C16-C17
2	A	373	BCL	C8-C10-C11-C12
2	A	371	BCL	C8-C10-C11-C12
2	A	371	BCL	C13-C15-C16-C17
2	A	373	BCL	C11-C12-C13-C15
2	A	372	BCL	C10-C11-C12-C13
2	A	373	BCL	C13-C15-C16-C17
2	A	368	BCL	C11-C10-C8-C7
2	A	372	BCL	C4-C3-C5-C6
2	A	372	BCL	C11-C10-C8-C9
2	A	368	BCL	C11-C10-C8-C9
2	A	368	BCL	C4-C3-C5-C6
2	A	371	BCL	C11-C12-C13-C15
2	A	372	BCL	C11-C10-C8-C7
2	A	372	BCL	C12-C13-C15-C16
2	A	369	BCL	C11-C10-C8-C7
2	A	368	BCL	C2-C3-C5-C6
2	A	368	BCL	C6-C7-C8-C10

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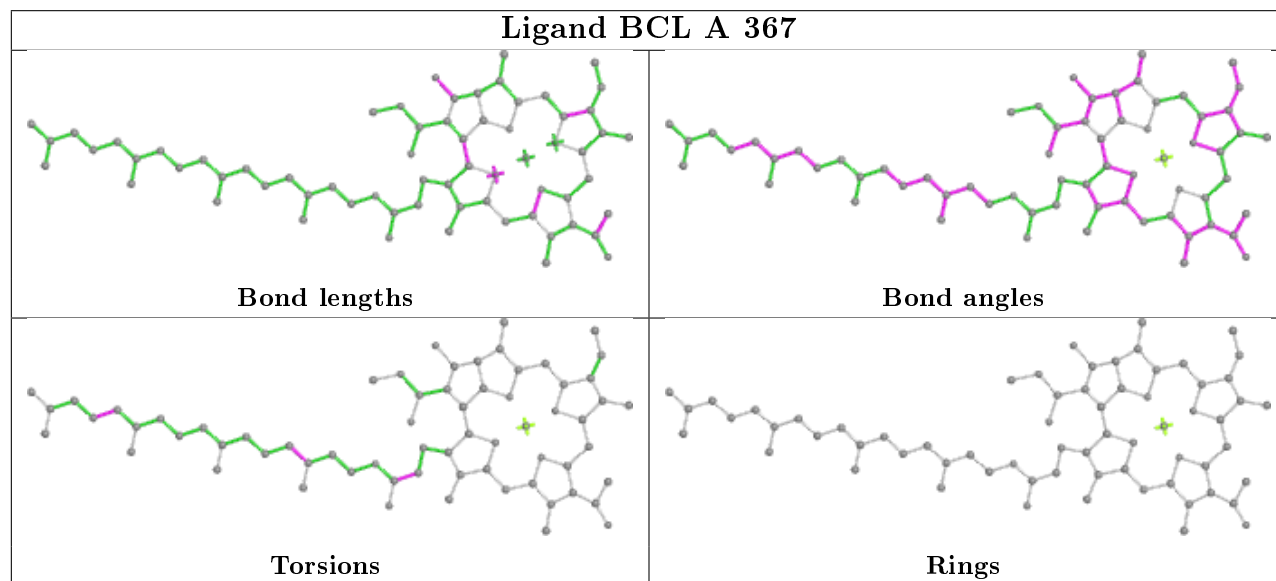
Mol	Chain	Res	Type	Atoms
2	A	372	BCL	C14-C13-C15-C16
2	A	373	BCL	C11-C10-C8-C9
2	A	373	BCL	C16-C17-C18-C20
2	A	369	BCL	C16-C17-C18-C20
2	A	371	BCL	C15-C16-C17-C18
2	A	369	BCL	C16-C17-C18-C19
2	A	373	BCL	C11-C10-C8-C7
2	A	373	BCL	C11-C12-C13-C14
2	A	370	BCL	C16-C17-C18-C19
2	A	372	BCL	C2-C3-C5-C6
2	A	370	BCL	C4-C3-C5-C6
2	A	370	BCL	C16-C17-C18-C20
2	A	372	BCL	C5-C6-C7-C8
2	A	373	BCL	CAA-CBA-CGA-O2A
2	A	373	BCL	C6-C7-C8-C10
2	A	369	BCL	C14-C13-C15-C16
2	A	368	BCL	C16-C17-C18-C20
2	A	367	BCL	C4-C3-C5-C6
2	A	367	BCL	C2-C3-C5-C6
2	A	370	BCL	C2-C3-C5-C6
2	A	372	BCL	O1A-CGA-O2A-C1
2	A	370	BCL	CAA-CBA-CGA-O2A
2	A	368	BCL	O1D-CGD-O2D-CED
2	A	369	BCL	C12-C13-C15-C16
2	A	371	BCL	C16-C17-C18-C20
2	A	372	BCL	C16-C17-C18-C19
2	A	373	BCL	CAD-CBD-CGD-O2D
2	A	367	BCL	CAA-CBA-CGA-O2A
2	A	370	BCL	CHA-CBD-CGD-O1D
2	A	370	BCL	CHA-CBD-CGD-O2D
2	A	371	BCL	CAA-CBA-CGA-O2A
2	A	371	BCL	C11-C10-C8-C9
2	A	370	BCL	CAA-CBA-CGA-O1A
2	A	367	BCL	CAA-CBA-CGA-O1A
2	A	367	BCL	C13-C15-C16-C17
2	A	373	BCL	C16-C17-C18-C19
2	A	373	BCL	CAA-CBA-CGA-O1A
2	A	369	BCL	C6-C7-C8-C9
2	A	373	BCL	C6-C7-C8-C9

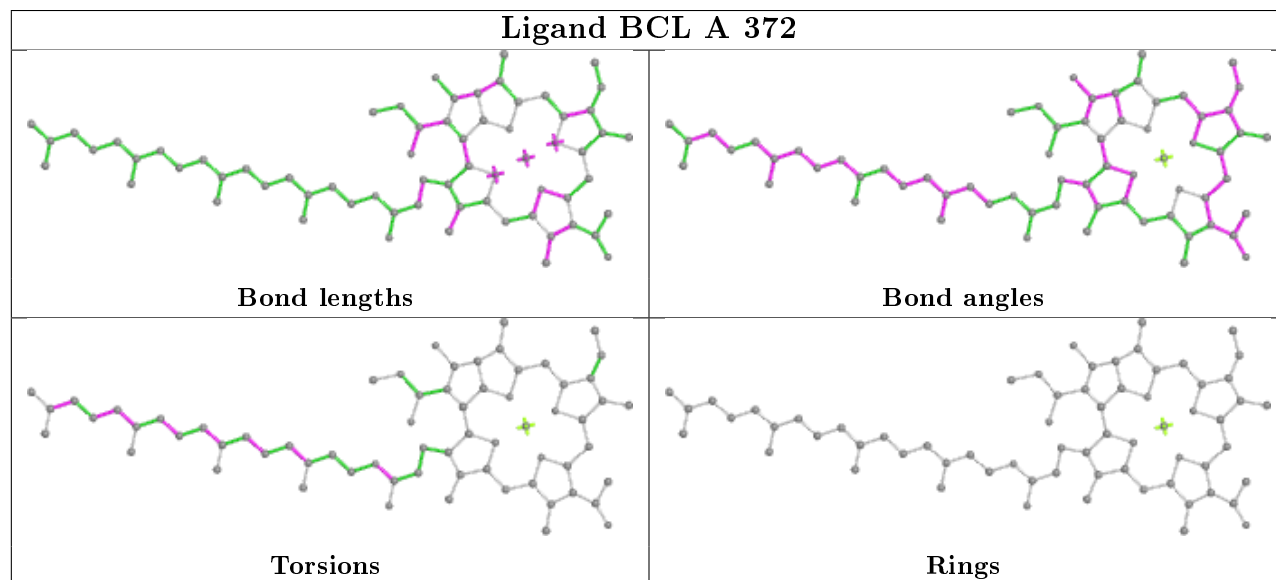
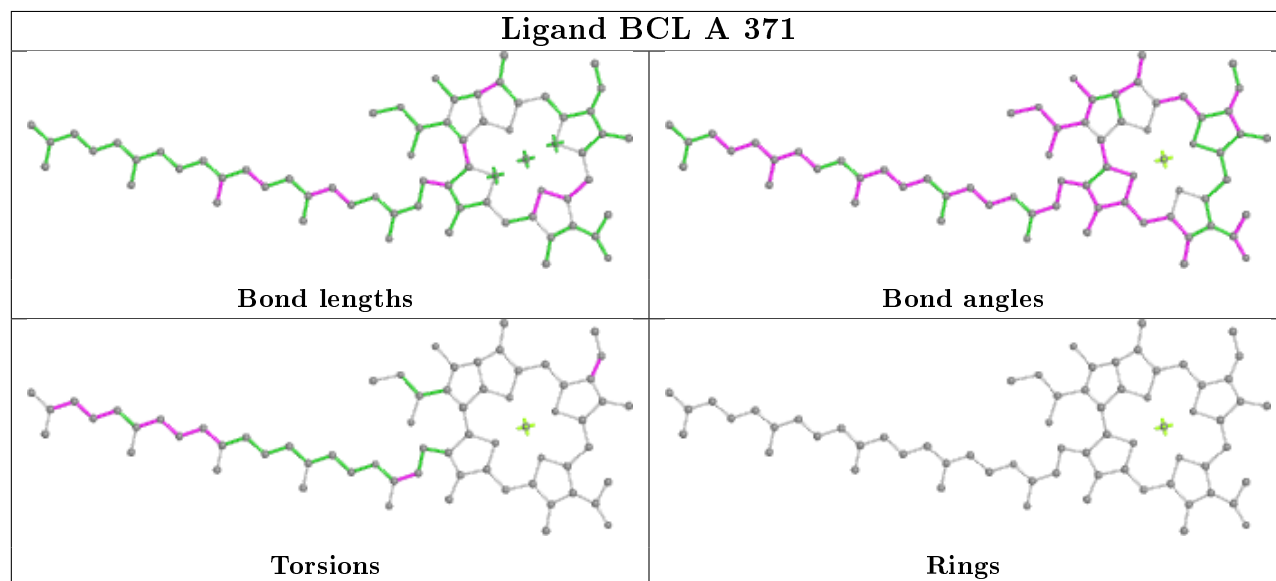
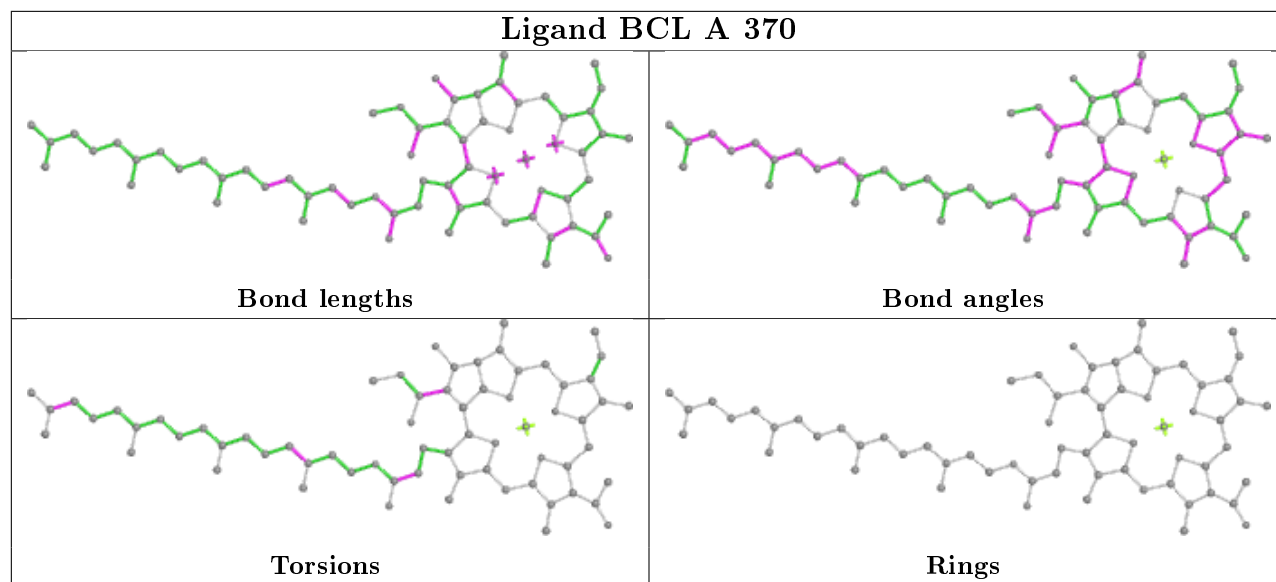
There are no ring outliers.

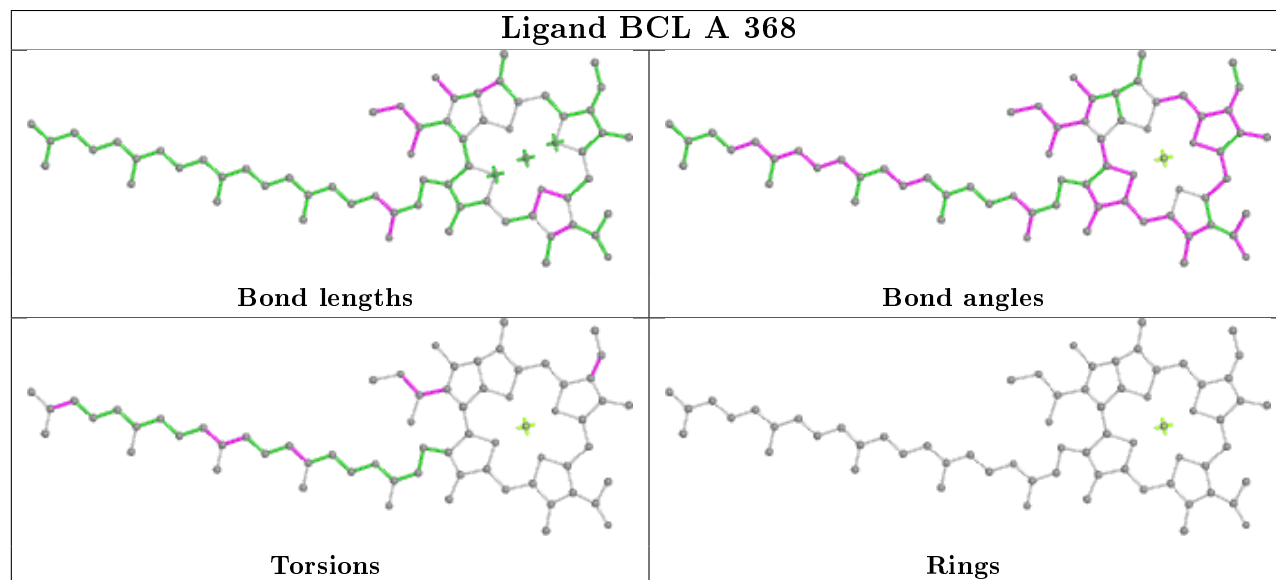
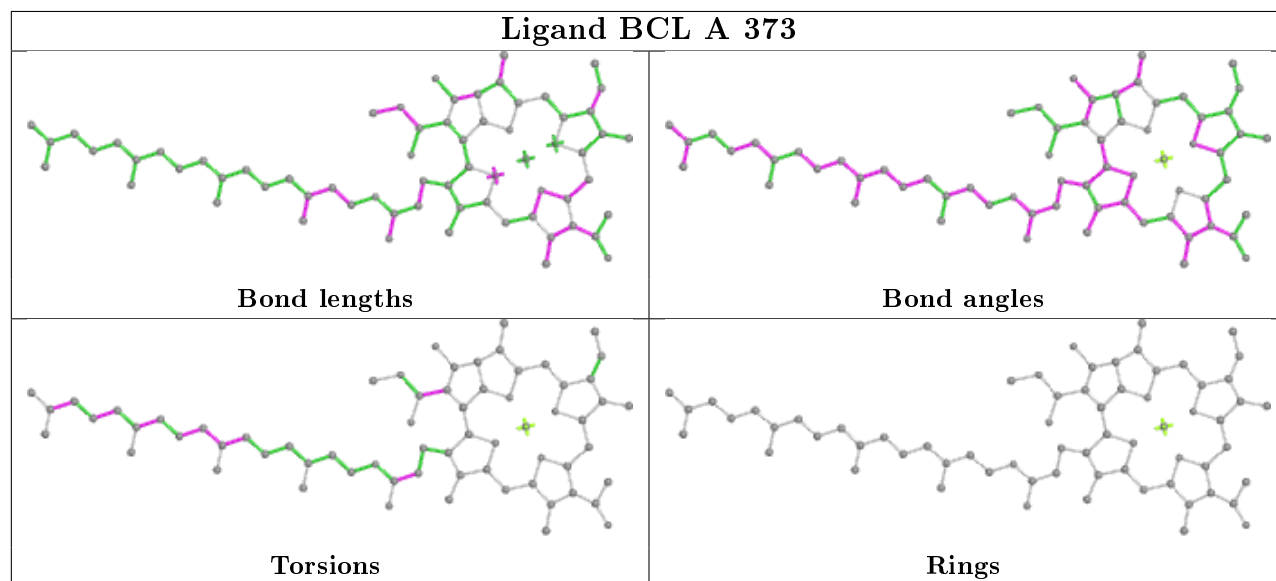
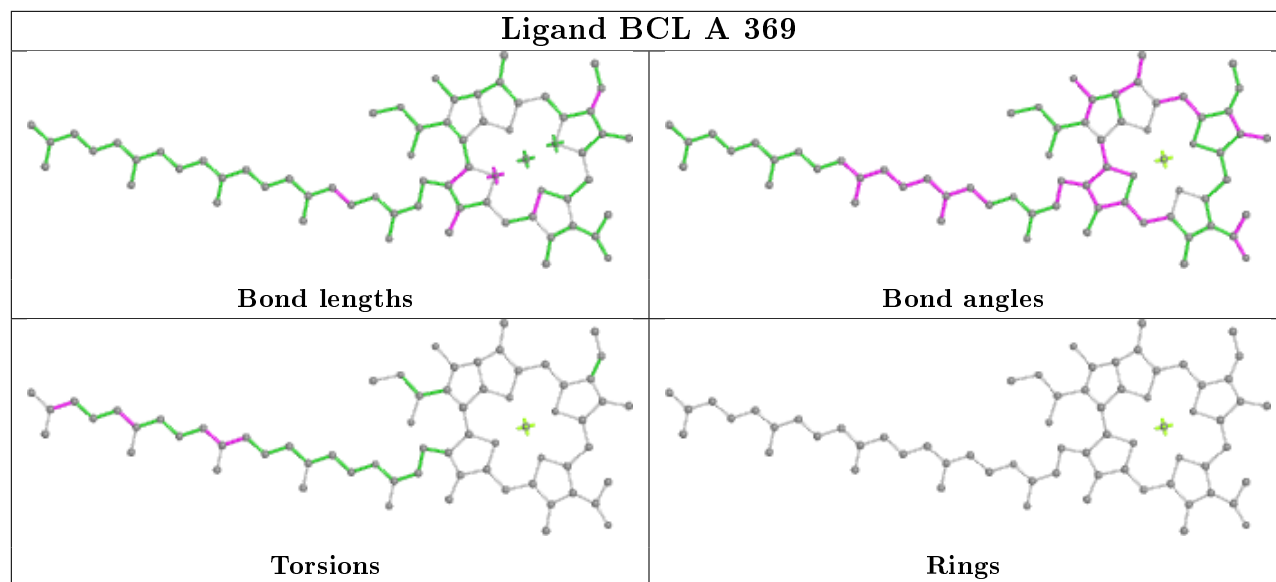
7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	367	BCL	4	0
2	A	370	BCL	5	0
2	A	371	BCL	6	0
2	A	372	BCL	3	0
2	A	369	BCL	5	0
2	A	373	BCL	4	0
2	A	368	BCL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	350/366 (95%)	-0.72	2 (0%) 89 90	8, 22, 56, 91	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	3.7
1	A	167	GLN	2.6

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BCL	A	370	66/66	0.97	0.07	3,15,41,50	0
2	BCL	A	373	66/66	0.97	0.08	8,18,37,48	0
2	BCL	A	371	66/66	0.98	0.08	6,15,32,60	0
2	BCL	A	372	66/66	0.98	0.07	4,18,37,46	0
2	BCL	A	369	66/66	0.98	0.07	6,13,24,33	0

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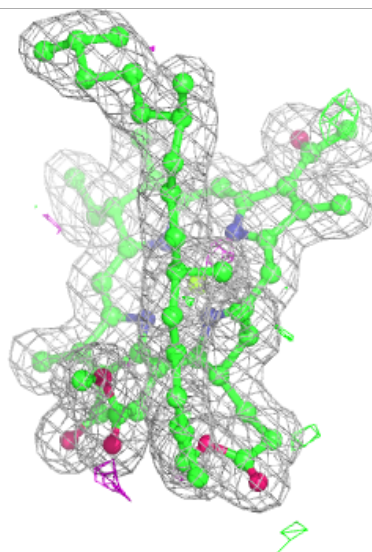
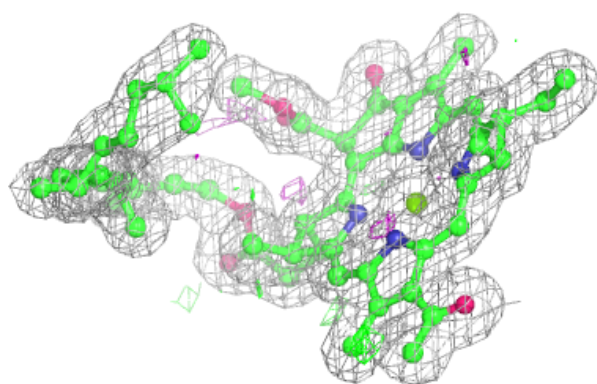
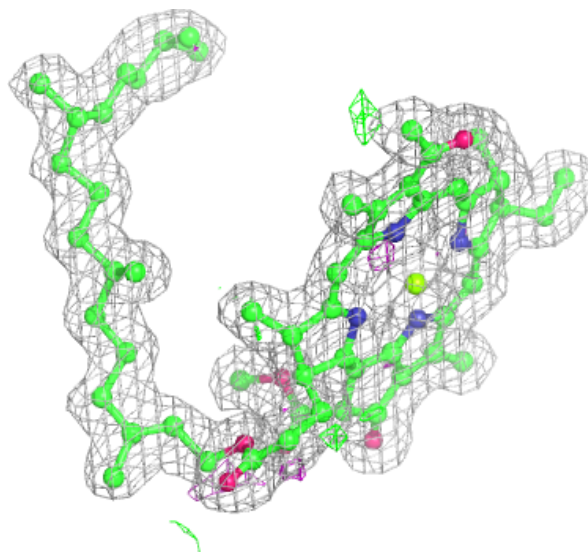
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BCL	A	367	66/66	0.98	0.09	9,20,35,47	0
2	BCL	A	368	66/66	0.98	0.09	6,18,35,53	0

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.

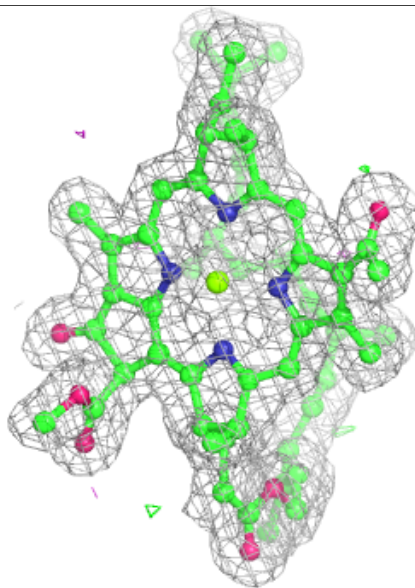
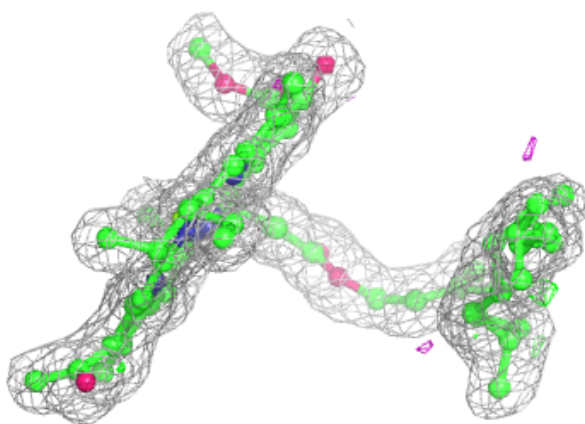
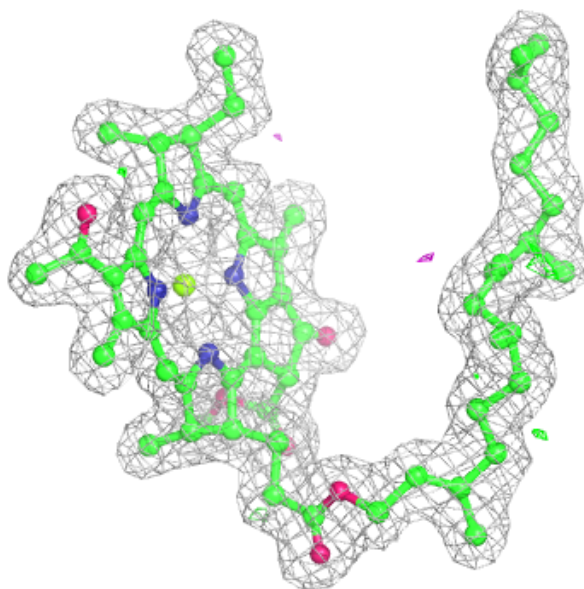
**Electron density around BCL A 370:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



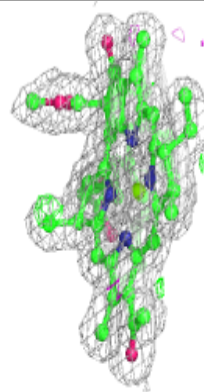
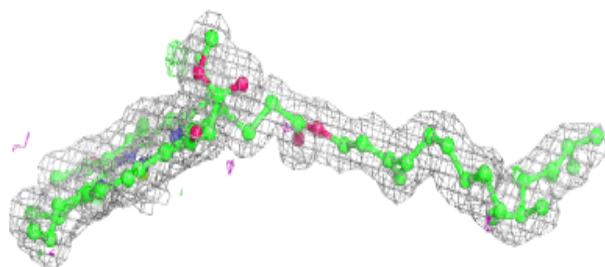
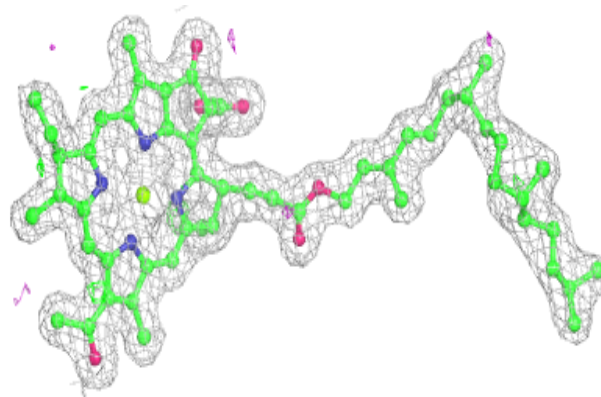
**Electron density around BCL A 373:**

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

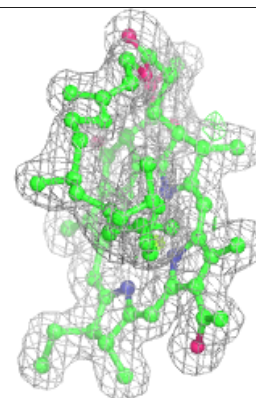
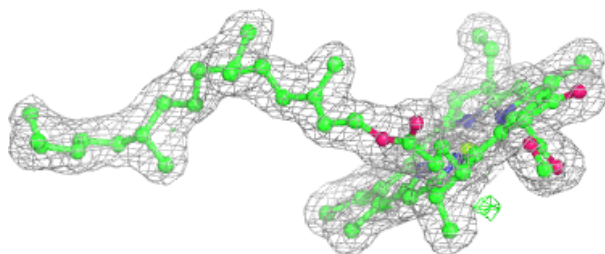
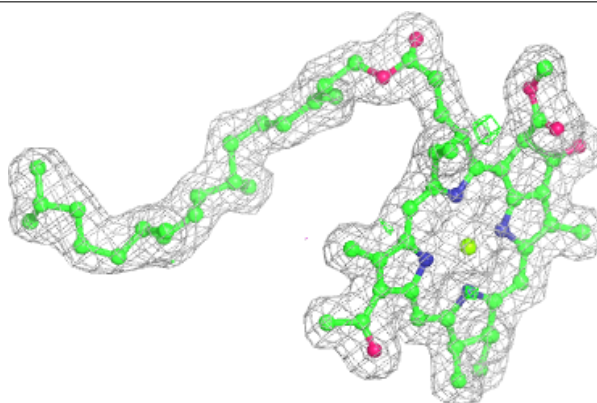


**Electron density around BCL A 371:**

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

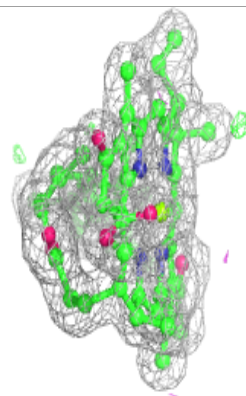
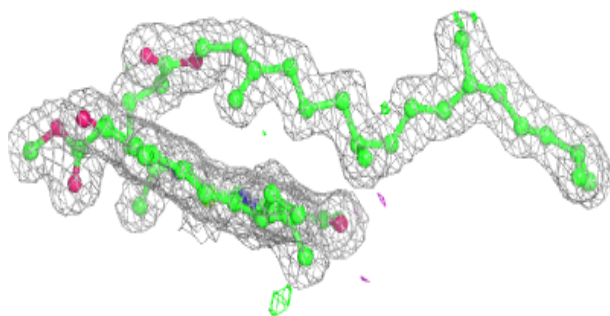
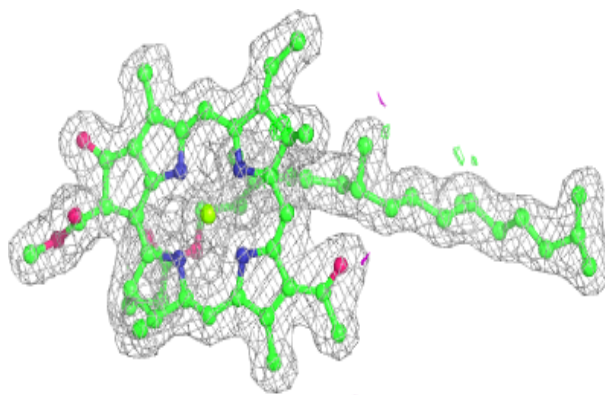
**Electron density around BCL A 372:**

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

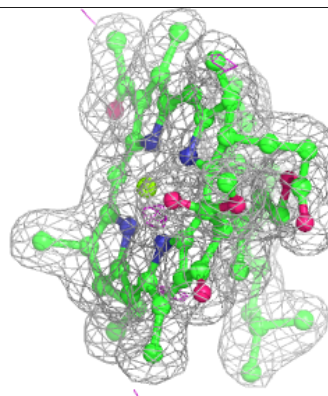
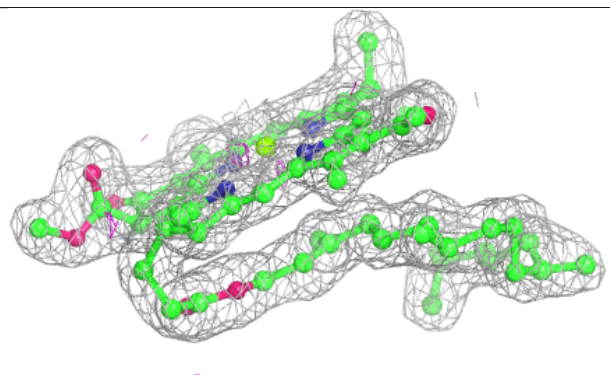
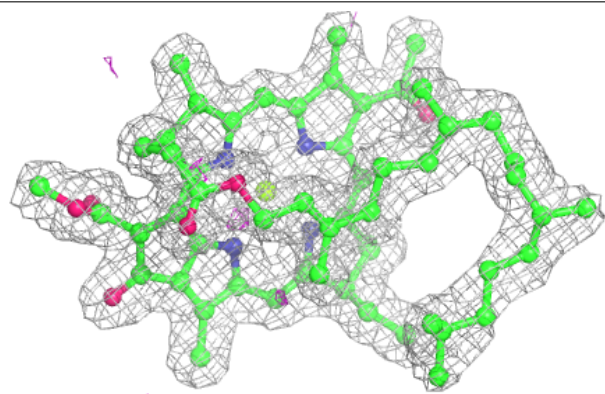


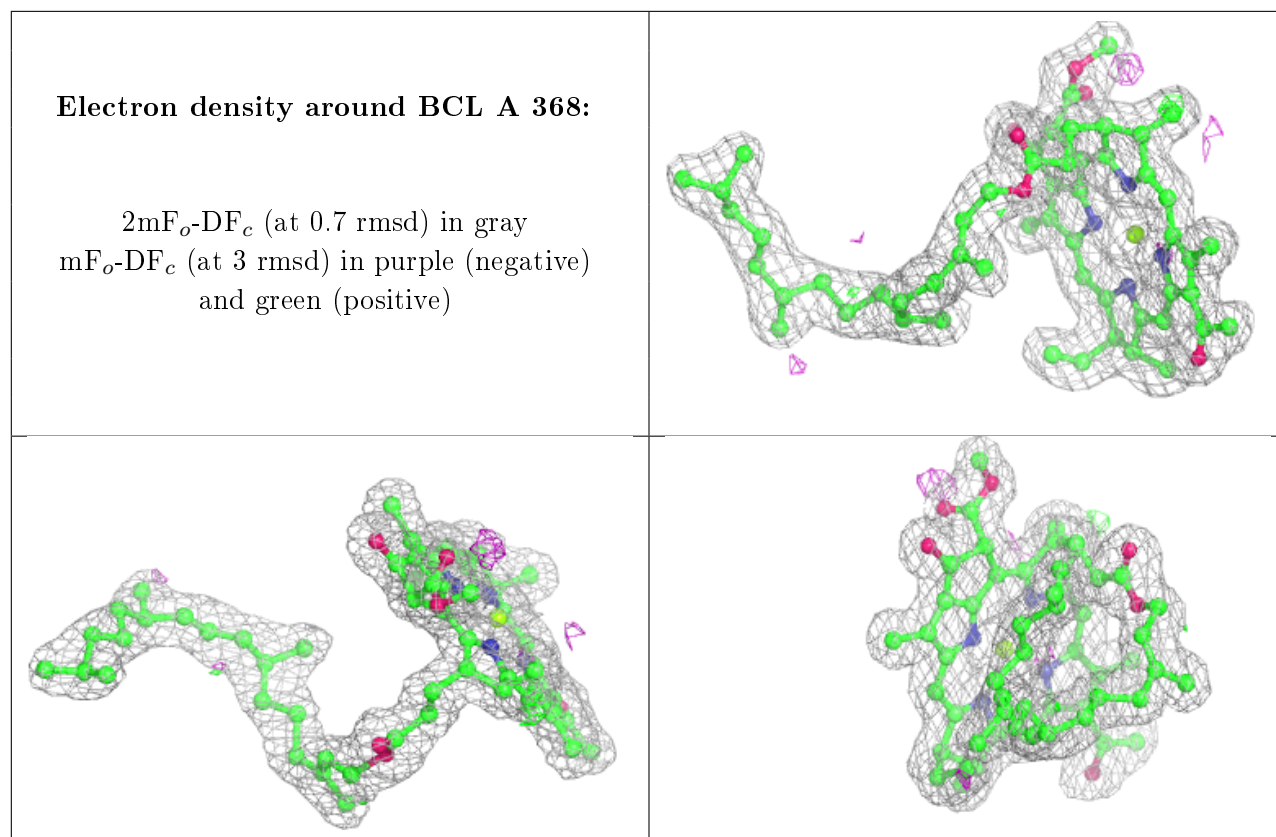
**Electron density around BCL A 369:**

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

**Electron density around BCL A 367:**

$2mF_o-DF_c$  (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.