



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:59 AM UTC

PDB ID : 4BCL / pdb_00004bcl
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

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

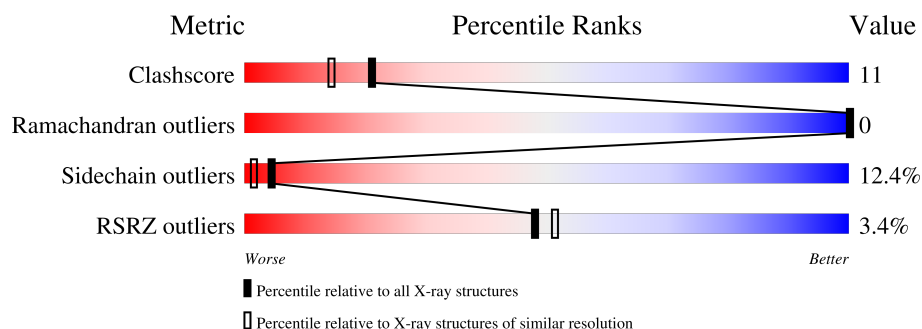
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	366	

2 Entry composition ⓘ

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.

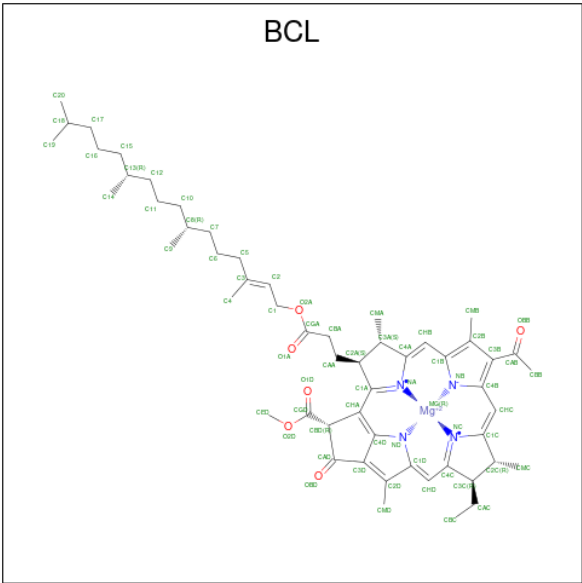
- Molecule 1 is a protein called BACTERIOCHLOROPHYLL A PROTEIN.

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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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		

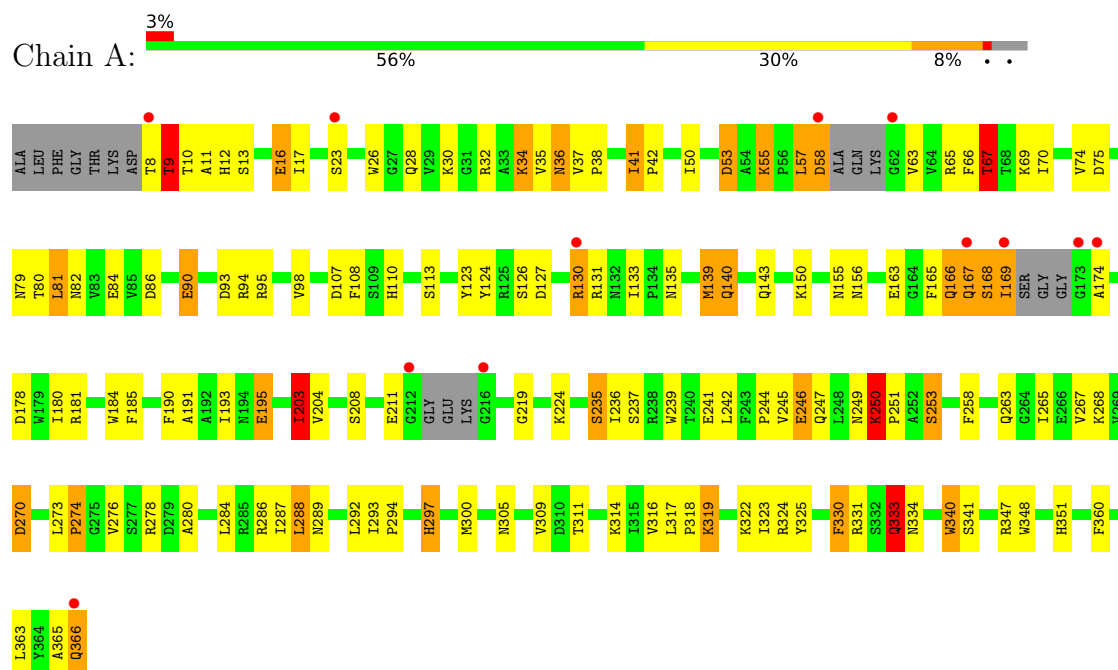
- Molecule 3 is water.

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, 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: BACTERIOCHLOROPHYLL A PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	111.90Å 111.90Å 98.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-1.90) 82.2 (20.00-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.84Å)	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 ²)	17.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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: 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	1.57	9/2783 (0.3%)	2.13	99/3771 (2.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ILE	CA-C	-8.06	1.46	1.53
1	A	124	TYR	CA-C	-7.37	1.42	1.52
1	A	274	PRO	N-CA	-6.94	1.40	1.46
1	A	297	HIS	CG-CD2	6.21	1.42	1.35
1	A	195	GLU	CD-OE1	5.63	1.36	1.25
1	A	84	GLU	C-O	5.59	1.30	1.24
1	A	191	ALA	C-O	-5.44	1.17	1.24
1	A	211	GLU	CD-OE1	5.40	1.35	1.25
1	A	86	ASP	CA-C	-5.14	1.46	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	TYR	O-C-N	11.47	137.85	122.59
1	A	185	PHE	CA-CB-CG	-10.27	103.53	113.80
1	A	124	TYR	CA-C-O	-8.89	107.79	120.51
1	A	123	TYR	CA-C-N	-8.73	104.86	121.54
1	A	123	TYR	C-N-CA	-8.73	104.86	121.54
1	A	124	TYR	CB-CA-C	-8.66	93.19	110.42
1	A	139	MET	CA-CB-CG	-8.21	97.67	114.10
1	A	156	ASN	CA-CB-CG	-8.00	104.60	112.60
1	A	250	LYS	N-CA-C	-7.92	101.09	108.22
1	A	53	ASP	CA-CB-CG	-7.46	105.14	112.60
1	A	10	THR	CA-C-N	-7.45	112.44	122.72
1	A	10	THR	C-N-CA	-7.45	112.44	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLN	CB-CG-CD	-7.21	100.35	112.60
1	A	330	PHE	CA-CB-CG	-7.18	106.62	113.80
1	A	155	ASN	N-CA-CB	7.07	122.51	111.56
1	A	319	LYS	CA-C-N	-7.02	112.61	122.86
1	A	319	LYS	C-N-CA	-7.02	112.61	122.86
1	A	11	ALA	CA-C-N	-7.01	113.33	123.00
1	A	11	ALA	C-N-CA	-7.01	113.33	123.00
1	A	184	TRP	N-CA-CB	-6.96	99.99	110.07
1	A	90	GLU	CB-CA-C	-6.84	98.04	110.56
1	A	42	PRO	N-CA-CB	6.81	110.40	103.25
1	A	190	PHE	CA-C-O	6.74	127.90	120.82
1	A	331	ARG	N-CA-CB	-6.70	100.28	110.26
1	A	314	LYS	CA-C-N	-6.68	114.39	123.14
1	A	314	LYS	C-N-CA	-6.68	114.39	123.14
1	A	110	HIS	CA-CB-CG	6.65	120.45	113.80
1	A	278	ARG	N-CA-CB	-6.60	99.24	111.52
1	A	8	THR	CA-CB-OG1	6.56	119.44	109.60
1	A	34	LYS	CB-CA-C	6.54	120.91	109.80
1	A	241	GLU	CA-C-O	6.53	127.47	120.55
1	A	107	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	93	ASP	CB-CA-C	-6.48	98.18	109.07
1	A	287	ILE	N-CA-C	-6.39	101.34	109.58
1	A	65	ARG	CA-CB-CG	-6.36	101.38	114.10
1	A	67	THR	N-CA-CB	-6.20	100.04	110.83
1	A	286	ARG	CD-NE-CZ	-6.15	115.78	124.40
1	A	366	GLN	CB-CG-CD	-6.04	102.33	112.60
1	A	250	LYS	CA-C-N	5.99	126.01	119.90
1	A	250	LYS	C-N-CA	5.99	126.01	119.90
1	A	79	ASN	CA-C-N	-5.95	112.57	122.21
1	A	79	ASN	C-N-CA	-5.95	112.57	122.21
1	A	12	HIS	CB-CA-C	-5.90	99.52	109.72
1	A	265	ILE	CA-C-N	-5.88	113.45	122.62
1	A	265	ILE	C-N-CA	-5.88	113.45	122.62
1	A	341	SER	N-CA-CB	5.86	120.55	111.24
1	A	347	ARG	CA-CB-CG	-5.81	102.48	114.10
1	A	131	ARG	CG-CD-NE	-5.79	99.26	112.00
1	A	108	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	193	ILE	O-C-N	5.77	127.56	121.91
1	A	270	ASP	CB-CA-C	-5.75	100.03	109.80
1	A	253	SER	CA-CB-OG	-5.75	99.61	111.10
1	A	245	VAL	CA-C-O	5.72	126.65	120.47
1	A	288	LEU	CA-C-O	-5.70	115.51	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASN	CA-CB-CG	-5.69	106.91	112.60
1	A	174	ALA	N-CA-C	-5.65	106.22	113.23
1	A	169	ILE	CA-CB-CG2	-5.62	100.94	110.50
1	A	130	ARG	CB-CG-CD	5.62	124.23	111.30
1	A	292	LEU	CA-C-N	-5.61	115.05	120.43
1	A	292	LEU	C-N-CA	-5.61	115.05	120.43
1	A	309	VAL	N-CA-CB	-5.59	104.29	110.99
1	A	181	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	340	TRP	CA-C-O	5.57	126.72	120.70
1	A	249	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	195	GLU	CB-CA-C	-5.54	100.38	110.63
1	A	280	ALA	N-CA-C	-5.50	105.92	113.30
1	A	90	GLU	N-CA-C	-5.49	104.14	112.04
1	A	273	LEU	N-CA-CB	-5.49	105.34	111.10
1	A	11	ALA	N-CA-C	-5.44	100.37	109.24
1	A	203	ILE	CB-CA-C	-5.42	103.61	111.68
1	A	66	PHE	CA-C-O	5.42	126.21	120.36
1	A	181	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	A	236	ILE	CA-C-N	-5.40	111.70	120.72
1	A	236	ILE	C-N-CA	-5.40	111.70	120.72
1	A	130	ARG	CA-C-N	-5.38	112.06	122.06
1	A	130	ARG	C-N-CA	-5.38	112.06	122.06
1	A	204	VAL	CB-CA-C	-5.38	102.48	110.33
1	A	316	VAL	CB-CA-C	-5.36	104.02	110.99
1	A	247	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	239	TRP	N-CA-C	5.35	117.53	111.11
1	A	63	VAL	O-C-N	5.34	128.59	122.93
1	A	235	SER	CB-CA-C	-5.34	100.11	110.46
1	A	143	GLN	N-CA-CB	-5.33	102.08	110.77
1	A	80	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	113	SER	CA-C-N	-5.25	112.83	121.80
1	A	113	SER	C-N-CA	-5.25	112.83	121.80
1	A	273	LEU	CA-C-O	5.24	125.24	120.26
1	A	190	PHE	N-CA-C	5.18	116.62	111.07
1	A	57	LEU	N-CA-C	-5.18	104.56	111.24
1	A	95	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	276	VAL	CA-C-N	-5.13	113.85	123.03
1	A	276	VAL	C-N-CA	-5.13	113.85	123.03
1	A	38	PRO	CB-CA-C	-5.10	104.42	111.21
1	A	204	VAL	CA-C-N	-5.09	116.38	122.90
1	A	204	VAL	C-N-CA	-5.09	116.38	122.90
1	A	297	HIS	N-CA-CB	-5.04	102.70	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LYS	CA-CB-CG	-5.02	104.06	114.10
1	A	9	THR	N-CA-CB	5.00	118.16	110.21
1	A	126	SER	CA-C-O	5.00	126.96	120.21

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	52	0
2	A	462	0	518	22	0
3	A	122	0	0	1	0
All	All	3304	0	3162	70	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 (70) 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:H	1:A:36:ASN:ND2	1.70	0.90
1:A:36:ASN:HD22	1:A:36:ASN:N	1.78	0.78
1:A:140:GLN:HE21	1:A:140:GLN:N	1.84	0.71
1:A:140:GLN:H	1:A:140:GLN:NE2	1.83	0.70
2:A:369:BCL:HBA2	2:A:369:BCL:C4A	2.21	0.69
1:A:139:MET:HB2	1:A:237:SER:HB2	1.75	0.68
1:A:246:GLU:H	1:A:246:GLU:CD	2.02	0.66
1:A:195:GLU:HG3	1:A:300:MET:SD	2.36	0.65
1:A:55:LYS:O	1:A:55:LYS:HG2	1.96	0.65
2:A:370:BCL:HBB2	2:A:370:BCL:HMB3	1.79	0.65
1:A:67:THR:HG22	3:A:446:HOH:O	1.97	0.64
1:A:135:ASN:HD21	1:A:289:ASN:HD21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:TRP:HA	1:A:274:PRO:HA	1.81	0.62
2:A:368:BCL:CBB	2:A:368:BCL:HMB1	2.33	0.59
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
1:A:250:LYS:HB2	1:A:251:PRO:CD	2.36	0.56
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:244:PRO:HG2	2:A:373:BCL:HMB2	1.91	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:166:GLN:O	1:A:167:GLN:C	2.50	0.50
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:368:BCL:HMB1	2:A:368:BCL:HBB2	1.96	0.48
1:A:325:TYR:HB3	1:A:363:LEU:HD12	1.98	0.46
2:A:371:BCL:H42	2:A:373:BCL:H171	1.98	0.45
2:A:371:BCL:HBB3	2:A:371:BCL:HHC	1.97	0.45
2:A:370:BCL:H2A	2:A:370:BCL:O2A	2.16	0.45
1:A:168:SER:O	1:A:169:ILE:C	2.58	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:9:THR:HG21	1:A:37:VAL:HG12	1.99	0.44
1:A:81:LEU:HG	1:A:82:ASN:N	2.30	0.44
1:A:330:PHE:HA	1:A:340:TRP:CD1	2.52	0.44
1:A:178:ASP:OD1	1:A:178:ASP:C	2.61	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
1:A:258:PHE:C	1:A:258:PHE:CD1	2.97	0.43
2:A:367:BCL:HAA1	2:A:367:BCL:CBF	2.49	0.43
2:A:369:BCL:CBB	2:A:369:BCL:HMB1	2.49	0.42
1:A:180:ILE:HG21	1:A:203:ILE:HD12	2.02	0.42
2:A:371:BCL:H2A	2:A:371:BCL:CGD	2.48	0.42
1:A:58:ASP:OD1	1:A:58:ASP:O	2.37	0.42
1:A:50:ILE:HD12	1:A:70:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:370:BCL:CBB	2:A:370:BCL:CMB	2.99	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
1:A:98:VAL:O	1:A:98:VAL:HG13	2.21	0.41
2:A:371:BCL:H62	2:A:371:BCL:H102	1.98	0.41
1:A:74:VAL:O	1:A:75:ASP:C	2.64	0.41
1:A:16:GLU:OE2	1:A:30:LYS:HD3	2.20	0.41
1:A:242:LEU:HD12	1:A:242:LEU:C	2.46	0.41
2:A:369:BCL:CBB	2:A:369:BCL:CMB	2.99	0.41
2:A:371:BCL:H112	2:A:371:BCL:H142	1.30	0.41
1:A:317:LEU:HB3	1:A:318:PRO:CD	2.49	0.41
2:A:372:BCL:CBB	2:A:372:BCL:HMB3	2.51	0.40
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:H111	2:A:370:BCL:H152	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%)	255 (88%)	36 (12%)	4 1

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
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	41	ILE
1	A	55	LYS
1	A	57	LEU
1	A	58	ASP
1	A	67	THR
1	A	81	LEU
1	A	140	GLN
1	A	163	GLU
1	A	166	GLN
1	A	167	GLN
1	A	168	SER
1	A	203	ILE
1	A	208	SER
1	A	224	LYS
1	A	235	SER
1	A	246	GLU
1	A	250	LYS
1	A	263	GLN
1	A	267	VAL
1	A	268	LYS
1	A	270	ASP
1	A	288	LEU
1	A	319	LYS
1	A	322	LYS
1	A	323	ILE
1	A	324	ARG
1	A	333	GLN
1	A	360	PHE
1	A	366	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	79	ASN
1	A	82	ASN
1	A	140	GLN
1	A	209	ASN
1	A	272	ASN
1	A	289	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](#)

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	369	1	69,74,74	1.43	12 (17%)	79,115,115	1.61	16 (20%)
2	BCL	A	370	1	69,74,74	1.58	15 (21%)	79,115,115	2.00	22 (27%)
2	BCL	A	373	1	69,74,74	1.72	17 (24%)	79,115,115	1.68	17 (21%)
2	BCL	A	372	3	69,74,74	1.96	16 (23%)	79,115,115	1.83	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BCL	A	367	1	69,74,74	1.76	12 (17%)	79,115,115	2.06	21 (26%)
2	BCL	A	371	1	69,74,74	1.66	15 (21%)	79,115,115	2.10	25 (31%)
2	BCL	A	368	1	69,74,74	1.68	13 (18%)	79,115,115	2.09	27 (34%)

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	369	1	-	3/41/137/137	-
2	BCL	A	370	1	-	8/41/137/137	-
2	BCL	A	373	1	-	11/41/137/137	-
2	BCL	A	372	3	-	11/41/137/137	-
2	BCL	A	367	1	-	5/41/137/137	-
2	BCL	A	371	1	-	11/41/137/137	-
2	BCL	A	368	1	-	10/41/137/137	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	372	BCL	MG-NB	-8.05	1.89	2.05
2	A	367	BCL	C3B-C4B	5.82	1.52	1.41
2	A	372	BCL	C3B-C4B	5.81	1.52	1.41
2	A	368	BCL	MG-ND	-5.38	1.95	2.05
2	A	367	BCL	MG-NB	-5.03	1.95	2.05
2	A	367	BCL	MG-ND	4.86	2.15	2.05
2	A	371	BCL	C1D-ND	4.79	1.44	1.37
2	A	368	BCL	OBD-CAD	4.77	1.30	1.22
2	A	372	BCL	C1D-ND	4.60	1.43	1.37
2	A	371	BCL	MG-NB	-4.57	1.96	2.05
2	A	370	BCL	O1D-CGD	-4.48	1.10	1.21
2	A	368	BCL	MG-NB	-4.44	1.97	2.05
2	A	373	BCL	MG-NB	-4.43	1.97	2.05
2	A	373	BCL	CAC-C3C	4.08	1.61	1.54
2	A	372	BCL	C3C-C4C	-4.01	1.46	1.51
2	A	368	BCL	O1D-CGD	-3.98	1.11	1.21
2	A	373	BCL	C3B-C4B	3.95	1.48	1.41
2	A	370	BCL	MG-ND	-3.87	1.98	2.05
2	A	367	BCL	MG-NA	3.81	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	369	BCL	C3D-C4D	-3.72	1.35	1.44
2	A	368	BCL	O2D-CED	3.59	1.53	1.45
2	A	369	BCL	MG-NA	3.50	2.14	2.06
2	A	370	BCL	OBB-CAB	-3.45	1.15	1.23
2	A	371	BCL	C3B-C4B	3.35	1.47	1.41
2	A	371	BCL	C1B-C2B	3.32	1.50	1.43
2	A	371	BCL	C4B-NB	3.25	1.42	1.37
2	A	370	BCL	MG-NC	3.25	2.14	2.06
2	A	373	BCL	O2D-CED	3.24	1.52	1.45
2	A	370	BCL	MG-NA	3.12	2.13	2.06
2	A	369	BCL	C2A-C1A	-3.07	1.45	1.52
2	A	370	BCL	C1D-C2D	3.06	1.51	1.45
2	A	367	BCL	C1B-C2B	3.06	1.50	1.43
2	A	367	BCL	C3D-C4D	-3.02	1.37	1.44
2	A	367	BCL	CBB-CAB	3.01	1.56	1.50
2	A	368	BCL	O2A-CGA	-2.98	1.24	1.33
2	A	368	BCL	O2D-CGD	-2.98	1.25	1.33
2	A	371	BCL	MG-ND	-2.98	1.99	2.05
2	A	372	BCL	CMB-C2B	2.94	1.56	1.50
2	A	367	BCL	C3C-C4C	-2.94	1.47	1.51
2	A	370	BCL	C1A-CHA	-2.91	1.31	1.43
2	A	370	BCL	O1A-CGA	-2.89	1.13	1.22
2	A	373	BCL	C1-C2	2.89	1.57	1.49
2	A	373	BCL	CHD-C1D	2.79	1.43	1.38
2	A	370	BCL	OBD-CAD	2.75	1.27	1.22
2	A	371	BCL	CBB-CAB	2.74	1.55	1.50
2	A	372	BCL	C1B-NB	2.74	1.41	1.37
2	A	368	BCL	O1A-CGA	-2.74	1.14	1.22
2	A	372	BCL	MG-ND	-2.73	2.00	2.05
2	A	373	BCL	C3B-C2B	-2.72	1.33	1.42
2	A	369	BCL	C1-C2	2.70	1.56	1.49
2	A	371	BCL	CAA-C2A	2.66	1.58	1.54
2	A	373	BCL	O1A-CGA	-2.64	1.14	1.22
2	A	369	BCL	C3B-C4B	2.62	1.46	1.41
2	A	371	BCL	C6-C7	2.61	1.63	1.52
2	A	372	BCL	CBD-CGD	-2.60	1.44	1.52
2	A	372	BCL	CHD-C1D	2.60	1.43	1.38
2	A	372	BCL	MG-NC	2.58	2.12	2.06
2	A	373	BCL	CMB-C2B	-2.57	1.45	1.50
2	A	370	BCL	C1-C2	2.56	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	373	BCL	C2-C3	2.51	1.38	1.33
2	A	372	BCL	CAA-CBA	2.48	1.60	1.52
2	A	371	BCL	C1A-CHA	-2.45	1.33	1.43
2	A	373	BCL	CMD-C2D	-2.45	1.45	1.50
2	A	372	BCL	CMA-C3A	-2.44	1.48	1.53
2	A	373	BCL	CHC-C4B	-2.41	1.34	1.39
2	A	370	BCL	C3B-C4B	2.41	1.45	1.41
2	A	369	BCL	CAC-C3C	2.38	1.58	1.54
2	A	368	BCL	C3B-C2B	-2.35	1.34	1.42
2	A	373	BCL	CAA-CBA	2.34	1.59	1.52
2	A	369	BCL	C1B-NB	2.34	1.40	1.37
2	A	368	BCL	OBB-CAB	-2.33	1.17	1.23
2	A	369	BCL	CMB-C2B	2.33	1.55	1.50
2	A	367	BCL	CHD-C1D	2.31	1.42	1.38
2	A	373	BCL	O2D-CGD	2.30	1.38	1.33
2	A	369	BCL	C1D-C2D	-2.28	1.40	1.45
2	A	371	BCL	CMB-C2B	2.27	1.55	1.50
2	A	367	BCL	CMD-C2D	2.24	1.55	1.50
2	A	371	BCL	CHC-C4B	-2.22	1.34	1.39
2	A	368	BCL	C1D-C2D	-2.21	1.41	1.45
2	A	370	BCL	C6-C5	2.21	1.60	1.52
2	A	370	BCL	O2A-CGA	-2.20	1.27	1.33
2	A	373	BCL	C4-C3	2.18	1.56	1.50
2	A	371	BCL	C9-C8	2.17	1.59	1.52
2	A	370	BCL	C3A-C2A	2.14	1.60	1.54
2	A	372	BCL	C1A-CHA	-2.13	1.34	1.43
2	A	369	BCL	CMA-C3A	-2.11	1.48	1.53
2	A	368	BCL	C1B-C2B	-2.11	1.38	1.43
2	A	367	BCL	C1A-CHA	-2.11	1.34	1.43
2	A	371	BCL	C1-C2	2.09	1.55	1.49
2	A	367	BCL	OBB-CAB	-2.09	1.18	1.23
2	A	370	BCL	C3B-C2B	-2.08	1.35	1.42
2	A	371	BCL	C2-C3	2.07	1.37	1.33
2	A	372	BCL	C3B-C2B	-2.05	1.35	1.42
2	A	369	BCL	MG-NB	-2.04	2.01	2.05
2	A	368	BCL	C3B-CAB	2.04	1.53	1.46
2	A	369	BCL	CHC-C1C	2.04	1.42	1.37
2	A	372	BCL	O1D-CGD	-2.03	1.16	1.21
2	A	373	BCL	C3A-C2A	2.01	1.59	1.54

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	367	BCL	C4A-NA-C1A	-8.44	102.83	106.68
2	A	371	BCL	C4A-NA-C1A	-7.42	103.30	106.68
2	A	370	BCL	C4A-NA-C1A	-7.18	103.40	106.68
2	A	368	BCL	C1D-ND-C4D	-6.66	101.64	106.31
2	A	372	BCL	C1-C2-C3	-5.89	116.55	126.20
2	A	370	BCL	CHA-C1A-NA	-5.37	114.23	126.39
2	A	368	BCL	O2D-CGD-CBD	5.21	120.33	111.23
2	A	368	BCL	C1C-NC-C4C	-5.02	104.39	106.68
2	A	368	BCL	O2D-CGD-O1D	-4.85	114.40	123.85
2	A	373	BCL	CBA-CAA-C2A	-4.84	99.39	113.79
2	A	367	BCL	C1D-ND-C4D	4.62	109.55	106.31
2	A	371	BCL	C3D-C2D-C1D	-4.47	99.73	105.83
2	A	372	BCL	C2C-C3C-C4C	4.39	107.92	101.34
2	A	370	BCL	C1C-NC-C4C	4.27	108.63	106.68
2	A	371	BCL	C2D-C1D-ND	4.23	114.31	110.13
2	A	370	BCL	O2D-CGD-CBD	4.17	118.53	111.23
2	A	371	BCL	C1-C2-C3	-4.12	119.45	126.20
2	A	369	BCL	CHD-C1D-ND	-4.08	119.06	124.80
2	A	369	BCL	C2A-C3A-C4A	4.05	108.41	101.87
2	A	369	BCL	C4-C3-C5	4.04	122.25	115.23
2	A	367	BCL	C11-C12-C13	-4.04	102.53	115.97
2	A	370	BCL	CMC-C2C-C1C	-4.02	100.97	111.77
2	A	371	BCL	CBA-CAA-C2A	-4.02	101.83	113.79
2	A	371	BCL	O2D-CGD-O1D	-4.01	116.04	123.85
2	A	371	BCL	CED-O2D-CGD	-3.99	106.87	115.92
2	A	372	BCL	CHC-C4B-NB	3.92	129.93	124.05
2	A	373	BCL	C4D-CHA-C1A	3.91	125.90	121.24
2	A	368	BCL	C2D-C1D-ND	3.87	113.96	110.13
2	A	373	BCL	C1C-NC-C4C	-3.82	104.94	106.68
2	A	367	BCL	C4D-CHA-C1A	3.72	125.68	121.24
2	A	367	BCL	CHD-C1D-ND	-3.71	119.59	124.80
2	A	372	BCL	C4-C3-C5	3.68	121.61	115.23
2	A	370	BCL	C3B-C4B-NB	-3.68	104.91	109.76
2	A	373	BCL	C4A-NA-C1A	-3.65	105.01	106.68
2	A	371	BCL	C11-C12-C13	-3.65	103.84	115.97
2	A	369	BCL	C3A-C2A-C1A	-3.63	95.90	101.34
2	A	373	BCL	C1-C2-C3	-3.61	120.28	126.20
2	A	371	BCL	CHA-C1A-NA	-3.60	118.24	126.39
2	A	373	BCL	C11-C10-C8	-3.59	104.03	115.97
2	A	373	BCL	C9-C8-C7	-3.54	98.65	111.27
2	A	371	BCL	C2B-C1B-NB	-3.53	106.67	110.33
2	A	367	BCL	CBC-CAC-C3C	-3.51	105.96	113.41
2	A	367	BCL	C4D-C3D-CAD	-3.50	104.31	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	373	BCL	CHA-C1A-NA	-3.44	118.59	126.39
2	A	369	BCL	C6-C7-C8	-3.44	104.52	115.97
2	A	370	BCL	C2B-C1B-NB	-3.39	106.81	110.33
2	A	367	BCL	C1-C2-C3	-3.33	120.74	126.20
2	A	370	BCL	C16-C17-C18	-3.31	101.16	115.94
2	A	372	BCL	C14-C13-C15	-3.28	99.57	111.27
2	A	368	BCL	C16-C15-C13	-3.26	105.12	115.97
2	A	369	BCL	CAA-C2A-C3A	-3.23	104.26	113.00
2	A	369	BCL	C4D-CHA-C1A	3.22	125.08	121.24
2	A	371	BCL	CMD-C2D-C1D	3.20	130.36	124.73
2	A	368	BCL	C4D-CHA-C1A	3.18	125.03	121.24
2	A	372	BCL	C2B-C1B-NB	3.17	113.61	110.33
2	A	367	BCL	C7-C6-C5	-3.14	104.89	113.26
2	A	372	BCL	C16-C17-C18	-3.10	102.09	115.94
2	A	370	BCL	C15-C13-C12	-3.07	96.49	112.07
2	A	368	BCL	CHD-C1D-ND	-3.06	120.49	124.80
2	A	372	BCL	CAA-C2A-C3A	-3.06	104.73	113.00
2	A	367	BCL	C16-C15-C13	-3.06	105.81	115.97
2	A	370	BCL	CAA-C2A-C1A	-3.05	101.99	111.97
2	A	368	BCL	CHA-C1A-NA	-2.94	119.74	126.39
2	A	373	BCL	O2A-CGA-O1A	-2.93	116.29	123.63
2	A	367	BCL	OBB-CAB-CBB	-2.93	113.22	119.77
2	A	368	BCL	C11-C10-C8	-2.92	106.25	115.97
2	A	371	BCL	C1D-ND-C4D	-2.91	104.27	106.31
2	A	368	BCL	C7-C6-C5	-2.91	105.50	113.26
2	A	371	BCL	C14-C13-C15	-2.88	101.00	111.27
2	A	372	BCL	CHD-C1D-ND	-2.87	120.76	124.80
2	A	367	BCL	CBB-CAB-C3B	2.84	126.39	120.40
2	A	367	BCL	CHA-C1A-NA	-2.81	120.03	126.39
2	A	369	BCL	C7-C6-C5	-2.81	105.78	113.26
2	A	368	BCL	CHB-C1B-NB	2.81	128.26	124.05
2	A	370	BCL	CMD-C2D-C3D	2.80	134.11	127.69
2	A	368	BCL	CMC-C2C-C3C	-2.79	103.21	113.98
2	A	372	BCL	CMD-C2D-C1D	2.77	129.61	124.73
2	A	372	BCL	C4A-NA-C1A	2.76	107.94	106.68
2	A	373	BCL	CHB-C4A-NA	-2.76	120.42	124.40
2	A	368	BCL	O2A-CGA-O1A	-2.75	116.74	123.63
2	A	373	BCL	C7-C6-C5	-2.75	105.94	113.26
2	A	371	BCL	O1D-CGD-CBD	2.73	129.91	124.52
2	A	367	BCL	CGD-CBD-CAD	-2.69	102.12	110.85
2	A	370	BCL	O2D-CGD-O1D	-2.68	118.64	123.85
2	A	372	BCL	CMB-C2B-C1B	2.67	129.48	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	BCL	C17-C16-C15	-2.65	101.42	113.28
2	A	367	BCL	C1C-NC-C4C	-2.65	105.47	106.68
2	A	368	BCL	C4A-NA-C1A	-2.64	105.47	106.68
2	A	367	BCL	CAC-C3C-C4C	-2.64	106.73	112.58
2	A	373	BCL	O2A-CGA-CBA	2.64	119.87	111.83
2	A	369	BCL	C9-C8-C10	-2.61	101.97	111.27
2	A	368	BCL	C3D-C2D-C1D	-2.59	102.29	105.83
2	A	368	BCL	C11-C12-C13	-2.56	107.44	115.97
2	A	367	BCL	O1D-CGD-CBD	2.56	129.57	124.52
2	A	371	BCL	CAA-CBA-CGA	-2.56	105.95	113.21
2	A	371	BCL	C7-C6-C5	-2.54	106.49	113.26
2	A	370	BCL	CMC-C2C-C3C	-2.53	104.20	113.98
2	A	368	BCL	CMA-C3A-C4A	-2.51	105.02	111.77
2	A	371	BCL	C4D-CHA-C1A	2.51	124.23	121.24
2	A	369	BCL	OBB-CAB-CBB	-2.49	114.20	119.77
2	A	373	BCL	C12-C11-C10	-2.47	102.20	113.28
2	A	370	BCL	O2A-CGA-CBA	2.46	119.33	111.83
2	A	370	BCL	C11-C12-C13	-2.45	107.83	115.97
2	A	373	BCL	C2A-C1A-CHA	2.44	128.10	123.87
2	A	371	BCL	C9-C8-C7	-2.43	102.61	111.27
2	A	368	BCL	C3B-C4B-NB	-2.42	106.56	109.76
2	A	368	BCL	OBB-CAB-CBB	-2.42	114.35	119.77
2	A	371	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
2	A	372	BCL	C11-C10-C8	-2.38	108.05	115.97
2	A	370	BCL	CHC-C1C-NC	-2.38	120.96	124.40
2	A	371	BCL	C17-C16-C15	-2.38	102.63	113.28
2	A	370	BCL	O2A-CGA-O1A	-2.38	117.69	123.63
2	A	371	BCL	CHD-C1D-ND	-2.37	121.47	124.80
2	A	372	BCL	C11-C12-C13	-2.35	108.14	115.97
2	A	369	BCL	C1-C2-C3	-2.34	122.36	126.20
2	A	369	BCL	CMC-C2C-C3C	-2.34	104.95	113.98
2	A	370	BCL	C12-C11-C10	-2.33	102.86	113.28
2	A	373	BCL	C16-C15-C13	-2.29	108.34	115.97
2	A	373	BCL	C20-C18-C19	-2.29	100.32	110.53
2	A	372	BCL	C7-C6-C5	-2.28	107.19	113.26
2	A	372	BCL	CHA-C1A-NA	-2.27	121.24	126.39
2	A	369	BCL	CHA-C1A-NA	-2.27	121.24	126.39
2	A	372	BCL	OBB-CAB-CBB	-2.27	114.69	119.77
2	A	372	BCL	CHC-C4B-C3B	-2.22	122.91	131.72
2	A	371	BCL	OBB-CAB-CBB	-2.20	114.84	119.77
2	A	368	BCL	C12-C11-C10	-2.20	103.41	113.28
2	A	368	BCL	C2A-C3A-C4A	-2.20	98.31	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	372	BCL	CBC-CAC-C3C	-2.19	108.77	113.41
2	A	371	BCL	C2A-C3A-C4A	-2.19	98.33	101.87
2	A	368	BCL	CHC-C1C-NC	2.18	127.54	124.40
2	A	370	BCL	C11-C10-C8	-2.16	108.79	115.97
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	367	BCL	CMD-C2D-C3D	2.14	132.60	127.69
2	A	368	BCL	CMB-C2B-C1B	-2.13	122.17	125.42
2	A	372	BCL	CHB-C1B-C2B	-2.13	121.24	127.43
2	A	372	BCL	C3B-C4B-NB	-2.12	106.96	109.76
2	A	373	BCL	CMA-C3A-C4A	-2.11	106.10	111.77
2	A	372	BCL	C4-C3-C2	-2.10	118.23	123.63
2	A	368	BCL	CED-O2D-CGD	-2.10	111.16	115.92
2	A	371	BCL	C19-C18-C17	-2.08	99.25	111.55
2	A	367	BCL	C2A-C3A-C4A	-2.06	98.55	101.87
2	A	369	BCL	CBA-CAA-C2A	-2.04	107.73	113.79
2	A	371	BCL	CHB-C1B-NB	2.02	127.09	124.05
2	A	370	BCL	C9-C8-C7	-2.02	104.06	111.27
2	A	368	BCL	CMD-C2D-C1D	2.02	128.29	124.73
2	A	369	BCL	CMA-C3A-C2A	-2.02	106.16	113.98
2	A	368	BCL	C2C-C3C-C4C	-2.01	98.32	101.34
2	A	367	BCL	C4-C3-C5	2.00	118.71	115.23
2	A	370	BCL	C1-C2-C3	-2.00	122.92	126.20

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	368	BCL	C4C-C3C-CAC-CBC
2	A	370	BCL	CHA-CBD-CGD-O1D
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	CBD-CGD-O2D-CED
2	A	368	BCL	C6-C7-C8-C9
2	A	371	BCL	C10-C11-C12-C13
2	A	373	BCL	C11-C12-C13-C15
2	A	373	BCL	C8-C10-C11-C12
2	A	371	BCL	C13-C15-C16-C17
2	A	371	BCL	C8-C10-C11-C12
2	A	372	BCL	C13-C15-C16-C17
2	A	372	BCL	C10-C11-C12-C13

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

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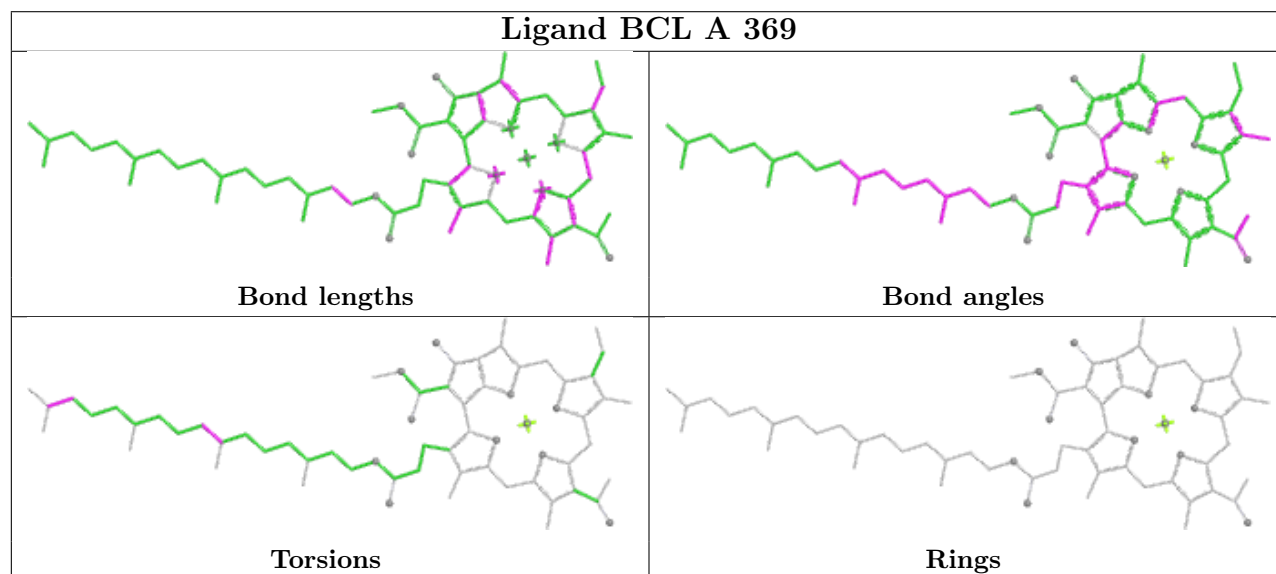
Mol	Chain	Res	Type	Atoms
2	A	373	BCL	CAA-CBA-CGA-O1A
2	A	371	BCL	C11-C10-C8-C9
2	A	367	BCL	CAA-CBA-CGA-O1A

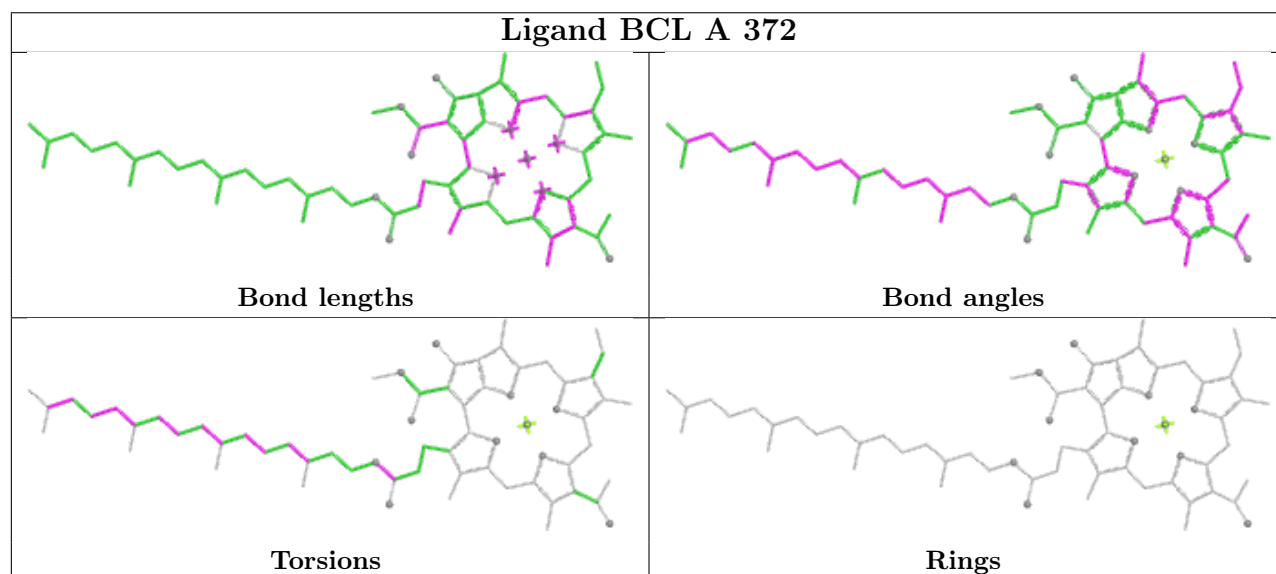
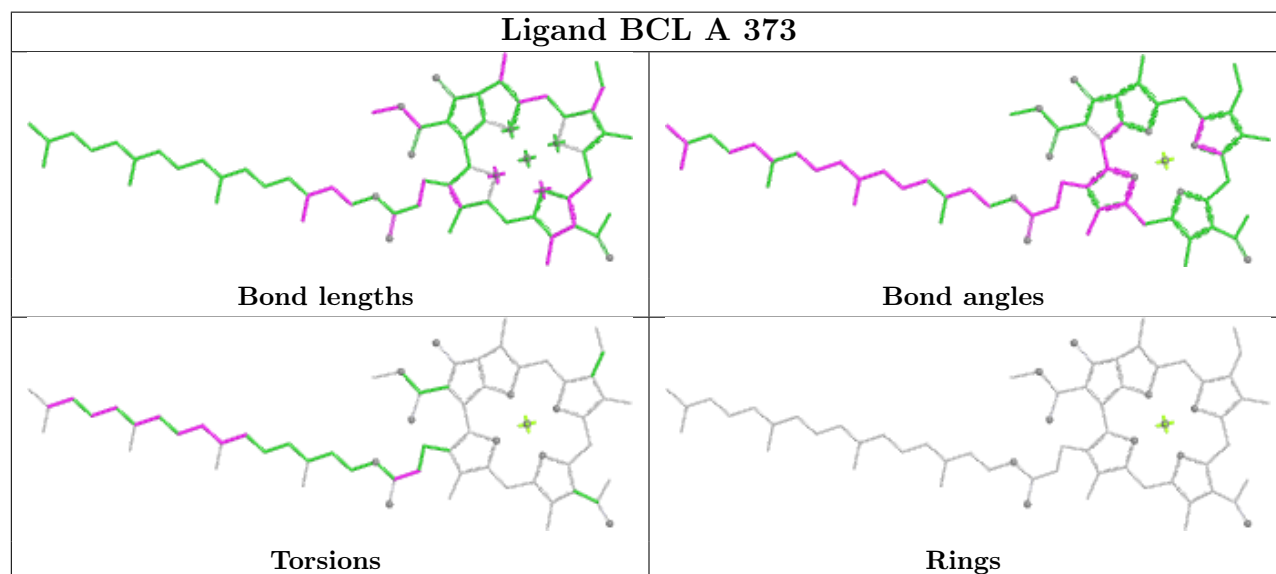
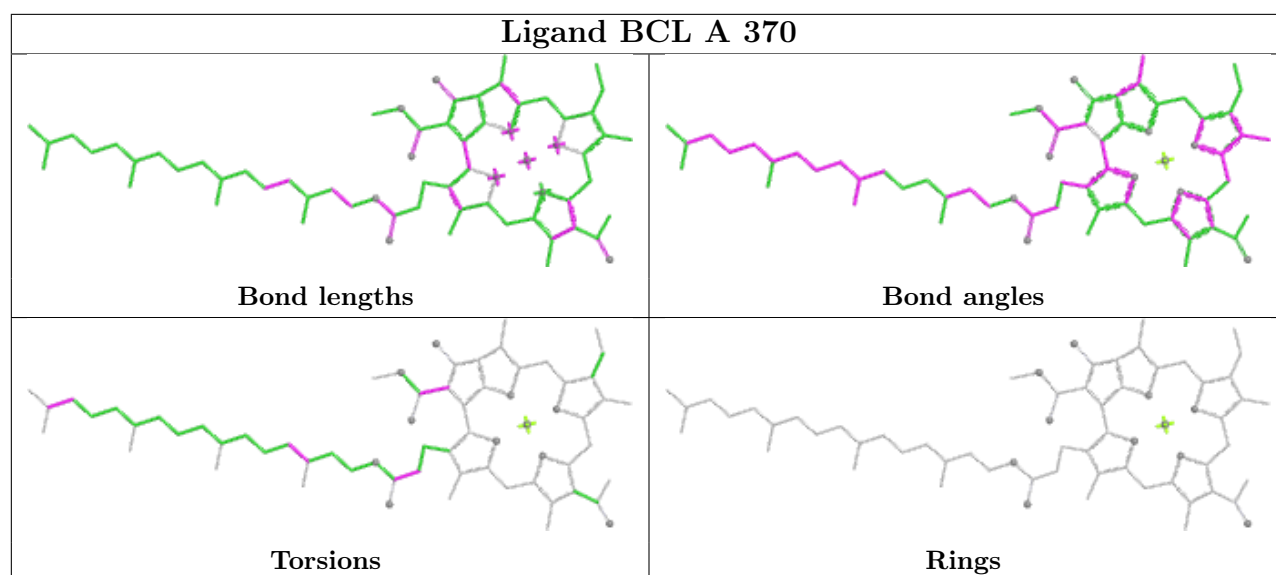
There are no ring outliers.

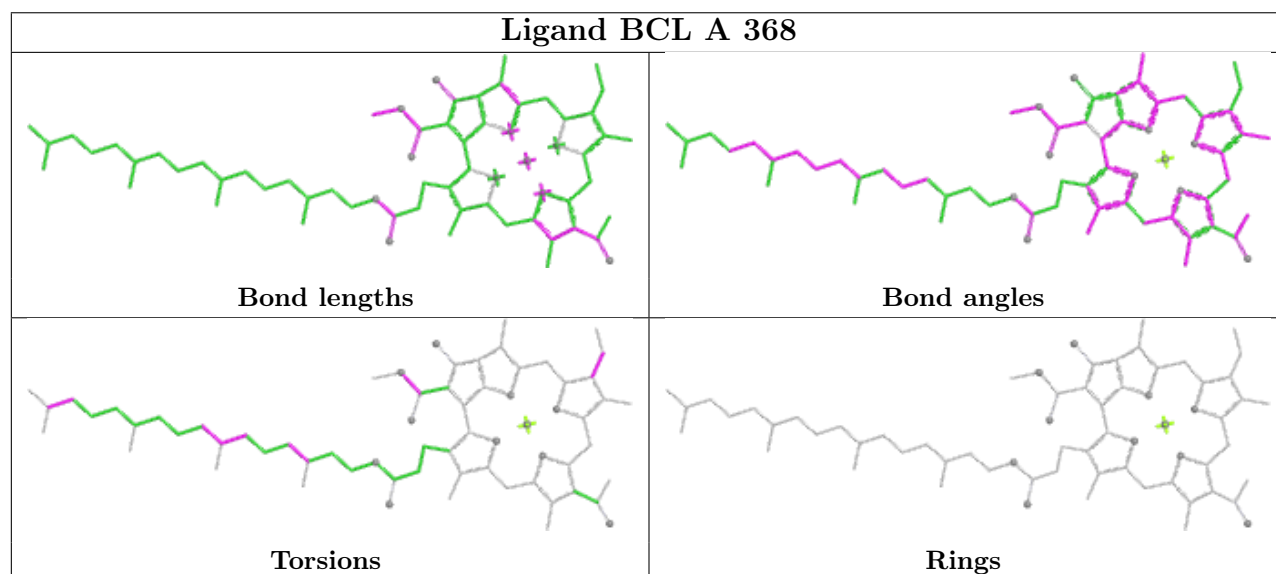
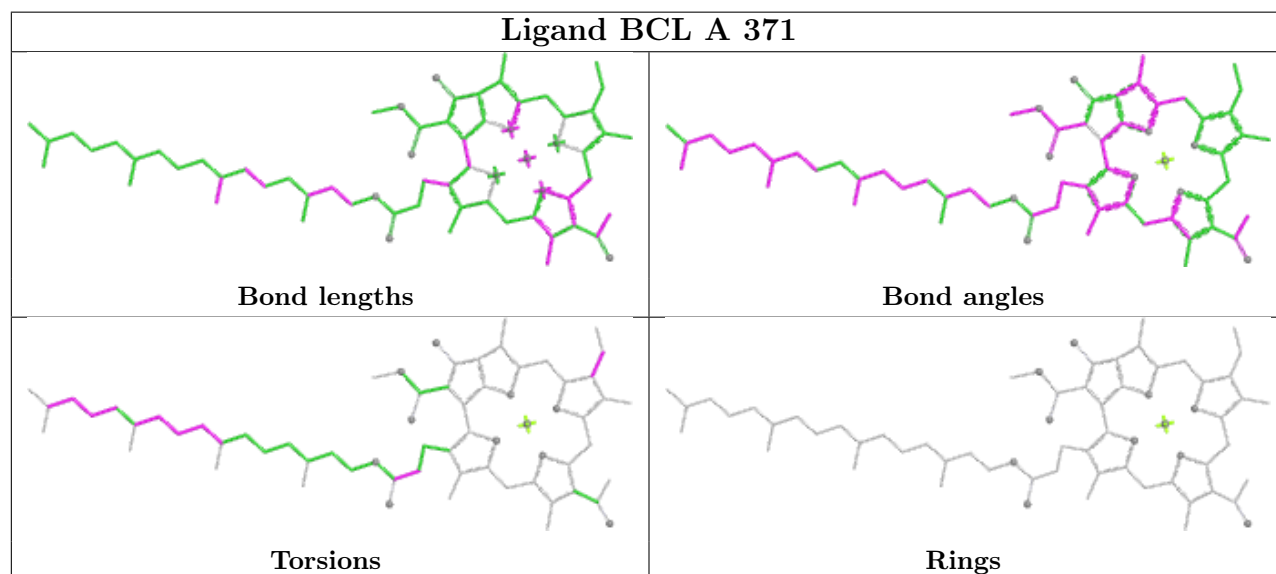
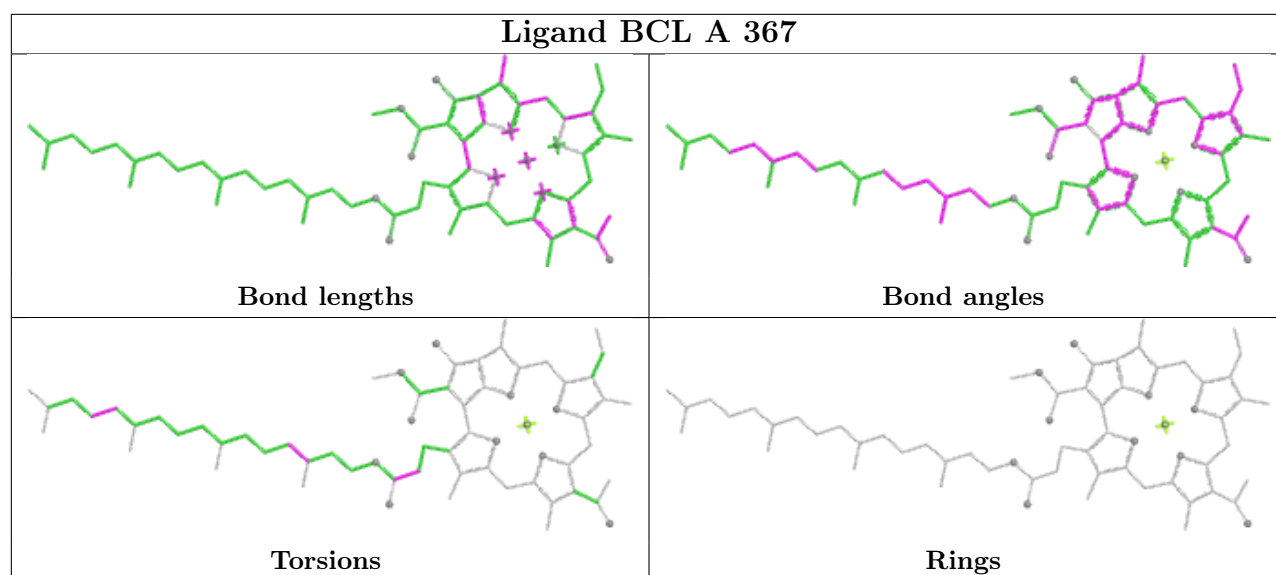
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	369	BCL	4	0
2	A	370	BCL	5	0
2	A	373	BCL	2	0
2	A	372	BCL	2	0
2	A	367	BCL	3	0
2	A	371	BCL	5	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, 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	350/366 (95%)	-0.19	12 (3%)	48 51	8, 22, 56, 91	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	5.3
1	A	174	ALA	5.1
1	A	212	GLY	4.6
1	A	173	GLY	4.4
1	A	58	ASP	3.7
1	A	169	ILE	3.4
1	A	62	GLY	3.1
1	A	130	ARG	3.0
1	A	366	GLN	2.5
1	A	23	SER	2.4
1	A	216	GLY	2.3
1	A	167	GLN	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.

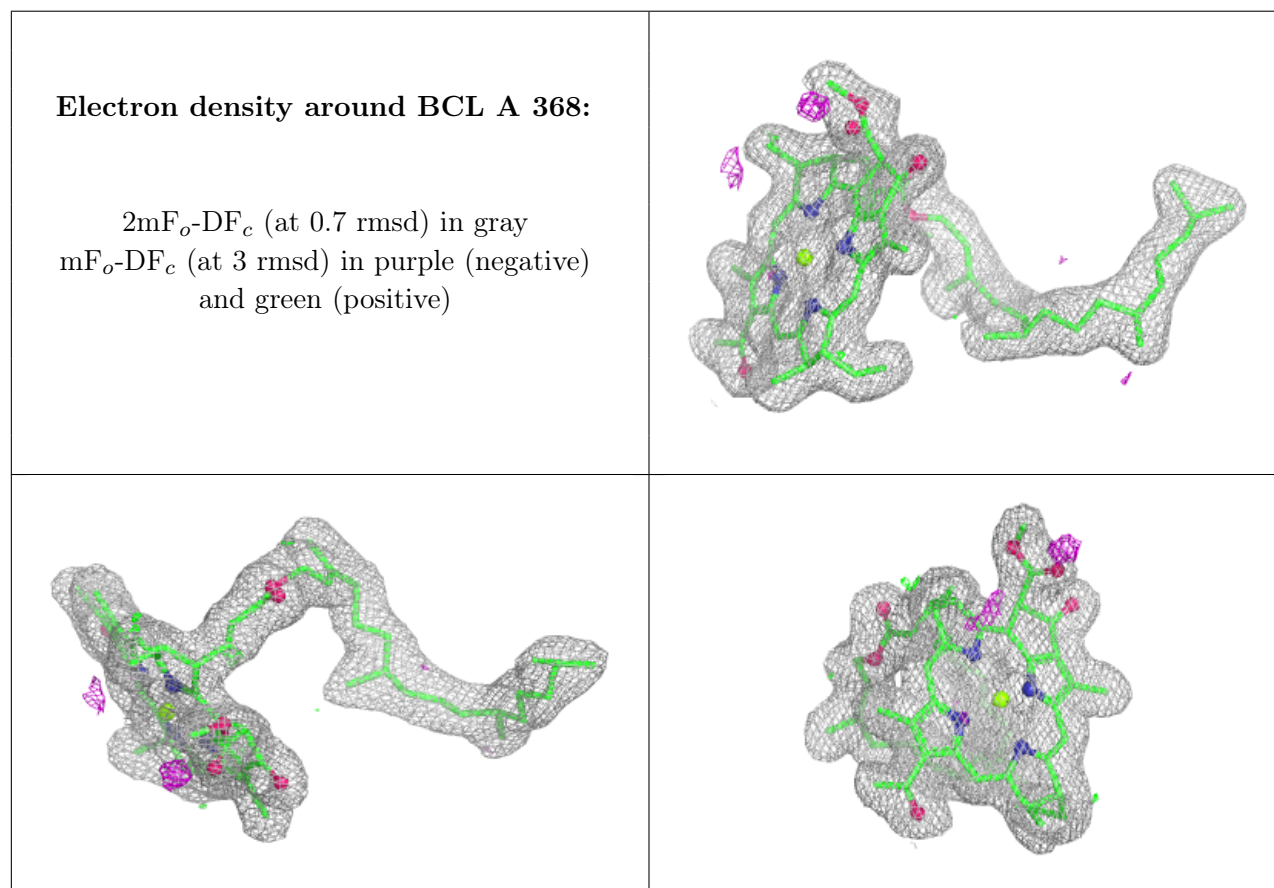
6.4 Ligands [i](#)

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.

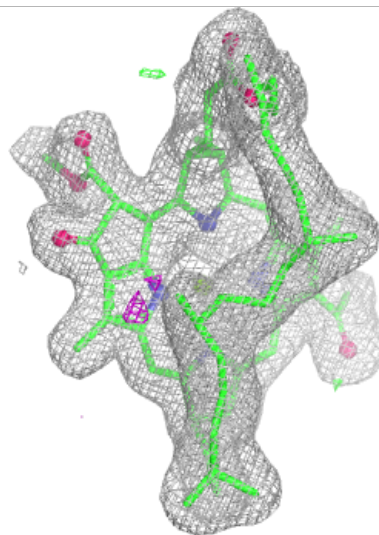
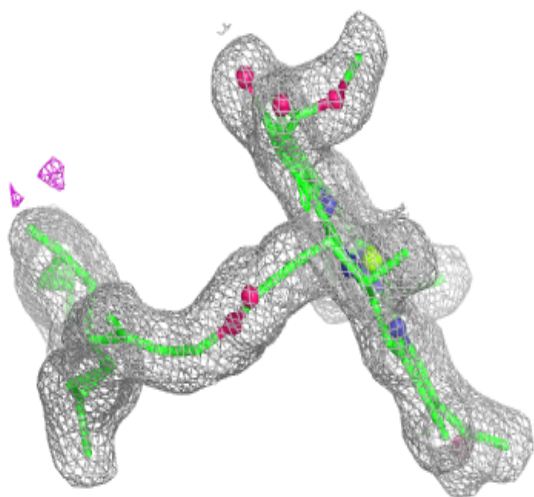
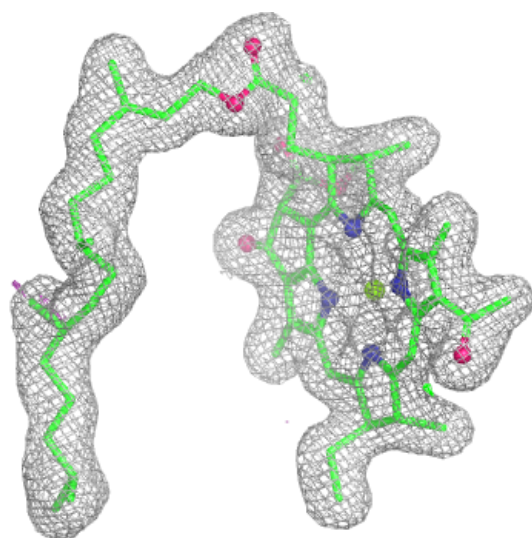
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BCL	A	368	66/66	0.97	0.05	6,18,35,53	0
2	BCL	A	373	66/66	0.97	0.06	8,18,37,48	0
2	BCL	A	369	66/66	0.98	0.04	6,13,24,33	0
2	BCL	A	370	66/66	0.98	0.05	3,15,41,50	0
2	BCL	A	371	66/66	0.98	0.05	6,15,32,60	0
2	BCL	A	372	66/66	0.98	0.05	4,18,37,46	0
2	BCL	A	367	66/66	0.98	0.05	9,20,35,47	0

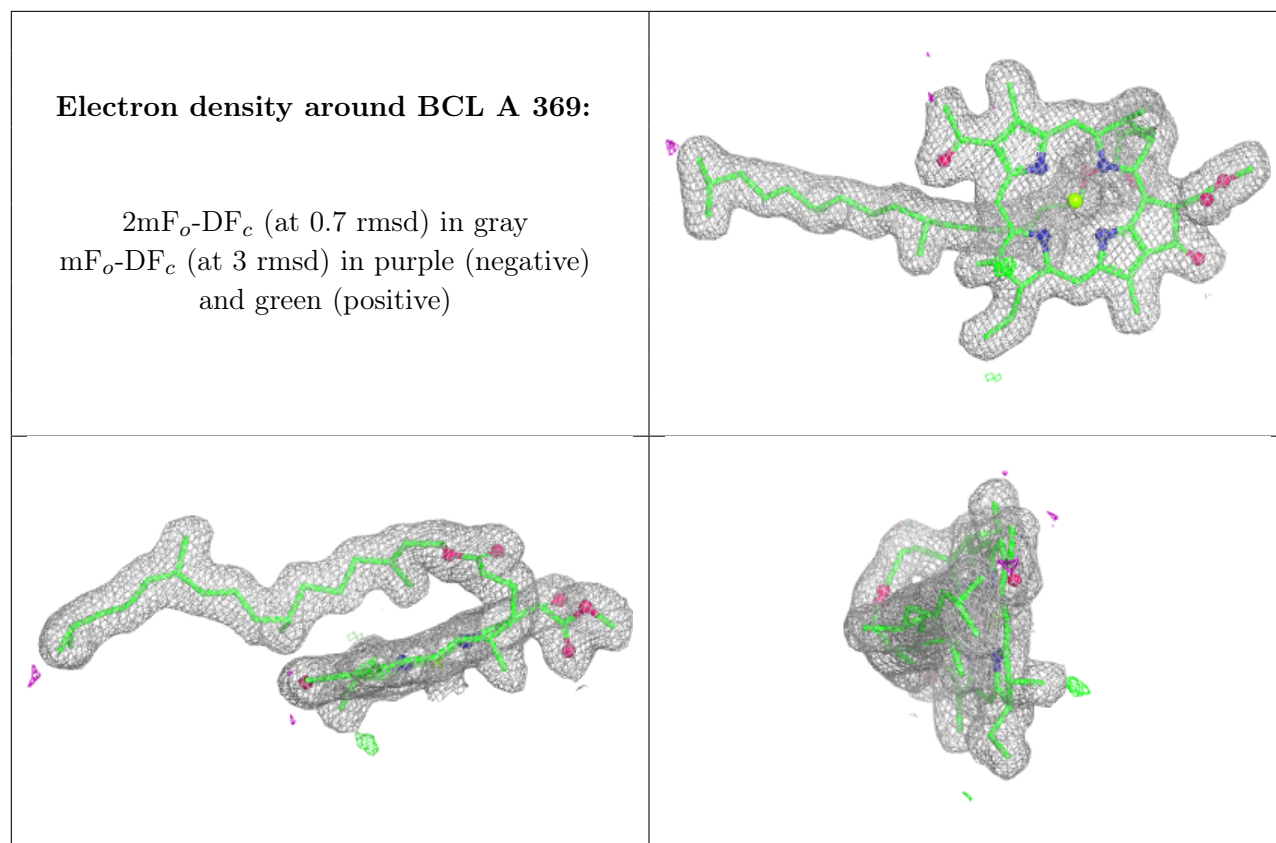
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around BCL A 373:

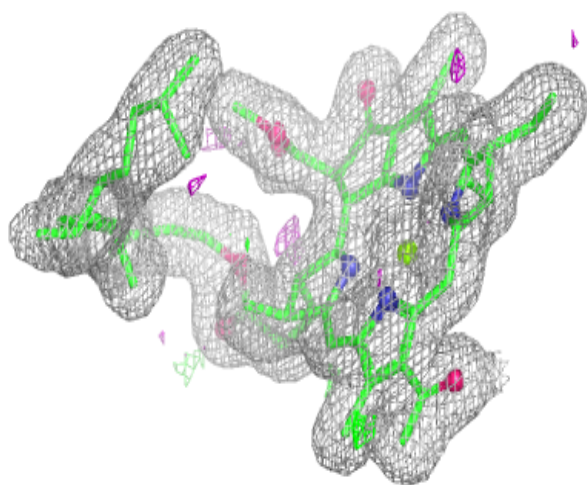
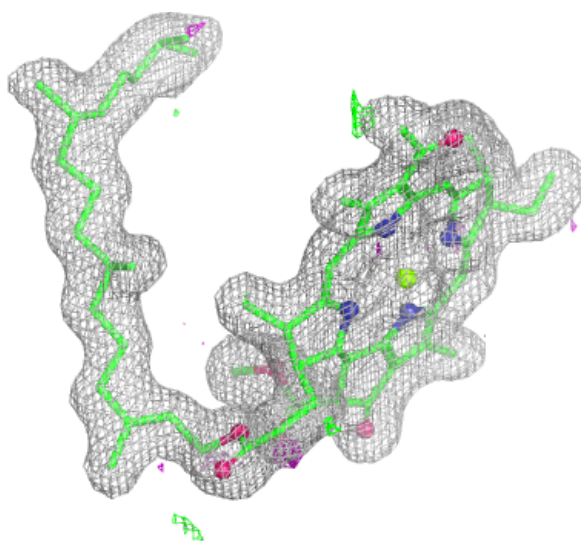
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





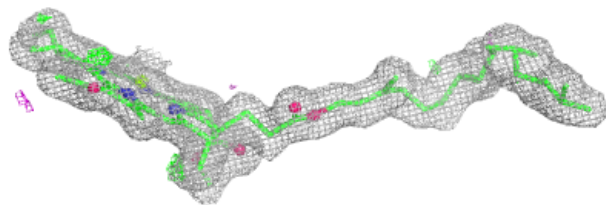
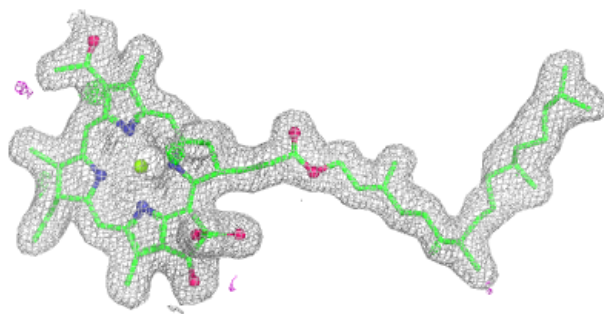
Electron density around BCL A 370:

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

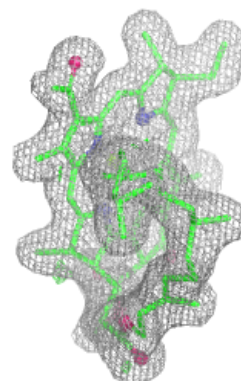
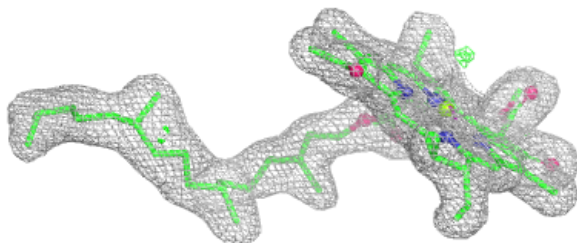
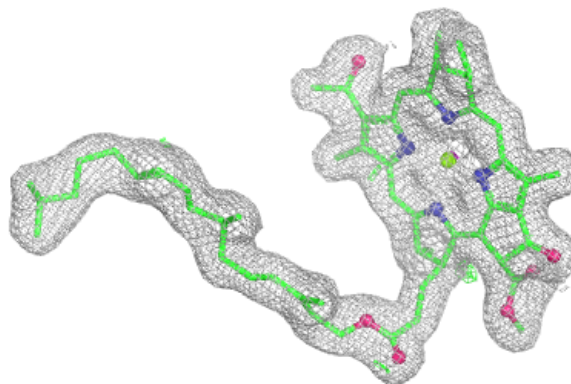


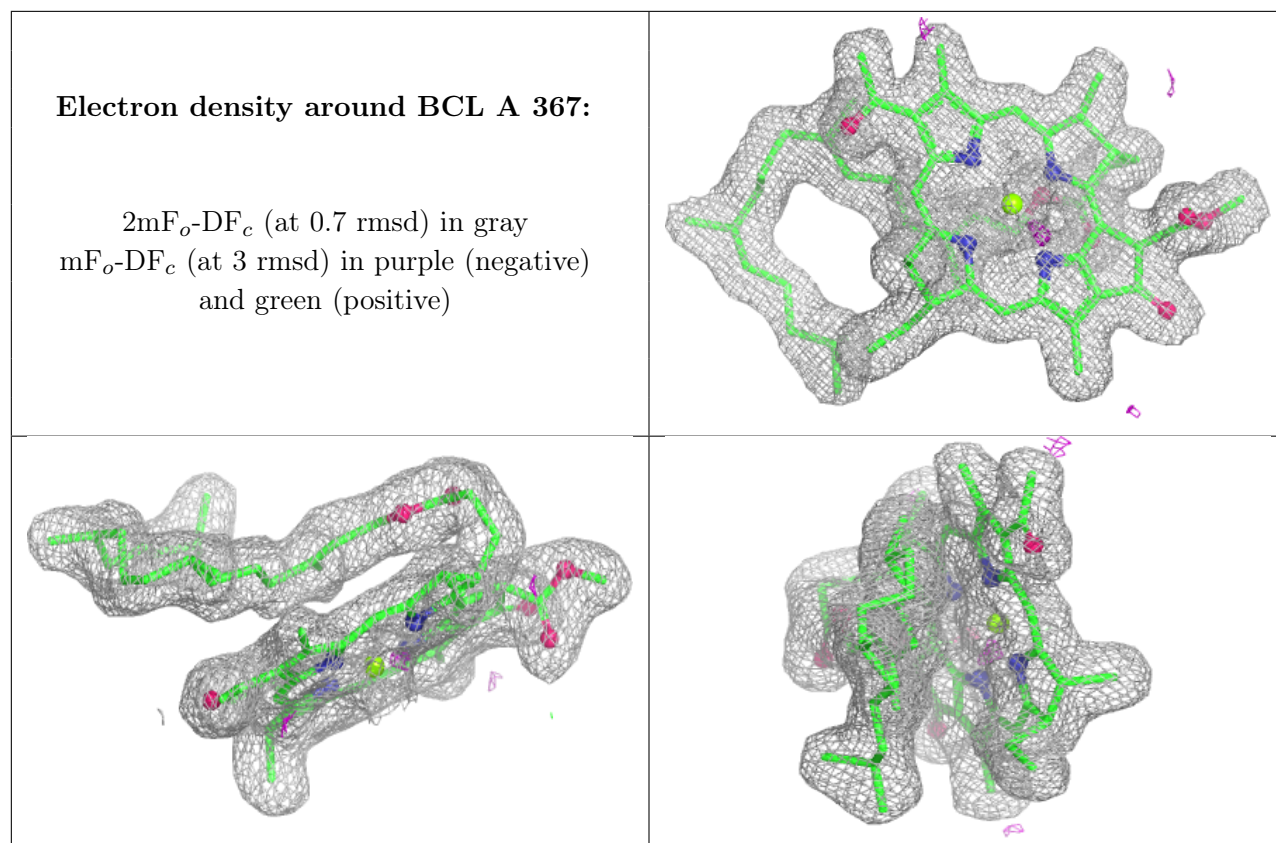
Electron density around BCL A 371:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.