Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 10:21 pm BST

PDB ID	:	6Q53 / pdb_00006q53
Title	:	CRYSTAL STRUCTURE OF THE LIGHT-HARVESTING COMPLEX II (B800-850) FROM Ectothiorhodospira haloalkaliphila
Authors	:	Gabdulkhakov, A.G.
Deposited on	:	2018-12-07
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

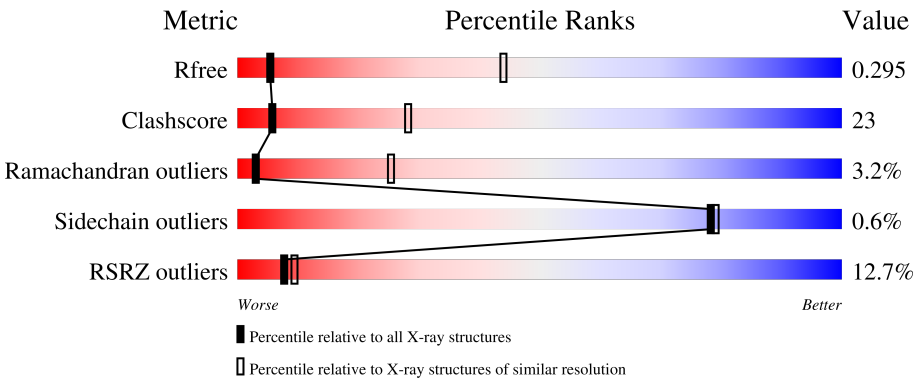
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 <=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	61	13% 48% 34% 7% 11%
1	D	61	18% 62% 30% • 7%
2	B	45	4% 62% 33% •
2	E	45	9% 47% 49% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2148 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.

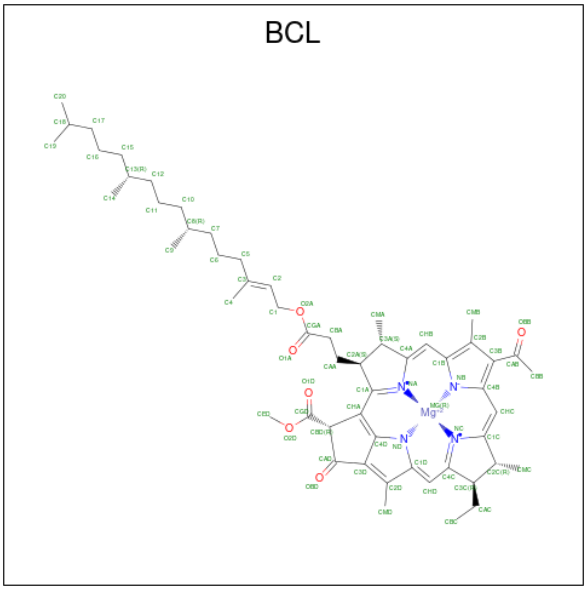
- Molecule 1 is a protein called light-harvesting protein subunit alpha.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	54	Total C N O 452 304 74 74	0	0	0
1	D	57	Total C N O S 475 317 77 80 1	0	0	0

- Molecule 2 is a protein called Light-harvesting protein B:800-850 subunit beta.

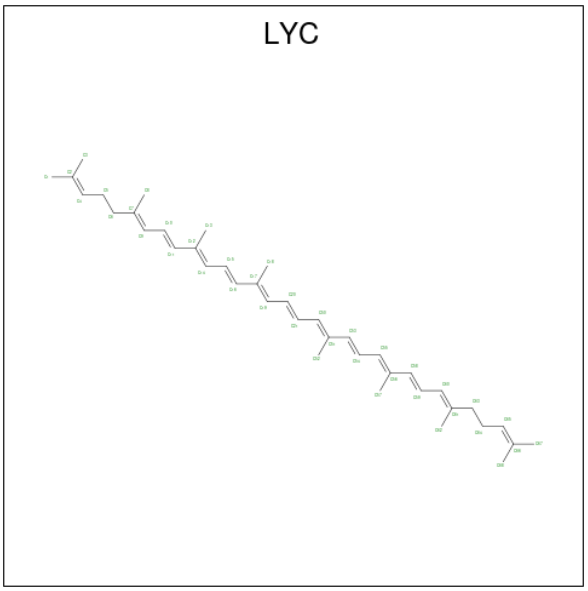
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	43	Total C N O 361 244 57 60	0	0	0
2	E	43	Total C N O 361 244 57 60	0	0	0

- Molecule 3 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



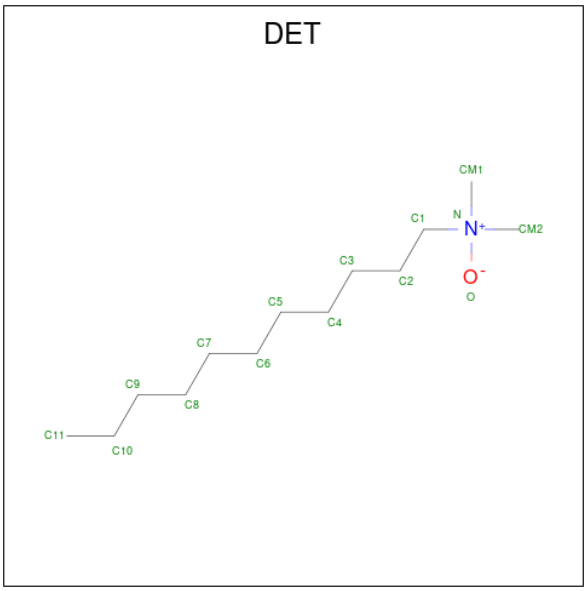
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
3	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
3	A	1	55	44	1	4	6	0	0
			Total	C	Mg	N	O		
3	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
3	D	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
3	D	1	55	44	1	4	6	0	0
			Total	C	Mg	N	O		
3	E	1	66	55	1	4	6	0	0

- Molecule 4 is LYCOPENE (CCD ID: LYC) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	40	40	0	0
			Total	C		
4	E	1	40	40	0	0

- Molecule 5 is UNDECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DET) (formula: $C_{13}H_{29}NO$).



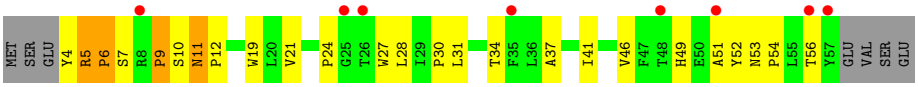
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	15	13	1	1	0	0
			Total	C	N	O		
5	E	1	15	13	1	1	0	0
			Total	C	N	O		
5	E	1	15	13	1	1	0	0

3 Residue-property plots (i)

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

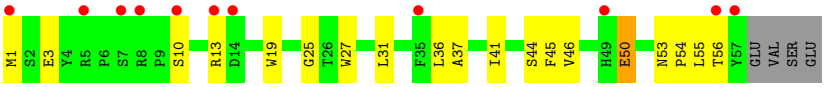
• Molecule 1: light-harvesting protein subunit alpha

Chain A:



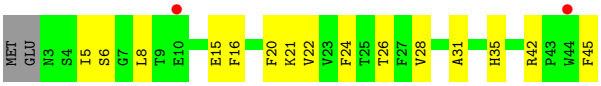
• Molecule 1: light-harvesting protein subunit alpha

Chain D:



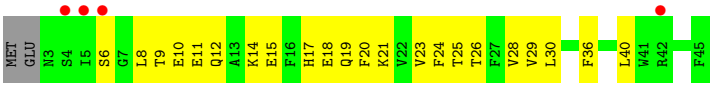
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain B:



• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	177.24Å 177.24Å 177.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.70 29.96 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.96-3.70) 99.6 (29.96-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.240 , 0.277 0.258 , 0.295	Depositor DCC
R_{free} test set	575 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	90.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	2148	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LYC, BCL, DET

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	0.69	0/471	0.93	1/651 (0.2%)
1	D	0.58	0/494	0.80	0/681
2	B	0.49	0/374	0.64	0/507
2	E	0.52	0/374	0.68	0/507
All	All	0.58	0/1713	0.78	1/2346 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	ARG	N-CA-C	7.83	120.75	109.48

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	452	0	448	36	0
1	D	475	0	471	14	0
2	B	361	0	347	15	0
2	E	361	0	347	29	0
3	A	121	0	124	17	0
3	B	66	0	74	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	121	0	124	11	0
3	E	66	0	74	5	0
4	A	40	0	56	5	0
4	E	40	0	56	8	0
5	B	15	0	29	2	0
5	E	30	0	58	1	0
All	All	2148	0	2208	101	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 23.

All (101) 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:5:ARG:HH22	1:A:7:SER:HB3	0.98	1.10
1:A:5:ARG:NH2	1:A:7:SER:HB3	1.84	0.91
1:A:5:ARG:HD2	2:E:11:GLU:HG3	1.52	0.89
1:A:5:ARG:HH22	1:A:7:SER:CB	1.86	0.85
2:E:19:GLN:HE21	2:E:23:VAL:HG23	1.52	0.72
1:A:5:ARG:HH21	1:A:5:ARG:HG2	1.58	0.69
1:A:56:THR:HG22	1:A:56:THR:O	1.94	0.67
1:A:5:ARG:CD	2:E:11:GLU:HG3	2.27	0.65
1:D:27:TRP:O	1:D:31:LEU:HG	1.99	0.63
2:E:11:GLU:OE2	2:E:11:GLU:N	2.30	0.62
1:A:49:HIS:CE1	1:A:51:ALA:HB3	2.36	0.60
3:A:102:BCL:HHC	2:E:23:VAL:HG22	1.83	0.59
4:A:103:LYC:H33	2:B:15:GLU:HG2	1.84	0.59
1:A:11:ASN:HB2	1:A:12:PRO:HA	1.83	0.59
3:B:101:BCL:H8	3:D:101:BCL:H91	1.85	0.59
1:A:11:ASN:OD1	2:E:19:GLN:NE2	2.35	0.58
1:A:5:ARG:HH21	1:A:5:ARG:CG	2.15	0.58
1:A:11:ASN:HD21	3:A:102:BCL:HBB3	1.69	0.57
3:B:101:BCL:H192	3:D:101:BCL:H61	1.87	0.56
1:A:5:ARG:HD2	2:E:11:GLU:CG	2.29	0.55
4:A:103:LYC:H14	2:B:20:PHE:HA	1.88	0.55
2:B:45:PHE:CE1	1:D:54:PRO:HB3	2.42	0.55
1:A:21:VAL:C	2:B:6:SER:HB3	2.32	0.54
2:E:20:PHE:HA	4:E:101:LYC:H14	1.87	0.54
2:E:23:VAL:HG12	4:E:101:LYC:H183	1.90	0.54
1:A:5:ARG:HD3	2:E:11:GLU:HA	1.90	0.54
1:D:10:SER:OG	1:D:13:ARG:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG23	3:D:101:BCL:HBC1	1.92	0.52
1:D:50:GLU:HA	1:D:53:ASN:HB3	1.91	0.51
1:A:37:ALA:O	1:A:41:ILE:HG12	2.10	0.51
3:D:102:BCL:HBC2	3:E:102:BCL:H91	1.92	0.51
1:A:11:ASN:HD21	3:A:102:BCL:CAB	2.24	0.51
2:E:15:GLU:HG2	4:E:101:LYC:H33	1.92	0.50
4:A:103:LYC:H59	1:D:36:LEU:HD21	1.94	0.50
2:E:24:PHE:O	2:E:28:VAL:HG23	2.12	0.50
1:A:19:TRP:O	2:B:6:SER:OG	2.25	0.49
3:B:101:BCL:HBA1	5:B:102:DET:H112	1.92	0.49
1:A:11:ASN:ND2	3:A:102:BCL:C3B	2.76	0.49
1:A:5:ARG:NH2	1:A:5:ARG:CG	2.72	0.48
2:B:24:PHE:CZ	2:B:28:VAL:HG21	2.49	0.48
2:E:25:THR:O	2:E:29:VAL:N	2.45	0.48
1:A:21:VAL:O	1:D:25:GLY:HA2	2.13	0.48
3:A:102:BCL:HED2	2:B:21:LYS:HB3	1.95	0.47
2:E:9:THR:HG23	2:E:12:GLN:OE1	2.14	0.47
1:A:5:ARG:NH2	1:A:6:PRO:O	2.48	0.47
3:A:101:BCL:HAA2	3:A:101:BCL:HBD	1.95	0.47
1:A:49:HIS:HE1	1:A:51:ALA:HB3	1.79	0.47
2:B:22:VAL:O	2:B:26:THR:HG23	2.15	0.47
2:B:35:HIS:HB3	5:B:102:DET:HM11	1.97	0.47
1:A:52:TYR:CE2	1:D:55:LEU:HB3	2.50	0.46
2:B:28:VAL:HA	2:B:31:ALA:HB3	1.96	0.46
1:A:53:ASN:HB2	1:A:54:PRO:HD2	1.96	0.46
4:E:101:LYC:C55	3:E:102:BCL:H11	2.46	0.46
3:A:102:BCL:H62	3:A:102:BCL:H41	1.73	0.46
1:D:3:GLU:HA	1:D:3:GLU:OE1	2.16	0.46
1:A:46:VAL:CG2	3:A:101:BCL:HBC1	2.45	0.45
1:D:44:SER:OG	1:D:45:PHE:N	2.48	0.45
1:A:11:ASN:HD21	3:A:102:BCL:CBB	2.28	0.45
1:D:36:LEU:HA	1:D:36:LEU:HD23	1.67	0.45
1:A:46:VAL:HG23	3:A:101:BCL:HBC1	1.99	0.45
2:E:30:LEU:HD23	2:E:30:LEU:HA	1.72	0.45
1:A:30:PRO:O	1:A:34:THR:HG23	2.17	0.45
2:E:36:PHE:CE2	2:E:40:LEU:HD11	2.51	0.45
1:A:53:ASN:OD1	1:A:56:THR:N	2.47	0.45
2:E:10:GLU:CG	2:E:14:LYS:HE3	2.47	0.44
1:A:4:TYR:O	1:A:6:PRO:HD3	2.18	0.44
3:A:101:BCL:H122	3:A:101:BCL:H161	1.71	0.44
1:D:37:ALA:O	1:D:41:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TRP:C	1:A:30:PRO:HD2	2.44	0.43
3:B:101:BCL:HBB3	3:D:101:BCL:CHC	2.48	0.43
4:A:103:LYC:H62	2:B:16:PHE:HD1	1.83	0.43
2:E:19:GLN:O	2:E:23:VAL:HG23	2.19	0.43
2:E:10:GLU:O	2:E:14:LYS:HG3	2.19	0.42
1:A:24:PRO:HD2	2:B:8:LEU:HD11	2.00	0.42
1:D:19:TRP:O	2:E:6:SER:OG	2.28	0.42
3:D:102:BCL:HMD2	3:E:102:BCL:H142	2.00	0.42
2:E:19:GLN:HB3	4:E:101:LYC:C9	2.49	0.42
4:E:101:LYC:H52	4:E:101:LYC:H31	1.82	0.42
3:A:101:BCL:H192	3:A:101:BCL:H162	1.82	0.42
3:A:102:BCL:HBB2	2:E:26:THR:HG21	2.02	0.42
3:B:101:BCL:HBB3	3:D:101:BCL:C4B	2.50	0.42
3:D:102:BCL:ND	3:E:102:BCL:H93	2.34	0.42
2:B:24:PHE:O	2:B:28:VAL:HG23	2.20	0.42
3:D:101:BCL:H162	3:D:101:BCL:H192	1.86	0.42
2:E:15:GLU:CG	4:E:101:LYC:H33	2.50	0.42
1:A:11:ASN:ND2	3:A:102:BCL:CAB	2.83	0.41
3:A:102:BCL:HMD2	3:B:101:BCL:H142	2.02	0.41
2:E:17:HIS:O	2:E:21:LYS:HG2	2.20	0.41
3:A:102:BCL:HHC	3:A:102:BCL:OBB	2.20	0.41
3:A:102:BCL:CBB	2:E:26:THR:HG21	2.50	0.41
3:E:102:BCL:H161	3:E:102:BCL:H192	1.78	0.41
2:E:10:GLU:HG3	2:E:14:LYS:HE3	2.03	0.41
1:A:28:LEU:O	1:A:31:LEU:HG	2.20	0.41
3:D:101:BCL:H142	2:E:23:VAL:HG13	2.02	0.41
4:A:103:LYC:H14	2:B:20:PHE:CD2	2.57	0.40
3:B:101:BCL:H92	3:D:101:BCL:H161	2.03	0.40
2:B:5:ILE:HG12	2:E:8:LEU:HD22	2.02	0.40
5:E:104:DET:H22	5:E:104:DET:HM12	1.76	0.40
1:A:9:PRO:HD3	2:E:18:GLU:HG3	2.04	0.40
4:E:101:LYC:H15	4:E:101:LYC:H131	1.80	0.40
1:D:1:MET:SD	1:D:1:MET:O	2.79	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	52/61 (85%)	42 (81%)	7 (14%)	3 (6%)	1 15
1	D	55/61 (90%)	49 (89%)	4 (7%)	2 (4%)	2 23
2	B	41/45 (91%)	36 (88%)	4 (10%)	1 (2%)	4 29
2	E	41/45 (91%)	38 (93%)	3 (7%)	0	100 100
All	All	189/212 (89%)	165 (87%)	18 (10%)	6 (3%)	3 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	D	50	GLU
1	A	6	PRO
1	A	9	PRO
1	D	56	THR
2	B	42	ARG

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	50/57 (88%)	49 (98%)	1 (2%)	48 64
1	D	53/57 (93%)	53 (100%)	0	100 100
2	B	37/39 (95%)	37 (100%)	0	100 100
2	E	37/39 (95%)	37 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	177/192 (92%)	176 (99%)	1 (1%)	78 79

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	19	GLN

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)

11 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	$\#\|Z\| > 2$
5	DET	E	104	-	11,14,14	2.18	1 (9%)	13,16,16	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BCL	E	102	2	69,74,74	1.39	8 (11%)	83,115,115	2.22	20 (24%)
5	DET	B	102	-	11,14,14	2.20	1 (9%)	13,16,16	3.93	3 (23%)
3	BCL	D	102	1	58,63,74	1.43	10 (17%)	69,101,115	1.95	16 (23%)
3	BCL	A	102	1	58,63,74	1.38	8 (13%)	69,101,115	1.86	17 (24%)
5	DET	E	103	-	11,14,14	2.09	1 (9%)	13,16,16	0.54	0
3	BCL	D	101	1	69,74,74	1.20	6 (8%)	83,115,115	1.60	15 (18%)
4	LYC	A	103	-	39,39,39	0.74	0	44,46,46	1.79	9 (20%)
4	LYC	E	101	-	39,39,39	1.00	1 (2%)	44,46,46	1.91	14 (31%)
3	BCL	A	101	1	69,74,74	1.20	4 (5%)	83,115,115	1.69	19 (22%)
3	BCL	B	101	2	69,74,74	1.18	3 (4%)	83,115,115	1.66	15 (18%)

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
5	DET	E	104	-	-	7/12/12/12	-
3	BCL	E	102	2	-	12/41/137/137	-
5	DET	B	102	-	-	3/12/12/12	-
3	BCL	D	102	1	-	8/28/124/137	-
3	BCL	A	102	1	-	8/28/124/137	-
5	DET	E	103	-	-	2/12/12/12	-
3	BCL	D	101	1	-	5/41/137/137	-
4	LYC	A	103	-	-	9/43/43/43	-
4	LYC	E	101	-	-	10/43/43/43	-
3	BCL	A	101	1	-	14/41/137/137	-
3	BCL	B	101	2	-	5/41/137/137	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	102	DET	O-N	-7.22	1.25	1.42
5	E	104	DET	O-N	-7.14	1.25	1.42
5	E	103	DET	O-N	-6.86	1.26	1.42
3	E	102	BCL	MG-NA	5.68	2.19	2.06
3	B	101	BCL	MG-NA	5.18	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	101	BCL	MG-NA	4.76	2.17	2.06
3	D	101	BCL	MG-NA	4.36	2.16	2.06
3	D	102	BCL	MG-NA	4.33	2.16	2.06
3	A	102	BCL	MG-NA	4.08	2.16	2.06
3	E	102	BCL	O1A-CGA	4.06	1.34	1.22
3	A	102	BCL	OBD-CAD	3.65	1.28	1.22
3	D	101	BCL	C3B-C4B	3.45	1.47	1.41
4	E	101	LYC	C60-C61	3.43	1.37	1.34
3	E	102	BCL	CAA-CBA	3.42	1.63	1.52
3	A	101	BCL	MG-NC	2.94	2.13	2.06
3	A	102	BCL	C5-C3	2.89	1.57	1.51
3	A	101	BCL	C3B-C4B	2.76	1.46	1.41
3	E	102	BCL	MG-NC	2.76	2.12	2.06
3	D	102	BCL	O2A-CGA	2.74	1.41	1.33
3	B	101	BCL	MG-NC	2.73	2.12	2.06
3	D	102	BCL	C3B-C4B	2.71	1.46	1.41
3	A	101	BCL	CHD-C1D	2.67	1.43	1.38
3	D	101	BCL	C1D-C2D	-2.66	1.40	1.45
3	E	102	BCL	C1D-C2D	-2.65	1.40	1.45
3	D	102	BCL	C1D-C2D	-2.53	1.40	1.45
3	D	102	BCL	OBD-CAD	2.52	1.26	1.22
3	D	101	BCL	C3D-C4D	-2.50	1.38	1.44
3	D	102	BCL	C1-C2	2.46	1.56	1.49
3	D	101	BCL	MG-NC	2.43	2.12	2.06
3	D	102	BCL	MG-NC	2.42	2.12	2.06
3	D	102	BCL	MG-ND	-2.41	2.01	2.05
3	E	102	BCL	C3B-C4B	2.40	1.45	1.41
3	A	102	BCL	MG-ND	-2.38	2.01	2.05
3	A	102	BCL	C6-C5	2.30	1.60	1.52
3	A	102	BCL	C3B-C4B	2.30	1.45	1.41
3	D	102	BCL	C3D-C4D	-2.26	1.39	1.44
3	A	102	BCL	MG-NC	2.25	2.11	2.06
3	B	101	BCL	CAA-CBA	2.25	1.59	1.52
3	A	102	BCL	CAC-C3C	2.23	1.58	1.54
3	D	101	BCL	CBD-CGD	-2.13	1.45	1.52
3	D	102	BCL	CBD-CGD	-2.12	1.45	1.52
3	E	102	BCL	C3D-C4D	-2.07	1.39	1.44
3	E	102	BCL	OBD-CAD	2.05	1.26	1.22

All (128) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	102	DET	CM1-N-C1	-10.13	88.94	110.23
3	D	102	BCL	C1-C2-C3	8.89	141.42	126.04
3	E	102	BCL	C1-C2-C3	-7.81	112.54	126.04
5	B	102	DET	O-N-C1	-7.49	90.91	109.27
3	E	102	BCL	C1-O2A-CGA	7.03	134.89	116.44
3	E	102	BCL	C6-C7-C8	-6.43	95.14	115.92
5	B	102	DET	CM2-N-C1	-6.08	97.47	110.23
3	A	102	BCL	C4D-CHA-C1A	5.51	127.96	121.25
3	A	102	BCL	C1-O2A-CGA	5.41	130.63	116.44
3	A	101	BCL	CHD-C1D-ND	-5.33	119.56	124.45
4	A	103	LYC	C21-C50-C51	-5.26	119.80	127.31
3	B	101	BCL	C4D-CHA-C1A	5.20	127.58	121.25
3	D	102	BCL	C4D-CHA-C1A	5.14	127.51	121.25
3	D	101	BCL	C4D-CHA-C1A	5.09	127.44	121.25
3	B	101	BCL	CHD-C1D-ND	-4.96	119.90	124.45
3	D	101	BCL	CHD-C1D-ND	-4.86	119.98	124.45
3	A	102	BCL	CHD-C1D-ND	-4.86	119.99	124.45
3	E	102	BCL	CHD-C1D-ND	-4.68	120.15	124.45
3	E	102	BCL	C4D-CHA-C1A	4.62	126.87	121.25
3	D	102	BCL	CHD-C1D-ND	-4.60	120.23	124.45
4	E	101	LYC	C21-C20-C19	-4.36	114.54	123.47
3	A	101	BCL	C4D-CHA-C1A	4.26	126.43	121.25
4	A	103	LYC	C8-C7-C6	4.25	122.42	115.27
4	E	101	LYC	C21-C50-C51	-4.17	121.35	127.31
3	E	102	BCL	CAA-CBA-CGA	3.99	124.90	113.25
3	B	101	BCL	C1-O2A-CGA	-3.98	106.01	116.44
3	A	102	BCL	C4A-NA-C1A	3.91	108.46	106.71
3	E	102	BCL	O2A-CGA-CBA	-3.86	99.79	111.91
3	E	102	BCL	OBB-CAB-C3B	3.82	127.48	120.41
3	A	101	BCL	C1D-ND-C4D	-3.67	103.73	106.33
3	E	102	BCL	CHA-C1A-NA	-3.64	118.07	126.40
3	E	102	BCL	C16-C15-C13	-3.57	104.39	115.92
4	E	101	LYC	C8-C7-C6	3.57	121.27	115.27
4	E	101	LYC	C13-C12-C11	3.55	123.67	118.08
3	E	102	BCL	CBA-CAA-C2A	3.51	124.23	113.86
4	E	101	LYC	C15-C14-C12	-3.51	122.30	127.31
3	D	101	BCL	C1D-ND-C4D	-3.49	103.86	106.33
3	B	101	BCL	CAB-C3B-C2B	3.46	133.53	128.34
3	D	101	BCL	C4A-NA-C1A	3.39	108.23	106.71
3	B	101	BCL	CHA-C1A-NA	-3.33	118.77	126.40
3	D	102	BCL	CBA-CAA-C2A	3.31	123.63	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	102	BCL	CHA-C1A-NA	-3.31	118.83	126.40
3	D	102	BCL	C1D-ND-C4D	-3.29	104.00	106.33
3	B	101	BCL	C1D-ND-C4D	-3.28	104.01	106.33
3	A	101	BCL	C11-C10-C8	3.26	126.46	115.92
4	A	103	LYC	C15-C14-C12	-3.23	122.70	127.31
3	A	102	BCL	CAB-C3B-C2B	3.22	133.16	128.34
4	E	101	LYC	C13-C12-C14	-3.20	118.45	122.92
3	A	101	BCL	C1-C2-C3	3.18	131.54	126.04
3	D	101	BCL	CHA-C1A-NA	-3.15	119.18	126.40
3	A	102	BCL	CHA-C1A-NA	-3.12	119.26	126.40
4	E	101	LYC	C3-C2-C1	3.07	121.39	114.60
3	E	102	BCL	C1D-ND-C4D	-3.02	104.19	106.33
4	A	103	LYC	C21-C20-C19	-3.02	117.29	123.47
3	B	101	BCL	CBA-CAA-C2A	3.00	122.72	113.86
3	B	101	BCL	CAA-CBA-CGA	3.00	122.02	113.25
3	E	102	BCL	C2A-C1A-CHA	2.98	129.07	123.86
3	B	101	BCL	C6-C7-C8	-2.94	106.41	115.92
3	A	101	BCL	O2D-CGD-CBD	2.94	116.50	111.27
3	A	101	BCL	CAC-C3C-C2C	-2.94	106.91	114.26
3	A	101	BCL	O2D-CGD-O1D	-2.87	118.23	123.84
3	A	101	BCL	CBC-CAC-C3C	-2.85	107.11	113.47
3	B	101	BCL	C17-C16-C15	-2.84	100.17	113.24
4	E	101	LYC	C18-C17-C16	2.83	122.54	118.08
3	A	101	BCL	CHA-C1A-NA	-2.82	119.95	126.40
3	A	101	BCL	C16-C15-C13	-2.81	106.84	115.92
3	D	101	BCL	CBA-CAA-C2A	-2.80	105.58	113.86
3	A	102	BCL	C1D-ND-C4D	-2.77	104.36	106.33
3	D	102	BCL	O2A-CGA-CBA	2.76	120.56	111.91
3	D	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
3	E	102	BCL	C4A-NA-C1A	2.67	107.91	106.71
3	B	101	BCL	C14-C13-C15	-2.66	101.66	111.29
4	A	103	LYC	C3-C2-C1	2.65	120.47	114.60
3	E	102	BCL	CHC-C4B-NB	-2.62	121.49	124.26
3	D	101	BCL	CMB-C2B-C1B	-2.62	121.39	125.37
3	D	102	BCL	O2A-CGA-O1A	-2.61	117.01	123.59
3	E	102	BCL	C11-C10-C8	-2.61	107.49	115.92
4	A	103	LYC	C9-C10-C11	-2.61	115.09	123.22
3	A	102	BCL	CMB-C2B-C1B	-2.60	121.41	125.37
3	A	101	BCL	C4A-NA-C1A	2.58	107.87	106.71
3	A	101	BCL	OBB-CAB-CBB	-2.56	114.06	119.73
3	D	101	BCL	CAC-C3C-C4C	-2.54	106.94	112.58
3	D	101	BCL	C4B-C3B-C2B	-2.54	104.27	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	102	BCL	O2A-CGA-O1A	2.53	129.97	123.59
4	E	101	LYC	C9-C10-C11	-2.53	115.34	123.22
3	B	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
3	E	102	BCL	C4B-C3B-C2B	-2.51	104.31	108.36
3	E	102	BCL	OBB-CAB-CBB	-2.50	114.20	119.73
3	E	102	BCL	C14-C13-C15	-2.47	102.35	111.29
3	D	102	BCL	CMA-C3A-C4A	-2.47	105.15	111.77
3	D	101	BCL	CHC-C4B-NB	-2.42	121.69	124.26
3	D	101	BCL	C11-C10-C8	2.41	123.72	115.92
3	A	102	BCL	O2D-CGD-CBD	2.40	115.53	111.27
4	E	101	LYC	C20-C19-C17	-2.40	123.89	127.31
3	D	101	BCL	OBB-CAB-CBB	-2.39	114.43	119.73
3	D	102	BCL	C2A-C1A-CHA	2.38	128.02	123.86
3	A	102	BCL	OBB-CAB-CBB	-2.38	114.46	119.73
3	A	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
3	A	102	BCL	CMA-C3A-C4A	-2.36	105.42	111.77
4	E	101	LYC	C18-C17-C19	-2.33	119.65	122.92
4	A	103	LYC	C13-C12-C11	2.33	121.75	118.08
3	A	101	BCL	C4B-C3B-C2B	-2.32	104.63	108.36
3	A	102	BCL	C2A-C1A-CHA	2.28	127.85	123.86
3	D	101	BCL	O2D-CGD-O1D	-2.28	119.39	123.84
4	A	103	LYC	C18-C17-C16	2.27	121.66	118.08
3	B	101	BCL	OBB-CAB-CBB	-2.27	114.70	119.73
3	B	101	BCL	CHC-C4B-NB	-2.25	121.88	124.26
4	A	103	LYC	C62-C61-C63	2.24	119.04	115.27
3	D	102	BCL	C6-C5-C3	2.23	119.31	113.45
3	D	102	BCL	C4A-NA-C1A	2.23	107.71	106.71
3	B	101	BCL	C4A-NA-C1A	2.22	107.71	106.71
4	E	101	LYC	C55-C54-C53	-2.21	116.31	123.22
3	A	102	BCL	C4B-C3B-C2B	-2.20	104.82	108.36
3	A	102	BCL	C2D-C1D-ND	2.19	111.72	110.10
3	A	102	BCL	CHC-C4B-NB	-2.17	121.96	124.26
3	A	101	BCL	CAB-C3B-C2B	2.17	131.59	128.34
3	A	101	BCL	OBB-CAB-C3B	2.16	124.40	120.41
3	A	102	BCL	O2A-CGA-CBA	-2.16	105.13	111.91
3	A	101	BCL	CAA-CBA-CGA	2.14	119.51	113.25
4	E	101	LYC	C1-C2-C4	-2.12	116.51	122.65
3	A	102	BCL	O2A-CGA-O1A	2.12	128.95	123.59
3	D	102	BCL	C4B-C3B-C2B	-2.08	105.01	108.36
3	D	102	BCL	OBB-CAB-CBB	-2.05	115.20	119.73
3	A	101	BCL	CMB-C2B-C1B	-2.04	122.27	125.37
3	D	102	BCL	CAB-C3B-C2B	2.03	131.38	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	101	LYC	C6-C5-C4	-2.02	105.23	111.88
3	D	101	BCL	CED-O2D-CGD	-2.02	111.36	115.94
3	D	102	BCL	CHC-C4B-NB	-2.01	122.13	124.26

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	101	BCL	C4C-C3C-CAC-CBC
3	A	101	BCL	CHA-CBD-CGD-O1D
3	A	101	BCL	CHA-CBD-CGD-O2D
3	A	102	BCL	C2-C3-C5-C6
3	A	102	BCL	C4-C3-C5-C6
3	B	101	BCL	CHA-CBD-CGD-O1D
3	B	101	BCL	CHA-CBD-CGD-O2D
3	D	102	BCL	O2A-C1-C2-C3
3	E	102	BCL	C2-C1-O2A-CGA
3	E	102	BCL	C2B-C3B-CAB-OBB
3	E	102	BCL	C2B-C3B-CAB-CBB
3	E	102	BCL	C4B-C3B-CAB-OBB
3	E	102	BCL	C4B-C3B-CAB-CBB
3	E	102	BCL	CHA-CBD-CGD-O1D
3	E	102	BCL	CHA-CBD-CGD-O2D
4	A	103	LYC	C15-C16-C17-C18
4	A	103	LYC	C15-C16-C17-C19
4	A	103	LYC	C52-C51-C53-C54
4	E	101	LYC	C5-C6-C7-C8
4	E	101	LYC	C15-C16-C17-C18
4	E	101	LYC	C15-C16-C17-C19
4	E	101	LYC	C55-C56-C58-C59
4	E	101	LYC	C57-C56-C58-C59
5	B	102	DET	C2-C1-N-O
5	B	102	DET	C2-C1-N-CM2
3	D	102	BCL	C4-C3-C5-C6
3	A	102	BCL	C2A-CAA-CBA-CGA
3	B	101	BCL	C2A-CAA-CBA-CGA
3	D	102	BCL	C2A-CAA-CBA-CGA
3	D	102	BCL	C5-C6-C7-C8
4	A	103	LYC	C5-C6-C7-C8
4	A	103	LYC	C5-C6-C7-C9
4	E	101	LYC	C5-C6-C7-C9
4	E	101	LYC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	D	102	BCL	C2-C3-C5-C6
4	A	103	LYC	C57-C56-C58-C59
3	D	101	BCL	C15-C16-C17-C18
3	A	101	BCL	C10-C11-C12-C13
3	A	102	BCL	C2-C1-O2A-CGA
4	A	103	LYC	C4-C5-C6-C7
5	B	102	DET	C3-C4-C5-C6
5	E	103	DET	C2-C3-C4-C5
5	E	103	DET	C6-C7-C8-C9
3	A	101	BCL	C16-C17-C18-C20
3	A	101	BCL	C13-C15-C16-C17
4	E	101	LYC	C52-C51-C53-C54
3	A	101	BCL	C2C-C3C-CAC-CBC
5	E	104	DET	C3-C4-C5-C6
3	A	101	BCL	C15-C16-C17-C18
3	A	102	BCL	C3-C5-C6-C7
4	A	103	LYC	C50-C51-C53-C54
5	E	104	DET	N-C1-C2-C3
3	A	101	BCL	C16-C17-C18-C19
5	E	104	DET	C4-C5-C6-C7
3	D	102	BCL	C6-C7-C8-C9
5	E	104	DET	C2-C3-C4-C5
3	B	101	BCL	C15-C16-C17-C18
5	E	104	DET	C11-C10-C9-C8
3	E	102	BCL	C11-C12-C13-C14
3	D	101	BCL	C10-C11-C12-C13
5	E	104	DET	C5-C6-C7-C8
3	A	101	BCL	C1A-C2A-CAA-CBA
4	A	103	LYC	C55-C56-C58-C59
3	E	102	BCL	CAA-CBA-CGA-O2A
3	A	101	BCL	C6-C7-C8-C9
3	D	101	BCL	CAD-CBD-CGD-O2D
3	A	101	BCL	C2-C1-O2A-CGA
4	E	101	LYC	C50-C51-C53-C54
3	D	101	BCL	CAA-CBA-CGA-O2A
4	E	101	LYC	C11-C10-C9-C7
3	D	101	BCL	CAA-CBA-CGA-O1A
3	A	102	BCL	C1A-C2A-CAA-CBA
3	E	102	BCL	C1A-C2A-CAA-CBA
3	E	102	BCL	CAA-CBA-CGA-O1A
3	A	102	BCL	C6-C7-C8-C9
3	E	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	101	BCL	CAA-CBA-CGA-O2A
5	E	104	DET	C1-C2-C3-C4
3	D	102	BCL	CAD-CBD-CGD-O1D
3	B	101	BCL	C8-C10-C11-C12
3	A	102	BCL	C3A-C2A-CAA-CBA
3	D	102	BCL	C2C-C3C-CAC-CBC
3	A	101	BCL	CAA-CBA-CGA-O1A

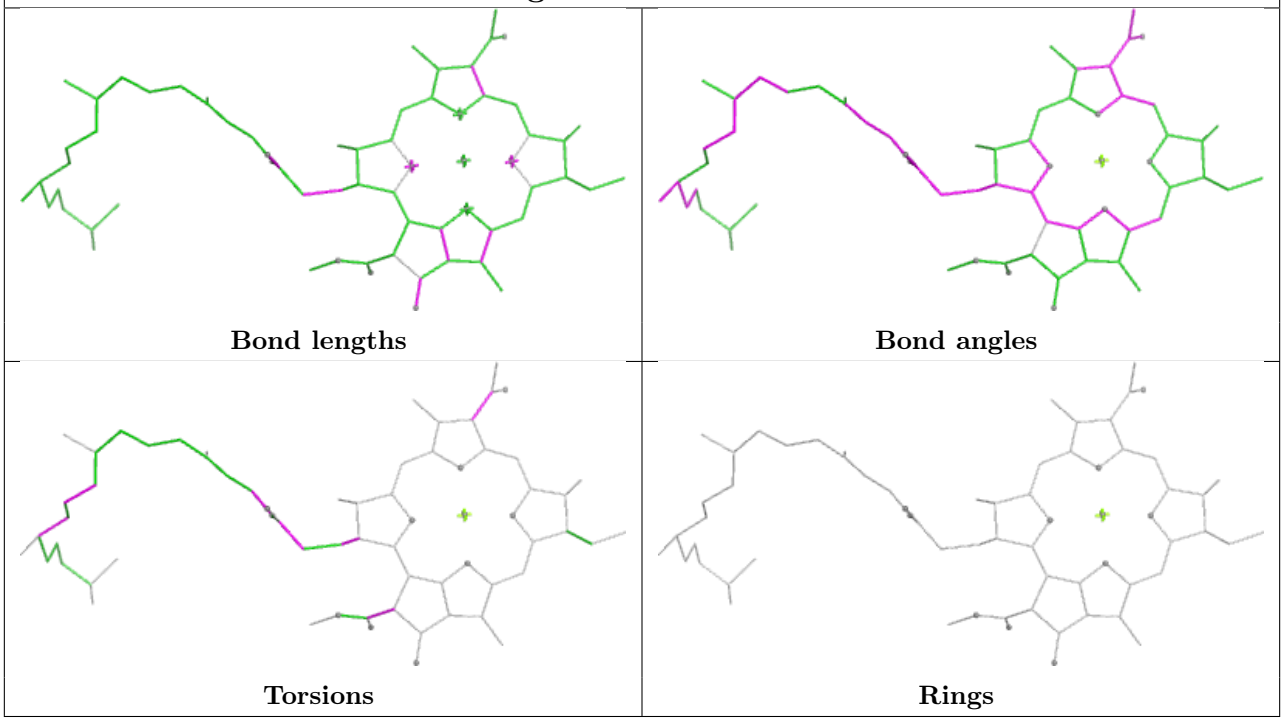
There are no ring outliers.

10 monomers are involved in 45 short contacts:

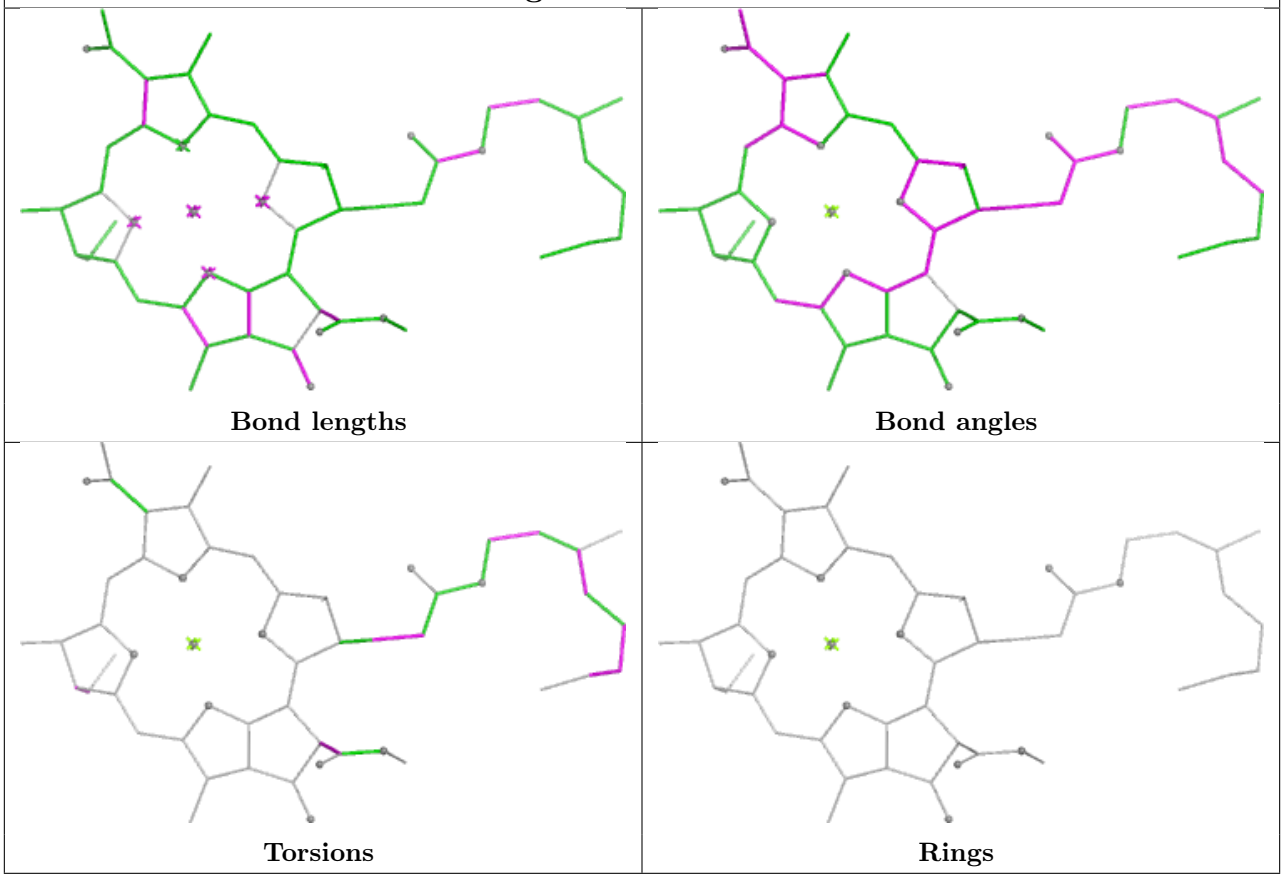
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	104	DET	1	0
3	E	102	BCL	5	0
5	B	102	DET	2	0
3	D	102	BCL	3	0
3	A	102	BCL	12	0
3	D	101	BCL	8	0
4	A	103	LYC	5	0
4	E	101	LYC	8	0
3	A	101	BCL	5	0
3	B	101	BCL	7	0

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

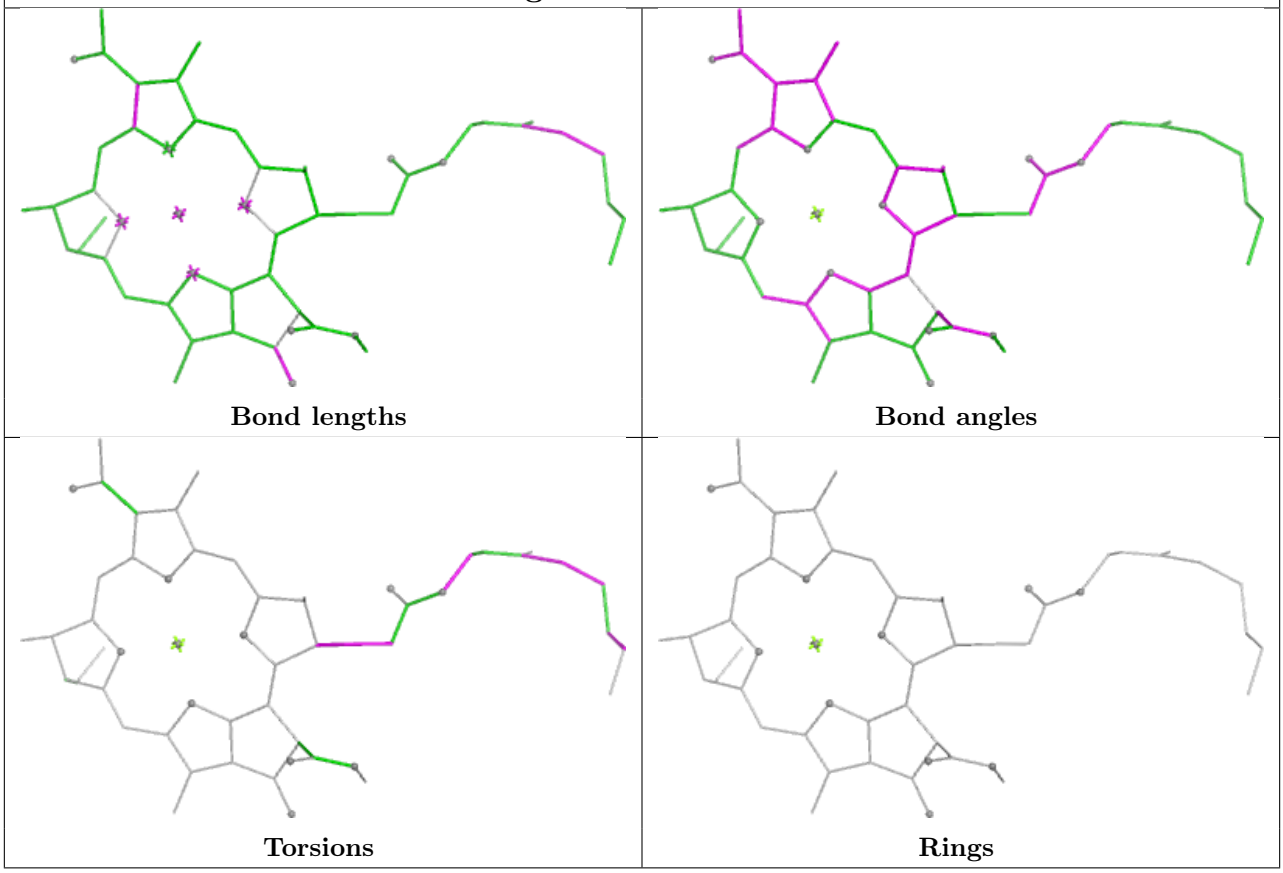
Ligand BCL E 102



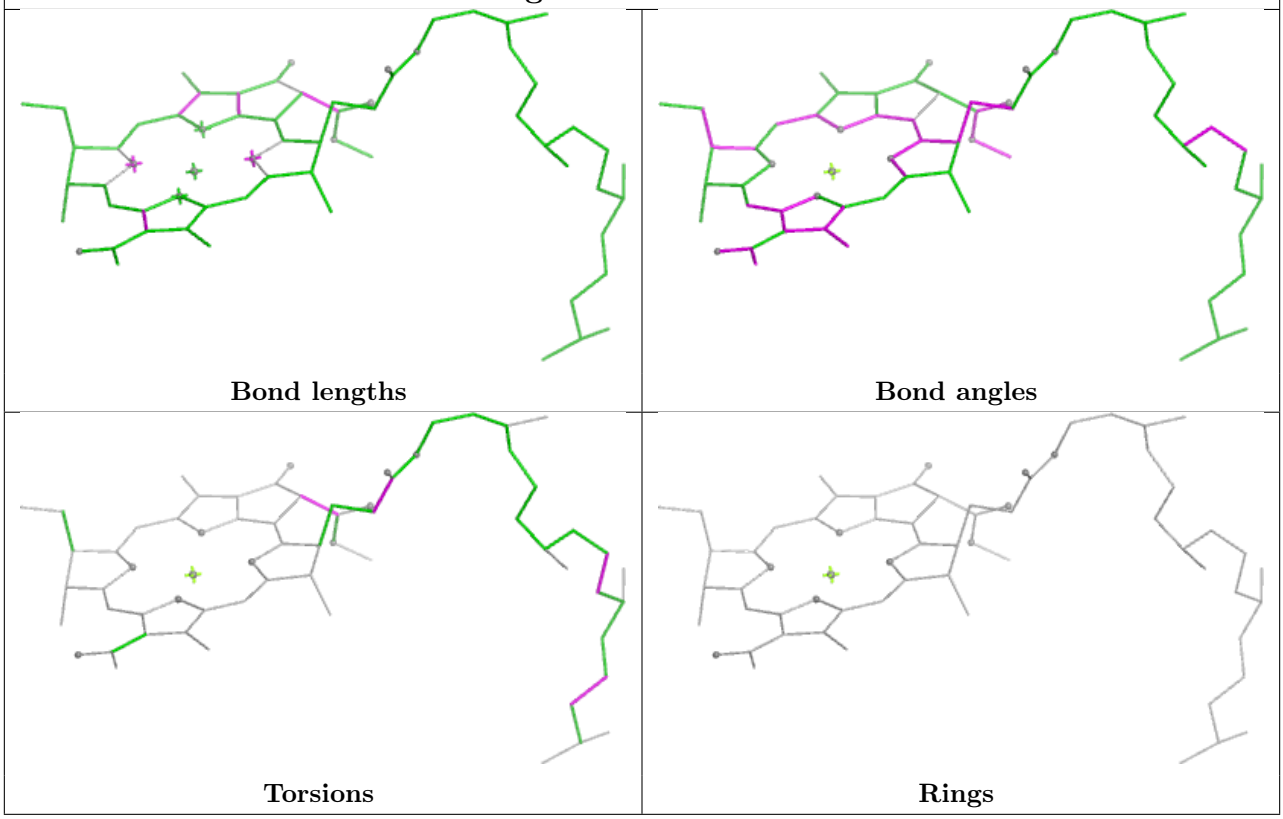
Ligand BCL D 102



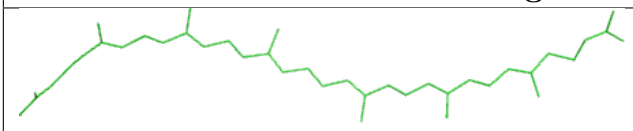
Ligand BCL A 102



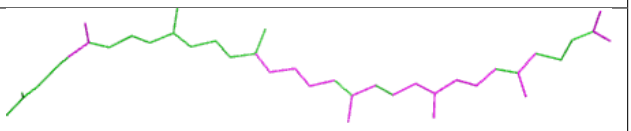
Ligand BCL D 101



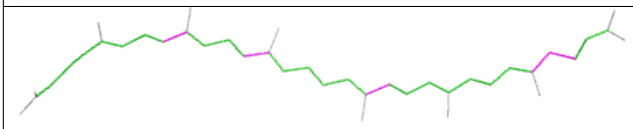
Ligand LYC A 103



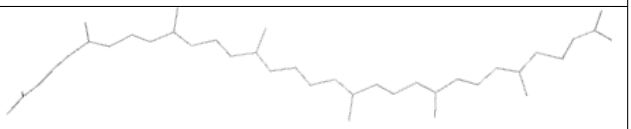
Bond lengths



Bond angles

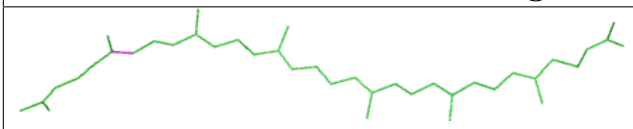


Torsions

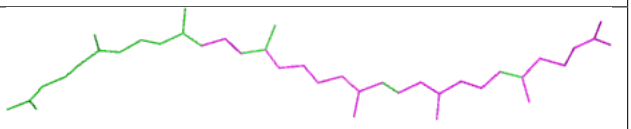


Rings

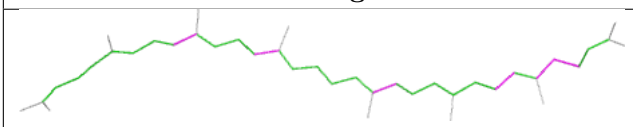
Ligand LYC E 101



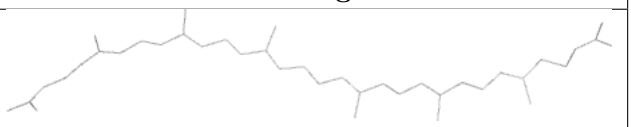
Bond lengths



Bond angles

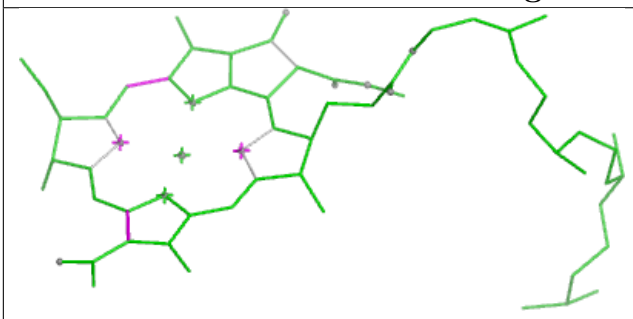


Torsions

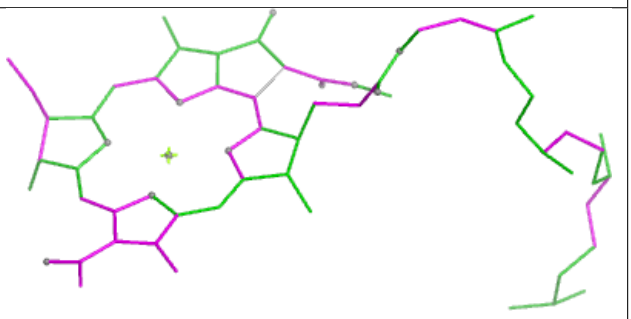


Rings

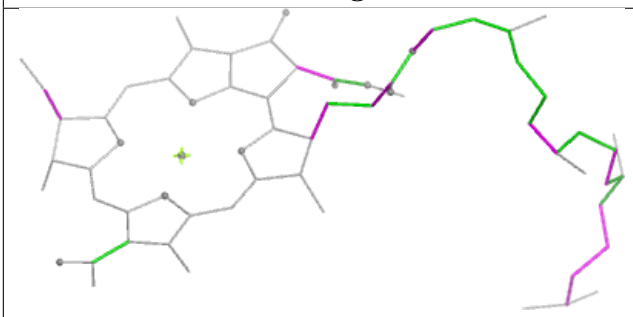
Ligand BCL A 101



Bond lengths



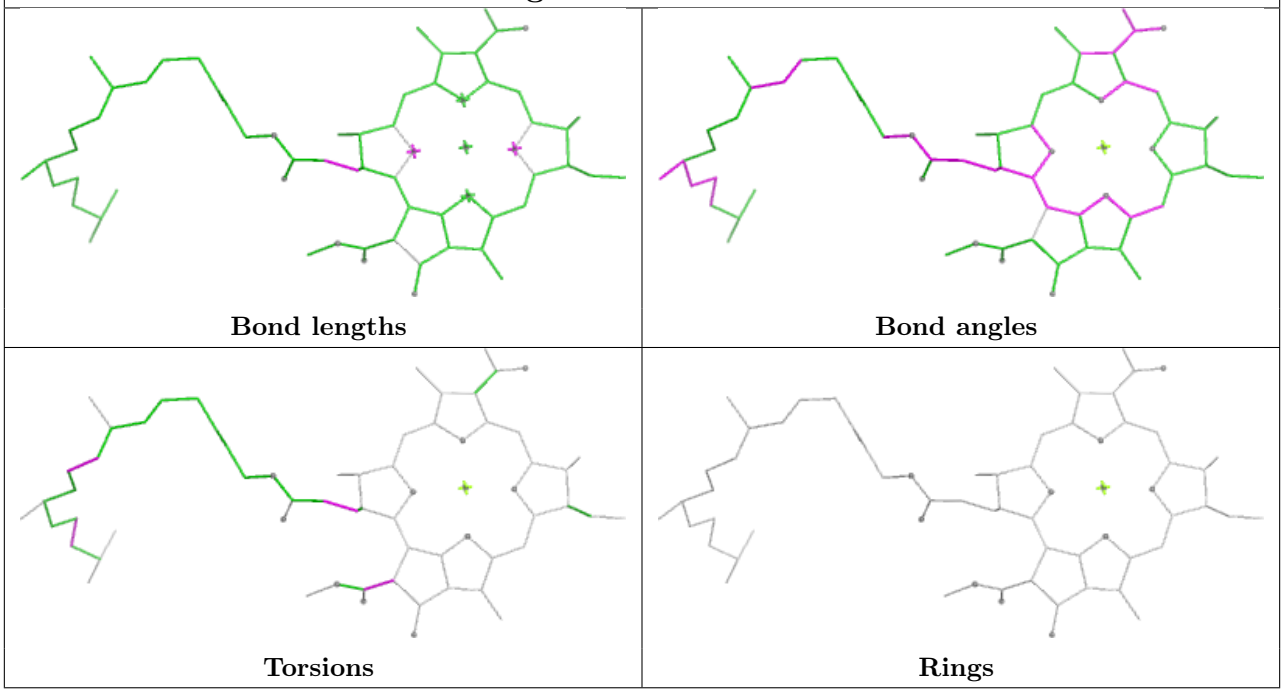
Bond angles



Torsions

Rings

Ligand BCL B 101



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	54/61 (88%)	0.87	8 (14%) 5 7	59, 74, 112, 171	0
1	D	57/61 (93%)	1.08	11 (19%) 3 4	54, 77, 132, 144	0
2	B	43/45 (95%)	0.30	2 (4%) 36 23	57, 76, 98, 120	0
2	E	43/45 (95%)	0.29	4 (9%) 14 13	60, 73, 89, 117	0
All	All	197/212 (92%)	0.68	25 (12%) 8 9	54, 76, 118, 171	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	TYR	9.2
1	D	57	TYR	7.1
1	D	1	MET	6.0
1	D	5	ARG	5.9
1	D	56	THR	5.8
1	A	8	ARG	5.3
1	D	49	HIS	5.0
1	D	8	ARG	4.9
1	A	25	GLY	4.0
1	A	56	THR	3.3
1	D	10	SER	3.3
1	D	14	ASP	3.0
1	D	13	ARG	3.0
1	A	26	THR	2.8
1	D	7	SER	2.7
2	E	6	SER	2.6
2	E	42	ARG	2.5
1	D	35	PHE	2.4
2	E	5	ILE	2.3
2	B	44	TRP	2.2
1	A	35	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	48	THR	2.2
1	A	51	ALA	2.2
2	B	10	GLU	2.2
2	E	4	SER	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)

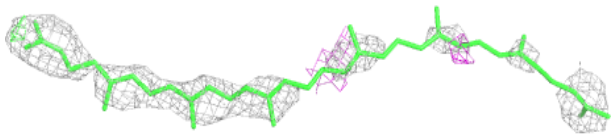
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

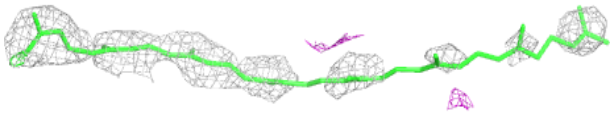
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DET	E	103	15/15	0.77	0.32	63,89,133,133	0
5	DET	B	102	15/15	0.85	0.29	73,102,134,137	0
5	DET	E	104	15/15	0.86	0.32	69,107,127,129	0
4	LYC	E	101	40/40	0.91	0.23	54,73,88,88	0
3	BCL	D	102	55/66	0.92	0.14	57,68,105,110	0
3	BCL	A	102	55/66	0.95	0.12	57,67,112,134	0
3	BCL	A	101	66/66	0.95	0.14	63,78,87,89	0
3	BCL	E	102	66/66	0.95	0.13	60,80,87,99	0
4	LYC	A	103	40/40	0.95	0.16	58,69,83,86	0
3	BCL	B	101	66/66	0.96	0.12	63,77,84,91	0
3	BCL	D	101	66/66	0.97	0.11	66,77,84,93	0

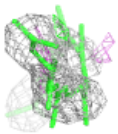
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LYC E 101:

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

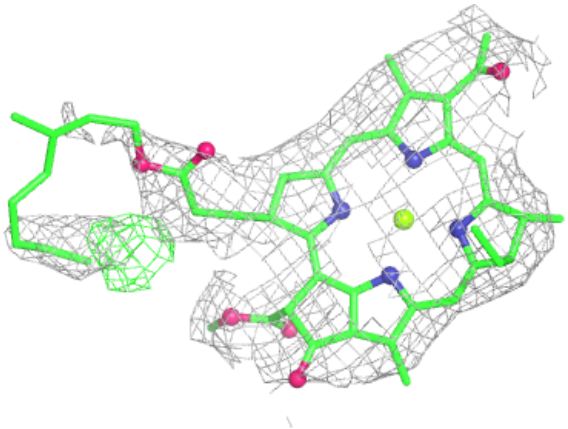


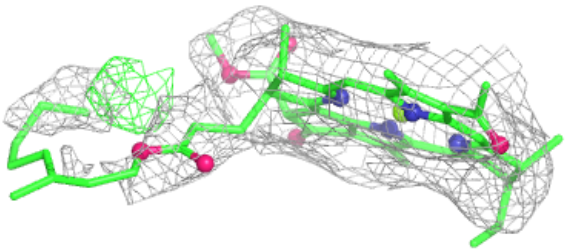


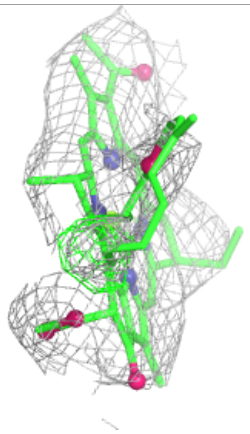


Electron density around BCL D 102:

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

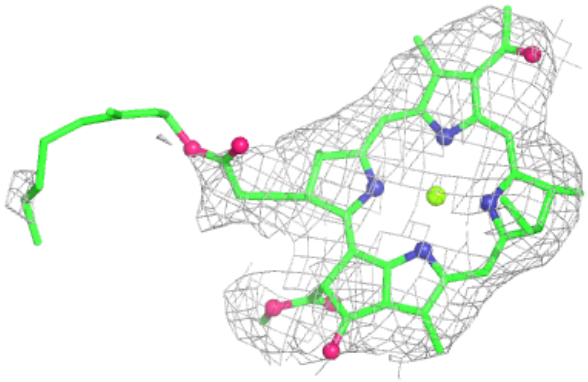


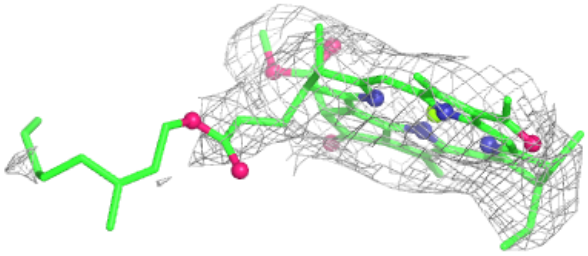




Electron density around BCL A 102:

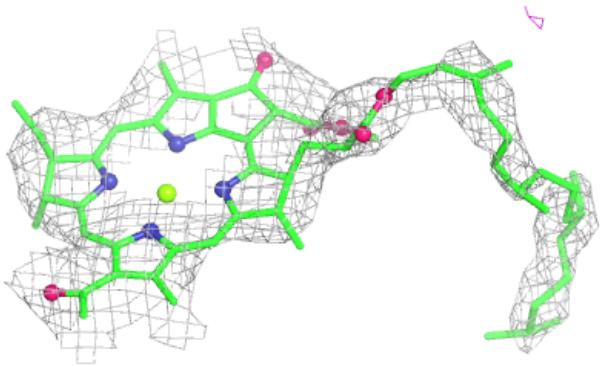
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

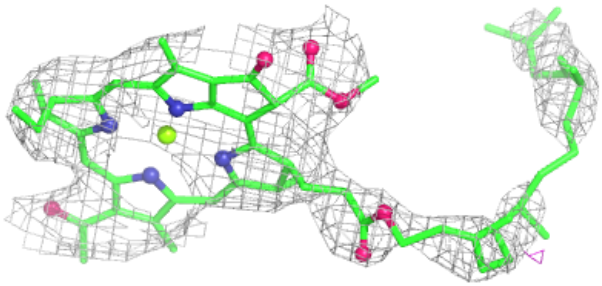


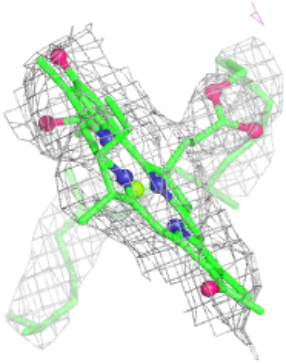


Electron density around BCL A 101:

$2mF_o$-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 E 102:

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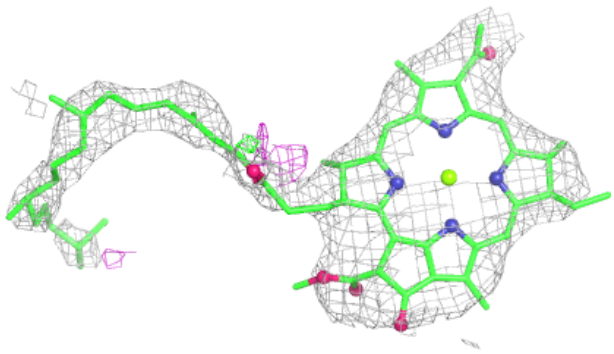
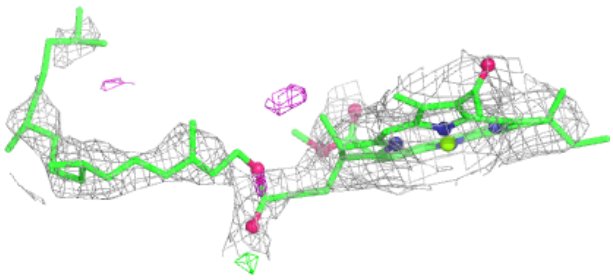
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around LYC A 103:

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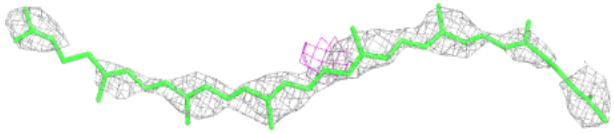
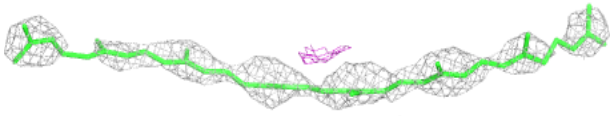
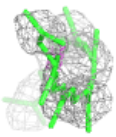
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL B 101:

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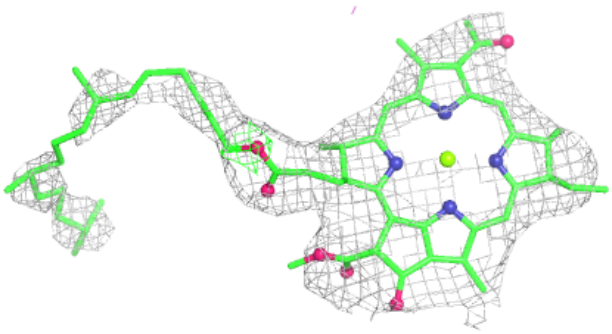
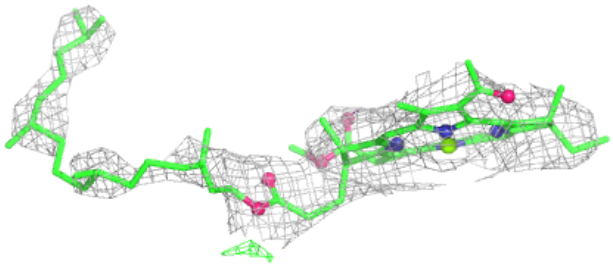
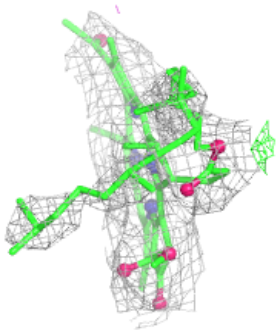
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

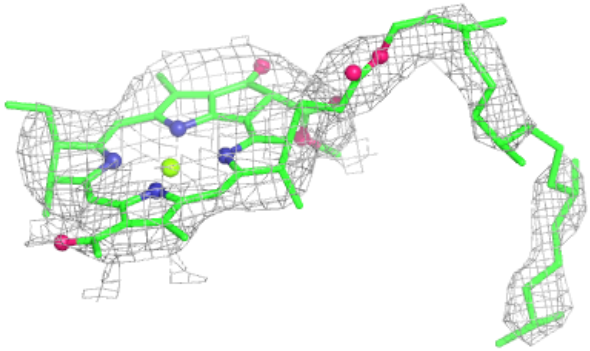


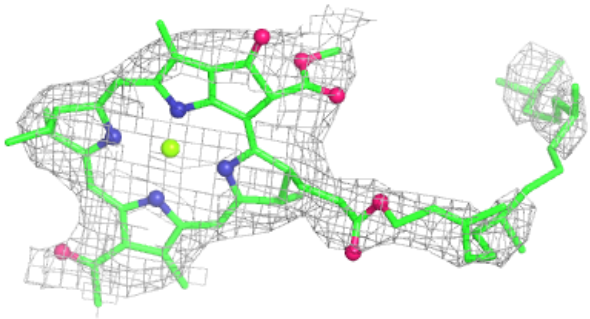


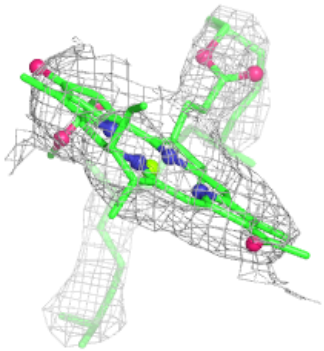


Electron density around BCL D 101:

$2mF_o$-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.