



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:01 AM UTC

PDB ID : 1IJD / pdb_00001ijd
Title : Crystallographic Structure of the LH3 Complex from Rhodopseudomonas acidophila strain 7050
Authors : McLuskey, K.; Prince, S.M.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2001-04-25
Resolution : 3.00 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:

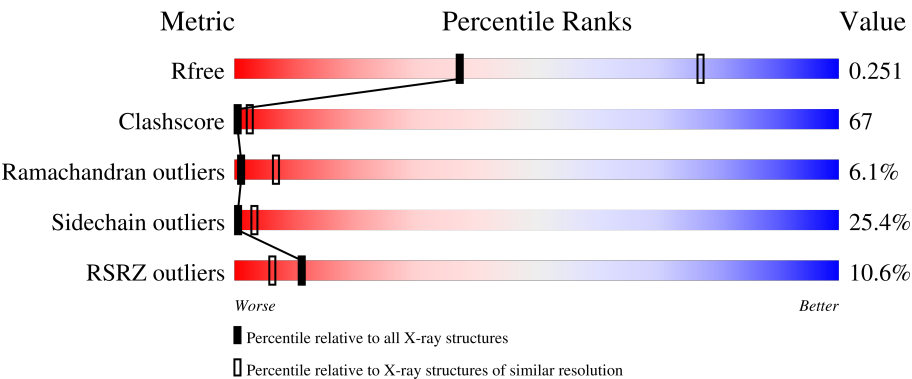
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	53	4% 34% 34% 19% 13%
1	C	53	4% 34% 34% 19% 13%
1	E	53	2% 40% 28% 19% 13%
2	B	42	21% 21% 45% 29% 5%
2	D	42	17% 21% 45% 29% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	42	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	FME	A	1	-	-	X	-
1	FME	C	1	-	-	X	-
1	FME	E	1	-	-	X	-
3	BCL	A	54	X	-	-	-
3	BCL	A	55	-	-	X	-
3	BCL	C	54	X	-	-	-
3	BCL	C	55	-	-	X	-
3	BCL	E	54	X	-	-	-
3	BCL	E	55	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2826 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 B-800/820, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	S	0	0	0
			350	236	56	56	2			
1	C	46	Total	C	N	O	S	0	0	0
			350	236	56	56	2			
1	E	46	Total	C	N	O	S	0	0	0
			350	236	56	56	2			

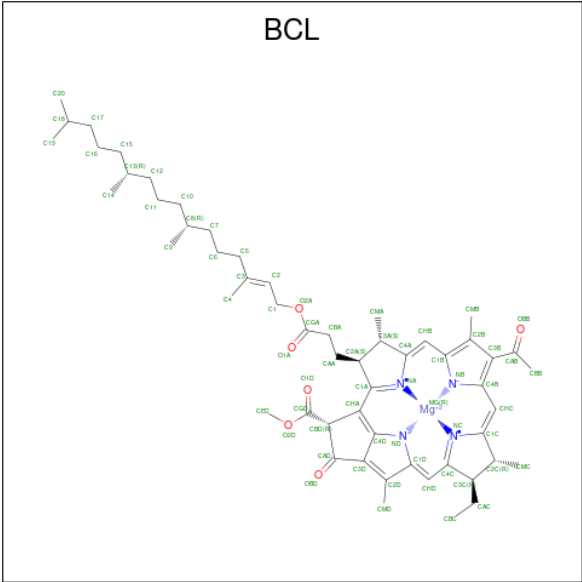
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	FME	MET	modified residue	UNP P35089
C	1	FME	MET	modified residue	UNP P35089
E	1	FME	MET	modified residue	UNP P35089

- Molecule 2 is a protein called LIGHT-HARVESTING PROTEIN B-800/820, BETA CHAIN.

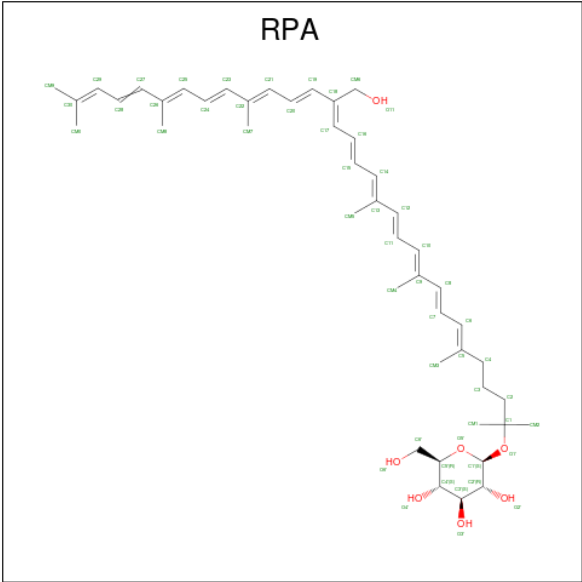
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	0	0	0
			317	209	52	56			
2	D	40	Total	C	N	O	0	0	0
			317	209	52	56			
2	F	40	Total	C	N	O	0	0	0
			317	209	52	56			

- Molecule 3 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



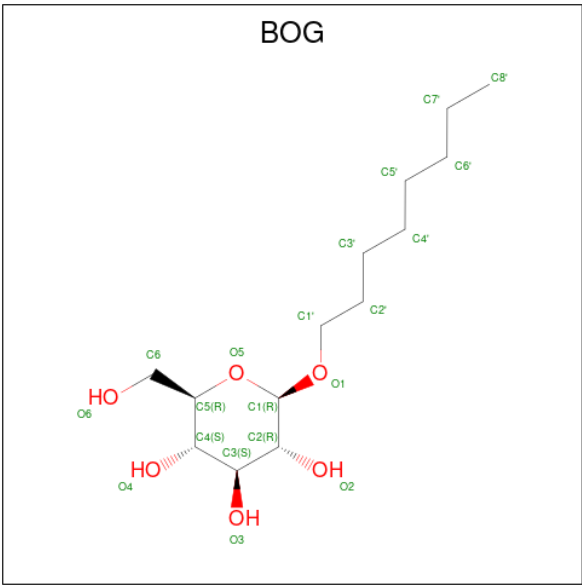
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	E	1	Total 66	C 55	Mg 1	N 4	O 6	0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

- Molecule 4 is RHODOPINAL GLUCOSIDE (CCD ID: RPA) (formula: C₄₆H₆₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			54	46	8		
4	D	1	Total	C	O	0	1
			54	46	8		
4	F	1	Total	C	O	0	1
			54	46	8		

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			9	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			9	8	1		
5	F	1	Total	C	O	0	0
			9	8	1		

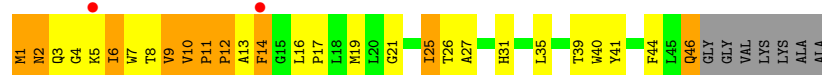
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	7	Total	O	0	0
			7	7		
6	C	9	Total	O	0	0
			9	9		
6	D	4	Total	O	0	0
			4	4		
6	E	10	Total	O	0	0
			10	10		
6	F	3	Total	O	0	0
			3	3		

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 B-800/820, ALPHA CHAIN



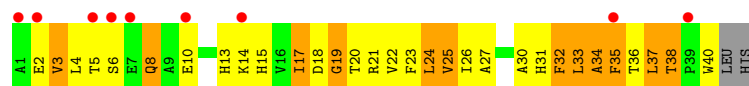
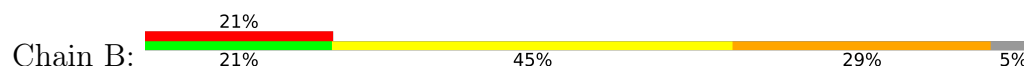
- Molecule 1: LIGHT-HARVESTING PROTEIN B-800/820, ALPHA CHAIN



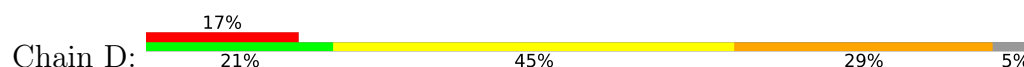
- Molecule 1: LIGHT-HARVESTING PROTEIN B-800/820, ALPHA CHAIN



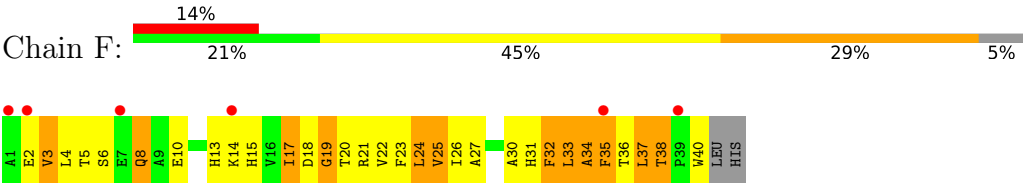
- Molecule 2: LIGHT-HARVESTING PROTEIN B-800/820, BETA CHAIN



- Molecule 2: LIGHT-HARVESTING PROTEIN B-800/820, BETA CHAIN



- Molecule 2: LIGHT-HARVESTING PROTEIN B-800/820, BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.26Å 117.26Å 295.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.00 – 3.00 42.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.00-3.00) 96.5 (42.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 3.01Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.243 , 0.256 0.227 , 0.251	Depositor DCC
R_{free} test set	744 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 135.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l, -k, 8/3^*h+4/3^*k+1/3^*l$ 0.007 for $-2/3^*h-1/3^*k-1/3^*l, -1/3^*h-2/3^*k+1/3^*l, -4/3^*h+4/3^*k+1/3^*l$ 0.000 for $-h, 1/3^*h-1/3^*k-1/3^*l, -4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2826	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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: BOG, FME, BCL, RPA

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	0.52	0/351	1.22	2/485 (0.4%)
1	C	0.52	0/351	1.22	2/485 (0.4%)
1	E	0.52	0/351	1.22	2/485 (0.4%)
2	B	0.48	0/325	1.18	0/444
2	D	0.48	0/325	1.18	0/444
2	F	0.48	0/325	1.18	0/444
All	All	0.50	0/2028	1.20	6/2787 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	VAL	CA-C-N	5.08	125.61	120.38
1	E	10	VAL	C-N-CA	5.08	125.61	120.38
1	C	10	VAL	CA-C-N	5.03	125.56	120.38
1	C	10	VAL	C-N-CA	5.03	125.56	120.38
1	A	10	VAL	CA-C-N	5.01	125.54	120.38
1	A	10	VAL	C-N-CA	5.01	125.54	120.38

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	350	0	364	47	4
1	C	350	0	364	46	0
1	E	350	0	364	44	0
2	B	317	0	319	59	0
2	D	317	0	319	67	0
2	F	317	0	319	65	0
3	A	132	0	148	37	0
3	B	66	0	74	12	0
3	C	132	0	148	40	0
3	D	66	0	74	12	0
3	E	132	0	148	32	0
3	F	66	0	74	13	0
4	B	54	0	14	2	0
4	D	54	0	14	2	0
4	F	54	0	14	2	0
5	B	9	0	17	0	0
5	D	9	0	17	0	0
5	F	9	0	17	0	0
6	A	9	0	0	1	0
6	B	7	0	0	1	0
6	C	9	0	0	2	0
6	D	4	0	0	0	0
6	E	10	0	0	2	4
6	F	3	0	0	0	0
All	All	2826	0	2808	386	4

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 67.

All (386) 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)
3:A:55:BCL:CBC	2:D:22:VAL:HG11	1.80	1.11
3:C:55:BCL:CBC	2:F:22:VAL:HG11	1.80	1.11
3:A:55:BCL:HHC	3:A:55:BCL:HBB2	1.30	1.08
3:C:55:BCL:HHC	3:C:55:BCL:HBB2	1.30	1.06
3:C:55:BCL:HBC1	2:F:22:VAL:CG1	1.86	1.05
3:E:55:BCL:HHC	3:E:55:BCL:HBB2	1.30	1.05
3:A:55:BCL:HBC1	2:D:22:VAL:CG1	1.86	1.04
3:C:55:BCL:CBC	2:F:22:VAL:CG1	2.42	0.97
3:A:55:BCL:CBC	2:D:22:VAL:CG1	2.42	0.97
3:A:55:BCL:HBC1	2:D:22:VAL:HG13	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:BCL:HBC1	2:F:22:VAL:HG13	1.45	0.95
3:C:55:BCL:HHC	3:C:55:BCL:CBB	1.98	0.94
3:E:55:BCL:HHC	3:E:55:BCL:CBB	1.98	0.93
2:F:37:LEU:N	2:F:37:LEU:HD23	1.85	0.91
3:A:55:BCL:HHC	3:A:55:BCL:CBB	1.98	0.91
2:D:37:LEU:N	2:D:37:LEU:HD23	1.85	0.91
2:B:37:LEU:HD23	2:B:37:LEU:N	1.85	0.89
3:A:55:BCL:H92	3:A:55:BCL:C5	2.06	0.86
3:C:55:BCL:H92	3:C:55:BCL:C5	2.06	0.85
1:A:19:MET:HE2	3:A:55:BCL:HED3	1.60	0.84
1:E:19:MET:HE2	3:E:55:BCL:HED3	1.60	0.84
3:E:55:BCL:C5	3:E:55:BCL:H92	2.06	0.84
1:C:19:MET:HE2	3:C:55:BCL:HED3	1.60	0.84
1:E:10:VAL:HG13	1:E:14:PHE:HE2	1.44	0.82
1:C:10:VAL:HG13	1:C:14:PHE:HE2	1.44	0.81
1:A:10:VAL:HG13	1:A:14:PHE:HE2	1.44	0.80
2:B:36:THR:HG22	2:B:37:LEU:HD23	1.63	0.80
1:A:10:VAL:HG13	1:A:14:PHE:CE2	2.18	0.79
1:C:10:VAL:HG13	1:C:14:PHE:CE2	2.18	0.79
2:D:36:THR:HG22	2:D:37:LEU:HD23	1.63	0.79
2:F:36:THR:HG22	2:F:37:LEU:HD23	1.63	0.79
1:E:10:VAL:HG13	1:E:14:PHE:CE2	2.18	0.78
1:E:19:MET:HE2	3:E:55:BCL:CED	2.15	0.77
1:C:19:MET:HE2	3:C:55:BCL:CED	2.15	0.76
1:A:1:FME:HCN	1:A:3:GLN:H	1.51	0.76
3:A:55:BCL:CHD	3:A:55:BCL:HBC3	2.16	0.75
3:E:55:BCL:HBC3	3:E:55:BCL:CHD	2.16	0.75
1:C:1:FME:HCN	1:C:3:GLN:H	1.51	0.75
1:E:1:FME:HCN	1:E:3:GLN:H	1.51	0.75
1:A:19:MET:HE2	3:A:55:BCL:CED	2.15	0.75
3:C:55:BCL:CHD	3:C:55:BCL:HBC3	2.16	0.74
3:C:55:BCL:CBC	3:C:55:BCL:CHD	2.66	0.74
2:F:32:PHE:CD2	2:F:33:LEU:N	2.56	0.74
2:D:32:PHE:CD2	2:D:33:LEU:N	2.56	0.74
2:D:18:ASP:O	2:D:22:VAL:HG23	1.88	0.74
3:E:55:BCL:CHD	3:E:55:BCL:CBC	2.66	0.73
3:A:55:BCL:CBC	3:A:55:BCL:CHD	2.66	0.73
2:B:32:PHE:CD2	2:B:33:LEU:N	2.56	0.73
2:B:18:ASP:O	2:B:22:VAL:HG23	1.88	0.73
3:C:55:BCL:C5	3:C:55:BCL:C9	2.67	0.73
2:F:18:ASP:O	2:F:22:VAL:HG23	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:PHE:HD2	2:F:33:LEU:N	1.87	0.73
2:B:32:PHE:HD2	2:B:33:LEU:N	1.87	0.73
2:B:38:THR:CG2	2:B:40:TRP:H	2.01	0.72
2:D:38:THR:CG2	2:D:40:TRP:H	2.01	0.72
3:E:55:BCL:C5	3:E:55:BCL:C9	2.67	0.72
1:A:1:FME:HE2	2:B:21:ARG:HH22	1.54	0.72
2:F:38:THR:CG2	2:F:40:TRP:H	2.01	0.72
1:E:1:FME:HE2	2:F:21:ARG:HH22	1.54	0.72
3:A:55:BCL:C5	3:A:55:BCL:C9	2.67	0.72
2:B:33:LEU:O	2:B:37:LEU:HG	1.90	0.71
1:C:1:FME:HE2	2:D:21:ARG:HH22	1.54	0.71
2:F:33:LEU:O	2:F:37:LEU:HG	1.90	0.71
2:B:32:PHE:CD2	2:B:32:PHE:C	2.69	0.71
2:D:32:PHE:HD2	2:D:33:LEU:N	1.87	0.70
2:D:33:LEU:O	2:D:37:LEU:HG	1.90	0.70
1:E:16:LEU:N	1:E:17:PRO:CD	2.54	0.70
1:C:16:LEU:N	1:C:17:PRO:CD	2.54	0.70
2:F:36:THR:HG22	2:F:37:LEU:CD2	2.21	0.70
3:A:55:BCL:HBC3	2:D:22:VAL:HG11	1.74	0.70
2:D:32:PHE:CD2	2:D:32:PHE:C	2.69	0.70
1:A:11:PRO:O	1:A:13:ALA:N	2.25	0.70
1:A:16:LEU:N	1:A:17:PRO:CD	2.54	0.70
2:B:36:THR:HG22	2:B:37:LEU:CD2	2.21	0.69
1:A:31:HIS:CE1	3:B:45:BCL:HMD3	2.27	0.69
2:D:36:THR:HG22	2:D:37:LEU:CD2	2.21	0.69
1:C:31:HIS:CE1	3:D:45:BCL:HMD3	2.27	0.69
1:C:11:PRO:O	1:C:13:ALA:N	2.25	0.69
3:C:55:BCL:HBC3	2:F:22:VAL:HG11	1.74	0.69
2:F:32:PHE:CD2	2:F:32:PHE:C	2.69	0.69
1:E:31:HIS:CE1	3:F:45:BCL:HMD3	2.27	0.69
3:C:55:BCL:CBB	3:C:55:BCL:CHC	2.71	0.68
1:E:11:PRO:O	1:E:13:ALA:N	2.25	0.68
3:E:55:BCL:H203	3:F:45:BCL:C2B	2.24	0.68
2:B:22:VAL:O	2:B:26:ILE:HG13	1.94	0.67
2:B:38:THR:HG23	2:B:40:TRP:H	1.58	0.67
3:C:55:BCL:H203	3:D:45:BCL:C2B	2.24	0.67
2:D:38:THR:HG23	2:D:40:TRP:H	1.58	0.67
2:F:22:VAL:O	2:F:26:ILE:HG13	1.94	0.67
3:A:55:BCL:H203	3:B:45:BCL:C2B	2.24	0.67
1:C:26:THR:OG1	3:E:54:BCL:C4	2.43	0.66
2:D:22:VAL:O	2:D:26:ILE:HG13	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:THR:HG23	2:F:40:TRP:H	1.58	0.66
1:A:1:FME:CN	2:B:13:HIS:HE1	2.09	0.66
1:C:26:THR:OG1	3:E:54:BCL:H41	1.96	0.66
1:A:26:THR:OG1	3:C:54:BCL:H41	1.96	0.66
1:E:1:FME:CN	2:F:13:HIS:HE1	2.09	0.66
1:C:1:FME:CN	2:D:13:HIS:HE1	2.09	0.66
1:A:26:THR:OG1	3:C:54:BCL:C4	2.43	0.65
2:D:34:ALA:O	2:D:38:THR:HB	1.97	0.65
2:B:34:ALA:O	2:B:38:THR:HB	1.96	0.65
2:B:17:ILE:O	2:B:21:ARG:HG3	1.97	0.64
3:E:55:BCL:H92	3:E:55:BCL:H51	1.77	0.64
3:C:55:BCL:H92	3:C:55:BCL:H51	1.77	0.64
1:C:1:FME:O1	6:C:114:HOH:O	2.15	0.64
1:A:6:ILE:O	1:A:9:VAL:HG23	1.98	0.64
2:F:17:ILE:O	2:F:21:ARG:HG3	1.97	0.64
1:C:6:ILE:O	1:C:9:VAL:HG23	1.98	0.64
2:D:17:ILE:O	2:D:21:ARG:HG3	1.97	0.64
2:F:34:ALA:O	2:F:38:THR:HB	1.97	0.64
2:F:36:THR:CG2	2:F:37:LEU:HD23	2.28	0.63
3:A:55:BCL:H92	3:A:55:BCL:H51	1.77	0.63
1:E:1:FME:O1	6:E:128:HOH:O	2.15	0.63
1:E:6:ILE:O	1:E:9:VAL:HG23	1.98	0.63
2:D:36:THR:CG2	2:D:37:LEU:HD23	2.28	0.63
3:A:55:BCL:CBB	3:A:55:BCL:CHC	2.71	0.62
1:C:41:TYR:O	1:C:44:PHE:HB3	2.00	0.62
1:A:41:TYR:O	1:A:44:PHE:HB3	2.00	0.61
2:B:36:THR:CG2	2:B:37:LEU:HD23	2.28	0.61
1:E:41:TYR:O	1:E:44:PHE:HB3	2.00	0.61
2:F:35:PHE:HB2	2:F:40:TRP:CZ3	2.36	0.61
2:B:24:LEU:HG	2:B:25:VAL:N	2.16	0.60
2:B:5:THR:OG1	2:B:8:GLN:HG3	2.02	0.60
2:F:5:THR:HG23	2:F:8:GLN:OE1	2.02	0.60
2:D:24:LEU:HG	2:D:25:VAL:N	2.16	0.60
2:B:35:PHE:HB2	2:B:40:TRP:CZ3	2.36	0.60
2:D:35:PHE:HB2	2:D:40:TRP:CZ3	2.36	0.60
2:D:5:THR:OG1	2:D:8:GLN:HG3	2.02	0.60
2:F:5:THR:OG1	2:F:8:GLN:HG3	2.02	0.60
2:F:24:LEU:HG	2:F:25:VAL:N	2.16	0.60
2:B:5:THR:HG23	2:B:8:GLN:OE1	2.02	0.59
2:D:5:THR:HG23	2:D:8:GLN:OE1	2.02	0.59
1:E:14:PHE:O	1:E:17:PRO:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:FME:O1	6:B:100:HOH:O	2.15	0.59
3:E:55:BCL:CBB	3:E:55:BCL:CHC	2.71	0.59
1:C:14:PHE:O	1:C:17:PRO:HD2	2.02	0.59
1:C:35:LEU:HA	1:C:41:TYR:CD2	2.39	0.58
3:A:55:BCL:H92	3:A:55:BCL:H52	1.86	0.58
1:E:35:LEU:HA	1:E:41:TYR:CD2	2.39	0.58
1:A:35:LEU:HA	1:A:41:TYR:CD2	2.39	0.58
1:A:14:PHE:O	1:A:17:PRO:HD2	2.02	0.57
3:C:55:BCL:H92	3:C:55:BCL:H52	1.86	0.56
2:F:37:LEU:N	2:F:37:LEU:CD2	2.60	0.56
1:C:16:LEU:N	1:C:17:PRO:HD3	2.20	0.56
1:E:16:LEU:N	1:E:17:PRO:HD3	2.20	0.56
1:A:16:LEU:N	1:A:17:PRO:HD3	2.20	0.56
2:B:36:THR:C	2:B:37:LEU:HD23	2.30	0.56
2:D:36:THR:C	2:D:37:LEU:HD23	2.30	0.56
2:F:36:THR:C	2:F:37:LEU:HD23	2.30	0.56
3:E:55:BCL:CBC	3:E:55:BCL:HHD	2.36	0.55
2:D:37:LEU:N	2:D:37:LEU:CD2	2.60	0.54
3:E:54:BCL:HMD3	2:F:31:HIS:CE1	2.42	0.54
3:E:55:BCL:H92	3:E:55:BCL:H52	1.86	0.54
3:A:55:BCL:CBC	3:A:55:BCL:HHD	2.36	0.54
3:C:55:BCL:CBC	3:C:55:BCL:HHD	2.36	0.54
3:A:54:BCL:HMD3	2:B:31:HIS:CE1	2.43	0.54
2:B:36:THR:CG2	2:B:37:LEU:CD2	2.85	0.54
1:A:8:THR:O	2:B:3:VAL:HG11	2.08	0.54
1:E:8:THR:O	2:F:3:VAL:HG11	2.08	0.54
2:F:36:THR:CG2	2:F:37:LEU:CD2	2.85	0.54
1:C:8:THR:O	2:D:3:VAL:HG11	2.08	0.54
3:C:54:BCL:HMD3	2:D:31:HIS:CE1	2.42	0.54
2:F:24:LEU:HB2	3:F:45:BCL:H11	1.90	0.54
2:D:36:THR:CG2	2:D:37:LEU:CD2	2.85	0.53
1:C:25:ILE:N	1:C:25:ILE:HD13	2.24	0.53
2:D:24:LEU:HB2	3:D:45:BCL:H11	1.90	0.53
2:B:37:LEU:N	2:B:37:LEU:CD2	2.60	0.53
3:C:55:BCL:HBC2	2:F:22:VAL:HG11	1.84	0.53
3:A:54:BCL:HED2	2:B:27:ALA:CA	2.39	0.53
2:B:18:ASP:O	2:B:19:GLY:C	2.51	0.52
3:E:54:BCL:HED2	2:F:27:ALA:CA	2.39	0.52
3:A:55:BCL:HAA1	3:A:55:BCL:HBD	1.91	0.52
1:A:25:ILE:N	1:A:25:ILE:HD13	2.24	0.52
1:A:40:TRP:CE3	1:A:41:TYR:N	2.78	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:HB2	3:B:45:BCL:H11	1.90	0.52
3:E:55:BCL:HBD	3:E:55:BCL:HAA1	1.91	0.52
1:C:11:PRO:C	1:C:13:ALA:N	2.68	0.52
1:E:11:PRO:C	1:E:13:ALA:N	2.68	0.52
1:C:40:TRP:CE3	1:C:41:TYR:N	2.78	0.52
3:C:54:BCL:HED2	2:D:27:ALA:CA	2.39	0.52
2:F:25:VAL:HG12	2:F:26:ILE:N	2.24	0.52
1:A:11:PRO:O	1:A:12:PRO:C	2.53	0.52
1:A:11:PRO:C	1:A:13:ALA:N	2.68	0.52
2:D:18:ASP:O	2:D:19:GLY:C	2.52	0.52
2:F:18:ASP:O	2:F:19:GLY:C	2.52	0.52
3:C:55:BCL:HBD	3:C:55:BCL:HAA1	1.91	0.52
1:E:25:ILE:HD13	1:E:25:ILE:N	2.24	0.52
1:E:40:TRP:CE3	1:E:41:TYR:N	2.78	0.52
2:F:38:THR:HG22	2:F:40:TRP:H	1.75	0.52
3:C:55:BCL:HHD	3:C:55:BCL:HBC2	1.93	0.51
2:D:25:VAL:HG12	2:D:26:ILE:N	2.24	0.51
3:E:55:BCL:HHD	3:E:55:BCL:HBC2	1.93	0.51
3:A:55:BCL:HHD	3:A:55:BCL:HBC2	1.93	0.51
3:B:45:BCL:HMB3	3:B:45:BCL:HBB2	1.93	0.50
3:F:45:BCL:HBB2	3:F:45:BCL:HMB3	1.93	0.50
2:B:25:VAL:HG12	2:B:26:ILE:N	2.24	0.50
2:B:24:LEU:O	2:B:27:ALA:HB3	2.12	0.50
2:D:24:LEU:O	2:D:27:ALA:HB3	2.12	0.49
1:A:2:ASN:OD1	1:A:2:ASN:N	2.44	0.49
1:E:11:PRO:O	1:E:12:PRO:C	2.53	0.49
1:E:1:FME:HE2	2:F:21:ARG:NH2	2.24	0.49
3:D:45:BCL:HBB2	3:D:45:BCL:HMB3	1.93	0.49
2:F:24:LEU:O	2:F:27:ALA:HB3	2.12	0.49
2:D:38:THR:CG2	2:D:40:TRP:HB3	2.43	0.48
2:B:38:THR:HG22	2:B:40:TRP:H	1.75	0.48
1:A:1:FME:HE2	2:B:21:ARG:NH2	2.24	0.48
1:C:11:PRO:C	1:C:13:ALA:H	2.22	0.48
1:A:11:PRO:C	1:A:13:ALA:H	2.22	0.48
3:A:55:BCL:HBC2	2:D:22:VAL:HG11	1.84	0.48
2:B:10:GLU:O	2:B:14:LYS:HG3	2.14	0.48
2:B:38:THR:CG2	2:B:40:TRP:HB3	2.43	0.48
1:E:25:ILE:N	1:E:25:ILE:CD1	2.77	0.48
2:F:38:THR:CG2	2:F:40:TRP:HB3	2.43	0.48
2:D:10:GLU:O	2:D:14:LYS:HG3	2.14	0.48
1:E:2:ASN:OD1	1:E:2:ASN:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:PRO:C	1:E:13:ALA:H	2.22	0.48
1:A:39:THR:HG23	1:C:46:GLN:OE1	2.14	0.47
2:D:38:THR:HG22	2:D:40:TRP:H	1.75	0.47
1:C:11:PRO:O	1:C:12:PRO:C	2.53	0.47
1:C:25:ILE:N	1:C:25:ILE:CD1	2.77	0.47
1:C:1:FME:HE2	2:D:21:ARG:NH2	2.24	0.47
1:A:25:ILE:N	1:A:25:ILE:CD1	2.77	0.47
1:C:39:THR:HG23	1:E:46:GLN:OE1	2.14	0.47
3:C:55:BCL:H201	3:D:45:BCL:CAB	2.44	0.47
1:A:4:GLY:HA2	2:B:13:HIS:CG	2.50	0.47
3:A:55:BCL:H201	3:B:45:BCL:CAB	2.44	0.47
1:C:1:FME:CN	2:D:13:HIS:CE1	2.94	0.47
1:E:19:MET:CE	3:E:55:BCL:CED	2.91	0.47
3:E:55:BCL:H201	3:F:45:BCL:CAB	2.44	0.47
2:B:27:ALA:O	2:B:30:ALA:HB3	2.15	0.47
1:C:41:TYR:HB3	6:C:116:HOH:O	2.15	0.47
1:C:4:GLY:HA2	2:D:13:HIS:CG	2.50	0.47
2:D:20:THR:O	2:D:23:PHE:HB3	2.15	0.47
2:F:10:GLU:O	2:F:14:LYS:HG3	2.14	0.47
2:F:20:THR:O	2:F:23:PHE:HB3	2.15	0.47
1:E:4:GLY:HA2	2:F:13:HIS:CG	2.50	0.46
1:C:14:PHE:C	1:C:17:PRO:HD2	2.41	0.46
2:F:36:THR:CB	2:F:37:LEU:HD23	2.45	0.46
2:D:27:ALA:O	2:D:30:ALA:HB3	2.15	0.46
2:F:27:ALA:O	2:F:30:ALA:HB3	2.15	0.46
1:A:1:FME:CN	2:B:13:HIS:CE1	2.94	0.46
1:E:41:TYR:HB3	6:E:130:HOH:O	2.14	0.46
1:A:14:PHE:C	1:A:17:PRO:HD2	2.41	0.46
2:D:36:THR:CB	2:D:37:LEU:HD23	2.45	0.46
1:A:1:FME:N	2:B:17:ILE:HD11	2.31	0.46
1:E:14:PHE:C	1:E:17:PRO:HD2	2.41	0.46
1:A:41:TYR:HB3	6:A:102:HOH:O	2.15	0.46
3:A:55:BCL:CMD	2:D:19:GLY:HA2	2.46	0.46
2:B:20:THR:O	2:B:23:PHE:HB3	2.15	0.46
1:E:16:LEU:H	1:E:17:PRO:HD3	1.81	0.46
1:C:16:LEU:H	1:C:17:PRO:HD3	1.81	0.45
1:E:1:FME:CN	2:F:13:HIS:CE1	2.94	0.45
3:E:55:BCL:C20	3:F:45:BCL:C2B	2.94	0.45
3:C:55:BCL:CMD	2:F:19:GLY:HA2	2.46	0.45
1:E:1:FME:N	2:F:17:ILE:HD11	2.31	0.45
1:C:1:FME:N	2:D:17:ILE:HD11	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:CE	3:C:55:BCL:CED	2.91	0.45
2:B:36:THR:CB	2:B:37:LEU:HD23	2.45	0.45
1:A:21:GLY:O	1:A:25:ILE:HD13	2.17	0.45
1:C:21:GLY:O	1:C:25:ILE:HD13	2.17	0.45
1:A:19:MET:CE	3:A:55:BCL:HED3	2.40	0.44
1:C:7:TRP:HE1	2:D:13:HIS:HD2	1.64	0.44
1:E:21:GLY:O	1:E:25:ILE:HD13	2.17	0.44
1:A:19:MET:CE	3:A:55:BCL:CED	2.91	0.44
1:E:7:TRP:HE1	2:F:13:HIS:HD2	1.64	0.44
1:A:16:LEU:H	1:A:17:PRO:HD3	1.81	0.44
3:C:55:BCL:C20	3:D:45:BCL:C2B	2.94	0.44
1:A:7:TRP:HE1	2:B:13:HIS:HD2	1.64	0.44
1:E:19:MET:CE	3:E:55:BCL:HED3	2.40	0.44
3:A:55:BCL:C20	3:B:45:BCL:C2B	2.94	0.44
3:E:54:BCL:H121	3:E:54:BCL:H161	1.47	0.44
1:A:35:LEU:HA	1:A:41:TYR:HD2	1.82	0.44
1:C:35:LEU:HA	1:C:41:TYR:HD2	1.82	0.44
3:A:54:BCL:H161	3:A:54:BCL:H121	1.47	0.44
3:A:55:BCL:C20	3:B:45:BCL:C3B	2.96	0.44
3:A:55:BCL:HMB1	2:B:21:ARG:HE	1.83	0.44
3:E:55:BCL:HMB1	2:F:21:ARG:HE	1.83	0.43
1:C:2:ASN:OD1	1:C:2:ASN:N	2.44	0.43
3:C:55:BCL:HMB1	2:D:21:ARG:HE	1.83	0.43
3:A:54:BCL:HED2	2:B:27:ALA:HA	2.00	0.43
3:C:54:BCL:HED2	2:D:27:ALA:HA	2.00	0.43
3:E:54:BCL:HED2	2:F:27:ALA:HA	2.00	0.43
1:A:1:FME:CN	1:A:3:GLN:H	2.26	0.43
3:E:55:BCL:C20	3:F:45:BCL:C3B	2.96	0.43
3:C:55:BCL:C20	3:D:45:BCL:C3B	2.96	0.43
3:C:54:BCL:H121	3:C:54:BCL:H161	1.47	0.43
3:C:54:BCL:H51	3:C:54:BCL:H12	1.79	0.42
1:C:40:TRP:CE3	1:C:40:TRP:C	2.97	0.42
1:C:1:FME:HCN	2:D:13:HIS:CE1	2.55	0.42
3:C:55:BCL:HBA1	3:C:55:BCL:H3A	1.89	0.42
1:A:6:ILE:C	1:A:9:VAL:HG23	2.44	0.42
1:C:6:ILE:C	1:C:9:VAL:HG23	2.44	0.42
1:E:35:LEU:HA	1:E:41:TYR:HD2	1.82	0.42
1:E:6:ILE:C	1:E:9:VAL:HG23	2.44	0.42
1:A:11:PRO:HA	1:A:12:PRO:HD2	1.85	0.42
1:A:40:TRP:CE3	1:A:40:TRP:C	2.97	0.42
1:E:40:TRP:CE3	1:E:40:TRP:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:45:BCL:HBB2	3:F:45:BCL:CMB	2.50	0.41
1:A:1:FME:N	2:B:17:ILE:CD1	2.84	0.41
1:C:1:FME:N	2:D:17:ILE:CD1	2.84	0.41
1:E:1:FME:N	2:F:17:ILE:CD1	2.83	0.41
1:A:1:FME:HCN	2:B:13:HIS:CE1	2.55	0.41
3:B:45:BCL:HBB2	3:B:45:BCL:CMB	2.50	0.41
1:E:1:FME:HCN	2:F:13:HIS:CE1	2.55	0.41
1:E:1:FME:CN	1:E:3:GLN:H	2.26	0.41
1:E:27:ALA:CA	3:F:45:BCL:HED2	2.51	0.41
2:B:38:THR:HG22	2:B:40:TRP:HB3	2.03	0.41
1:C:16:LEU:HD12	1:C:16:LEU:HA	1.87	0.41
1:C:27:ALA:CA	3:D:45:BCL:HED2	2.51	0.41
2:D:35:PHE:HA	2:D:40:TRP:CE3	2.56	0.41
3:D:45:BCL:HBB2	3:D:45:BCL:CMB	2.50	0.41
1:A:27:ALA:CA	3:B:45:BCL:HED2	2.51	0.41
3:A:55:BCL:H61	3:A:55:BCL:H93	1.73	0.40
3:F:45:BCL:H2A	3:F:45:BCL:O1D	2.21	0.40
2:D:32:PHE:CE2	2:D:33:LEU:HD23	2.57	0.40
3:A:55:BCL:HBA1	3:A:55:BCL:H3A	1.89	0.40
2:F:35:PHE:HA	2:F:40:TRP:CE3	2.56	0.40
2:B:35:PHE:HA	2:B:40:TRP:CE3	2.56	0.40
2:D:38:THR:HG22	2:D:40:TRP:HB3	2.02	0.40
1:E:10:VAL:CG1	1:E:14:PHE:CE2	2.99	0.40
3:A:54:BCL:H51	3:A:54:BCL:H12	1.79	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:OE1	6:E:131:HOH:O[3_555]	0.82	1.38
1:A:46:GLN:CD	6:E:131:HOH:O[3_555]	0.85	1.35
1:A:46:GLN:CG	6:E:131:HOH:O[3_555]	1.60	0.60
1:A:46:GLN:NE2	6:E:131:HOH:O[3_555]	2.14	0.06

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	44/53 (83%)	36 (82%)	6 (14%)	2 (4%)	2	12
1	C	44/53 (83%)	37 (84%)	5 (11%)	2 (4%)	2	12
1	E	44/53 (83%)	37 (84%)	5 (11%)	2 (4%)	2	12
2	B	38/42 (90%)	25 (66%)	10 (26%)	3 (8%)	1	3
2	D	38/42 (90%)	25 (66%)	10 (26%)	3 (8%)	1	3
2	F	38/42 (90%)	25 (66%)	10 (26%)	3 (8%)	1	3
All	All	246/285 (86%)	185 (75%)	46 (19%)	15 (6%)	1	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	PHE
2	D	35	PHE
2	F	35	PHE
1	A	12	PRO
1	C	12	PRO
1	E	12	PRO
2	B	34	ALA
2	D	34	ALA
2	F	34	ALA
1	A	11	PRO
1	C	11	PRO
1	E	11	PRO
2	B	19	GLY
2	D	19	GLY
2	F	19	GLY

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	34/37 (92%)	28 (82%)	6 (18%)	2	10
1	C	34/37 (92%)	28 (82%)	6 (18%)	2	10
1	E	34/37 (92%)	28 (82%)	6 (18%)	2	10
2	B	33/35 (94%)	22 (67%)	11 (33%)	0	1
2	D	33/35 (94%)	22 (67%)	11 (33%)	0	1
2	F	33/35 (94%)	22 (67%)	11 (33%)	0	1
All	All	201/216 (93%)	150 (75%)	51 (25%)	0	3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	ILE
1	A	9	VAL
1	A	14	PHE
1	A	25	ILE
1	A	46	GLN
2	B	2	GLU
2	B	3	VAL
2	B	6	SER
2	B	8	GLN
2	B	17	ILE
2	B	24	LEU
2	B	25	VAL
2	B	32	PHE
2	B	33	LEU
2	B	37	LEU
2	B	38	THR
1	C	2	ASN
1	C	6	ILE
1	C	9	VAL
1	C	14	PHE
1	C	25	ILE
1	C	46	GLN
2	D	2	GLU
2	D	3	VAL
2	D	6	SER
2	D	8	GLN
2	D	17	ILE
2	D	24	LEU
2	D	25	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	32	PHE
2	D	33	LEU
2	D	37	LEU
2	D	38	THR
1	E	2	ASN
1	E	6	ILE
1	E	9	VAL
1	E	14	PHE
1	E	25	ILE
1	E	46	GLN
2	F	2	GLU
2	F	3	VAL
2	F	6	SER
2	F	8	GLN
2	F	17	ILE
2	F	24	LEU
2	F	25	VAL
2	F	32	PHE
2	F	33	LEU
2	F	37	LEU
2	F	38	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
2	B	13	HIS
2	B	31	HIS
1	C	31	HIS
2	D	13	HIS
2	D	31	HIS
1	E	31	HIS
2	F	13	HIS
2	F	31	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	FME	A	1	1,3	8,9,10	2.48	2 (25%)	8,9,11	2.08	1 (12%)
1	FME	C	1	1,3	8,9,10	2.48	2 (25%)	8,9,11	2.08	1 (12%)
1	FME	E	1	1,3	8,9,10	2.48	2 (25%)	8,9,11	2.08	1 (12%)

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
1	FME	A	1	1,3	-	4/7/9/11	-
1	FME	C	1	1,3	-	4/7/9/11	-
1	FME	E	1	1,3	-	4/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	FME	O1-CN	5.88	1.46	1.22
1	C	1	FME	O1-CN	5.87	1.46	1.22
1	A	1	FME	O1-CN	5.87	1.46	1.22
1	A	1	FME	CN-N	3.62	1.45	1.33
1	C	1	FME	CN-N	3.61	1.45	1.33
1	E	1	FME	CN-N	3.61	1.45	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O1-CN-N	-5.46	111.22	125.32
1	C	1	FME	O1-CN-N	-5.46	111.23	125.32
1	E	1	FME	O1-CN-N	-5.45	111.23	125.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	C-CA-CB-CG
1	E	1	FME	O1-CN-N-CA
1	E	1	FME	C-CA-CB-CG
1	A	1	FME	N-CA-CB-CG
1	C	1	FME	N-CA-CB-CG
1	E	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
1	C	1	FME	CB-CG-SD-CE
1	E	1	FME	CB-CG-SD-CE

There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	10	0
1	C	1	FME	9	0
1	E	1	FME	10	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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
3	BCL	E	55	1	69,74,74	1.07	4 (5%)	79,115,115	1.38	9 (11%)
3	BCL	C	55	1	69,74,74	1.07	4 (5%)	79,115,115	1.38	9 (11%)
5	BOG	D	44	-	8,8,20	0.23	0	7,7,25	1.11	0
3	BCL	F	45	2	69,74,74	0.92	4 (5%)	79,115,115	1.46	14 (17%)
4	RPA	D	43[A]	-	52,53,53	2.18	8 (15%)	65,68,68	2.33	16 (24%)
3	BCL	A	54	1	69,74,74	1.01	5 (7%)	79,115,115	1.30	11 (13%)
5	BOG	B	44	-	8,8,20	0.23	0	7,7,25	1.11	0
3	BCL	E	54	1	69,74,74	1.01	5 (7%)	79,115,115	1.31	10 (12%)
4	RPA	B	43[A]	-	52,53,53	2.18	8 (15%)	65,68,68	2.33	17 (26%)
5	BOG	F	44	-	8,8,20	0.24	0	7,7,25	1.11	0
3	BCL	C	54	1	69,74,74	1.01	5 (7%)	79,115,115	1.30	10 (12%)
4	RPA	F	43[A]	-	52,53,53	2.17	8 (15%)	65,68,68	2.33	17 (26%)
4	RPA	D	43[B]	-	52,53,53	4.24	7 (13%)	65,68,68	2.23	15 (23%)
3	BCL	D	45	2	69,74,74	0.92	4 (5%)	79,115,115	1.47	14 (17%)
4	RPA	B	43[B]	-	52,53,53	4.25	7 (13%)	65,68,68	2.23	16 (24%)
3	BCL	A	55	1	69,74,74	1.07	4 (5%)	79,115,115	1.38	9 (11%)
3	BCL	B	45	2	69,74,74	0.92	3 (4%)	79,115,115	1.47	14 (17%)
4	RPA	F	43[B]	-	52,53,53	4.24	7 (13%)	65,68,68	2.23	16 (24%)

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
3	BCL	E	55	1	-	17/41/137/137	-
3	BCL	C	55	1	-	17/41/137/137	-
5	BOG	D	44	-	-	3/6/6/31	-
3	BCL	F	45	2	-	15/41/137/137	-
4	RPA	D	43[A]	-	-	19/53/73/73	0/1/1/1
3	BCL	A	54	1	1/1/21/25	19/41/137/137	-
5	BOG	B	44	-	-	3/6/6/31	-
3	BCL	E	54	1	1/1/21/25	19/41/137/137	-
4	RPA	B	43[A]	-	-	19/53/73/73	0/1/1/1
5	BOG	F	44	-	-	3/6/6/31	-
3	BCL	C	54	1	1/1/21/25	19/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RPA	F	43[A]	-	-	19/53/73/73	0/1/1/1
4	RPA	D	43[B]	-	-	19/53/73/73	0/1/1/1
3	BCL	D	45	2	-	15/41/137/137	-
4	RPA	B	43[B]	-	-	19/53/73/73	0/1/1/1
3	BCL	A	55	1	-	17/41/137/137	-
3	BCL	B	45	2	-	15/41/137/137	-
4	RPA	F	43[B]	-	-	19/53/73/73	0/1/1/1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	43[B]	RPA	O1'-C1	27.98	1.83	1.46
4	D	43[B]	RPA	O1'-C1	27.97	1.83	1.46
4	F	43[B]	RPA	O1'-C1	27.95	1.83	1.46
4	D	43[A]	RPA	O1'-C1'	7.28	1.70	1.40
4	F	43[A]	RPA	O1'-C1'	7.28	1.70	1.40
4	B	43[A]	RPA	O1'-C1'	7.27	1.70	1.40
4	B	43[A]	RPA	C28-C27	6.64	1.52	1.34
4	B	43[B]	RPA	C28-C27	6.64	1.52	1.34
4	D	43[A]	RPA	C28-C27	6.63	1.52	1.34
4	D	43[B]	RPA	C28-C27	6.63	1.52	1.34
4	F	43[A]	RPA	C28-C27	6.61	1.51	1.34
4	F	43[B]	RPA	C28-C27	6.61	1.51	1.34
4	B	43[A]	RPA	O1'-C1	6.35	1.55	1.46
4	D	43[A]	RPA	O1'-C1	6.34	1.55	1.46
4	F	43[A]	RPA	O1'-C1	6.34	1.55	1.46
4	B	43[A]	RPA	O11-CM6	-6.05	1.22	1.41
4	B	43[B]	RPA	O11-CM6	-6.05	1.22	1.41
4	D	43[A]	RPA	O11-CM6	-6.03	1.22	1.41
4	D	43[B]	RPA	O11-CM6	-6.03	1.22	1.41
4	F	43[A]	RPA	O11-CM6	-6.03	1.22	1.41
4	F	43[B]	RPA	O11-CM6	-6.03	1.22	1.41
4	F	43[A]	RPA	C16-C15	-5.55	1.21	1.36
4	F	43[B]	RPA	C16-C15	-5.55	1.21	1.36
4	B	43[A]	RPA	C16-C15	-5.55	1.21	1.36
4	B	43[B]	RPA	C16-C15	-5.55	1.21	1.36
4	D	43[A]	RPA	C16-C15	-5.52	1.21	1.36
4	D	43[B]	RPA	C16-C15	-5.52	1.21	1.36
3	E	55	BCL	MG-NC	4.92	2.18	2.06
3	C	55	BCL	MG-NC	4.91	2.17	2.06
3	A	55	BCL	MG-NC	4.91	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	43[A]	RPA	C2-C1	4.54	1.59	1.53
4	B	43[B]	RPA	C2-C1	4.54	1.59	1.53
4	D	43[A]	RPA	C2-C1	4.52	1.59	1.53
4	D	43[B]	RPA	C2-C1	4.52	1.59	1.53
4	F	43[A]	RPA	C2-C1	4.49	1.59	1.53
4	F	43[B]	RPA	C2-C1	4.49	1.59	1.53
3	E	54	BCL	MG-NC	4.15	2.16	2.06
3	C	54	BCL	MG-NC	4.15	2.16	2.06
3	A	54	BCL	MG-NC	4.14	2.16	2.06
3	A	55	BCL	MG-NA	3.80	2.15	2.06
3	E	55	BCL	MG-NA	3.80	2.15	2.06
3	C	55	BCL	MG-NA	3.80	2.15	2.06
3	A	54	BCL	MG-NA	3.62	2.14	2.06
3	E	54	BCL	MG-NA	3.62	2.14	2.06
3	C	54	BCL	MG-NA	3.62	2.14	2.06
3	B	45	BCL	MG-NC	3.27	2.14	2.06
3	D	45	BCL	MG-NC	3.26	2.14	2.06
3	F	45	BCL	MG-NC	3.26	2.14	2.06
3	B	45	BCL	MG-NA	3.06	2.13	2.06
3	D	45	BCL	MG-NA	3.06	2.13	2.06
3	F	45	BCL	MG-NA	3.05	2.13	2.06
4	F	43[A]	RPA	C28-C29	2.24	1.50	1.43
4	F	43[B]	RPA	C28-C29	2.24	1.50	1.43
4	D	43[A]	RPA	C28-C29	2.22	1.50	1.43
4	D	43[B]	RPA	C28-C29	2.22	1.50	1.43
4	B	43[A]	RPA	C28-C29	2.21	1.50	1.43
4	B	43[B]	RPA	C28-C29	2.21	1.50	1.43
3	A	54	BCL	C3B-C4B	2.17	1.45	1.41
3	C	54	BCL	C3B-C4B	2.17	1.45	1.41
3	E	54	BCL	C3B-C4B	2.16	1.45	1.41
3	E	55	BCL	C3B-C4B	2.15	1.45	1.41
3	A	55	BCL	C3B-C4B	2.14	1.45	1.41
3	C	55	BCL	C3B-C4B	2.13	1.45	1.41
3	F	45	BCL	C1-C2	2.07	1.55	1.49
3	B	45	BCL	C1-C2	2.07	1.55	1.49
3	D	45	BCL	C1-C2	2.06	1.55	1.49
4	F	43[A]	RPA	C4-C5	-2.05	1.47	1.51
4	F	43[B]	RPA	C4-C5	-2.05	1.47	1.51
4	B	43[A]	RPA	C4-C5	-2.04	1.47	1.51
4	B	43[B]	RPA	C4-C5	-2.04	1.47	1.51
3	A	54	BCL	C1-C2	2.04	1.55	1.49
3	A	55	BCL	C1-C2	2.03	1.54	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	43[A]	RPA	C4-C5	-2.03	1.47	1.51
4	D	43[B]	RPA	C4-C5	-2.03	1.47	1.51
3	C	54	BCL	C1-C2	2.03	1.54	1.49
3	C	55	BCL	C1-C2	2.02	1.54	1.49
3	A	54	BCL	CHC-C1C	2.02	1.42	1.37
3	E	55	BCL	C1-C2	2.01	1.54	1.49
3	E	54	BCL	C1-C2	2.01	1.54	1.49
3	C	54	BCL	CHC-C1C	2.01	1.42	1.37
3	D	45	BCL	CHC-C1C	2.01	1.42	1.37
3	F	45	BCL	CHC-C1C	2.00	1.42	1.37
3	E	54	BCL	CHC-C1C	2.00	1.42	1.37

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	43[A]	RPA	C1-O1'-C1'	8.91	138.01	119.78
4	D	43[A]	RPA	C1-O1'-C1'	8.90	138.00	119.78
4	F	43[A]	RPA	C1-O1'-C1'	8.90	137.99	119.78
4	F	43[A]	RPA	C15-C16-C17	8.70	141.32	123.52
4	F	43[B]	RPA	C15-C16-C17	8.70	141.32	123.52
4	B	43[A]	RPA	C15-C16-C17	8.69	141.29	123.52
4	B	43[B]	RPA	C15-C16-C17	8.69	141.29	123.52
4	D	43[A]	RPA	C15-C16-C17	8.68	141.27	123.52
4	D	43[B]	RPA	C15-C16-C17	8.68	141.27	123.52
4	D	43[B]	RPA	C1-O1'-C1'	7.49	135.10	119.78
4	B	43[B]	RPA	C1-O1'-C1'	7.49	135.10	119.78
4	F	43[B]	RPA	C1-O1'-C1'	7.48	135.07	119.78
4	F	43[A]	RPA	C16-C15-C14	6.32	136.45	123.52
4	F	43[B]	RPA	C16-C15-C14	6.32	136.45	123.52
4	B	43[A]	RPA	C16-C15-C14	6.32	136.44	123.52
4	B	43[B]	RPA	C16-C15-C14	6.32	136.44	123.52
4	D	43[A]	RPA	C16-C15-C14	6.30	136.40	123.52
4	D	43[B]	RPA	C16-C15-C14	6.30	136.40	123.52
3	A	55	BCL	C4D-CHA-C1A	5.72	128.06	121.24
3	C	55	BCL	C4D-CHA-C1A	5.70	128.04	121.24
3	E	55	BCL	C4D-CHA-C1A	5.68	128.02	121.24
3	D	45	BCL	C4A-NA-C1A	4.65	108.80	106.68
3	B	45	BCL	C4A-NA-C1A	4.63	108.79	106.68
3	F	45	BCL	C4A-NA-C1A	4.62	108.79	106.68
4	F	43[A]	RPA	C29-C28-C27	-4.60	109.86	123.20
4	F	43[B]	RPA	C29-C28-C27	-4.60	109.86	123.20
4	B	43[A]	RPA	C29-C28-C27	-4.60	109.88	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	43[B]	RPA	C29-C28-C27	-4.60	109.88	123.20
4	D	43[A]	RPA	C29-C28-C27	-4.60	109.88	123.20
4	D	43[B]	RPA	C29-C28-C27	-4.60	109.88	123.20
4	D	43[A]	RPA	CM3-C5-C4	3.67	121.61	115.23
4	D	43[B]	RPA	CM3-C5-C4	3.67	121.61	115.23
3	B	45	BCL	C1C-NC-C4C	3.67	108.35	106.68
3	D	45	BCL	C1C-NC-C4C	3.66	108.35	106.68
4	B	43[A]	RPA	CM3-C5-C4	3.66	121.58	115.23
4	B	43[B]	RPA	CM3-C5-C4	3.66	121.58	115.23
3	F	45	BCL	C1C-NC-C4C	3.66	108.35	106.68
4	F	43[A]	RPA	CM3-C5-C4	3.65	121.57	115.23
4	F	43[B]	RPA	CM3-C5-C4	3.65	121.57	115.23
3	E	54	BCL	C1C-NC-C4C	3.55	108.30	106.68
4	B	43[A]	RPA	C15-C14-C13	3.52	132.22	127.28
4	B	43[B]	RPA	C15-C14-C13	3.52	132.22	127.28
4	F	43[A]	RPA	C15-C14-C13	3.52	132.22	127.28
4	F	43[B]	RPA	C15-C14-C13	3.52	132.22	127.28
3	A	54	BCL	C1C-NC-C4C	3.51	108.28	106.68
3	C	54	BCL	C1C-NC-C4C	3.51	108.28	106.68
4	D	43[A]	RPA	C15-C14-C13	3.51	132.20	127.28
4	D	43[B]	RPA	C15-C14-C13	3.51	132.20	127.28
3	B	45	BCL	C3B-C4B-NB	-3.48	105.16	109.76
3	D	45	BCL	C3B-C4B-NB	-3.46	105.19	109.76
3	F	45	BCL	C3B-C4B-NB	-3.45	105.20	109.76
4	B	43[A]	RPA	C21-C20-C19	3.38	132.98	123.20
4	B	43[B]	RPA	C21-C20-C19	3.38	132.98	123.20
4	D	43[A]	RPA	C21-C20-C19	3.37	132.97	123.20
4	D	43[B]	RPA	C21-C20-C19	3.37	132.97	123.20
4	F	43[A]	RPA	C21-C20-C19	3.36	132.95	123.20
4	F	43[B]	RPA	C21-C20-C19	3.36	132.95	123.20
3	C	55	BCL	CHC-C4B-NB	3.34	129.06	124.05
3	A	55	BCL	CHC-C4B-NB	3.34	129.06	124.05
3	E	54	BCL	C4A-NA-C1A	3.34	108.20	106.68
3	E	55	BCL	CHC-C4B-NB	3.34	129.06	124.05
3	F	45	BCL	C1D-ND-C4D	3.32	108.64	106.31
4	D	43[A]	RPA	O1'-C1'-C2'	3.32	117.67	108.42
4	B	43[A]	RPA	O1'-C1'-C2'	3.32	117.66	108.42
3	A	54	BCL	C1-C2-C3	-3.32	120.76	126.20
3	D	45	BCL	C1D-ND-C4D	3.32	108.64	106.31
4	F	43[A]	RPA	O1'-C1'-C2'	3.31	117.64	108.42
3	A	54	BCL	C4A-NA-C1A	3.31	108.19	106.68
3	C	54	BCL	C4A-NA-C1A	3.30	108.19	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	45	BCL	C1D-ND-C4D	3.29	108.62	106.31
3	C	54	BCL	C2B-C1B-NB	-3.29	106.92	110.33
3	C	54	BCL	C1-C2-C3	-3.29	120.81	126.20
3	A	54	BCL	C2B-C1B-NB	-3.29	106.92	110.33
3	E	54	BCL	C2B-C1B-NB	-3.28	106.92	110.33
3	E	54	BCL	C1-C2-C3	-3.28	120.83	126.20
4	B	43[A]	RPA	CM4-C9-C8	3.18	122.94	118.09
4	B	43[B]	RPA	CM4-C9-C8	3.18	122.94	118.09
4	F	43[A]	RPA	CM4-C9-C8	3.17	122.93	118.09
4	F	43[B]	RPA	CM4-C9-C8	3.17	122.93	118.09
4	D	43[A]	RPA	CM4-C9-C8	3.16	122.92	118.09
4	D	43[B]	RPA	CM4-C9-C8	3.16	122.92	118.09
3	A	54	BCL	C4D-CHA-C1A	3.12	124.96	121.24
3	E	54	BCL	C4D-CHA-C1A	3.12	124.96	121.24
3	B	45	BCL	CHD-C1D-ND	-3.11	120.43	124.80
3	C	54	BCL	C4D-CHA-C1A	3.11	124.95	121.24
3	D	45	BCL	CHD-C1D-ND	-3.09	120.45	124.80
3	F	45	BCL	CHD-C1D-ND	-3.09	120.45	124.80
4	B	43[A]	RPA	C20-C21-C22	3.02	131.51	127.28
4	B	43[B]	RPA	C20-C21-C22	3.02	131.51	127.28
3	B	45	BCL	C4D-CHA-C1A	3.01	124.84	121.24
4	F	43[A]	RPA	C20-C21-C22	3.01	131.50	127.28
4	F	43[B]	RPA	C20-C21-C22	3.01	131.50	127.28
3	D	45	BCL	C4D-CHA-C1A	3.00	124.83	121.24
4	D	43[A]	RPA	C20-C21-C22	3.00	131.49	127.28
4	D	43[B]	RPA	C20-C21-C22	3.00	131.49	127.28
3	F	45	BCL	C4D-CHA-C1A	2.99	124.81	121.24
3	C	54	BCL	C3B-C4B-NB	-2.95	105.87	109.76
3	E	54	BCL	C3B-C4B-NB	-2.94	105.87	109.76
3	A	54	BCL	C3B-C4B-NB	-2.94	105.88	109.76
3	E	55	BCL	C3B-C4B-NB	-2.92	105.91	109.76
3	C	55	BCL	C3B-C4B-NB	-2.91	105.92	109.76
3	A	55	BCL	C3B-C4B-NB	-2.90	105.93	109.76
3	E	55	BCL	CHD-C1D-ND	-2.90	120.72	124.80
3	A	55	BCL	CHD-C1D-ND	-2.88	120.75	124.80
3	C	55	BCL	CHD-C1D-ND	-2.88	120.75	124.80
3	E	54	BCL	CHD-C1D-ND	-2.81	120.84	124.80
3	C	54	BCL	CHD-C1D-ND	-2.79	120.88	124.80
3	A	54	BCL	CHD-C1D-ND	-2.77	120.91	124.80
3	B	45	BCL	C2B-C1B-NB	-2.72	107.51	110.33
3	D	45	BCL	C2B-C1B-NB	-2.70	107.53	110.33
3	F	45	BCL	C2B-C1B-NB	-2.69	107.53	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	54	BCL	C4-C3-C5	2.66	119.84	115.23
3	E	54	BCL	C4-C3-C5	2.65	119.83	115.23
3	E	55	BCL	C4A-NA-C1A	2.62	107.88	106.68
3	A	54	BCL	C4-C3-C5	2.61	119.77	115.23
3	A	54	BCL	C12-C11-C10	-2.60	101.61	113.28
3	E	54	BCL	C12-C11-C10	-2.60	101.62	113.28
3	C	54	BCL	C12-C11-C10	-2.60	101.63	113.28
4	B	43[A]	RPA	C25-C24-C23	2.57	130.65	123.20
4	B	43[B]	RPA	C25-C24-C23	2.57	130.65	123.20
4	D	43[A]	RPA	C25-C24-C23	2.57	130.63	123.20
4	D	43[B]	RPA	C25-C24-C23	2.57	130.63	123.20
4	F	43[A]	RPA	C25-C24-C23	2.57	130.63	123.20
4	F	43[B]	RPA	C25-C24-C23	2.57	130.63	123.20
3	C	55	BCL	C4A-NA-C1A	2.56	107.85	106.68
3	A	55	BCL	C12-C11-C10	-2.55	101.84	113.28
3	A	55	BCL	C4A-NA-C1A	2.55	107.84	106.68
3	E	55	BCL	C12-C11-C10	-2.55	101.86	113.28
3	C	55	BCL	C12-C11-C10	-2.55	101.86	113.28
4	D	43[A]	RPA	C28-C29-C30	-2.49	123.68	127.48
4	D	43[B]	RPA	C28-C29-C30	-2.49	123.68	127.48
4	F	43[A]	RPA	C28-C29-C30	-2.48	123.69	127.48
4	F	43[B]	RPA	C28-C29-C30	-2.48	123.69	127.48
4	B	43[A]	RPA	C28-C29-C30	-2.47	123.71	127.48
4	B	43[B]	RPA	C28-C29-C30	-2.47	123.71	127.48
3	B	45	BCL	CHB-C1B-NB	2.40	127.64	124.05
3	D	45	BCL	CHB-C1B-NB	2.38	127.61	124.05
3	F	45	BCL	CHB-C1B-NB	2.35	127.58	124.05
3	C	54	BCL	CHA-C1A-NA	-2.35	121.07	126.39
3	E	54	BCL	CHA-C1A-NA	-2.35	121.07	126.39
3	A	54	BCL	CHA-C1A-NA	-2.35	121.08	126.39
3	A	55	BCL	C1-C2-C3	-2.34	122.36	126.20
3	E	55	BCL	C1-C2-C3	-2.30	122.42	126.20
3	C	55	BCL	C1-C2-C3	-2.30	122.43	126.20
3	B	45	BCL	C7-C6-C5	-2.28	107.18	113.26
3	D	45	BCL	C1-C2-C3	-2.27	122.47	126.20
3	F	45	BCL	C7-C6-C5	-2.27	107.21	113.26
3	D	45	BCL	C7-C6-C5	-2.27	107.21	113.26
3	B	45	BCL	C1-C2-C3	-2.27	122.48	126.20
4	F	43[A]	RPA	C24-C25-C26	-2.24	124.13	127.28
4	F	43[B]	RPA	C24-C25-C26	-2.24	124.13	127.28
3	F	45	BCL	C1-C2-C3	-2.24	122.53	126.20
4	B	43[A]	RPA	CM5-C13-C12	2.24	121.51	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	43[B]	RPA	CM5-C13-C12	2.24	121.51	118.09
4	D	43[A]	RPA	C24-C25-C26	-2.23	124.15	127.28
4	D	43[B]	RPA	C24-C25-C26	-2.23	124.15	127.28
3	F	45	BCL	C12-C11-C10	-2.22	103.34	113.28
3	D	45	BCL	C12-C11-C10	-2.21	103.36	113.28
4	D	43[A]	RPA	CM5-C13-C12	2.21	121.47	118.09
4	D	43[B]	RPA	CM5-C13-C12	2.21	121.47	118.09
3	B	45	BCL	C12-C11-C10	-2.21	103.36	113.28
4	F	43[A]	RPA	CM5-C13-C12	2.21	121.47	118.09
4	F	43[B]	RPA	CM5-C13-C12	2.21	121.47	118.09
4	B	43[A]	RPA	C24-C25-C26	-2.20	124.19	127.28
4	B	43[B]	RPA	C24-C25-C26	-2.20	124.19	127.28
3	A	55	BCL	C2B-C1B-NB	-2.19	108.05	110.33
3	C	55	BCL	C2B-C1B-NB	-2.19	108.06	110.33
3	E	55	BCL	C2B-C1B-NB	-2.17	108.07	110.33
3	B	45	BCL	O2D-CGD-CBD	2.16	115.01	111.23
3	B	45	BCL	CHD-C1D-C2D	2.16	129.98	125.49
3	F	45	BCL	CHD-C1D-C2D	2.15	129.97	125.49
3	D	45	BCL	CHD-C1D-C2D	2.15	129.96	125.49
4	B	43[A]	RPA	C19-C18-C17	-2.15	115.66	119.00
4	B	43[B]	RPA	C19-C18-C17	-2.15	115.66	119.00
3	D	45	BCL	O2D-CGD-CBD	2.15	114.98	111.23
4	D	43[A]	RPA	C19-C18-C17	-2.14	115.67	119.00
4	D	43[B]	RPA	C19-C18-C17	-2.14	115.67	119.00
3	F	45	BCL	O2D-CGD-CBD	2.13	114.96	111.23
4	F	43[A]	RPA	C19-C18-C17	-2.13	115.68	119.00
4	F	43[B]	RPA	C19-C18-C17	-2.13	115.68	119.00
3	F	45	BCL	CHA-C1A-NA	-2.07	121.71	126.39
3	D	45	BCL	CHA-C1A-NA	-2.06	121.72	126.39
3	B	45	BCL	CHA-C1A-NA	-2.06	121.72	126.39
4	B	43[A]	RPA	C12-C13-C14	-2.06	115.78	119.01
4	B	43[B]	RPA	C12-C13-C14	-2.06	115.78	119.01
3	C	55	BCL	C6-C7-C8	-2.04	109.20	115.97
4	D	43[A]	RPA	C12-C13-C14	-2.03	115.81	119.01
4	D	43[B]	RPA	C12-C13-C14	-2.03	115.81	119.01
4	F	43[A]	RPA	C12-C13-C14	-2.03	115.82	119.01
4	F	43[B]	RPA	C12-C13-C14	-2.03	115.82	119.01
3	E	55	BCL	C6-C7-C8	-2.03	109.22	115.97
3	A	55	BCL	C6-C7-C8	-2.03	109.23	115.97
3	A	54	BCL	C1D-ND-C4D	2.01	107.72	106.31
4	B	43[A]	RPA	CM8-C26-C25	-2.01	119.56	122.82
4	B	43[B]	RPA	CM8-C26-C25	-2.01	119.56	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	43[A]	RPA	CM8-C26-C25	-2.00	119.57	122.82
4	F	43[B]	RPA	CM8-C26-C25	-2.00	119.57	122.82

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	54	BCL	C13
3	C	54	BCL	C13
3	E	54	BCL	C13

All (276) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	54	BCL	C2C-C3C-CAC-CBC
3	A	55	BCL	C1A-C2A-CAA-CBA
3	A	55	BCL	C3A-C2A-CAA-CBA
3	A	55	BCL	C2C-C3C-CAC-CBC
3	A	55	BCL	C4C-C3C-CAC-CBC
3	B	45	BCL	C2C-C3C-CAC-CBC
3	B	45	BCL	C4C-C3C-CAC-CBC
3	C	54	BCL	C2C-C3C-CAC-CBC
3	C	55	BCL	C1A-C2A-CAA-CBA
3	C	55	BCL	C3A-C2A-CAA-CBA
3	C	55	BCL	C2C-C3C-CAC-CBC
3	C	55	BCL	C4C-C3C-CAC-CBC
3	D	45	BCL	C2C-C3C-CAC-CBC
3	D	45	BCL	C4C-C3C-CAC-CBC
3	E	54	BCL	C2C-C3C-CAC-CBC
3	E	55	BCL	C1A-C2A-CAA-CBA
3	E	55	BCL	C3A-C2A-CAA-CBA
3	E	55	BCL	C2C-C3C-CAC-CBC
3	E	55	BCL	C4C-C3C-CAC-CBC
3	F	45	BCL	C2C-C3C-CAC-CBC
3	F	45	BCL	C4C-C3C-CAC-CBC
4	B	43[A]	RPA	C1-C2-C3-C4
4	B	43[A]	RPA	C7-C8-C9-CM4
4	B	43[A]	RPA	C7-C8-C9-C10
4	B	43[A]	RPA	CM6-C18-C19-C20
4	B	43[A]	RPA	C19-C20-C21-C22
4	B	43[A]	RPA	C26-C27-C28-C29
4	B	43[A]	RPA	C27-C28-C29-C30
4	B	43[B]	RPA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	43[B]	RPA	C7-C8-C9-CM4
4	B	43[B]	RPA	C7-C8-C9-C10
4	B	43[B]	RPA	CM6-C18-C19-C20
4	B	43[B]	RPA	C19-C20-C21-C22
4	B	43[B]	RPA	C26-C27-C28-C29
4	B	43[B]	RPA	C27-C28-C29-C30
4	D	43[A]	RPA	C1-C2-C3-C4
4	D	43[A]	RPA	C7-C8-C9-CM4
4	D	43[A]	RPA	C7-C8-C9-C10
4	D	43[A]	RPA	CM6-C18-C19-C20
4	D	43[A]	RPA	C19-C20-C21-C22
4	D	43[A]	RPA	C26-C27-C28-C29
4	D	43[A]	RPA	C27-C28-C29-C30
4	D	43[B]	RPA	C1-C2-C3-C4
4	D	43[B]	RPA	C7-C8-C9-CM4
4	D	43[B]	RPA	C7-C8-C9-C10
4	D	43[B]	RPA	CM6-C18-C19-C20
4	D	43[B]	RPA	C19-C20-C21-C22
4	D	43[B]	RPA	C26-C27-C28-C29
4	D	43[B]	RPA	C27-C28-C29-C30
4	F	43[A]	RPA	C1-C2-C3-C4
4	F	43[A]	RPA	C7-C8-C9-CM4
4	F	43[A]	RPA	C7-C8-C9-C10
4	F	43[A]	RPA	CM6-C18-C19-C20
4	F	43[A]	RPA	C19-C20-C21-C22
4	F	43[A]	RPA	C26-C27-C28-C29
4	F	43[A]	RPA	C27-C28-C29-C30
4	F	43[B]	RPA	C1-C2-C3-C4
4	F	43[B]	RPA	C7-C8-C9-CM4
4	F	43[B]	RPA	C7-C8-C9-C10
4	F	43[B]	RPA	CM6-C18-C19-C20
4	F	43[B]	RPA	C19-C20-C21-C22
4	F	43[B]	RPA	C26-C27-C28-C29
4	F	43[B]	RPA	C27-C28-C29-C30
3	A	55	BCL	CBD-CGD-O2D-CED
3	C	55	BCL	CBD-CGD-O2D-CED
3	E	55	BCL	CBD-CGD-O2D-CED
3	A	54	BCL	CBD-CGD-O2D-CED
3	C	54	BCL	CBD-CGD-O2D-CED
3	E	54	BCL	CBD-CGD-O2D-CED
3	A	55	BCL	C3-C5-C6-C7
3	C	55	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	55	BCL	C3-C5-C6-C7
3	B	45	BCL	C4-C3-C5-C6
3	D	45	BCL	C4-C3-C5-C6
3	F	45	BCL	C4-C3-C5-C6
3	B	45	BCL	C2-C3-C5-C6
3	D	45	BCL	C2-C3-C5-C6
3	F	45	BCL	C2-C3-C5-C6
3	A	55	BCL	C6-C7-C8-C9
3	C	55	BCL	C6-C7-C8-C9
3	E	55	BCL	C6-C7-C8-C9
4	B	43[A]	RPA	CM7-C22-C23-C24
4	B	43[A]	RPA	CM8-C26-C27-C28
4	B	43[B]	RPA	CM7-C22-C23-C24
4	B	43[B]	RPA	CM8-C26-C27-C28
4	D	43[A]	RPA	CM7-C22-C23-C24
4	D	43[A]	RPA	CM8-C26-C27-C28
4	D	43[B]	RPA	CM7-C22-C23-C24
4	D	43[B]	RPA	CM8-C26-C27-C28
4	F	43[A]	RPA	CM7-C22-C23-C24
4	F	43[A]	RPA	CM8-C26-C27-C28
4	F	43[B]	RPA	CM7-C22-C23-C24
4	F	43[B]	RPA	CM8-C26-C27-C28
4	B	43[A]	RPA	C21-C22-C23-C24
4	B	43[B]	RPA	C21-C22-C23-C24
4	D	43[A]	RPA	C21-C22-C23-C24
4	D	43[B]	RPA	C21-C22-C23-C24
4	F	43[A]	RPA	C21-C22-C23-C24
4	F	43[B]	RPA	C21-C22-C23-C24
4	B	43[A]	RPA	O5'-C5'-C6'-O6'
4	B	43[B]	RPA	O5'-C5'-C6'-O6'
4	D	43[A]	RPA	O5'-C5'-C6'-O6'
4	D	43[B]	RPA	O5'-C5'-C6'-O6'
4	F	43[A]	RPA	O5'-C5'-C6'-O6'
4	F	43[B]	RPA	O5'-C5'-C6'-O6'
3	A	55	BCL	O1D-CGD-O2D-CED
3	C	55	BCL	O1D-CGD-O2D-CED
3	E	55	BCL	O1D-CGD-O2D-CED
3	B	45	BCL	CBD-CGD-O2D-CED
3	D	45	BCL	CBD-CGD-O2D-CED
3	F	45	BCL	CBD-CGD-O2D-CED
3	A	54	BCL	C6-C7-C8-C10
3	A	54	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	54	BCL	C6-C7-C8-C10
3	C	54	BCL	C12-C13-C15-C16
3	E	54	BCL	C6-C7-C8-C10
3	E	54	BCL	C12-C13-C15-C16
3	B	45	BCL	C8-C10-C11-C12
3	D	45	BCL	C8-C10-C11-C12
3	F	45	BCL	C8-C10-C11-C12
3	A	54	BCL	C10-C11-C12-C13
3	C	54	BCL	C10-C11-C12-C13
3	E	54	BCL	C10-C11-C12-C13
4	B	43[A]	RPA	C17-C18-C19-C20
4	B	43[B]	RPA	C17-C18-C19-C20
4	D	43[A]	RPA	C17-C18-C19-C20
4	D	43[B]	RPA	C17-C18-C19-C20
4	F	43[A]	RPA	C17-C18-C19-C20
4	F	43[B]	RPA	C17-C18-C19-C20
4	B	43[A]	RPA	C25-C26-C27-C28
4	B	43[B]	RPA	C25-C26-C27-C28
4	D	43[A]	RPA	C25-C26-C27-C28
4	D	43[B]	RPA	C25-C26-C27-C28
4	F	43[A]	RPA	C25-C26-C27-C28
4	F	43[B]	RPA	C25-C26-C27-C28
3	B	45	BCL	O1D-CGD-O2D-CED
3	D	45	BCL	O1D-CGD-O2D-CED
3	F	45	BCL	O1D-CGD-O2D-CED
3	A	55	BCL	C10-C11-C12-C13
3	C	55	BCL	C10-C11-C12-C13
3	E	55	BCL	C10-C11-C12-C13
4	B	43[A]	RPA	C4'-C5'-C6'-O6'
4	B	43[B]	RPA	C4'-C5'-C6'-O6'
4	D	43[A]	RPA	C4'-C5'-C6'-O6'
4	D	43[B]	RPA	C4'-C5'-C6'-O6'
4	F	43[A]	RPA	C4'-C5'-C6'-O6'
4	F	43[B]	RPA	C4'-C5'-C6'-O6'
3	A	54	BCL	C13-C15-C16-C17
3	E	54	BCL	C13-C15-C16-C17
3	C	54	BCL	C13-C15-C16-C17
3	B	45	BCL	C16-C17-C18-C19
3	B	45	BCL	C16-C17-C18-C20
3	D	45	BCL	C16-C17-C18-C19
3	D	45	BCL	C16-C17-C18-C20
3	F	45	BCL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	45	BCL	C16-C17-C18-C20
5	B	44	BOG	O1-C1'-C2'-C3'
5	D	44	BOG	O1-C1'-C2'-C3'
5	F	44	BOG	O1-C1'-C2'-C3'
3	A	55	BCL	C6-C7-C8-C10
3	C	55	BCL	C6-C7-C8-C10
3	E	55	BCL	C6-C7-C8-C10
3	A	54	BCL	C11-C10-C8-C9
3	A	54	BCL	C14-C13-C15-C16
3	C	54	BCL	C11-C10-C8-C9
3	C	54	BCL	C14-C13-C15-C16
3	E	54	BCL	C11-C10-C8-C9
3	E	54	BCL	C14-C13-C15-C16
3	A	54	BCL	C5-C6-C7-C8
3	C	54	BCL	C5-C6-C7-C8
3	E	54	BCL	C5-C6-C7-C8
5	B	44	BOG	C5'-C6'-C7'-C8'
5	D	44	BOG	C5'-C6'-C7'-C8'
5	F	44	BOG	C5'-C6'-C7'-C8'
3	A	54	BCL	C11-C10-C8-C7
3	A	54	BCL	C11-C12-C13-C15
3	C	54	BCL	C11-C10-C8-C7
3	C	54	BCL	C11-C12-C13-C15
3	E	54	BCL	C11-C10-C8-C7
3	E	54	BCL	C11-C12-C13-C15
3	B	45	BCL	CBA-CGA-O2A-C1
3	D	45	BCL	CBA-CGA-O2A-C1
3	F	45	BCL	CBA-CGA-O2A-C1
4	B	43[A]	RPA	C5-C6-C7-C8
4	B	43[B]	RPA	C5-C6-C7-C8
4	D	43[A]	RPA	C5-C6-C7-C8
4	D	43[B]	RPA	C5-C6-C7-C8
4	F	43[A]	RPA	C5-C6-C7-C8
4	F	43[B]	RPA	C5-C6-C7-C8
3	B	45	BCL	C1-C2-C3-C4
3	D	45	BCL	C1-C2-C3-C4
3	F	45	BCL	C1-C2-C3-C4
3	A	55	BCL	C2-C3-C5-C6
3	C	55	BCL	C2-C3-C5-C6
3	E	55	BCL	C2-C3-C5-C6
3	A	54	BCL	C4C-C3C-CAC-CBC
3	C	54	BCL	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	54	BCL	C4C-C3C-CAC-CBC
3	A	55	BCL	C16-C17-C18-C20
3	C	55	BCL	C16-C17-C18-C20
3	E	55	BCL	C16-C17-C18-C20
3	B	45	BCL	C13-C15-C16-C17
3	D	45	BCL	C13-C15-C16-C17
3	F	45	BCL	C10-C11-C12-C13
3	F	45	BCL	C13-C15-C16-C17
3	D	45	BCL	C10-C11-C12-C13
3	A	55	BCL	C16-C17-C18-C19
3	C	55	BCL	C16-C17-C18-C19
3	E	55	BCL	C16-C17-C18-C19
3	B	45	BCL	C10-C11-C12-C13
4	B	43[A]	RPA	C3-C4-C5-CM3
4	B	43[B]	RPA	C3-C4-C5-CM3
4	D	43[A]	RPA	C3-C4-C5-CM3
4	D	43[B]	RPA	C3-C4-C5-CM3
4	F	43[A]	RPA	C3-C4-C5-CM3
4	F	43[B]	RPA	C3-C4-C5-CM3
5	B	44	BOG	C2'-C3'-C4'-C5'
5	D	44	BOG	C2'-C3'-C4'-C5'
5	F	44	BOG	C2'-C3'-C4'-C5'
3	A	54	BCL	C11-C12-C13-C14
3	C	54	BCL	C11-C12-C13-C14
3	E	54	BCL	C11-C12-C13-C14
3	A	55	BCL	C4-C3-C5-C6
3	C	55	BCL	C4-C3-C5-C6
3	E	55	BCL	C4-C3-C5-C6
4	B	43[A]	RPA	C23-C24-C25-C26
4	B	43[B]	RPA	C23-C24-C25-C26
4	D	43[A]	RPA	C23-C24-C25-C26
4	D	43[B]	RPA	C23-C24-C25-C26
4	F	43[A]	RPA	C23-C24-C25-C26
4	F	43[B]	RPA	C23-C24-C25-C26
3	A	54	BCL	C8-C10-C11-C12
3	C	54	BCL	C8-C10-C11-C12
3	E	54	BCL	C8-C10-C11-C12
3	A	54	BCL	C6-C7-C8-C9
3	C	54	BCL	C6-C7-C8-C9
3	E	54	BCL	C6-C7-C8-C9
3	F	45	BCL	C2A-CAA-CBA-CGA
3	C	54	BCL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

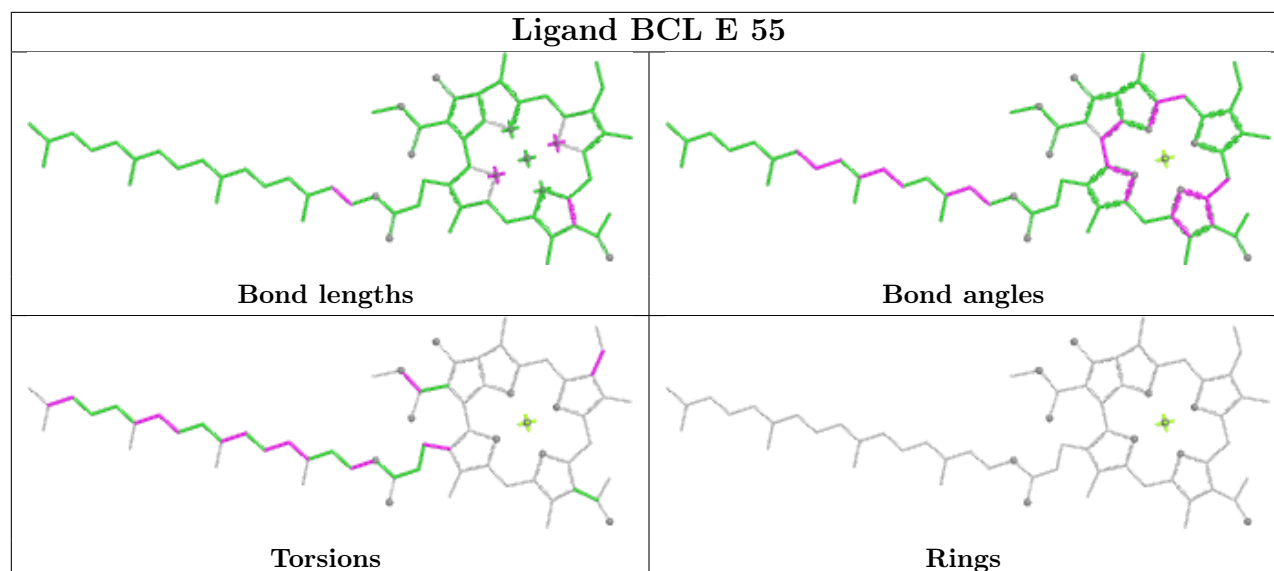
Mol	Chain	Res	Type	Atoms
3	E	54	BCL	C16-C17-C18-C19
3	A	54	BCL	C16-C17-C18-C19
3	B	45	BCL	C2A-CAA-CBA-CGA
3	D	45	BCL	C2A-CAA-CBA-CGA
3	B	45	BCL	C6-C7-C8-C10
3	D	45	BCL	C6-C7-C8-C10
3	F	45	BCL	C6-C7-C8-C10
3	A	55	BCL	C2-C1-O2A-CGA
3	C	55	BCL	C2-C1-O2A-CGA
3	E	55	BCL	C2-C1-O2A-CGA
4	B	43[A]	RPA	C9-C10-C11-C12
4	B	43[B]	RPA	C9-C10-C11-C12
4	D	43[A]	RPA	C9-C10-C11-C12
4	D	43[B]	RPA	C9-C10-C11-C12
4	F	43[A]	RPA	C9-C10-C11-C12
4	F	43[B]	RPA	C9-C10-C11-C12
3	A	55	BCL	C11-C12-C13-C15
3	C	55	BCL	C11-C12-C13-C15
3	E	55	BCL	C11-C12-C13-C15
3	A	55	BCL	C11-C12-C13-C14
3	C	55	BCL	C11-C12-C13-C14
3	E	55	BCL	C11-C12-C13-C14
3	A	54	BCL	CAA-CBA-CGA-O1A
3	C	54	BCL	CAA-CBA-CGA-O1A
3	E	54	BCL	CAA-CBA-CGA-O1A
4	B	43[A]	RPA	C3-C4-C5-C6
4	B	43[B]	RPA	C3-C4-C5-C6
4	D	43[A]	RPA	C3-C4-C5-C6
4	D	43[B]	RPA	C3-C4-C5-C6
4	F	43[A]	RPA	C3-C4-C5-C6
4	F	43[B]	RPA	C3-C4-C5-C6
3	A	54	BCL	C2-C1-O2A-CGA
3	C	54	BCL	C2-C1-O2A-CGA
3	E	54	BCL	C2-C1-O2A-CGA
3	A	54	BCL	CAA-CBA-CGA-O2A
3	C	54	BCL	CAA-CBA-CGA-O2A
3	E	54	BCL	CAA-CBA-CGA-O2A

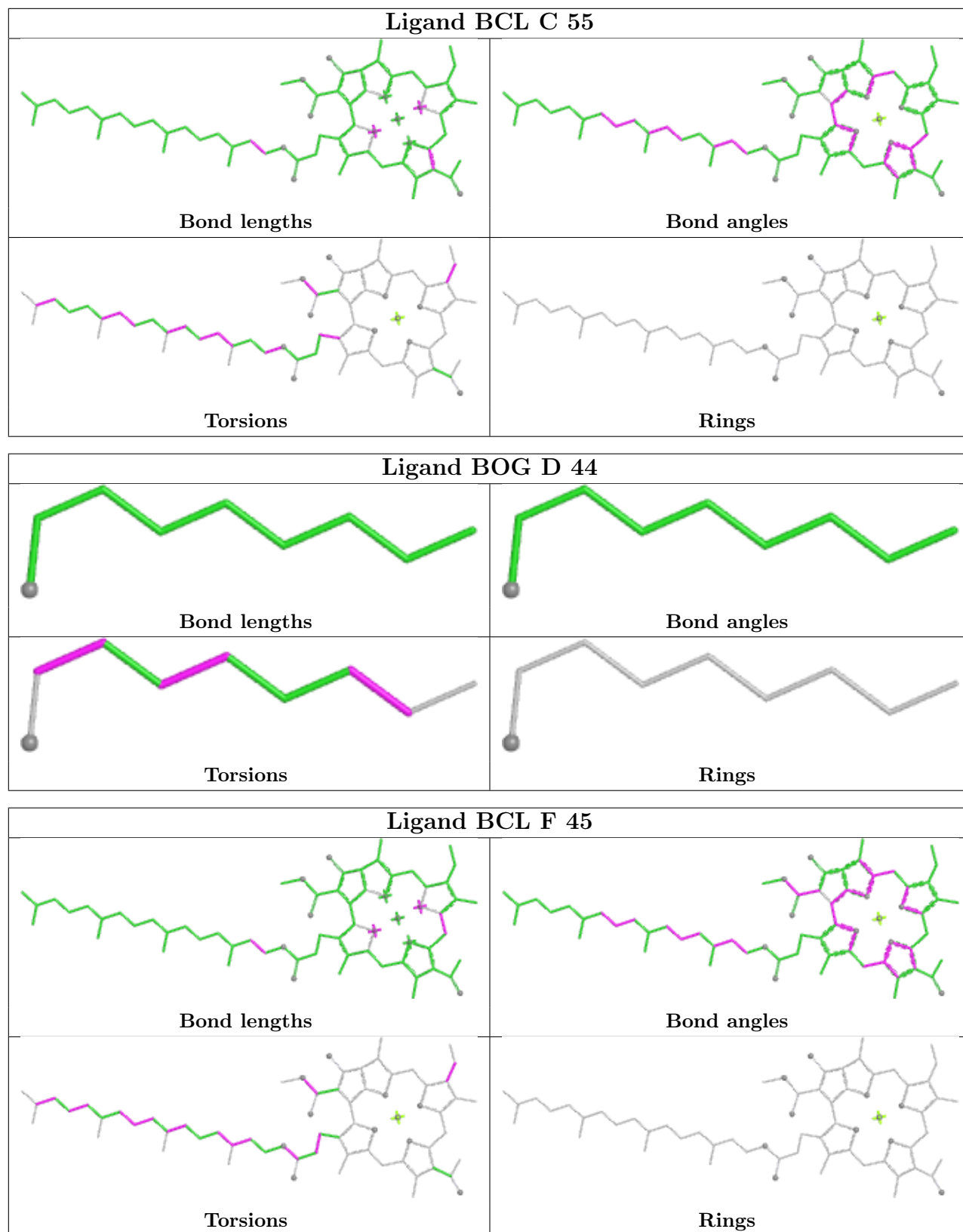
There are no ring outliers.

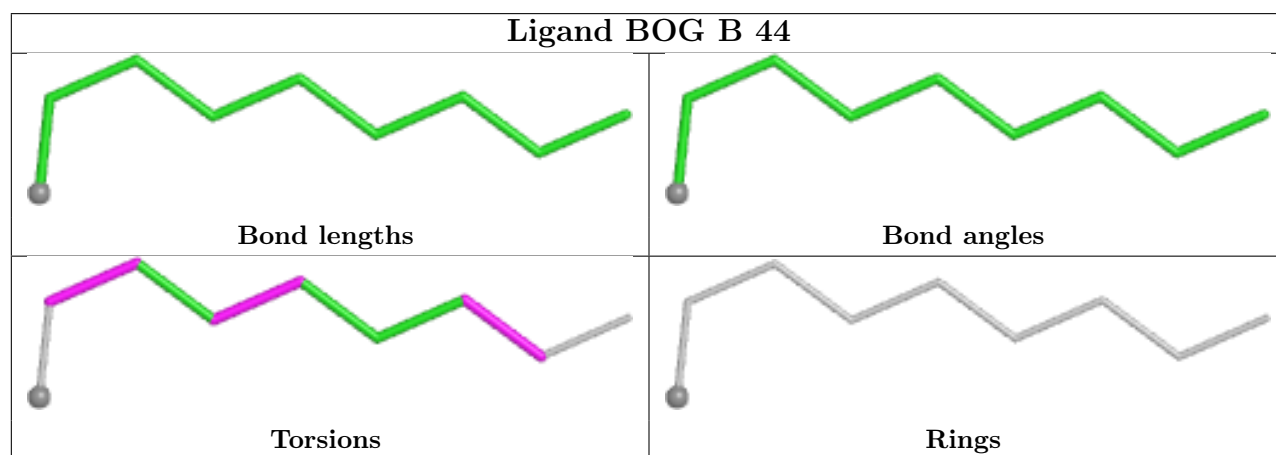
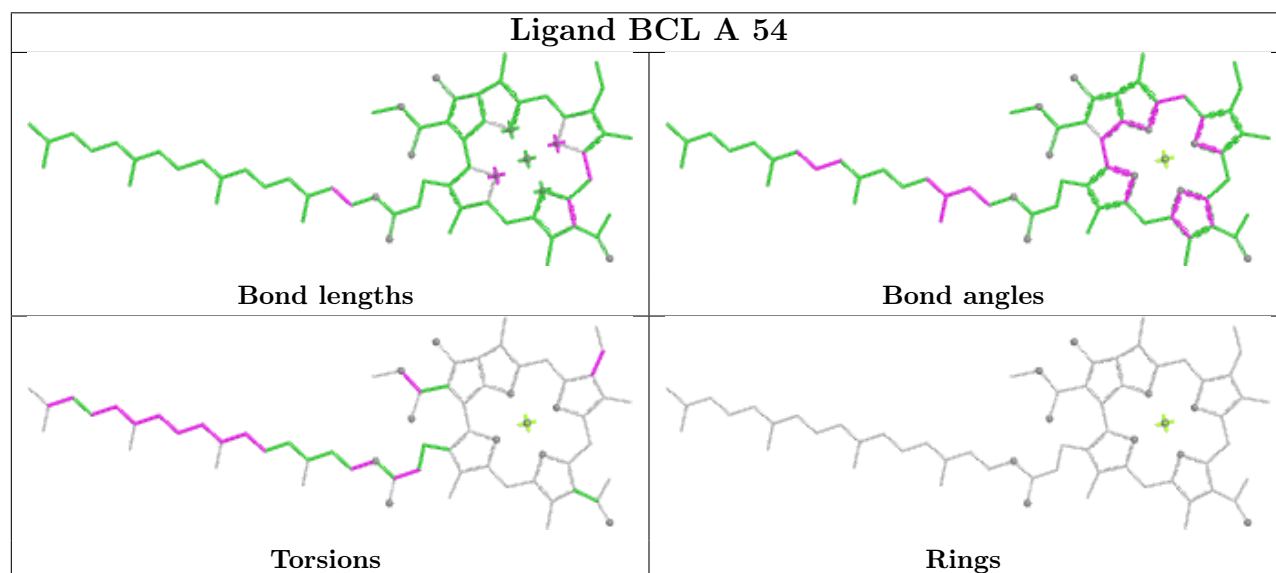
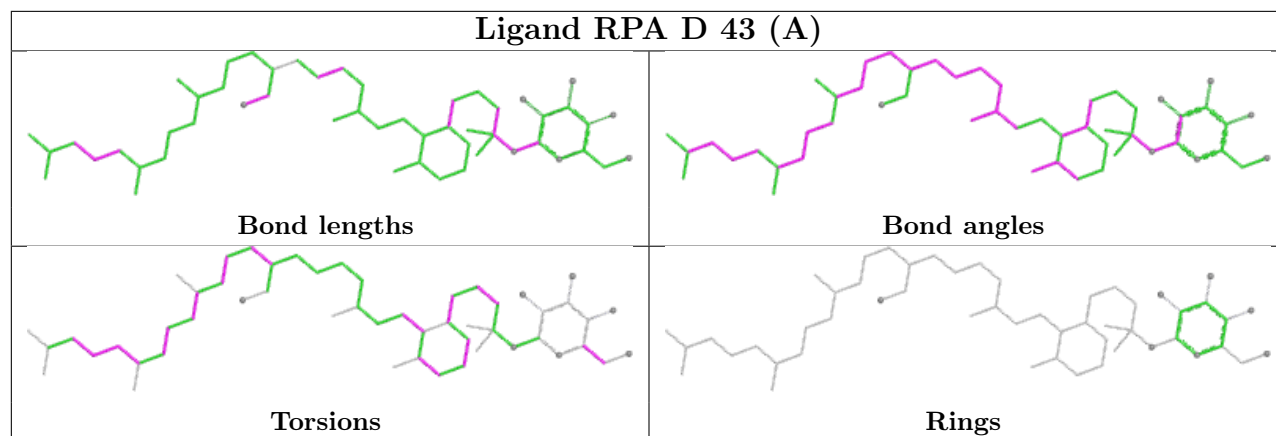
15 monomers are involved in 140 short contacts:

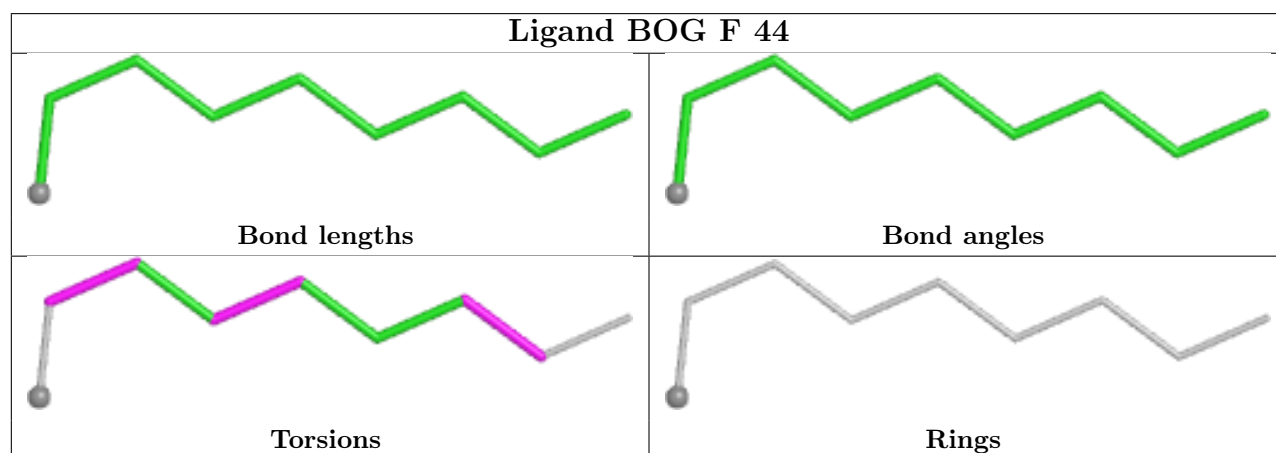
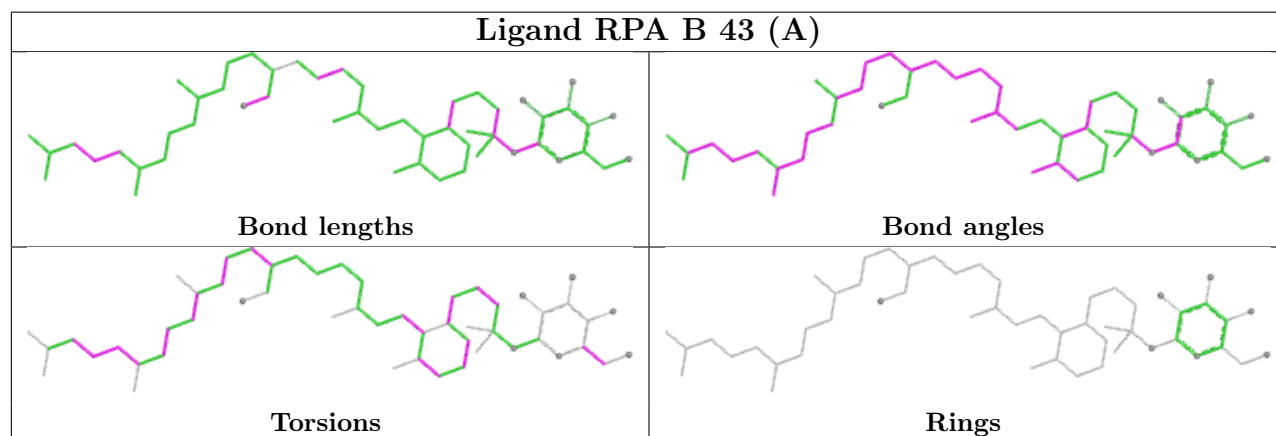
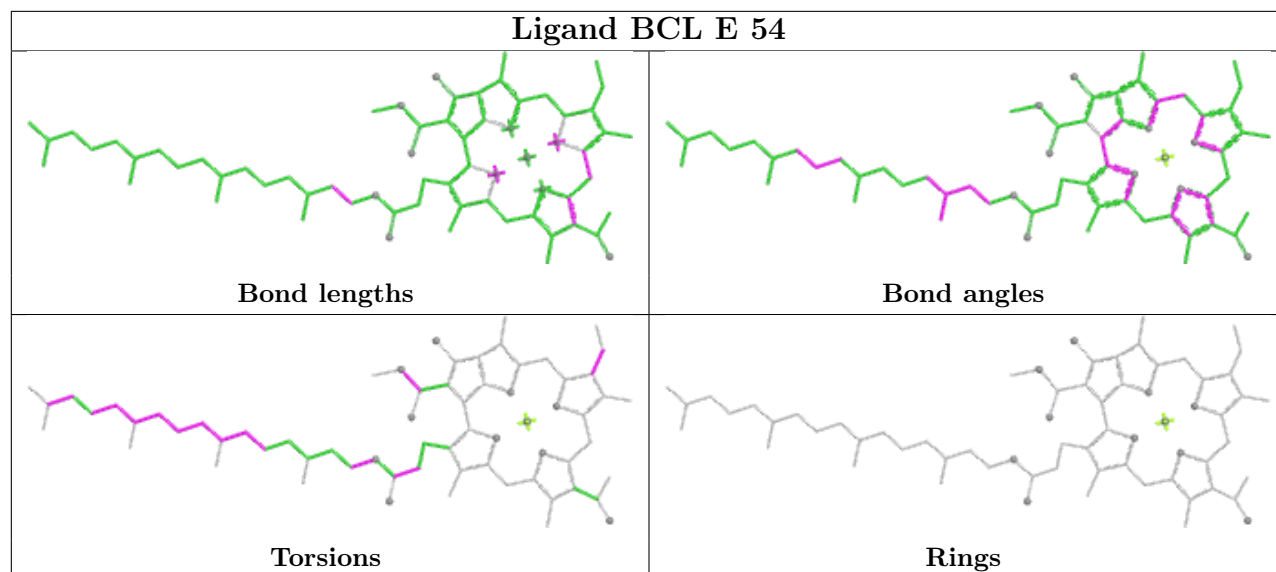
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	55	BCL	23	0
3	C	55	BCL	30	0
3	F	45	BCL	13	0
4	D	43[A]	RPA	1	0
3	A	54	BCL	5	0
3	E	54	BCL	9	0
4	B	43[A]	RPA	1	0
3	C	54	BCL	10	0
4	F	43[A]	RPA	1	0
4	D	43[B]	RPA	1	0
3	D	45	BCL	12	0
4	B	43[B]	RPA	1	0
3	A	55	BCL	32	0
3	B	45	BCL	12	0
4	F	43[B]	RPA	1	0

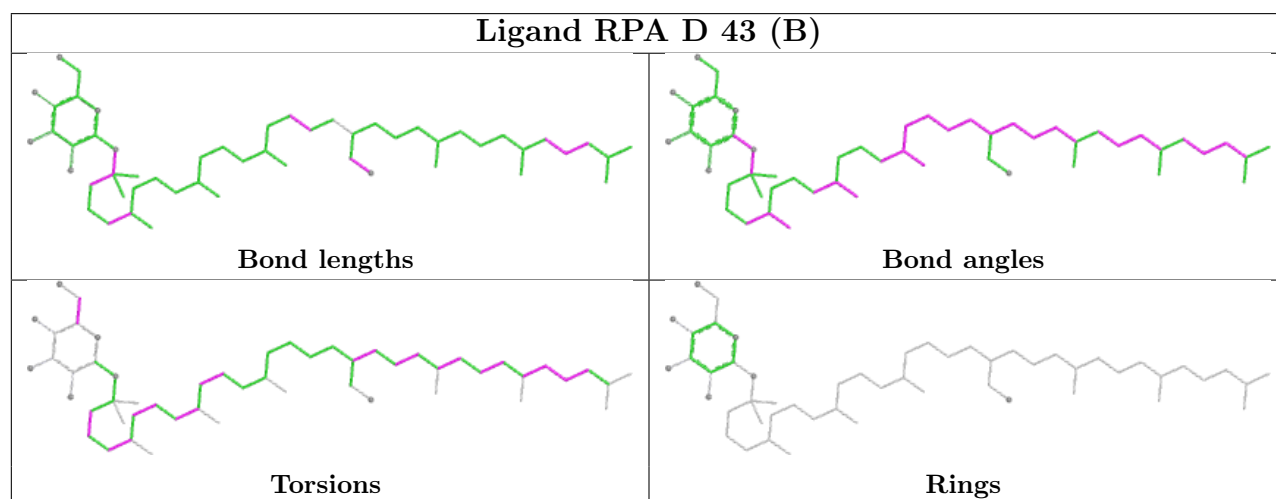
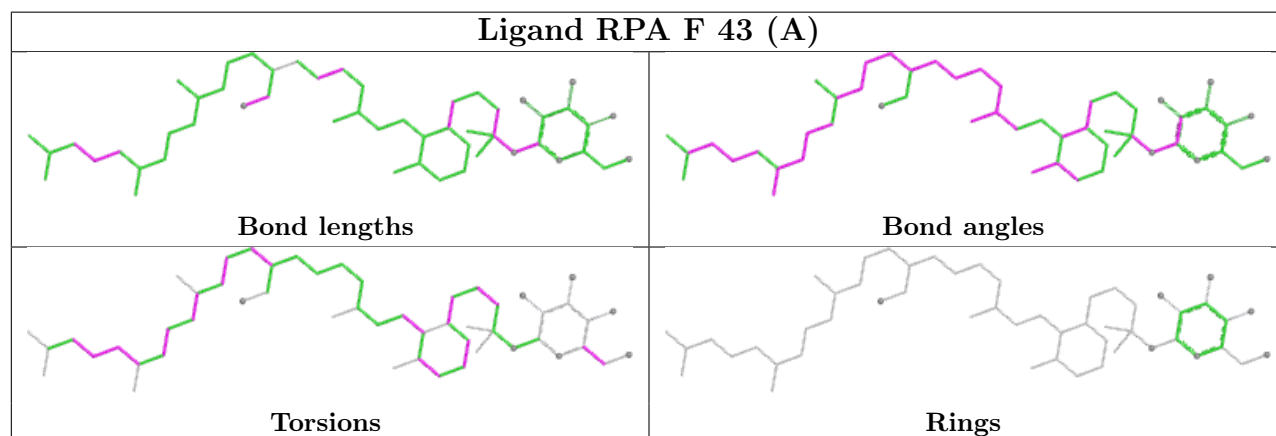
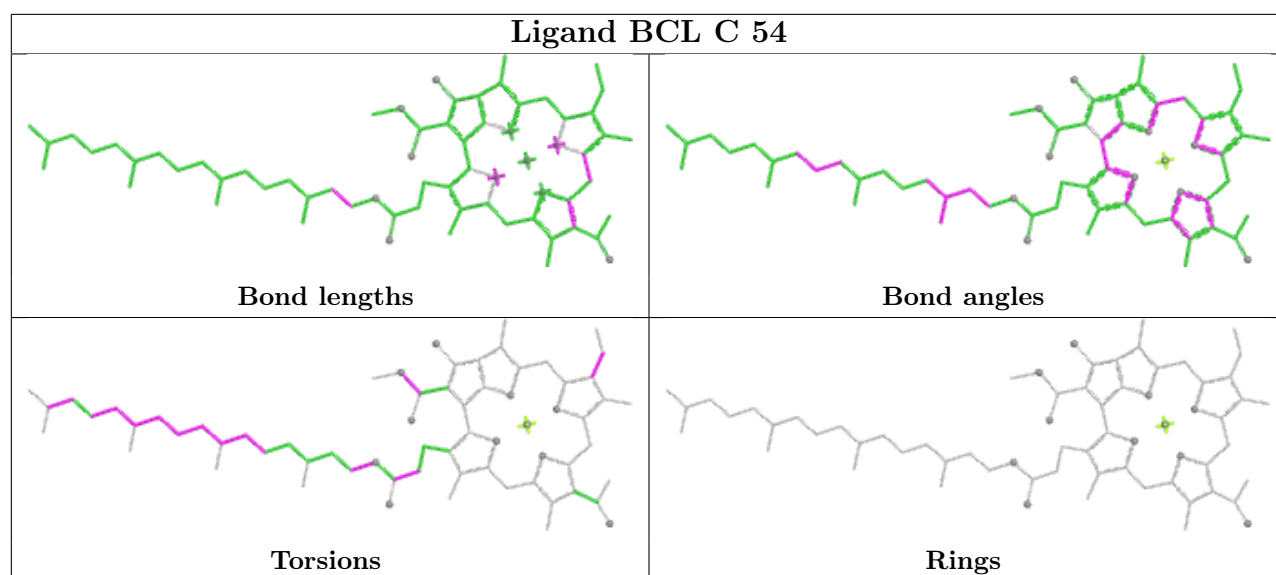
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

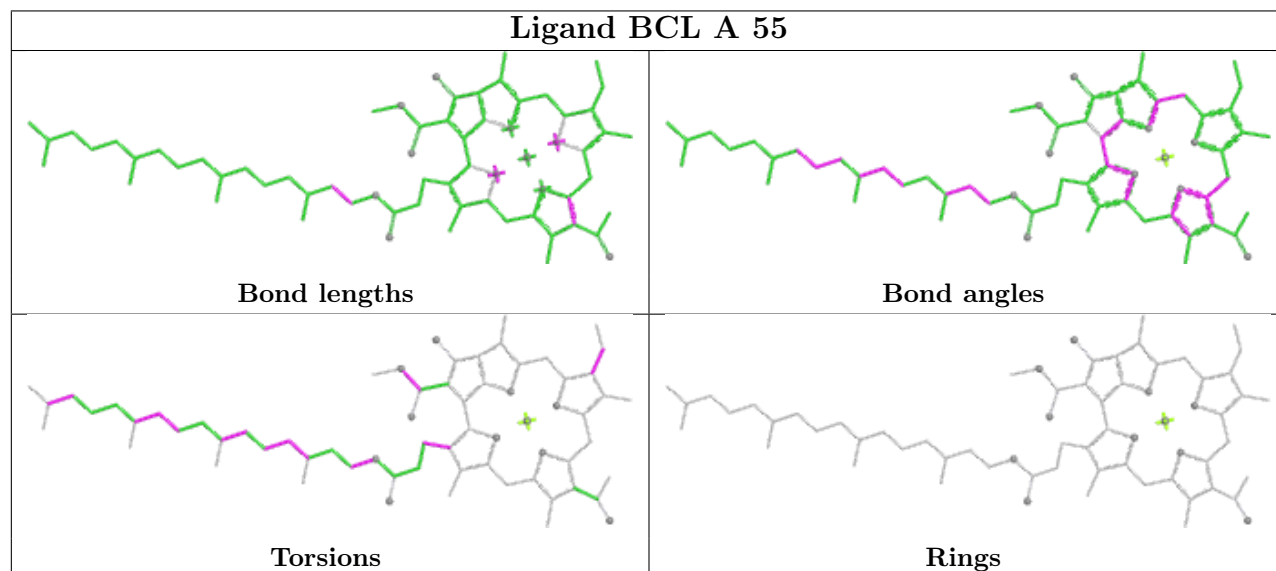
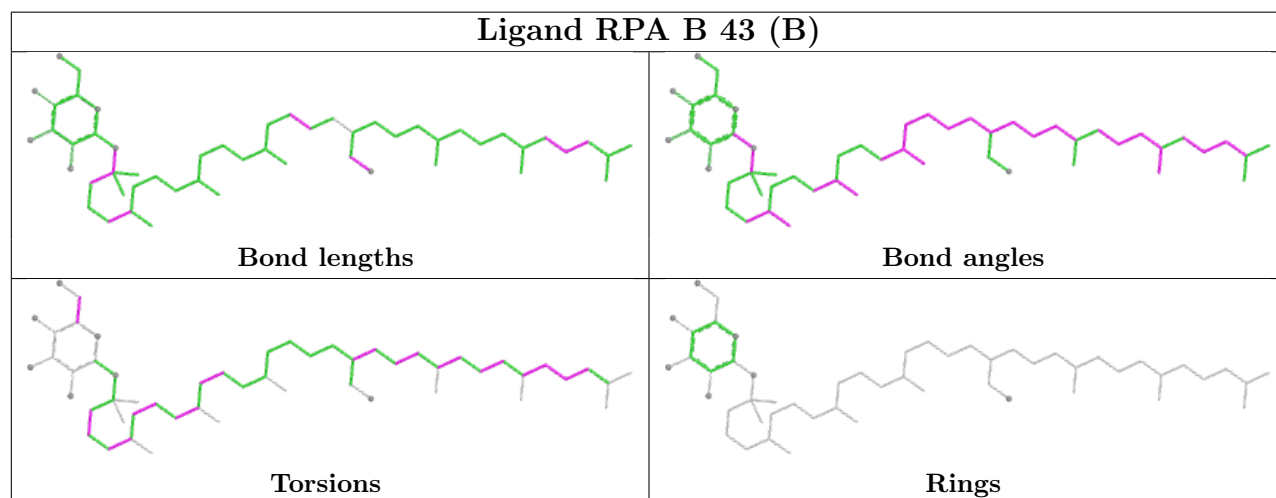
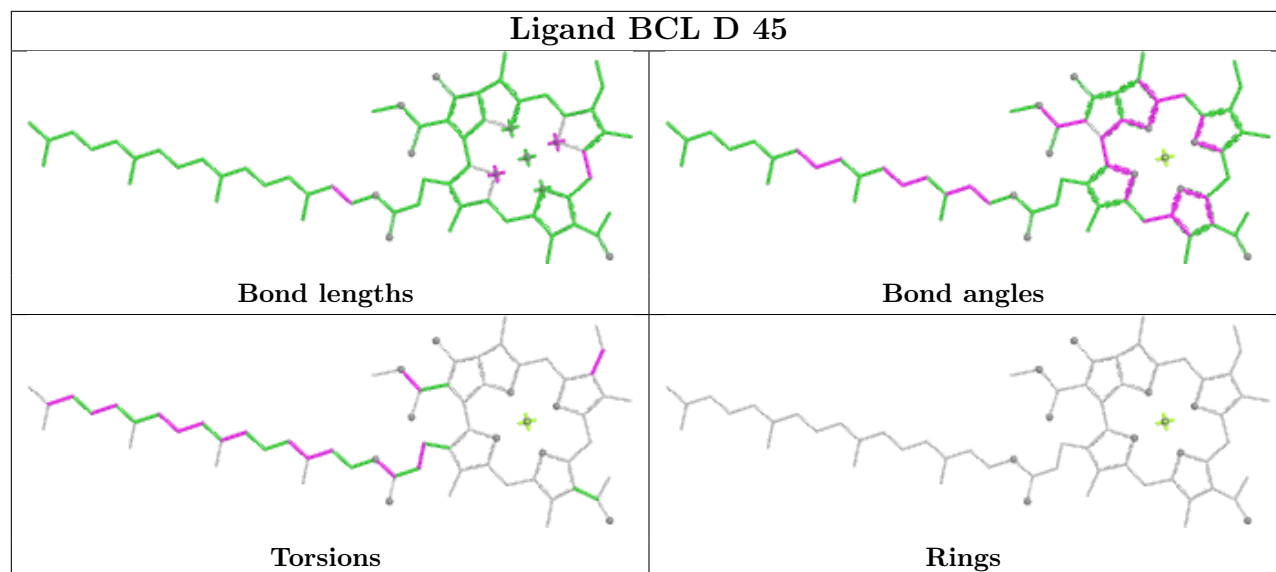


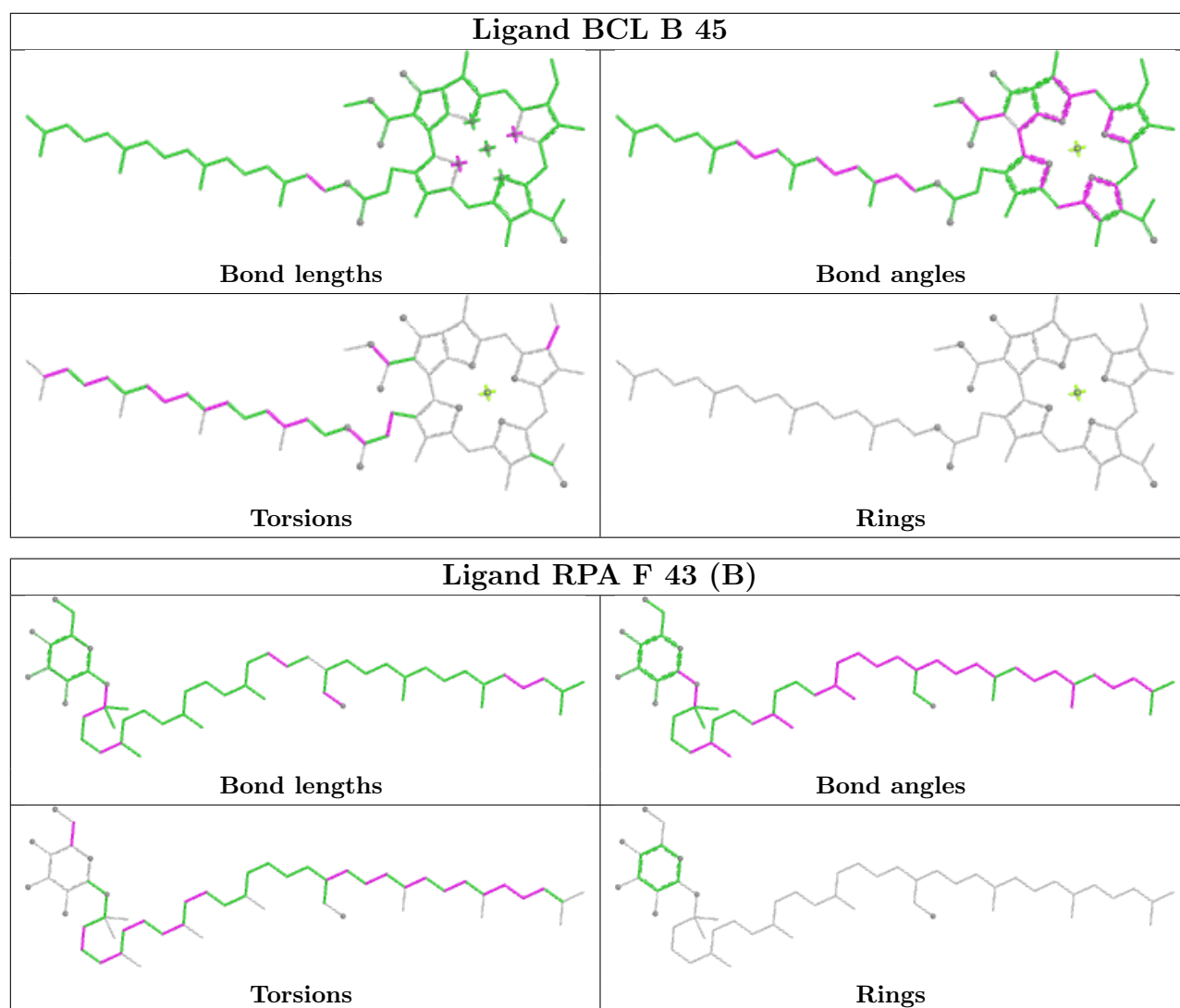












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	45/53 (84%)	-0.11	2 (4%) 39 21	14, 25, 65, 109	0
1	C	45/53 (84%)	-0.12	2 (4%) 39 21	14, 25, 65, 109	0
1	E	45/53 (84%)	-0.28	1 (2%) 62 39	14, 25, 65, 109	0
2	B	40/42 (95%)	1.11	9 (22%) 2 1	22, 51, 126, 135	0
2	D	40/42 (95%)	0.89	7 (17%) 4 3	22, 51, 126, 135	0
2	F	40/42 (95%)	0.61	6 (15%) 5 3	22, 51, 126, 135	0
All	All	255/285 (89%)	0.32	27 (10%) 11 6	14, 34, 115, 135	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	ALA	6.6
2	B	1	ALA	5.6
2	F	1	ALA	5.2
2	B	7	GLU	5.2
2	D	7	GLU	4.5
2	B	6	SER	4.4
2	B	39	PRO	4.0
1	C	14	PHE	3.9
2	D	14	LYS	3.9
2	F	2	GLU	3.6
2	B	2	GLU	3.6
2	B	14	LYS	3.5
1	A	14	PHE	3.3
2	D	39	PRO	3.2
2	B	10	GLU	3.2
2	D	2	GLU	3.0
2	D	35	PHE	2.9
2	B	35	PHE	2.7
1	C	46	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	14	LYS	2.5
2	F	39	PRO	2.4
1	E	46	GLN	2.4
2	F	35	PHE	2.4
2	B	5	THR	2.2
2	D	10	GLU	2.1
1	A	5	LYS	2.1
2	F	7	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	FME	E	1	10/11	0.91	0.18	15,42,118,197	0
1	FME	C	1	10/11	0.92	0.18	15,42,118,197	0
1	FME	A	1	10/11	0.92	0.16	15,42,118,197	0

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	BOG	F	44	9/20	0.84	0.27	30,60,93,105	0
5	BOG	D	44	9/20	0.85	0.29	30,60,93,105	0
5	BOG	B	44	9/20	0.85	0.27	30,60,93,105	0
4	RPA	F	43[B]	53/53	0.92	0.17	20,37,197,197	1
4	RPA	F	43[A]	53/53	0.92	0.17	20,37,197,197	1
4	RPA	B	43[B]	53/53	0.93	0.16	20,37,197,197	1
4	RPA	B	43[A]	53/53	0.93	0.16	20,37,197,197	1

Continued on next page...

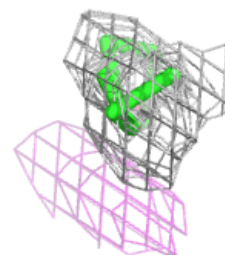
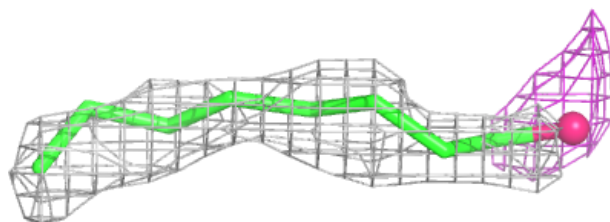
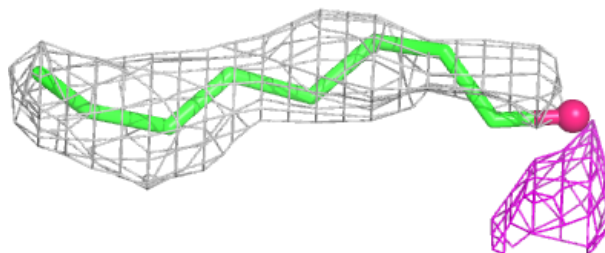
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BCL	D	45	66/66	0.94	0.10	7,27,49,78	0
4	RPA	D	43[A]	53/53	0.94	0.16	20,37,197,197	1
4	RPA	D	43[B]	53/53	0.94	0.16	20,37,197,197	1
3	BCL	A	55	66/66	0.94	0.14	14,22,124,197	0
3	BCL	B	45	66/66	0.95	0.09	7,27,49,78	0
3	BCL	E	55	66/66	0.95	0.13	14,22,124,197	0
3	BCL	F	45	66/66	0.95	0.09	7,27,49,78	0
3	BCL	C	55	66/66	0.95	0.12	14,22,124,197	0
3	BCL	E	54	66/66	0.96	0.09	13,28,44,124	0
3	BCL	A	54	66/66	0.96	0.09	13,28,44,124	0
3	BCL	C	54	66/66	0.96	0.10	13,28,44,124	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.

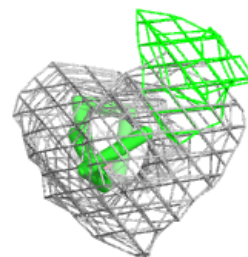
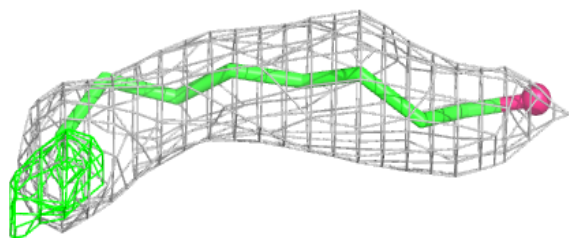
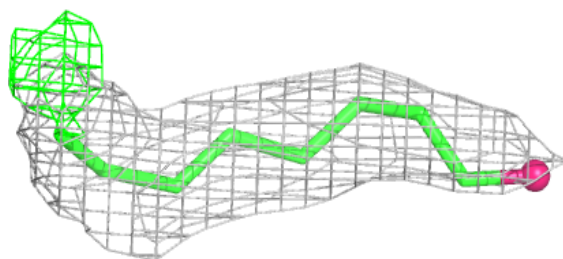
Electron density around BOG F 44:

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

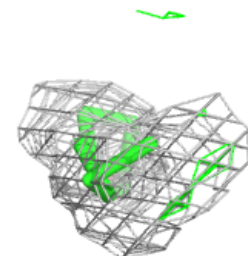
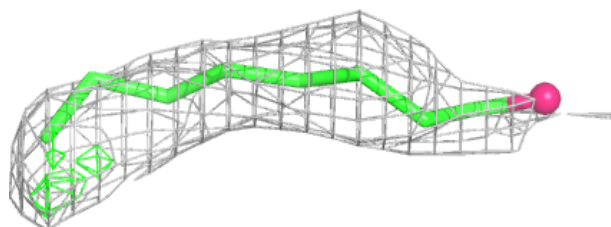
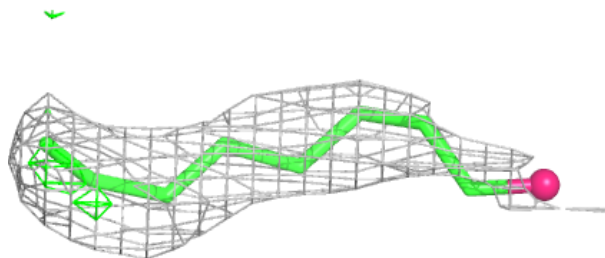


Electron density around BOG D 44:

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

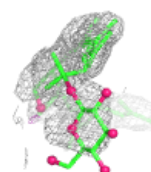
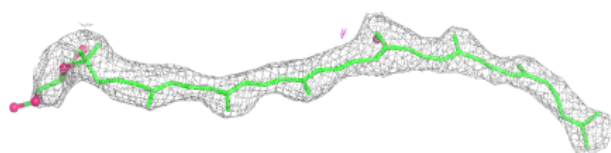
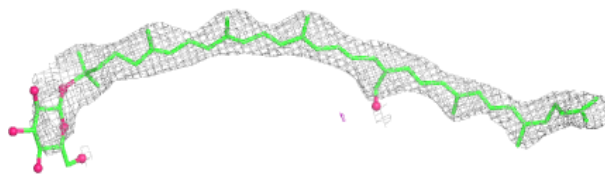
**Electron density around BOG B 44:**

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

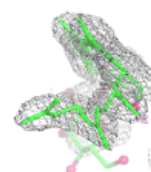
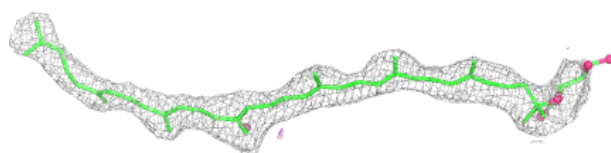
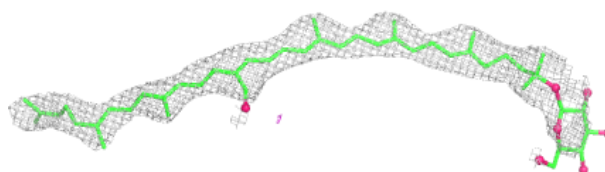


Electron density around RPA F 43 (B):

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

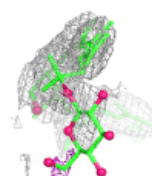
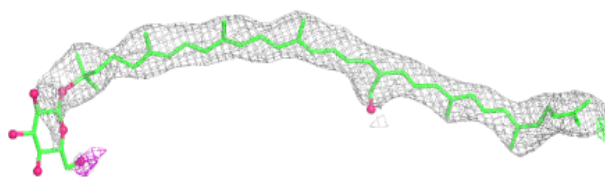
**Electron density around RPA F 43 (A):**

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

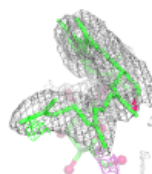
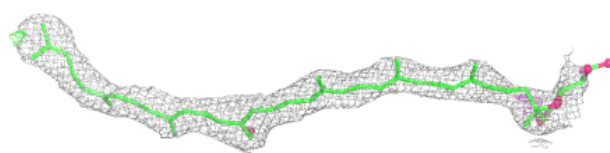
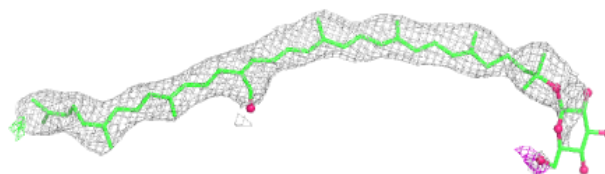


Electron density around RPA B 43 (B):

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

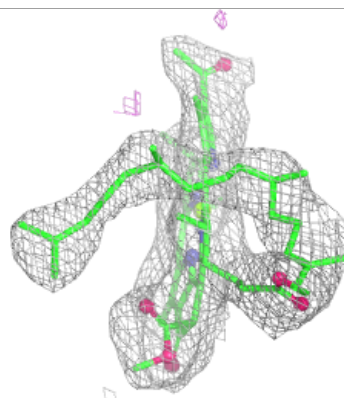
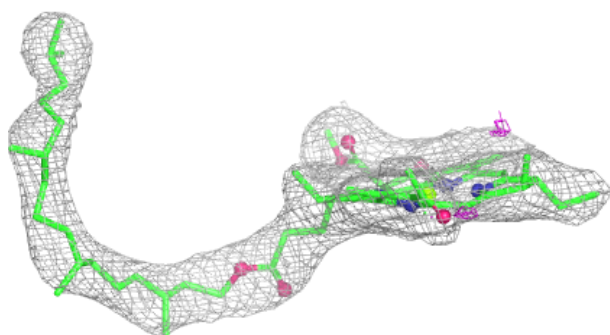
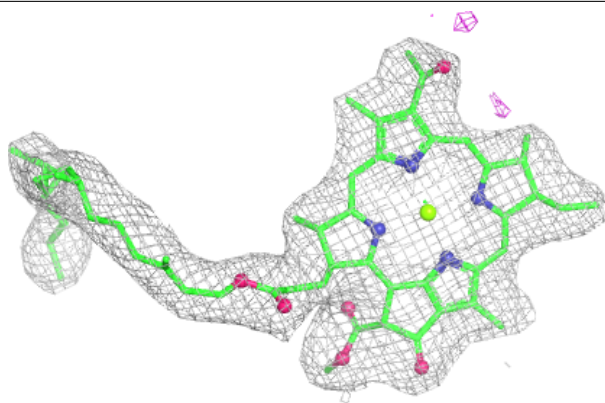
**Electron density around RPA B 43 (A):**

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

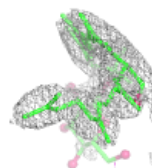
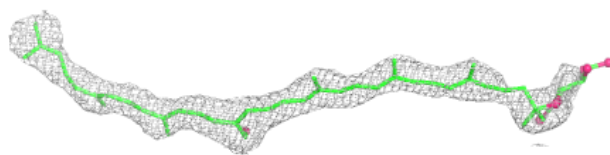
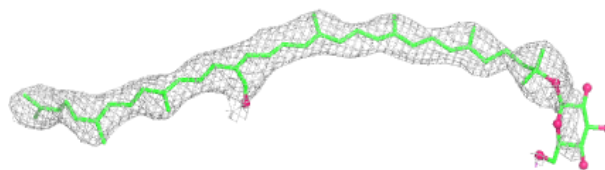


Electron density around BCL D 45:

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

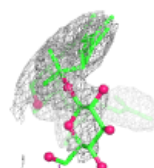
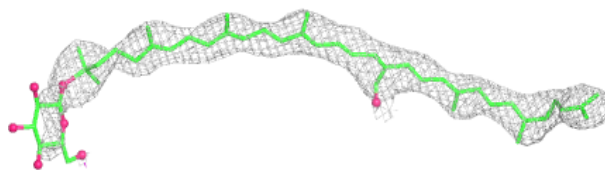
**Electron density around RPA D 43 (A):**

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

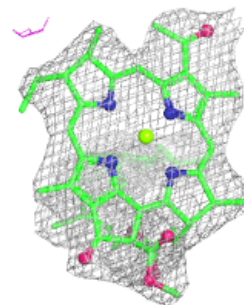
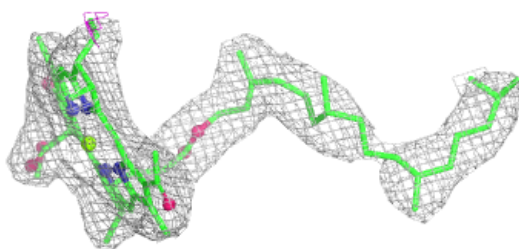
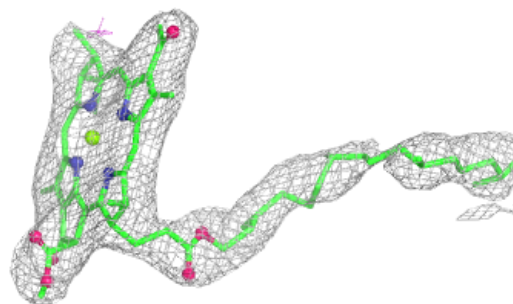


Electron density around RPA D 43 (B):

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

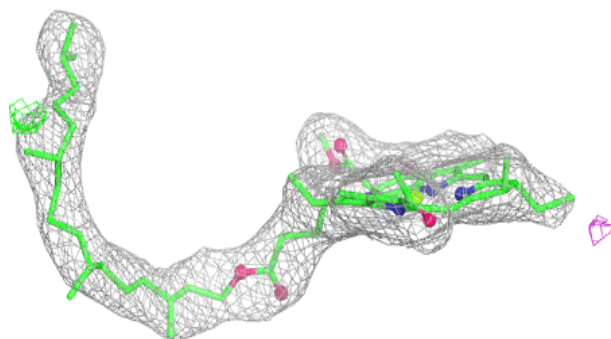
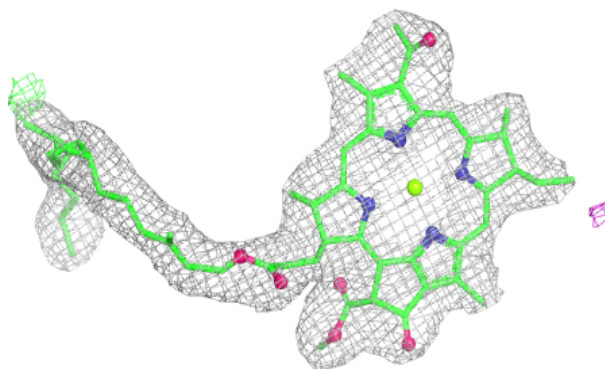
**Electron density around BCL A 55:**

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

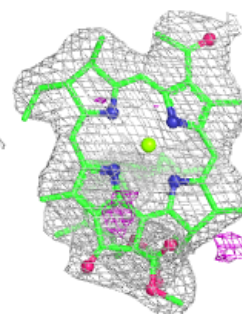
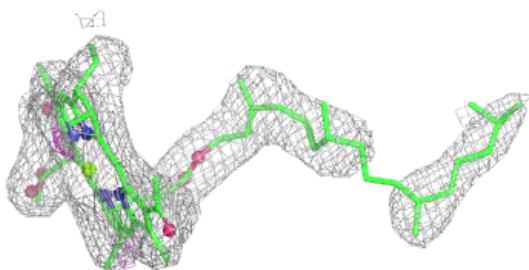
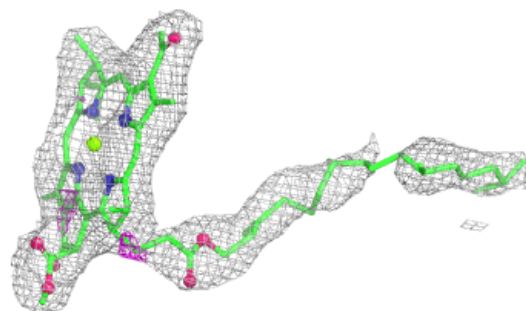


Electron density around BCL B 45:

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

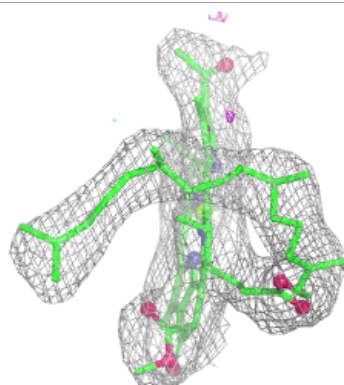
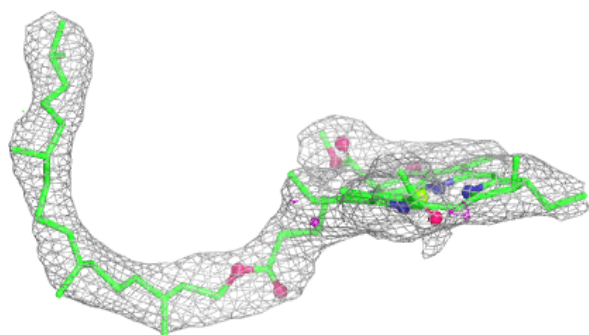
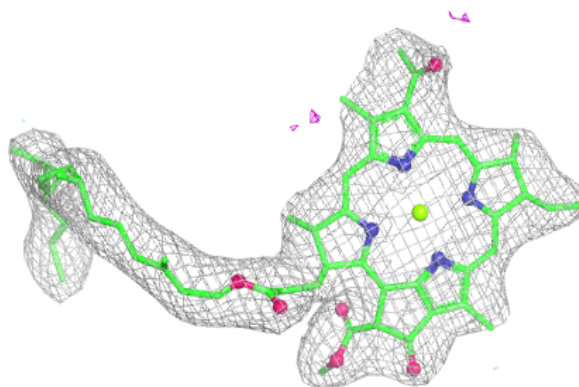
**Electron density around BCL E 55:**

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

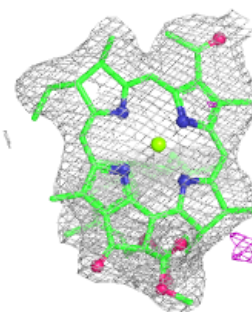
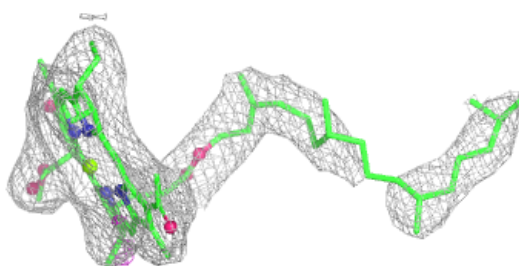
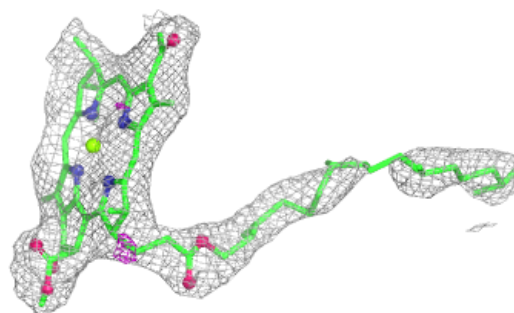


Electron density around BCL F 45:

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

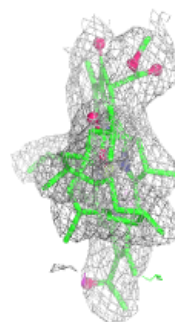
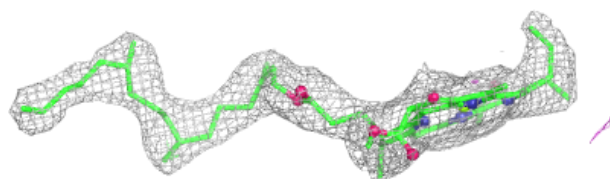
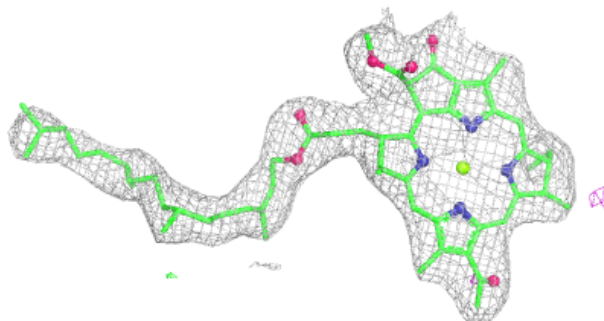
**Electron density around BCL C 55:**

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

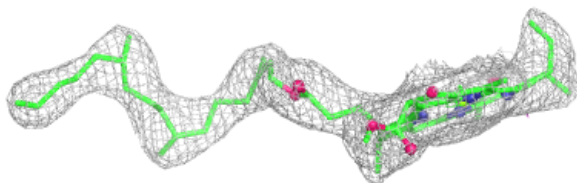
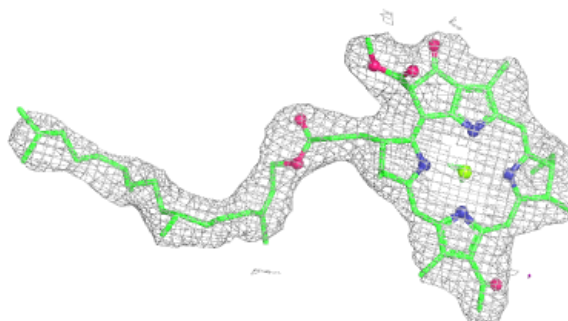


Electron density around BCL E 54:

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

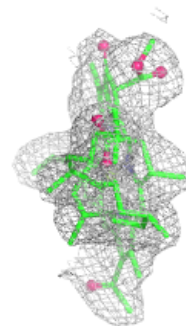
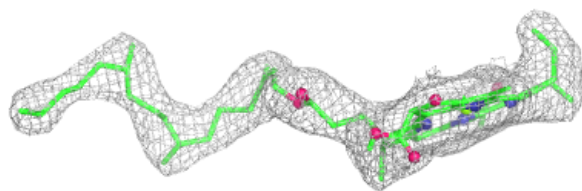
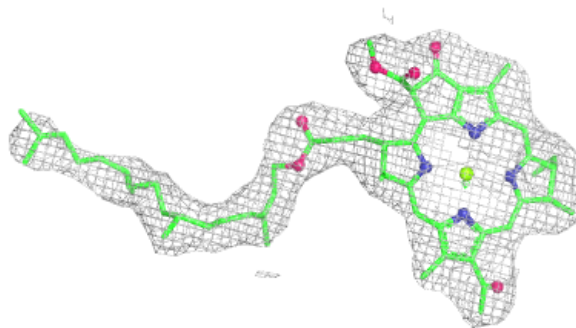
**Electron density around BCL A 54:**

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



Electron density around BCL C 54:

$2mF_o-DF_c$ (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.