



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 1RQK / pdb_00001rqk
Title : Structure of the reaction centre from Rhodobacter sphaeroides carotenoidless strain R-26.1 reconstituted with 3,4-dihydrospheroidene
Authors : Roszak, A.W.; Hashimoto, H.; Gardiner, A.T.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2003-12-05
Resolution : 2.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

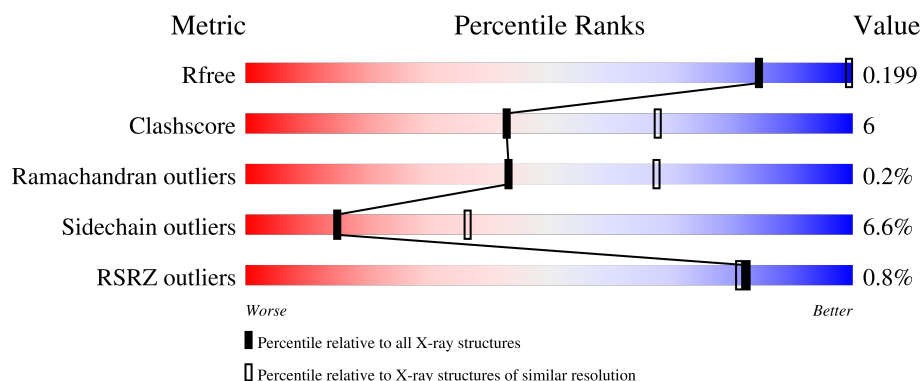
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	L	281	
2	M	307	
3	H	260	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7522 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	5	0
			2249	1518	355	368	8			

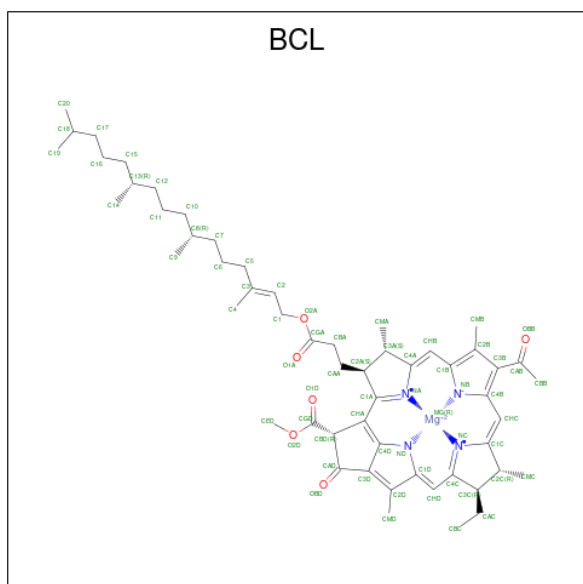
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	3	0
			2423	1615	400	397	11			

- Molecule 3 is a protein called Reaction center protein H chain.

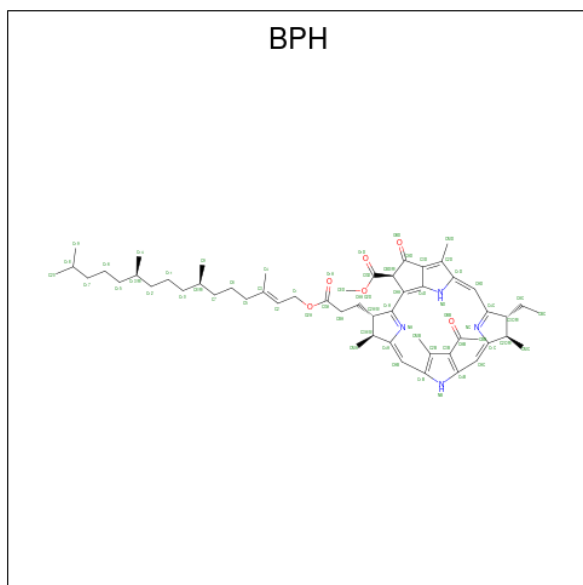
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1868	1190	324	345	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



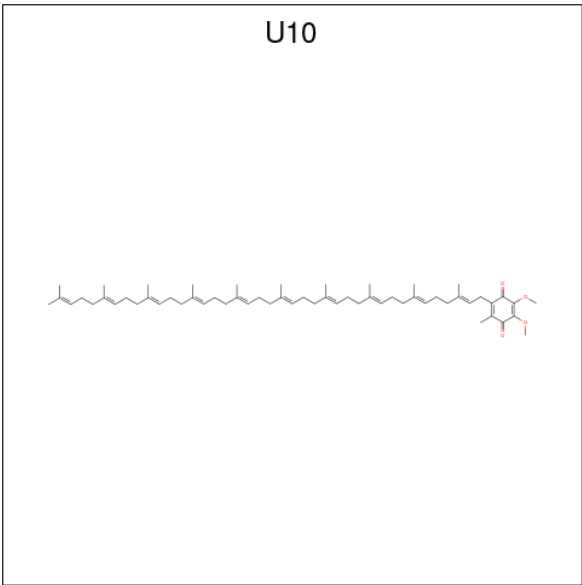
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



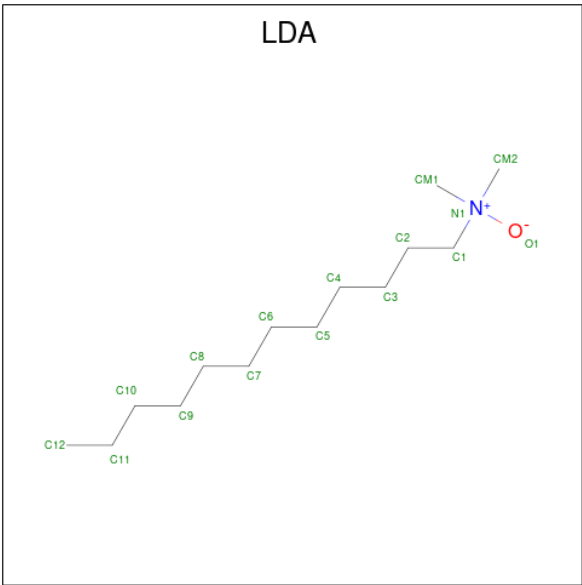
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	1
			96	88	8		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		

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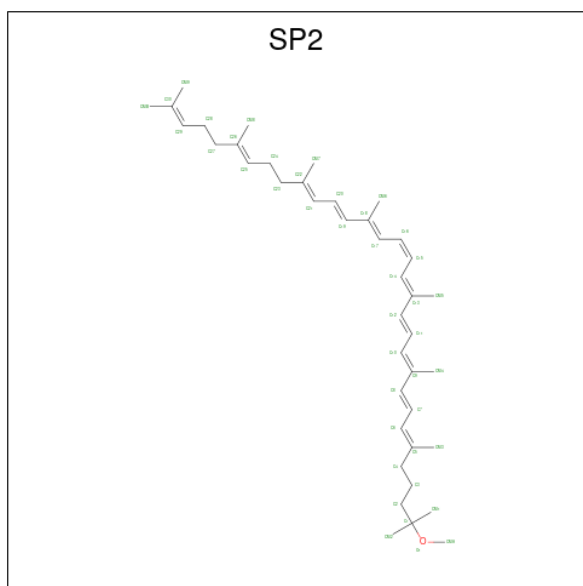
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

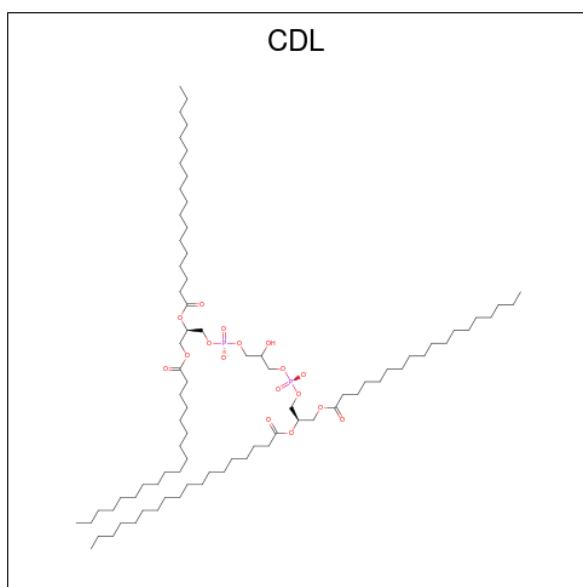
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is 3,4-DIHYDROSPHEROIDENE (CCD ID: SP2) (formula: C₄₁H₆₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

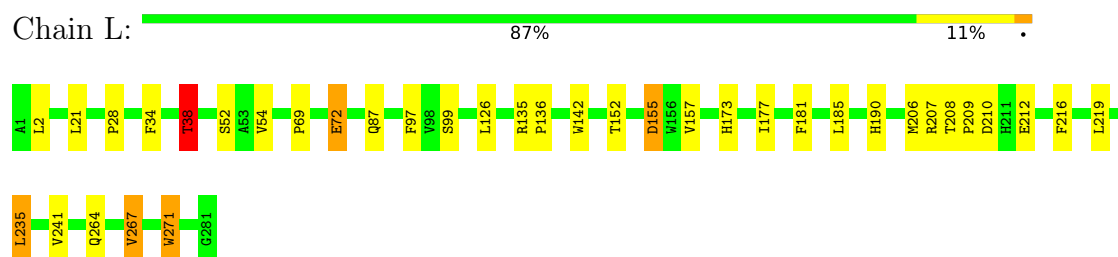
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	57	Total	O	0	0
			57	57		
11	M	66	Total	O	0	0
			66	66		
11	H	85	Total	O	0	0
			85	85		

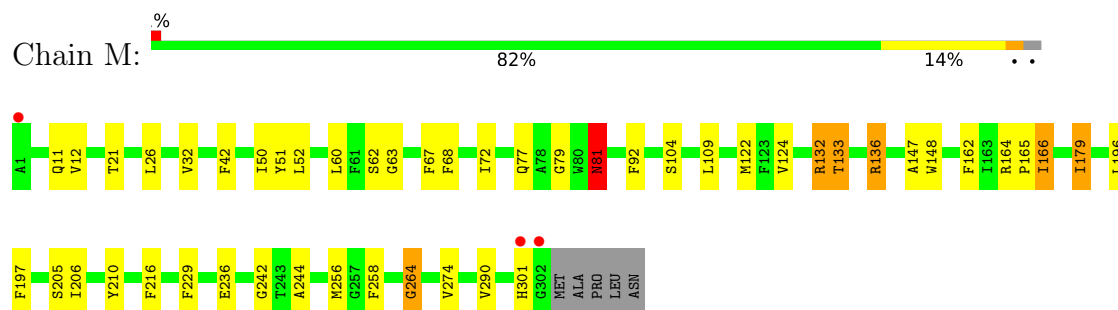
3 Residue-property plots [i](#)

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.

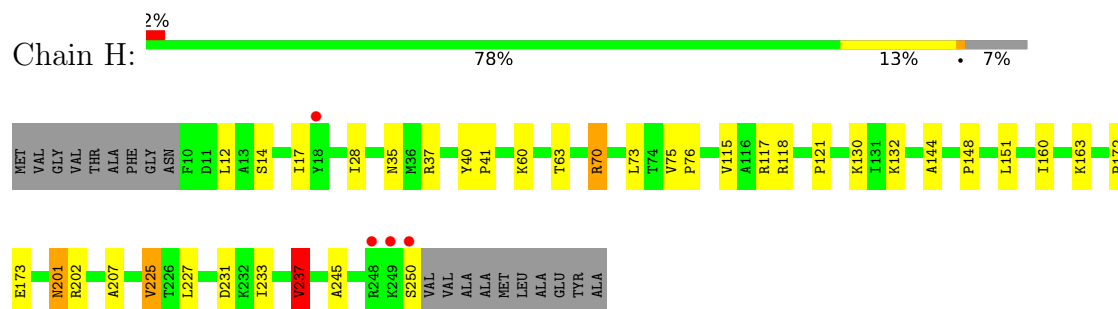
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.72Å 141.72Å 187.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.29 – 2.70 15.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (15.29-2.70) 95.7 (15.29-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.162 , 0.194 0.169 , 0.199	Depositor DCC
R_{free} test set	2864 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7522	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, FE, U10, CDL, BPH, SP2, LDA

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	L	0.91	1/2362 (0.0%)	0.95	1/3232 (0.0%)
2	M	0.92	0/2530	0.97	3/3452 (0.1%)
3	H	1.01	2/1956 (0.1%)	1.01	1/2657 (0.0%)
All	All	0.94	3/6848 (0.0%)	0.98	5/9341 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	38	THR	CA-CB	5.34	1.61	1.53
3	H	160	ILE	CA-CB	5.11	1.60	1.54
3	H	237	VAL	CA-CB	5.00	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	264	GLY	N-CA-C	6.46	120.46	112.64
3	H	225	VAL	CB-CA-C	-6.16	101.44	110.62
2	M	166	ILE	CB-CA-C	-5.52	104.90	111.97
2	M	81	ASN	CB-CA-C	5.40	116.16	108.76
1	L	38	THR	N-CA-CB	5.31	118.02	110.16

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	L	2249	0	2205	29	0
2	M	2423	0	2344	35	0
3	H	1868	0	1880	20	0
4	L	132	0	148	3	0
4	M	132	0	148	10	0
5	L	65	0	76	5	0
5	M	65	0	76	9	0
6	L	96	0	126	9	0
6	M	48	0	63	0	0
7	H	16	0	31	1	0
7	L	32	0	62	0	0
7	M	64	0	124	4	0
8	M	1	0	0	0	0
9	M	42	0	62	0	0
10	M	81	0	106	2	0
11	H	85	0	0	2	0
11	L	57	0	0	0	0
11	M	66	0	0	1	0
All	All	7522	0	7451	91	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 6.

All (91) 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:H:130[A]:LYS:NZ	3:H:173[A]:GLU:OE2	2.04	0.90
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.55	0.88
1:L:241:VAL:HG21	5:L:402:BPH:HAC1	1.72	0.71
1:L:271:TRP:H	1:L:271:TRP:CD1	2.06	0.71
3:H:117[A]:ARG:NH2	3:H:227:LEU:HD22	2.06	0.71
2:M:51:TYR:O	2:M:132:ARG:NH2	2.24	0.70
2:M:197:PHE:CZ	4:M:502:BCL:HBB2	2.27	0.70
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.75	0.68
1:L:34:PHE:O	1:L:38:THR:HG23	1.94	0.67
2:M:179:ILE:HG23	4:M:501:BCL:HED1	1.75	0.67
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.76	0.66
1:L:219:LEU:O	2:M:132:ARG:NH1	2.27	0.65
1:L:271:TRP:CD1	1:L:271:TRP:N	2.65	0.64
2:M:197:PHE:HZ	4:M:502:BCL:HBB2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:132:LYS:NZ	11:H:976:HOH:O	2.30	0.61
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.35	0.61
4:M:502:BCL:CBB	4:M:502:BCL:HHC	2.31	0.60
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.84	0.59
3:H:37:ARG:NH2	3:H:60:LYS:O	2.36	0.58
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.57
2:M:236:GLU:OE2	3:H:118[A]:ARG:NH2	2.34	0.57
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.87	0.56
3:H:14:SER:HA	3:H:17:ILE:HG22	1.88	0.56
3:H:70:ARG:NH2	3:H:121:PRO:O	2.39	0.56
1:L:216:PHE:CD1	6:L:502[B]:U10:H4M2	2.41	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
1:L:235[A]:LEU:HD22	2:M:42:PHE:CZ	2.41	0.55
2:M:63:GLY:HA3	5:M:401:BPH:H5C1	1.90	0.54
1:L:216:PHE:CG	6:L:502[B]:U10:H4M2	2.43	0.53
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.38	0.53
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.91	0.52
2:M:301:HIS:NE2	11:M:968:HOH:O	2.34	0.52
2:M:67:PHE:CD1	5:M:401:BPH:C9	2.93	0.51
2:M:242:GLY:CA	3:H:117[A]:ARG:HD3	2.39	0.51
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.11	0.51
1:L:38:THR:HG22	1:L:99:SER:HB3	1.93	0.51
5:L:402:BPH:HHC	5:L:402:BPH:CBB	2.33	0.50
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.47	0.50
1:L:181:PHE:HB3	5:M:401:BPH:CBB	2.42	0.49
2:M:67:PHE:CD1	5:M:401:BPH:H9C3	2.47	0.49
1:L:28:PRO:HG3	7:M:903:LDA:HM13	1.94	0.49
2:M:68:PHE:O	2:M:72:ILE:HG12	2.12	0.49
1:L:97:PHE:CE1	4:L:302:BCL:H121	2.48	0.49
1:L:152:THR:O	1:L:155[B]:ASP:HB2	2.13	0.48
4:M:501:BCL:H61	5:M:401:BPH:HMB2	1.95	0.48
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.48
5:L:402:BPH:HBB3	5:L:402:BPH:CHC	2.38	0.48
3:H:201:ASN:H	3:H:201:ASN:HD22	1.61	0.48
1:L:212:GLU:OE2	6:L:502[A]:U10:C3M	2.62	0.48
1:L:216:PHE:CD2	6:L:502[A]:U10:H102	2.50	0.47
3:H:130[B]:LYS:HE3	3:H:172:PRO:HG2	1.96	0.47
7:M:903:LDA:HM21	7:H:901:LDA:HM22	1.96	0.47
1:L:235[A]:LEU:HD11	6:L:502[A]:U10:H403	1.97	0.47
4:M:502:BCL:HHC	4:M:502:BCL:HBB3	1.95	0.46
3:H:63:THR:HA	3:H:73:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:VAL:HG11	4:M:502:BCL:HBB1	1.97	0.46
2:M:162:PHE:O	2:M:166:ILE:HG12	2.16	0.46
1:L:181:PHE:HB3	5:M:401:BPH:HBB2	1.98	0.46
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.51	0.45
2:M:206:ILE:HD12	4:M:502:BCL:HMA1	1.98	0.45
2:M:77:GLN:NE2	2:M:92:PHE:HB3	2.30	0.45
3:H:40:TYR:HA	3:H:41:PRO:C	2.40	0.45
3:H:207:ALA:HB1	3:H:237:VAL:O	2.17	0.45
6:L:502[B]:U10:C10	7:M:905:LDA:C12	2.94	0.45
2:M:133:THR:HG21	2:M:147:ALA:HA	1.99	0.45
2:M:197:PHE:CE1	4:M:502:BCL:HBB2	2.50	0.45
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.99	0.44
2:M:136:ARG:NE	2:M:136:ARG:HA	2.33	0.44
2:M:81:ASN:OD1	2:M:81:ASN:C	2.61	0.44
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.48	0.43
6:L:502[B]:U10:H271	6:L:502[B]:U10:H251	1.78	0.43
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.54	0.43
7:M:902:LDA:HM22	11:H:958:HOH:O	2.19	0.43
1:L:190:HIS:HA	6:L:502[A]:U10:O2	2.18	0.43
2:M:122:MET:HE1	4:M:501:BCL:HBB3	2.01	0.43
2:M:290:VAL:HG21	3:H:12:LEU:HD23	2.00	0.42
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.38	0.42
2:M:148:TRP:CE2	10:M:800:CDL:H511	2.54	0.42
3:H:233:ILE:O	3:H:237:VAL:HG13	2.19	0.42
1:L:38:THR:HG22	1:L:99:SER:HB2	2.00	0.42
4:L:302:BCL:HBB3	4:L:302:BCL:HMB3	2.02	0.42
2:M:11:GLN:HB2	3:H:144:ALA:HB3	2.02	0.41
2:M:148:TRP:CD1	10:M:800:CDL:OB6	2.74	0.41
2:M:133:THR:CG2	2:M:147:ALA:HA	2.50	0.41
1:L:208:THR:HB	1:L:209:PRO:HD2	2.03	0.41
2:M:164[A]:ARG:HB3	2:M:165:PRO:HD3	2.03	0.41
4:L:302:BCL:HMB3	4:L:302:BCL:CBB	2.50	0.41
6:L:502[A]:U10:H372	6:L:502[A]:U10:H351	1.84	0.40
2:M:242:GLY:HA2	3:H:117[A]:ARG:HD3	2.04	0.40
2:M:164[B]:ARG:HB3	2:M:165:PRO:HD3	2.04	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	L	284/281 (101%)	278 (98%)	6 (2%)	0	100	100
2	M	303/307 (99%)	288 (95%)	14 (5%)	1 (0%)	36	60
3	H	247/260 (95%)	242 (98%)	4 (2%)	1 (0%)	30	54
All	All	834/848 (98%)	808 (97%)	24 (3%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	79	GLY
3	H	245	ALA

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	L	225/220 (102%)	206 (92%)	19 (8%)	10	26
2	M	239/240 (100%)	221 (92%)	18 (8%)	12	31
3	H	203/208 (98%)	193 (95%)	10 (5%)	22	49
All	All	667/668 (100%)	620 (93%)	47 (7%)	15	34

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU

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Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	52	SER
1	L	54	VAL
1	L	72[A]	GLU
1	L	72[B]	GLU
1	L	126[A]	LEU
1	L	126[B]	LEU
1	L	155[A]	ASP
1	L	155[B]	ASP
1	L	185	LEU
1	L	206	MET
1	L	207	ARG
1	L	210	ASP
1	L	235[A]	LEU
1	L	235[B]	LEU
1	L	267	VAL
1	L	271	TRP
2	M	12	VAL
2	M	32	VAL
2	M	50	ILE
2	M	52	LEU
2	M	60	LEU
2	M	62	SER
2	M	81	ASN
2	M	104	SER
2	M	109	LEU
2	M	124	VAL
2	M	132	ARG
2	M	133	THR
2	M	136	ARG
2	M	179	ILE
2	M	196	LEU
2	M	205	SER
2	M	216	PHE
2	M	274	VAL
3	H	28	ILE
3	H	70	ARG
3	H	115	VAL
3	H	163	LYS
3	H	201	ASN
3	H	202	ARG

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Mol	Chain	Res	Type
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL
3	H	250	SER

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

Mol	Chain	Res	Type
1	L	258	GLN
2	M	4	GLN
2	M	44	ASN
2	M	77	GLN
2	M	299	GLN
3	H	44	ASN
3	H	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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
10	CDL	M	800	-	80,80,99	1.15	4 (5%)	86,92,111	1.17	9 (10%)
6	U10	M	503	-	48,48,63	1.13	4 (8%)	60,61,79	1.28	9 (15%)
9	SP2	M	600	-	41,41,41	1.12	2 (4%)	49,50,50	1.66	12 (24%)
4	BCL	L	302	1	69,74,74	1.19	4 (5%)	79,115,115	1.43	14 (17%)
6	U10	L	502[B]	-	48,48,63	1.05	2 (4%)	60,61,79	1.44	7 (11%)
7	LDA	L	904	-	13,15,15	2.30	2 (15%)	14,17,17	0.56	0
4	BCL	L	304	1	69,74,74	0.96	3 (4%)	79,115,115	1.36	14 (17%)
7	LDA	L	908	-	13,15,15	1.80	1 (7%)	14,17,17	0.52	0
7	LDA	H	901	-	13,15,15	2.31	2 (15%)	14,17,17	0.81	0
4	BCL	M	501	2	69,74,74	1.13	3 (4%)	79,115,115	1.77	22 (27%)
7	LDA	M	902	-	13,15,15	1.96	2 (15%)	14,17,17	0.80	0
7	LDA	M	905	-	13,15,15	2.07	2 (15%)	14,17,17	0.69	0
7	LDA	M	906	-	13,15,15	1.93	2 (15%)	14,17,17	0.57	0
5	BPH	M	401	-	59,70,70	1.06	3 (5%)	59,101,101	1.77	14 (23%)
6	U10	L	502[A]	-	48,48,63	1.12	2 (4%)	60,61,79	1.32	9 (15%)
4	BCL	M	502	2	69,74,74	1.14	3 (4%)	79,115,115	1.39	11 (13%)
7	LDA	M	903	-	13,15,15	1.95	2 (15%)	14,17,17	0.66	0
5	BPH	L	402	-	59,70,70	1.04	3 (5%)	59,101,101	1.92	13 (22%)

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
10	CDL	M	800	-	-	28/91/91/110	-
6	U10	M	503	-	-	9/45/69/87	0/1/1/1
9	SP2	M	600	-	-	8/47/47/47	-
4	BCL	L	302	1	-	5/41/137/137	-
6	U10	L	502[B]	-	-	13/45/69/87	0/1/1/1
7	LDA	L	904	-	-	6/13/13/13	-
4	BCL	L	304	1	-	2/41/137/137	-
7	LDA	L	908	-	-	4/13/13/13	-
7	LDA	H	901	-	-	5/13/13/13	-
4	BCL	M	501	2	-	8/41/137/137	-
7	LDA	M	902	-	-	4/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	M	905	-	-	6/13/13/13	-
7	LDA	M	906	-	-	4/13/13/13	-
5	BPH	M	401	-	-	12/37/105/105	0/5/6/6
6	U10	L	502[A]	-	-	16/45/69/87	0/1/1/1
4	BCL	M	502	2	-	3/41/137/137	-
7	LDA	M	903	-	-	5/13/13/13	-
5	BPH	L	402	-	-	5/37/105/105	0/5/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	904	LDA	O1-N1	-7.05	1.24	1.42
7	H	901	LDA	O1-N1	-7.04	1.24	1.42
4	L	302	BCL	MG-NA	6.43	2.21	2.06
7	M	902	LDA	O1-N1	-6.26	1.26	1.42
7	M	905	LDA	O1-N1	-6.25	1.26	1.42
7	M	903	LDA	O1-N1	-6.24	1.26	1.42
7	M	906	LDA	O1-N1	-6.16	1.27	1.42
4	M	501	BCL	MG-NA	6.05	2.20	2.06
7	L	908	LDA	O1-N1	-5.97	1.27	1.42
4	M	502	BCL	MG-NA	5.73	2.19	2.06
9	M	600	SP2	C16-C17	4.94	1.58	1.43
10	M	800	CDL	OB6-CB5	4.89	1.48	1.34
10	M	800	CDL	OA8-CA7	4.59	1.46	1.33
10	M	800	CDL	OB8-CB7	4.43	1.46	1.33
7	H	901	LDA	C1-N1	-4.35	1.47	1.51
5	M	401	BPH	C1B-C2B	4.23	1.44	1.39
10	M	800	CDL	OA6-CA5	4.20	1.46	1.34
6	M	503	U10	O3-C3	4.14	1.46	1.36
7	L	904	LDA	C1-N1	-4.12	1.47	1.51
5	L	402	BPH	C1B-C2B	4.05	1.44	1.39
7	M	905	LDA	C1-N1	-3.95	1.47	1.51
6	L	502[B]	U10	O3-C3	3.88	1.46	1.36
6	L	502[A]	U10	O3-C3	3.86	1.46	1.36
6	L	502[B]	U10	O4-C4	3.85	1.46	1.36
4	M	502	BCL	MG-NB	3.31	2.12	2.05
5	M	401	BPH	C3A-C2A	-3.26	1.51	1.54
6	M	503	U10	O4-C4	3.17	1.44	1.36
7	M	903	LDA	C1-N1	-3.10	1.48	1.51
5	L	402	BPH	C1D-C2D	3.06	1.42	1.39
7	M	906	LDA	C1-N1	-2.98	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502[A]	U10	O4-C4	2.86	1.43	1.36
4	L	304	BCL	MG-NA	2.73	2.12	2.06
7	M	902	LDA	C1-N1	-2.73	1.48	1.51
4	M	501	BCL	C3B-C4B	2.70	1.46	1.41
4	L	302	BCL	C3B-C4B	2.67	1.46	1.41
5	L	402	BPH	C2C-C3C	2.47	1.56	1.54
5	M	401	BPH	C1D-C2D	2.37	1.42	1.39
4	L	304	BCL	C3B-C4B	2.35	1.45	1.41
4	M	501	BCL	MG-NB	2.28	2.10	2.05
4	M	502	BCL	CBA-CGA	-2.27	1.44	1.50
4	L	302	BCL	MG-NB	2.25	2.10	2.05
4	L	304	BCL	MG-NB	2.19	2.10	2.05
9	M	600	SP2	C15-C14	2.19	1.50	1.43
6	M	503	U10	O4-C4M	-2.11	1.40	1.45
6	M	503	U10	O3-C3M	-2.05	1.40	1.45
4	L	302	BCL	MG-NC	2.01	2.11	2.06

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	C4D-CHA-CBD	-7.22	104.99	108.45
5	L	402	BPH	C2B-C1B-NB	-6.07	105.04	109.43
5	M	401	BPH	C4D-CHA-CBD	-5.70	105.72	108.45
5	M	401	BPH	C2B-C1B-NB	-5.37	105.55	109.43
4	M	501	BCL	C1-O2A-CGA	5.36	129.63	116.65
10	M	800	CDL	OB6-CB5-C51	4.77	121.80	111.48
10	M	800	CDL	OA6-CA5-C11	4.12	120.39	111.48
6	L	502[B]	U10	C20-C19-C21	4.09	122.33	115.23
4	M	502	BCL	C4D-CHA-C1A	4.07	126.10	121.24
5	L	402	BPH	O2D-CGD-CBD	4.05	115.39	110.95
4	M	502	BCL	O2D-CGD-CBD	3.93	118.10	111.23
5	L	402	BPH	C1-C2-C3	-3.89	119.83	126.20
9	M	600	SP2	CM3-C5-C4	3.88	121.95	115.23
4	M	502	BCL	C2B-C1B-NB	-3.84	106.35	110.33
4	M	502	BCL	O2D-CGD-O1D	-3.80	116.45	123.85
4	M	501	BCL	CMB-C2B-C1B	-3.76	119.69	125.42
6	M	503	U10	C30-C29-C31	3.74	121.73	115.23
9	M	600	SP2	C15-C14-C13	-3.70	122.08	127.28
5	M	401	BPH	O2D-CGD-CBD	3.58	114.88	110.95
5	M	401	BPH	CMA-C3A-C4A	-3.58	106.91	114.61
4	M	501	BCL	C4D-CHA-C1A	3.56	125.50	121.24
6	M	503	U10	C32-C33-C34	-3.54	119.52	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	501	BCL	C2C-C3C-C4C	3.50	106.59	101.34
6	L	502[B]	U10	C30-C29-C31	3.44	121.20	115.23
4	M	501	BCL	C2B-C1B-NB	-3.44	106.76	110.33
4	M	501	BCL	CHD-C1D-ND	-3.36	120.07	124.80
6	L	502[B]	U10	C15-C14-C16	3.35	121.03	115.23
4	M	501	BCL	C6-C5-C3	-3.31	105.39	113.47
5	L	402	BPH	C1B-NB-C4B	3.26	113.56	108.82
10	M	800	CDL	OA8-CA7-C31	3.22	121.66	111.83
4	L	302	BCL	CAC-C3C-C4C	-3.21	105.46	112.58
9	M	600	SP2	C16-C17-C18	-3.19	122.80	127.28
4	M	502	BCL	CHA-C1A-NA	-3.19	119.16	126.39
4	M	501	BCL	C1D-ND-C4D	3.14	108.52	106.31
6	L	502[B]	U10	C25-C24-C26	3.11	120.63	115.23
4	M	501	BCL	CHD-C1D-C2D	3.11	131.95	125.49
6	L	502[A]	U10	O2-C2-C3	-3.10	114.46	121.03
4	L	302	BCL	CHA-C1A-NA	-3.10	119.36	126.39
5	L	402	BPH	CMA-C3A-C4A	-3.10	107.93	114.61
4	L	304	BCL	O2D-CGD-CBD	3.10	116.65	111.23
9	M	600	SP2	CM7-C22-C23	3.09	120.58	115.23
4	M	501	BCL	O2A-C1-C2	3.05	119.86	108.11
4	L	304	BCL	C2B-C1B-NB	-3.03	107.18	110.33
4	L	302	BCL	CAA-C2A-C3A	-3.02	104.84	113.00
4	L	302	BCL	C4D-CHA-C1A	3.02	124.84	121.24
5	M	401	BPH	C1-O2A-CGA	3.01	123.94	116.65
4	M	501	BCL	CHA-C1A-NA	-2.98	119.64	126.39
9	M	600	SP2	CM4-C9-C8	2.96	122.61	118.09
5	M	401	BPH	C2D-C1D-ND	-2.96	107.29	109.43
5	M	401	BPH	CAA-C2A-C3A	-2.93	105.08	113.00
4	M	502	BCL	CAC-C3C-C4C	-2.93	106.09	112.58
5	M	401	BPH	C4A-C3A-C2A	2.92	105.61	102.84
10	M	800	CDL	OA6-CA5-OA7	-2.89	116.96	123.70
4	L	304	BCL	C2C-C3C-C4C	2.81	105.55	101.34
4	L	302	BCL	C17-C16-C15	-2.77	100.88	113.28
9	M	600	SP2	CM4-C9-C10	-2.75	118.36	122.82
4	L	304	BCL	CAC-C3C-C4C	-2.75	106.49	112.58
6	L	502[A]	U10	C25-C24-C26	2.74	119.98	115.23
4	L	302	BCL	C11-C12-C13	-2.72	106.93	115.97
4	M	501	BCL	C3B-C4B-NB	-2.71	106.18	109.76
6	L	502[A]	U10	C17-C18-C19	-2.71	121.43	127.62
5	L	402	BPH	C3B-C4B-NB	-2.70	104.13	108.05
4	L	304	BCL	C4A-NA-C1A	2.70	107.91	106.68
4	M	502	BCL	OBB-CAB-CBB	-2.65	113.84	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	503	U10	C6-C1-C2	2.65	121.26	119.17
5	M	401	BPH	C1-C2-C3	-2.64	121.87	126.20
4	L	302	BCL	C3B-C4B-NB	-2.63	106.28	109.76
4	L	302	BCL	C4-C3-C5	2.60	119.74	115.23
4	L	304	BCL	CAA-C2A-C3A	-2.59	105.99	113.00
4	M	501	BCL	C1C-NC-C4C	2.59	107.86	106.68
5	L	402	BPH	OBD-CAD-CBD	-2.57	122.05	125.82
10	M	800	CDL	OA8-CA7-OA9	-2.55	117.26	123.63
4	M	501	BCL	CAA-CBA-CGA	2.54	120.42	113.21
4	M	501	BCL	C11-C12-C13	-2.53	107.55	115.97
4	M	502	BCL	OBB-CAB-C3B	2.53	124.90	120.43
4	M	501	BCL	CHB-C1B-NB	2.51	127.82	124.05
4	L	304	BCL	C4D-CHA-C1A	2.51	124.24	121.24
6	M	503	U10	C31-C29-C28	-2.50	115.54	121.17
4	L	302	BCL	C2B-C1B-NB	-2.49	107.75	110.33
9	M	600	SP2	C20-C21-C22	-2.48	124.20	127.69
6	L	502[B]	U10	C35-C34-C33	-2.48	117.26	123.63
6	M	503	U10	C22-C23-C24	-2.43	122.06	127.62
4	L	304	BCL	O1D-CGD-CBD	-2.42	119.74	124.52
6	L	502[B]	U10	C31-C29-C28	-2.42	115.73	121.17
6	M	503	U10	C26-C27-C28	-2.41	100.12	112.02
5	L	402	BPH	C2D-C1D-ND	-2.37	107.72	109.43
6	L	502[A]	U10	C1M-C1-C6	-2.36	120.57	124.45
4	M	501	BCL	OBB-CAB-CBB	-2.33	114.56	119.77
4	L	304	BCL	OBB-CAB-C3B	2.32	124.54	120.43
5	M	401	BPH	CMA-C3A-C2A	-2.31	105.19	114.13
4	M	501	BCL	O2D-CGD-CBD	2.31	115.27	111.23
9	M	600	SP2	C11-C10-C9	-2.30	124.05	127.28
9	M	600	SP2	C19-C18-C17	-2.29	115.40	119.01
6	M	503	U10	C35-C34-C36	2.27	119.17	115.23
5	M	401	BPH	C1A-C2A-C3A	-2.27	100.68	102.84
9	M	600	SP2	C10-C11-C12	-2.27	116.64	123.20
5	M	401	BPH	CMD-C2D-C3D	2.26	129.21	124.68
5	M	401	BPH	C1B-NB-C4B	2.26	112.11	108.82
5	L	402	BPH	O2D-CGD-O1D	-2.26	119.45	123.85
5	M	401	BPH	C3B-C4B-NB	-2.25	104.78	108.05
4	L	304	BCL	CHD-C1D-ND	-2.25	121.63	124.80
4	L	304	BCL	CAA-C2A-C1A	-2.25	104.59	111.97
4	L	302	BCL	O2A-CGA-O1A	-2.25	118.00	123.63
9	M	600	SP2	C21-C20-C19	-2.24	116.70	123.20
4	M	502	BCL	CHD-C1D-ND	-2.23	121.67	124.80
5	L	402	BPH	OBD-CAD-C3D	2.22	131.35	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	501	BCL	C2D-C1D-ND	-2.20	107.95	110.13
4	M	501	BCL	OBB-CAB-C3B	2.19	124.31	120.43
4	L	304	BCL	CBC-CAC-C3C	2.18	118.03	113.41
6	L	502[A]	U10	C30-C29-C31	2.17	118.99	115.23
6	L	502[B]	U10	C22-C23-C24	-2.16	122.67	127.62
4	L	304	BCL	C6-C5-C3	-2.15	108.24	113.47
6	L	502[A]	U10	C3M-O3-C3	2.14	124.00	116.47
10	M	800	CDL	OB8-CB7-C71	2.14	118.35	111.83
4	L	302	BCL	CMA-C3A-C2A	-2.13	105.73	113.98
6	M	503	U10	C4M-O4-C4	2.13	123.94	116.47
6	L	502[A]	U10	C36-C34-C33	2.12	125.93	121.17
6	L	502[A]	U10	C22-C23-C24	-2.12	122.77	127.62
6	L	502[A]	U10	C3-C2-C1	2.12	122.28	118.10
9	M	600	SP2	CM8-C26-C27	2.11	118.90	115.23
10	M	800	CDL	CB6-OB8-CB7	2.11	124.83	117.12
10	M	800	CDL	CB6-CB4-CB3	-2.09	106.91	111.78
5	L	402	BPH	CMA-C3A-C2A	-2.08	106.11	114.13
5	L	402	BPH	CBC-CAC-C3C	2.07	117.86	113.78
4	L	302	BCL	C5-C3-C2	-2.05	116.57	121.17
4	L	302	BCL	CMA-C3A-C4A	-2.05	106.27	111.77
10	M	800	CDL	OB8-CB7-OB9	-2.04	118.51	123.63
4	M	501	BCL	C5-C3-C2	2.04	125.74	121.17
4	M	502	BCL	CHB-C1B-NB	2.03	127.09	124.05
6	M	503	U10	C15-C14-C16	2.02	118.73	115.23
4	M	502	BCL	C2C-C3C-C4C	2.02	104.36	101.34
4	L	304	BCL	C5-C3-C2	-2.02	116.64	121.17
4	L	302	BCL	C1D-ND-C4D	2.01	107.72	106.31
4	M	501	BCL	CAA-C2A-C3A	-2.01	107.58	113.00

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	302	BCL	C14-C13-C15-C16
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
6	L	502[B]	U10	C15-C14-C16-C17
6	L	502[B]	U10	C18-C19-C21-C22
6	L	502[B]	U10	C20-C19-C21-C22
7	L	904	LDA	C2-C1-N1-O1
7	L	904	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
7	H	901	LDA	C2-C1-N1-O1
7	H	901	LDA	C2-C1-N1-CM1
7	H	901	LDA	C2-C1-N1-CM2
9	M	600	SP2	CM1-C1-C2-C3
9	M	600	SP2	CM2-C1-C2-C3
6	L	502[A]	U10	C30-C29-C31-C32
6	L	502[B]	U10	C25-C24-C26-C27
6	L	502[A]	U10	C28-C29-C31-C32
6	L	502[B]	U10	C13-C14-C16-C17
6	L	502[B]	U10	C23-C24-C26-C27
6	L	502[A]	U10	C25-C24-C26-C27
6	L	502[B]	U10	C30-C29-C31-C32
6	L	502[A]	U10	C23-C24-C26-C27
6	L	502[B]	U10	C28-C29-C31-C32
6	L	502[A]	U10	C9-C11-C12-C13
6	L	502[A]	U10	C19-C21-C22-C23
6	L	502[B]	U10	C14-C16-C17-C18
6	L	502[B]	U10	C24-C26-C27-C28
6	M	503	U10	C29-C31-C32-C33
9	M	600	SP2	C3-C4-C5-CM3
9	M	600	SP2	C3-C4-C5-C6
4	M	501	BCL	C6-C7-C8-C10
6	L	502[A]	U10	C14-C16-C17-C18
6	L	502[A]	U10	C34-C36-C37-C38
10	M	800	CDL	CB7-C71-C72-C73
10	M	800	CDL	O1-C1-CA2-OA2
10	M	800	CDL	C11-CA5-OA6-CA4
5	M	401	BPH	C11-C12-C13-C14
10	M	800	CDL	OA7-CA5-OA6-CA4
4	M	501	BCL	C16-C17-C18-C19
7	M	903	LDA	C3-C4-C5-C6
10	M	800	CDL	C80-C81-C82-C83
7	M	905	LDA	C2-C3-C4-C5
7	M	903	LDA	C6-C7-C8-C9
7	M	905	LDA	C11-C10-C9-C8
10	M	800	CDL	C79-C80-C81-C82
10	M	800	CDL	C38-C39-C40-C41
5	M	401	BPH	C15-C16-C17-C18
7	M	902	LDA	C1-C2-C3-C4
9	M	600	SP2	CM6-C18-C19-C20
9	M	600	SP2	C17-C18-C19-C20
7	M	906	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	M	501	BCL	C16-C17-C18-C20
7	L	908	LDA	C7-C8-C9-C10
10	M	800	CDL	C14-C15-C16-C17
10	M	800	CDL	C19-C20-C21-C22
4	L	304	BCL	C13-C15-C16-C17
10	M	800	CDL	OA5-CA3-CA4-CA6
4	L	302	BCL	C11-C12-C13-C15
4	L	302	BCL	C12-C13-C15-C16
5	M	401	BPH	C6-C7-C8-C10
6	L	502[A]	U10	C15-C14-C16-C17
6	L	502[A]	U10	C13-C14-C16-C17
7	M	906	LDA	C1-C2-C3-C4
7	M	902	LDA	C11-C10-C9-C8
4	M	501	BCL	C14-C13-C15-C16
5	M	401	BPH	C6-C7-C8-C9
4	M	501	BCL	C13-C15-C16-C17
10	M	800	CDL	C18-C19-C20-C21
10	M	800	CDL	C71-C72-C73-C74
7	M	905	LDA	C9-C10-C11-C12
10	M	800	CDL	C17-C18-C19-C20
7	M	903	LDA	N1-C1-C2-C3
7	H	901	LDA	C9-C10-C11-C12
5	M	401	BPH	C5-C6-C7-C8
5	L	402	BPH	C4-C3-C5-C6
5	M	401	BPH	C4-C3-C5-C6
6	M	503	U10	C35-C34-C36-C37
4	L	302	BCL	C11-C12-C13-C14
4	M	501	BCL	C6-C7-C8-C9
10	M	800	CDL	C77-C78-C79-C80
4	M	501	BCL	C12-C13-C15-C16
5	M	401	BPH	C12-C13-C15-C16
6	M	503	U10	C30-C29-C31-C32
7	L	904	LDA	C4-C5-C6-C7
5	L	402	BPH	C2-C3-C5-C6
6	M	503	U10	C28-C29-C31-C32
5	M	401	BPH	C2-C3-C5-C6
6	M	503	U10	C33-C34-C36-C37
7	M	906	LDA	C4-C5-C6-C7
6	M	503	U10	C24-C26-C27-C28
7	H	901	LDA	C1-C2-C3-C4
4	M	502	BCL	C13-C15-C16-C17
4	M	501	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	M	401	BPH	O2A-C1-C2-C3
7	M	903	LDA	C5-C6-C7-C8
6	L	502[B]	U10	C29-C31-C32-C33
7	L	908	LDA	C9-C10-C11-C12
7	M	902	LDA	C5-C6-C7-C8
7	L	904	LDA	C2-C1-N1-CM1
6	L	502[B]	U10	C19-C21-C22-C23
10	M	800	CDL	C20-C21-C22-C23
5	L	402	BPH	C8-C10-C11-C12
10	M	800	CDL	OA5-CA3-CA4-OA6
5	M	401	BPH	C4C-C3C-CAC-CBC
10	M	800	CDL	C13-C14-C15-C16
4	M	502	BCL	CAD-CBD-CGD-O1D
6	M	503	U10	C25-C24-C26-C27
7	M	903	LDA	C2-C3-C4-C5
10	M	800	CDL	C51-C52-C53-C54
10	M	800	CDL	C72-C71-CB7-OB8
5	M	401	BPH	C14-C13-C15-C16
10	M	800	CDL	C81-C82-C83-C84
7	M	905	LDA	C1-C2-C3-C4
10	M	800	CDL	C35-C36-C37-C38
10	M	800	CDL	C72-C73-C74-C75
10	M	800	CDL	O1-C1-CB2-OB2
9	M	600	SP2	C5-C6-C7-C8
4	L	304	BCL	C3-C5-C6-C7
6	M	503	U10	C23-C24-C26-C27
10	M	800	CDL	CB2-C1-CA2-OA2
6	L	502[B]	U10	C5-C4-O4-C4M
7	M	902	LDA	C3-C4-C5-C6
7	L	908	LDA	C1-C2-C3-C4
4	M	502	BCL	C16-C17-C18-C19
6	L	502[A]	U10	C35-C34-C36-C37
7	L	904	LDA	C5-C6-C7-C8
10	M	800	CDL	C78-C79-C80-C81
7	L	908	LDA	C11-C10-C9-C8
7	L	904	LDA	C2-C3-C4-C5
7	M	906	LDA	C5-C6-C7-C8
6	L	502[A]	U10	C33-C34-C36-C37
6	M	503	U10	C14-C16-C17-C18
7	M	905	LDA	C2-C1-N1-CM1
10	M	800	CDL	C37-C38-C39-C40
10	M	800	CDL	C32-C31-CA7-OA8

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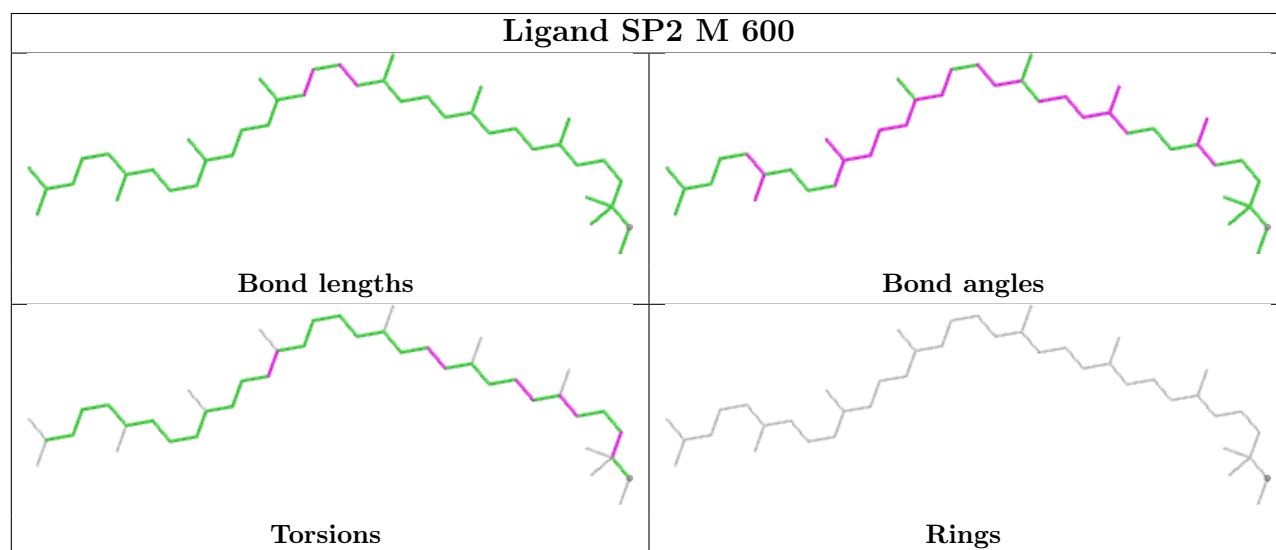
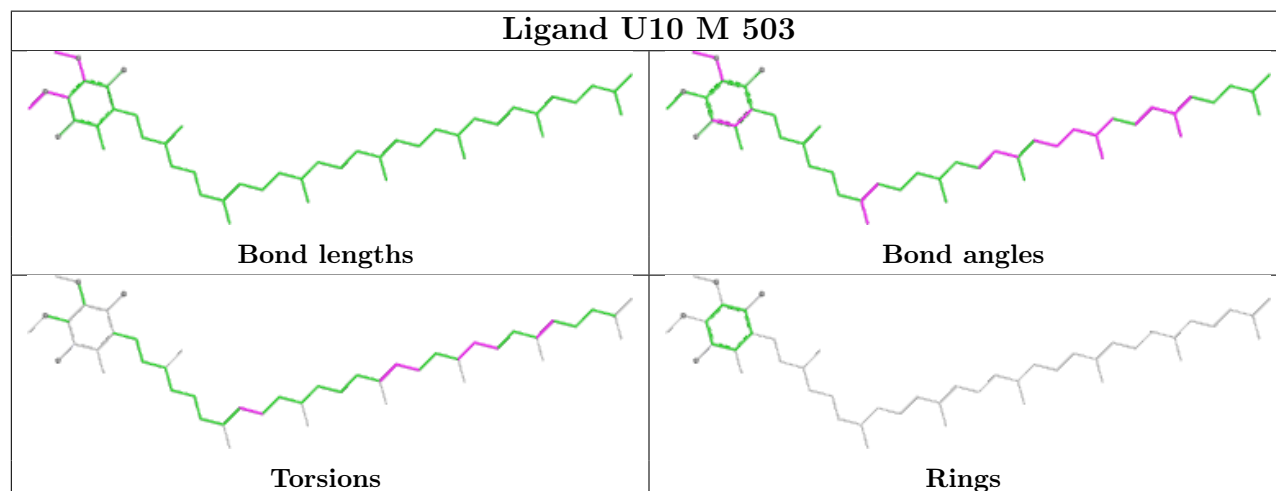
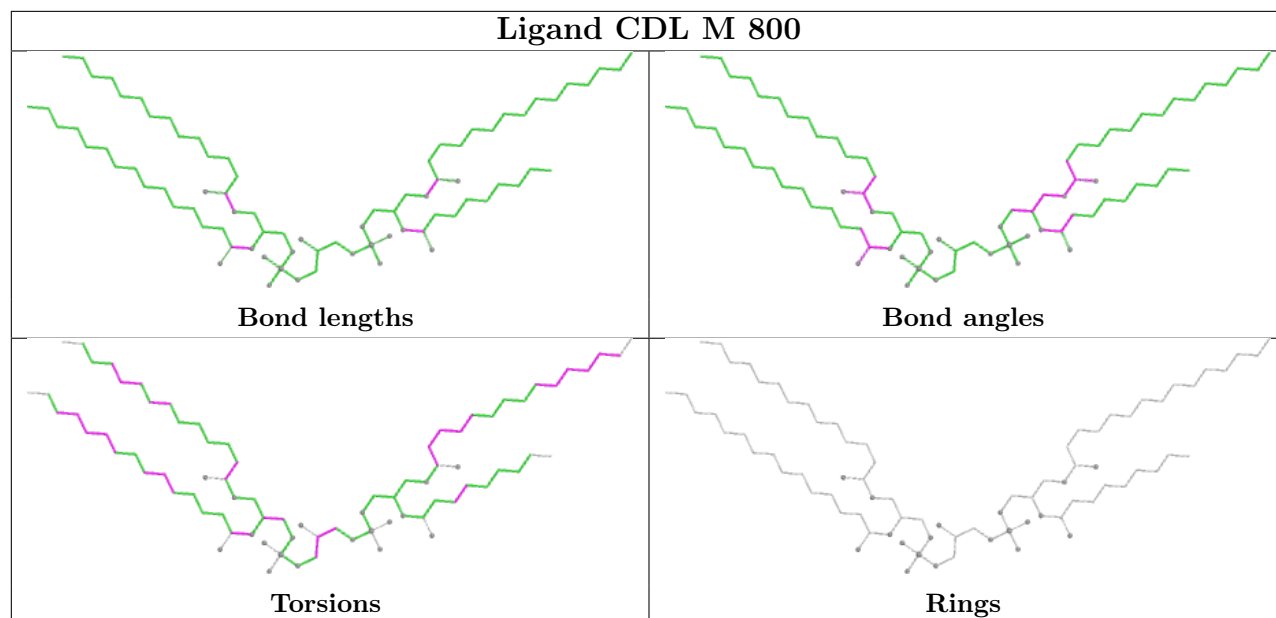
Mol	Chain	Res	Type	Atoms
6	L	502[A]	U10	C11-C12-C13-C14
4	L	302	BCL	C16-C17-C18-C19
6	L	502[A]	U10	C26-C27-C28-C29
6	L	502[A]	U10	C21-C22-C23-C24
6	L	502[A]	U10	C2-C3-O3-C3M
7	M	905	LDA	C2-C1-N1-O1
10	M	800	CDL	C32-C31-CA7-OA9
9	M	600	SP2	C9-C10-C11-C12

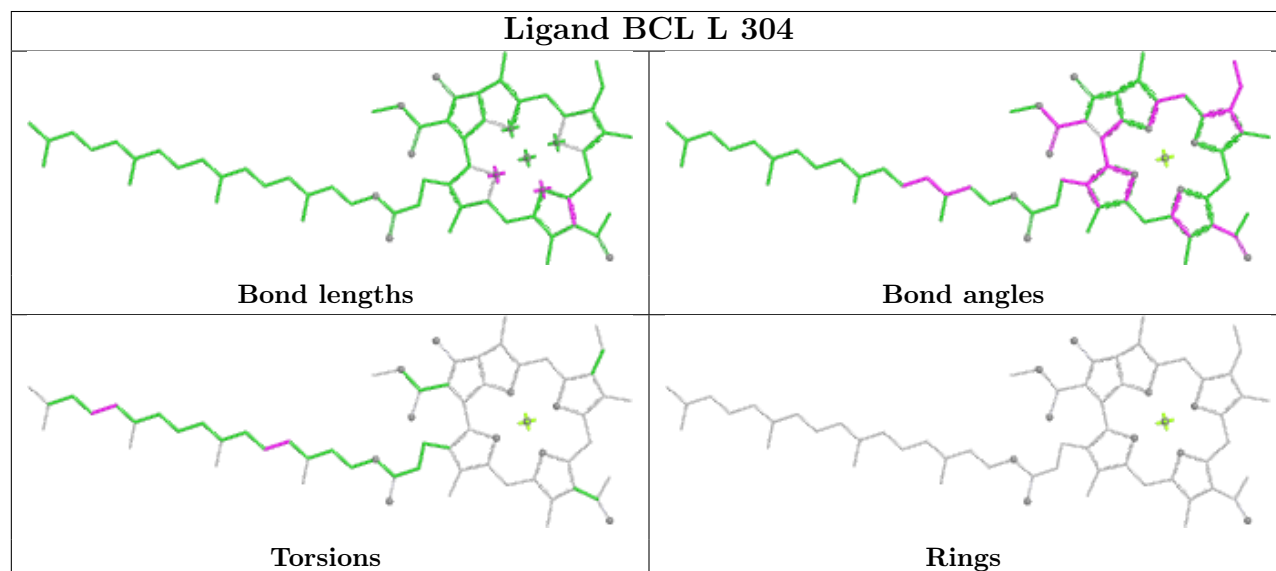
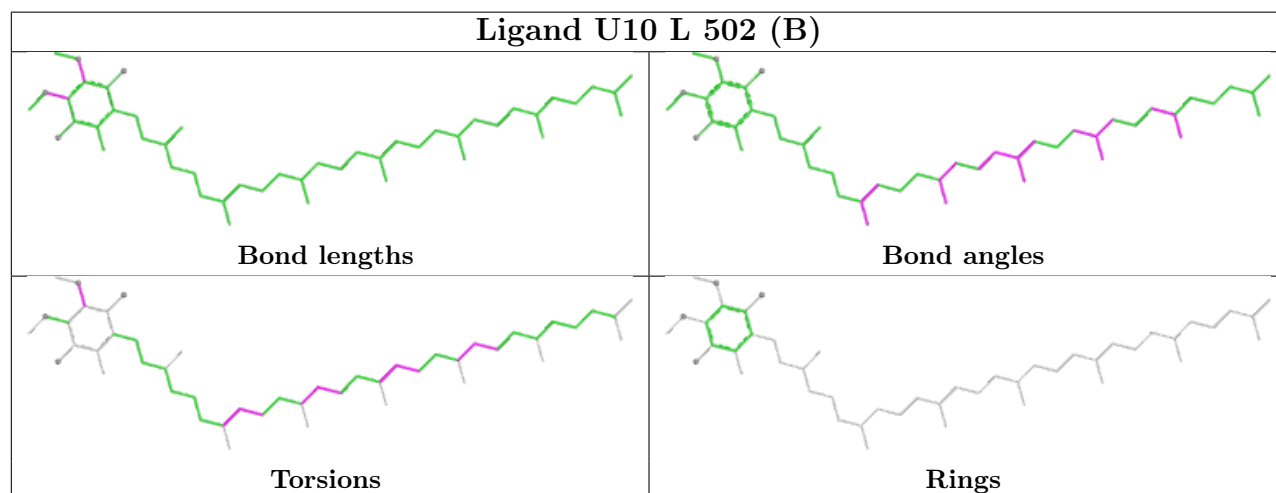
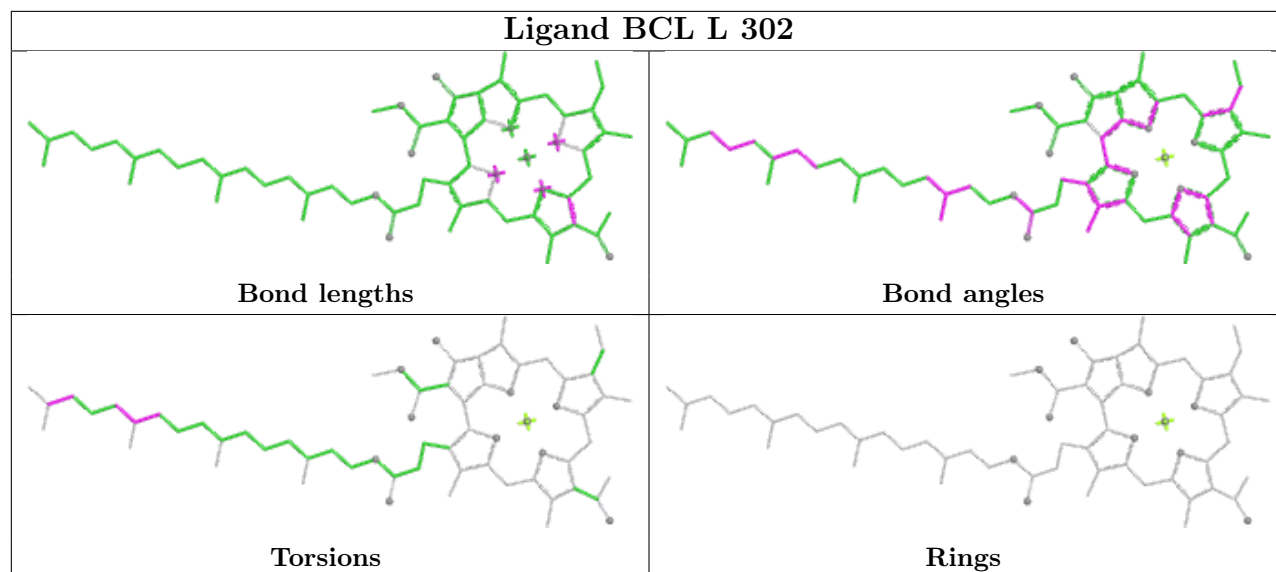
There are no ring outliers.

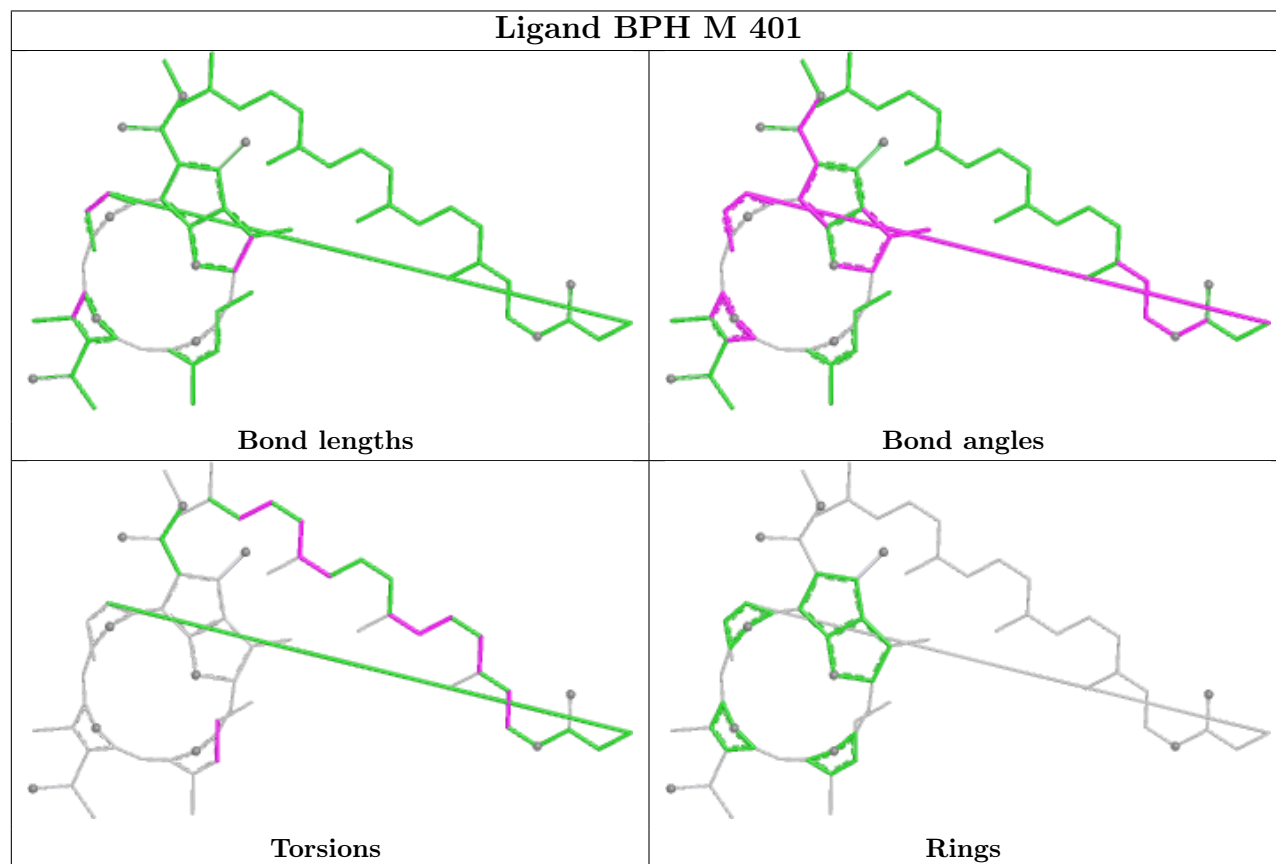
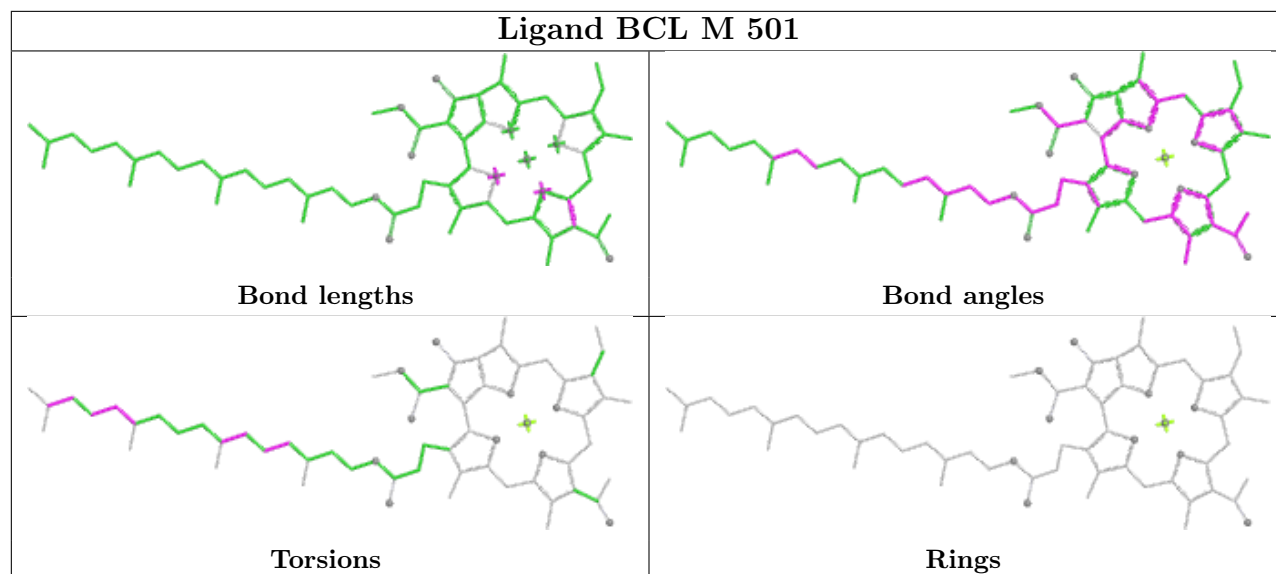
12 monomers are involved in 40 short contacts:

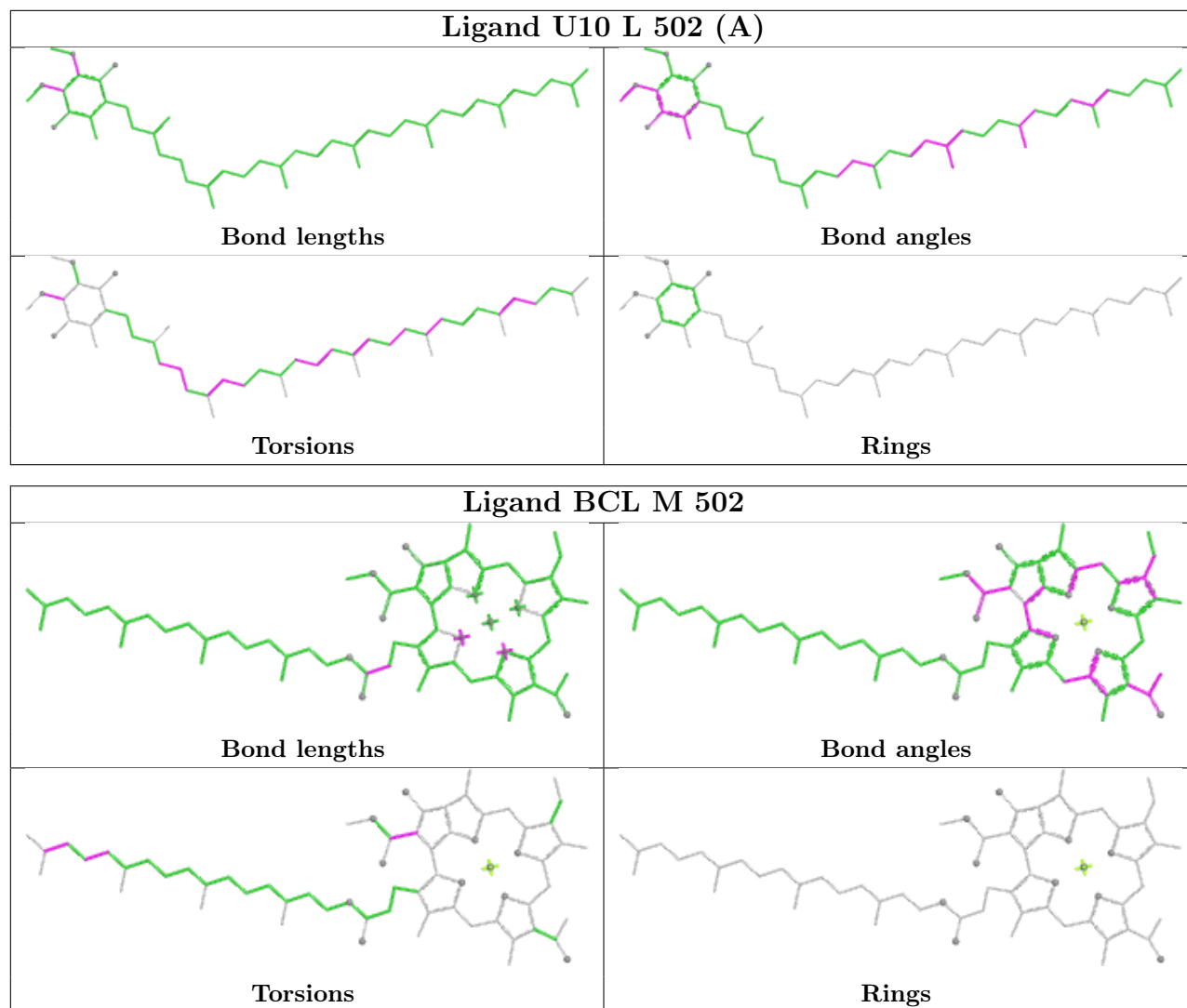
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	800	CDL	2	0
4	L	302	BCL	3	0
6	L	502[B]	U10	4	0
7	H	901	LDA	1	0
4	M	501	BCL	3	0
7	M	902	LDA	1	0
7	M	905	LDA	1	0
5	M	401	BPH	9	0
6	L	502[A]	U10	5	0
4	M	502	BCL	7	0
7	M	903	LDA	2	0
5	L	402	BPH	5	0

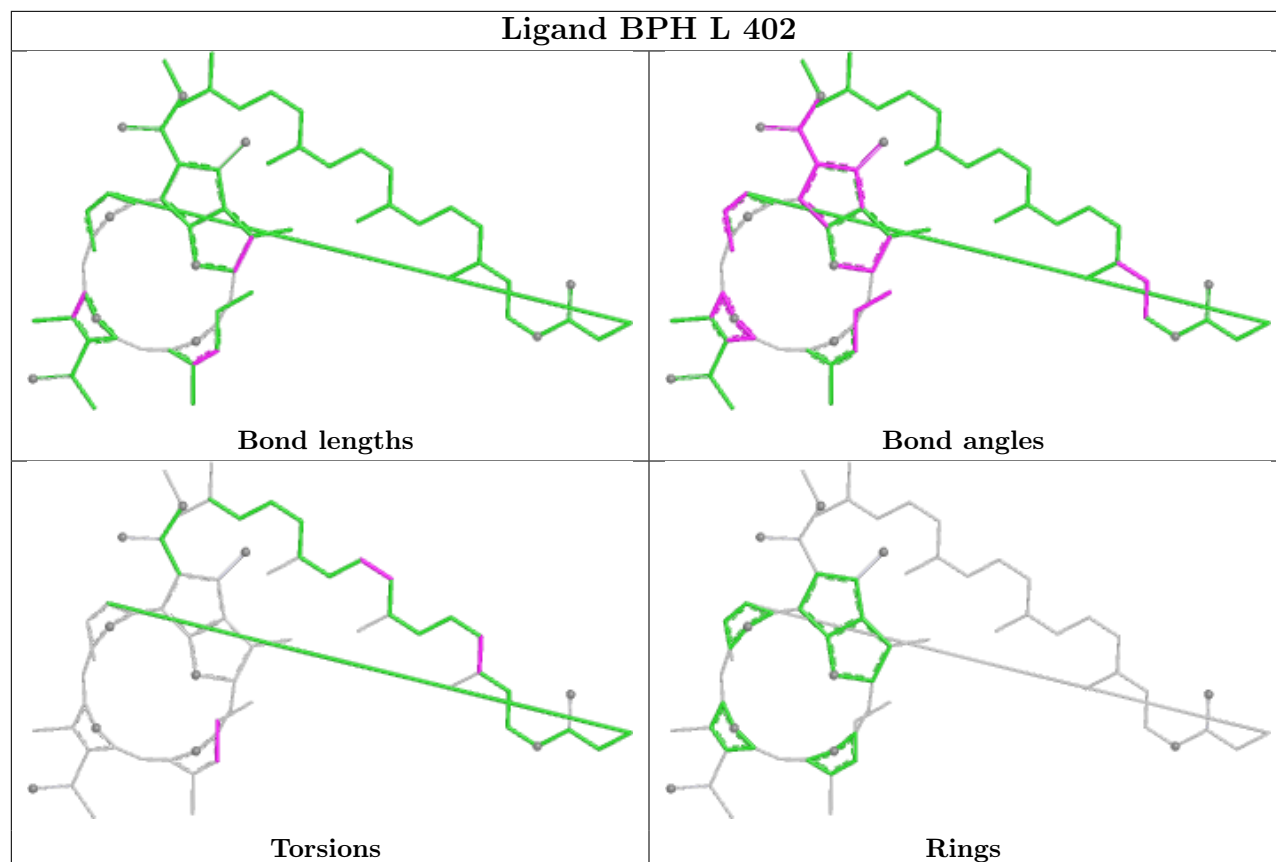
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	-0.47	0 100 100	32, 47, 61, 67	5 (1%)
2	M	302/307 (98%)	-0.40	3 (0%) 79 78	29, 47, 59, 85	3 (0%)
3	H	241/260 (92%)	-0.36	4 (1%) 69 67	27, 46, 60, 94	8 (3%)
All	All	824/848 (97%)	-0.41	7 (0%) 82 81	27, 47, 60, 94	16 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	4.1
3	H	249	LYS	3.7
2	M	1	ALA	3.1
3	H	250	SER	2.6
2	M	301	HIS	2.4
3	H	248	ARG	2.4
3	H	18	TYR	2.2

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,

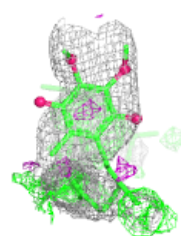
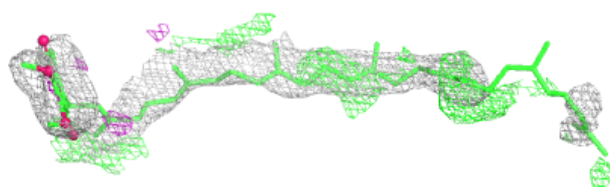
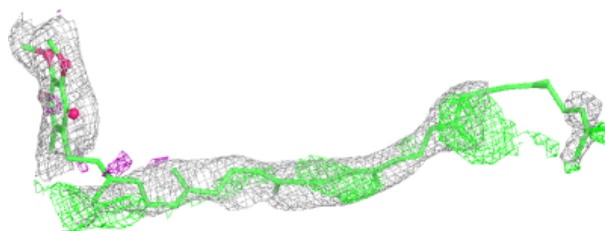
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	M	906	16/16	0.71	0.19	53,56,63,63	16
7	LDA	L	908	16/16	0.77	0.21	57,61,77,78	16
7	LDA	M	905	16/16	0.80	0.17	52,56,60,61	16
6	U10	L	502[B]	48/63	0.81	0.23	52,61,74,74	48
6	U10	L	502[A]	48/63	0.81	0.23	61,69,71,72	48
7	LDA	M	903	16/16	0.82	0.27	52,57,64,65	16
10	CDL	M	800	81/100	0.85	0.18	47,60,68,71	81
7	LDA	L	904	16/16	0.86	0.20	52,55,57,57	16
7	LDA	M	902	16/16	0.90	0.12	61,62,68,69	16
9	SP2	M	600	42/42	0.91	0.11	52,61,83,84	0
7	LDA	H	901	16/16	0.92	0.11	60,64,71,72	16
6	U10	M	503	48/63	0.93	0.10	44,56,82,83	0
4	BCL	M	501	66/66	0.94	0.10	42,48,101,103	0
5	BPH	M	401	65/65	0.95	0.08	47,51,100,102	0
4	BCL	L	302	66/66	0.97	0.07	35,43,60,65	0
4	BCL	M	502	66/66	0.97	0.07	40,43,68,78	0
5	BPH	L	402	65/65	0.97	0.06	39,46,54,55	0
4	BCL	L	304	66/66	0.97	0.06	36,44,62,65	0
8	FE	M	500	1/1	1.00	0.03	49,49,49,49	0

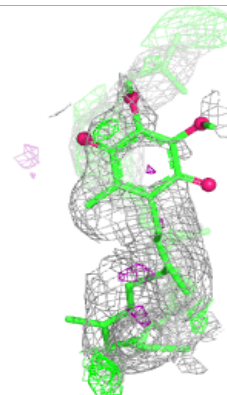
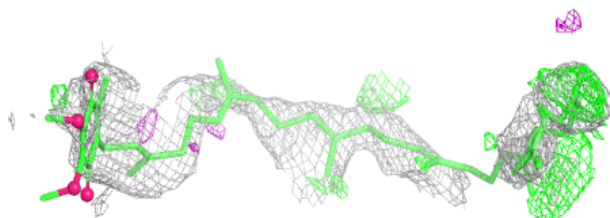
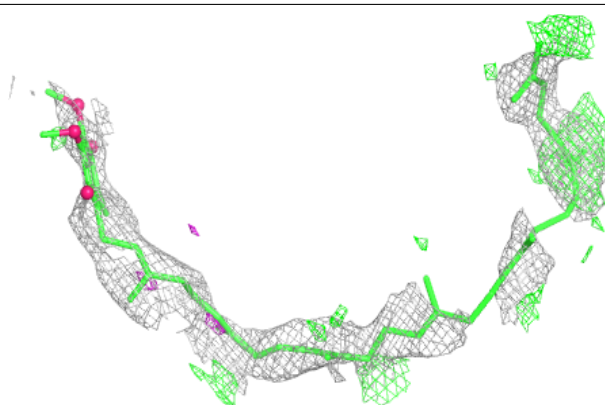
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 502 (B):

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

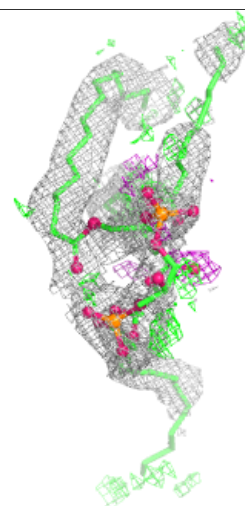
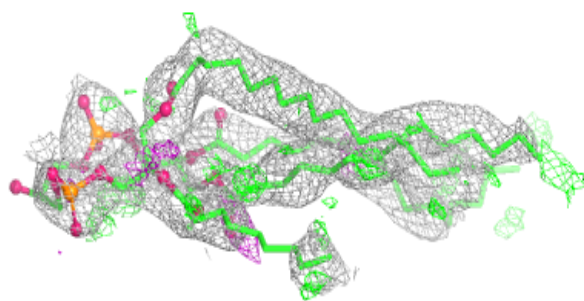
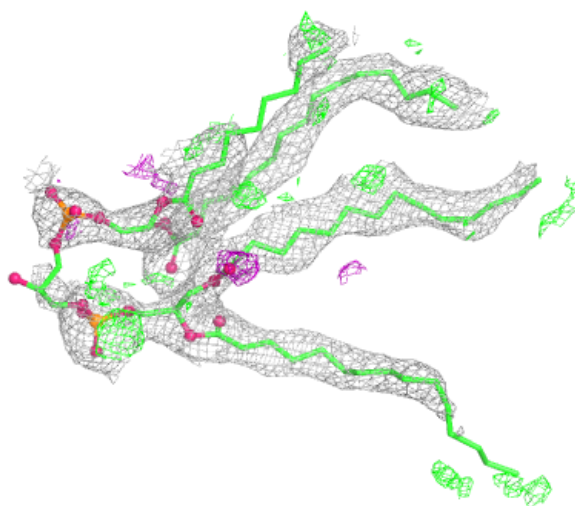
**Electron density around U10 L 502 (A):**

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



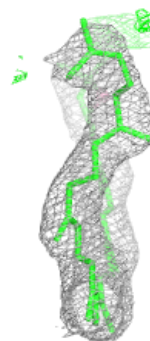
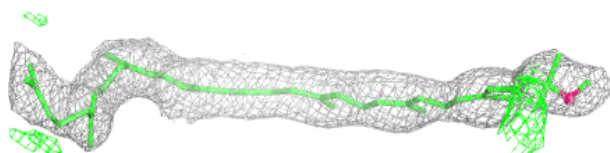
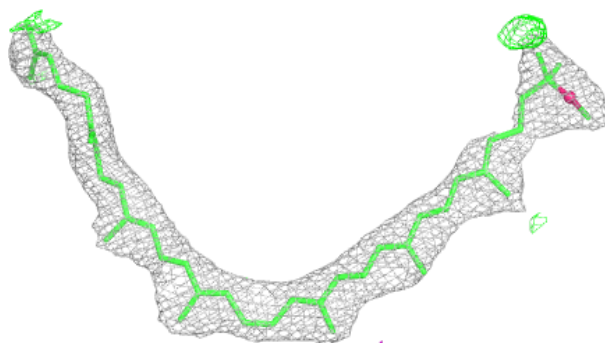
Electron density around CDL M 800:

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

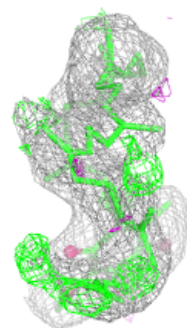
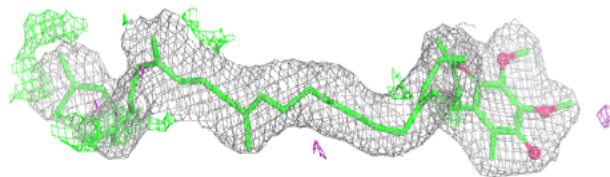
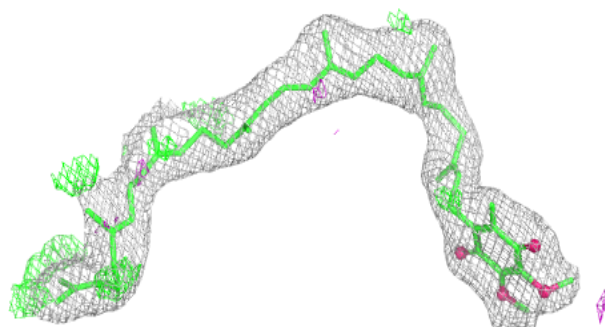


Electron density around SP2 M 600:

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

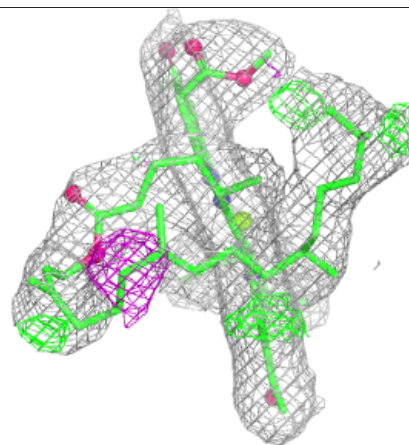
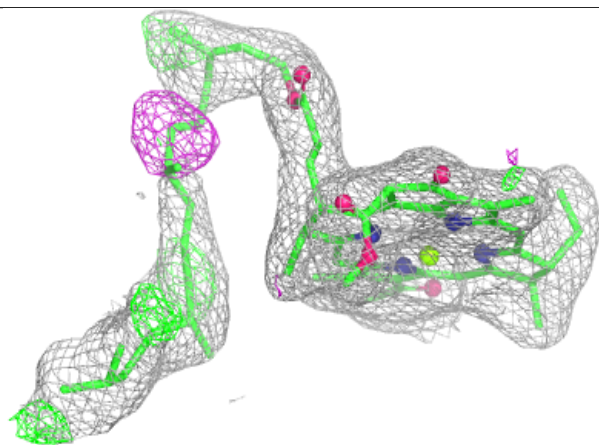
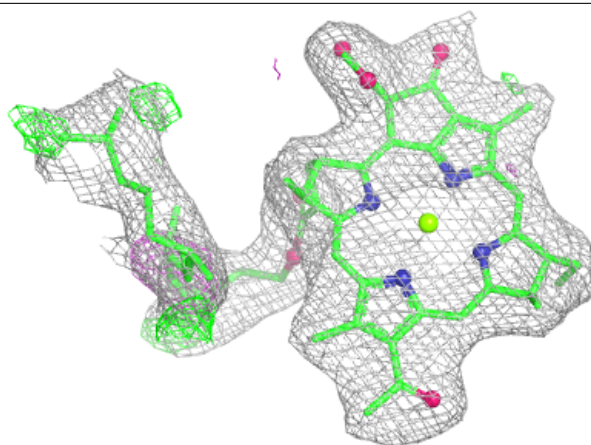
**Electron density around U10 M 503:**

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



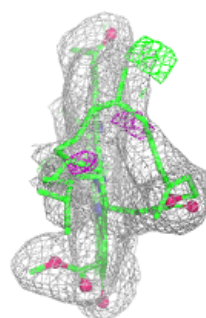
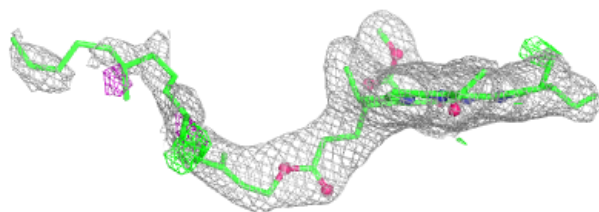
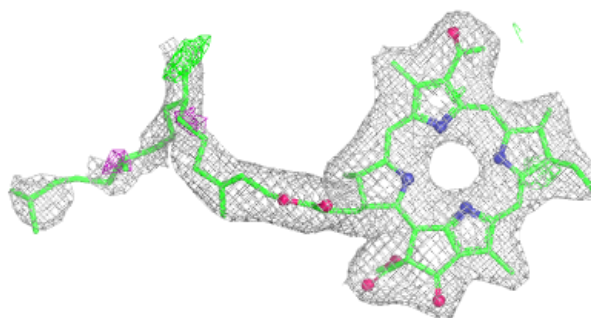
Electron density around BCL M 501:

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

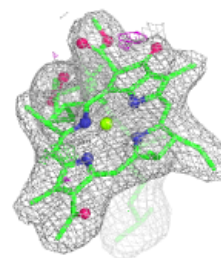
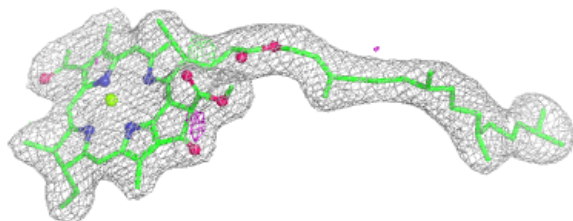
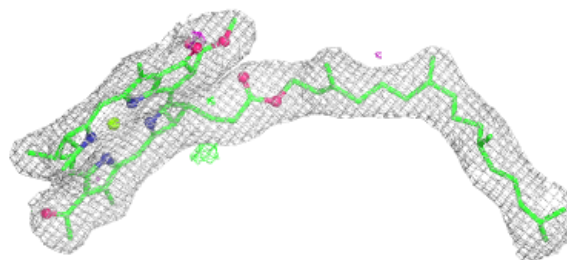


Electron density around BPH M 401:

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

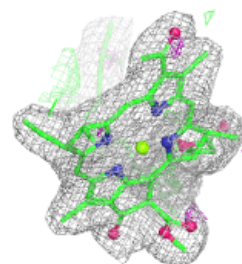
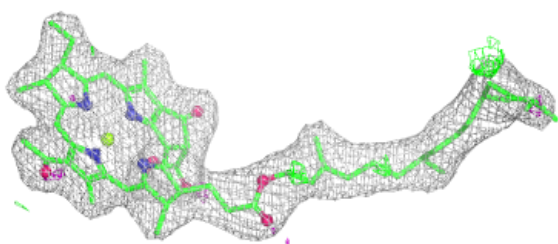
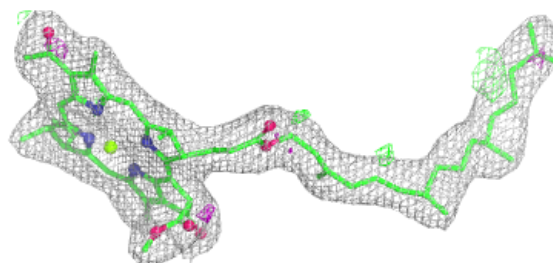
**Electron density around BCL L 302:**

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



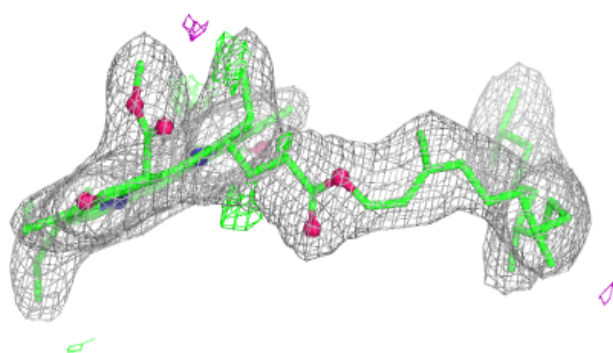
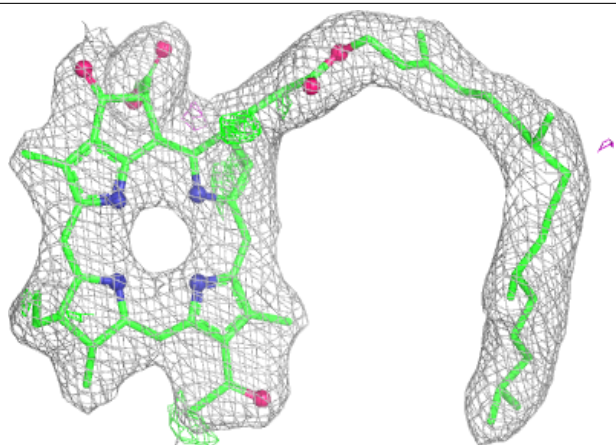
Electron density around BCL M 502:

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



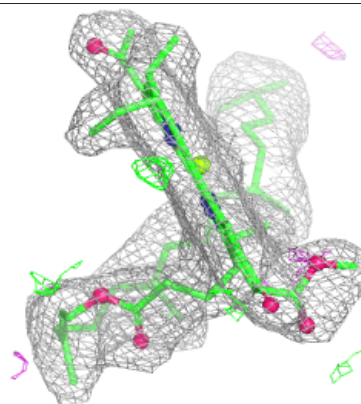
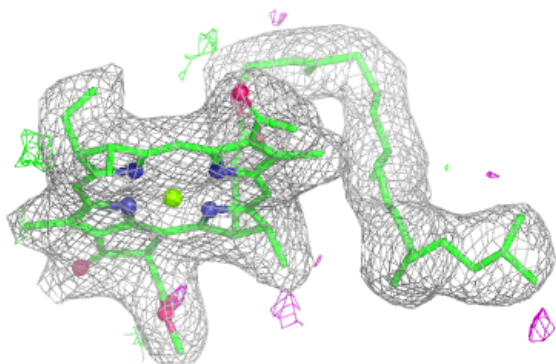
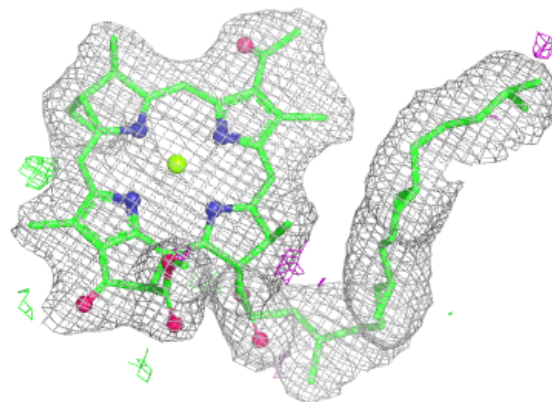
Electron density around BPH L 402:

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



Electron density around BCL L 304:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.