Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 10:27 am BST

PDB ID	:	7Z8D / pdb_00007z8d
Title	:	Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV by fixed-target serial synchrotron crystallography (room temperature, 26keV)
Authors	:	Gabdulkhakov, A.G.; Selikhanov, G.K.; Guenther, S.; Petrova, T.; Meents, A.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on	:	2022-03-17
Resolution	:	2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

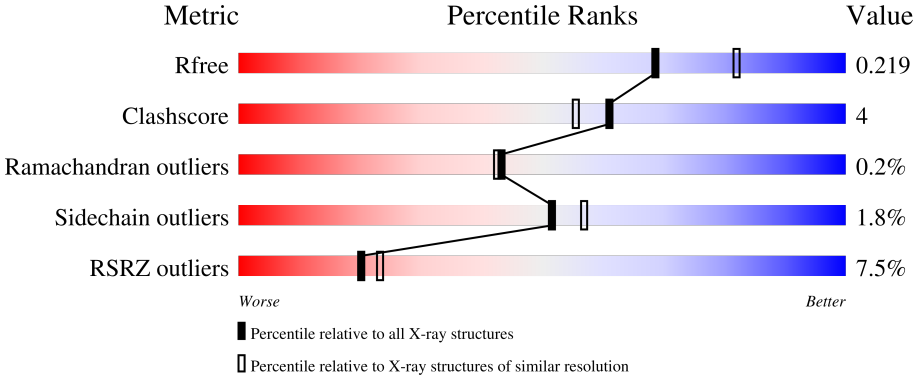
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	242	7% 88% 12%
2	L	281	10% 91% 9% •
3	M	302	5% 89% 11%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7660 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	242	1875	1198	322	345	10	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2430	1645	387	390	8	0	22	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP P0C0Y8

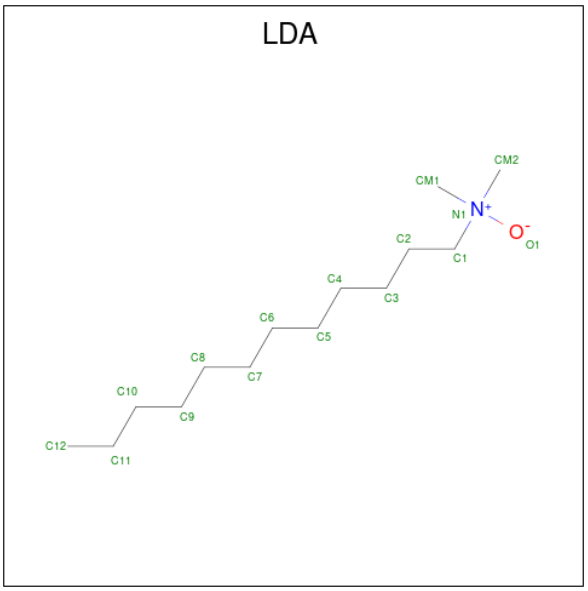
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2464	1643	405	405	11	0	7	0

There is a discrepancy between the modelled and reference sequences:

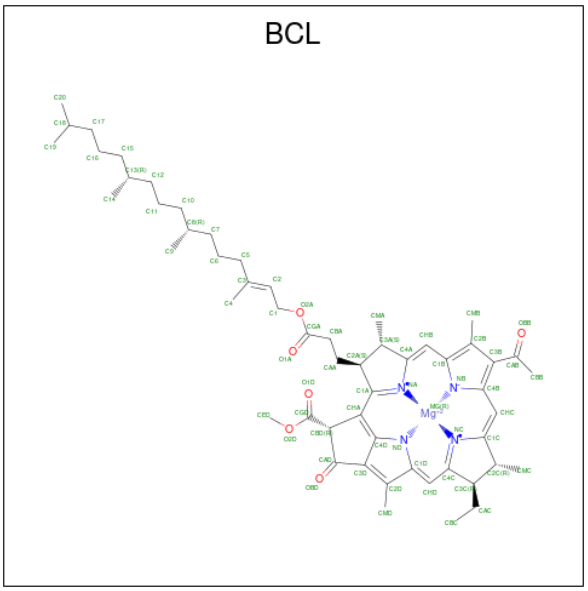
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



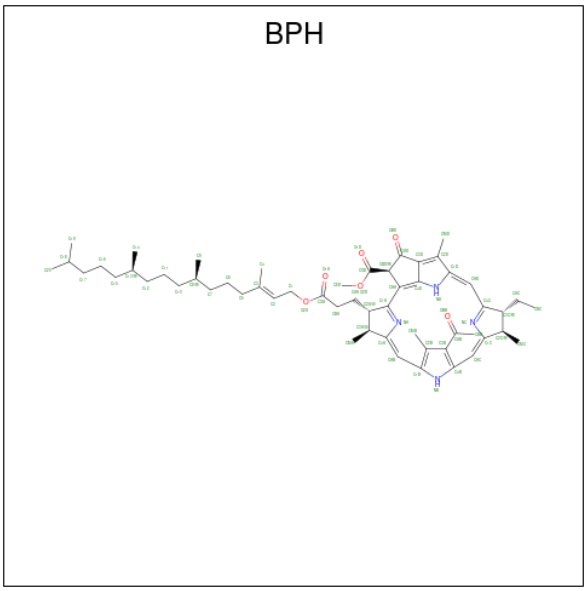
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



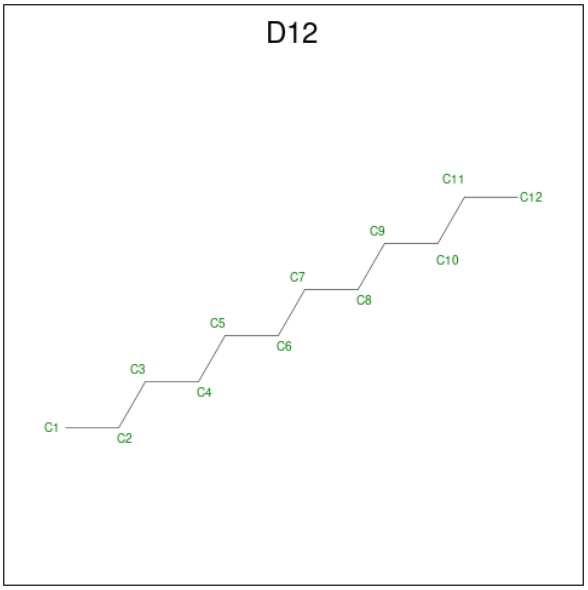
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



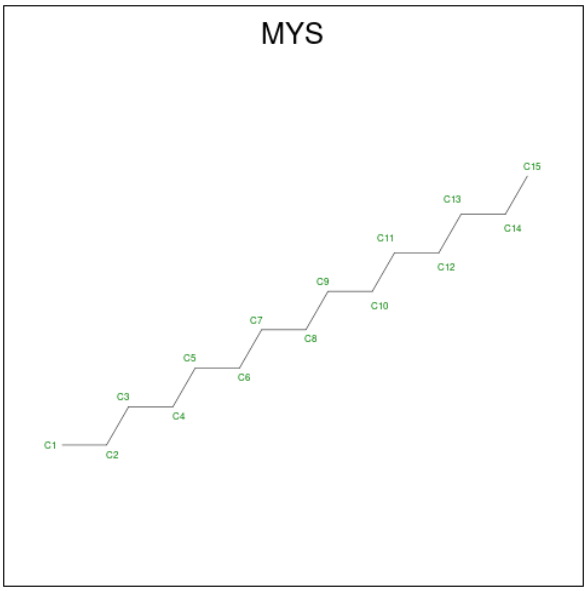
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	65	55	4	6	0	0
6	M	1	65	55	4	6	0	0

- Molecule 7 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



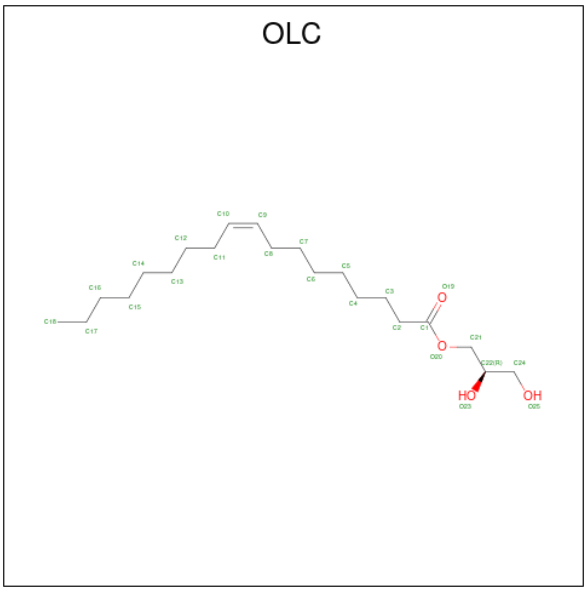
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
7	L	1	12	12	0	0
7	M	1	12	12	0	0

- Molecule 8 is PENTADECANE (CCD ID: MYS) (formula: $C_{15}H_{32}$).



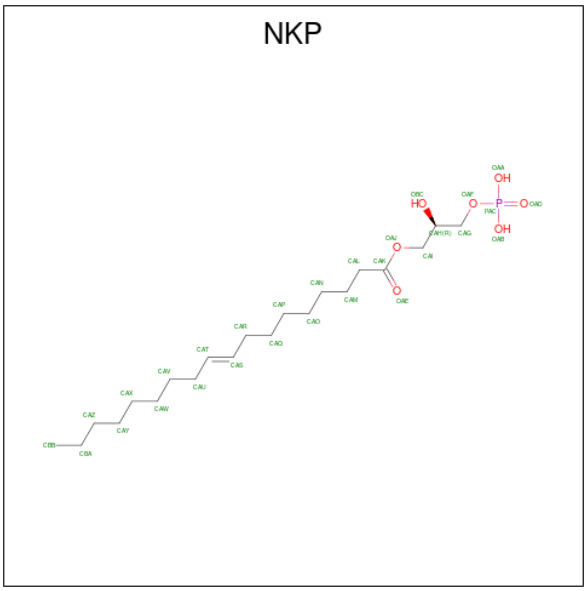
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C 15 15	0	0

- Molecule 9 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



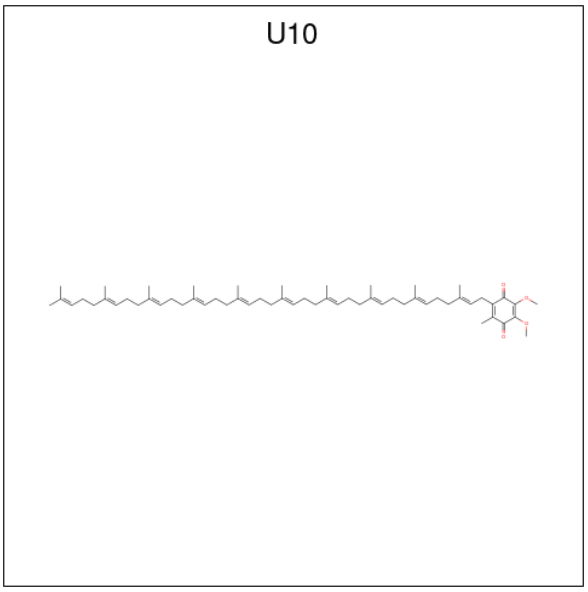
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C O 25 21 4	0	0

- Molecule 10 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: $C_{21}H_{41}O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
10	M	1	29	21	7	1	0	0
			Total	C	O	P		
10	M	1	29	21	7	1	0	0

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

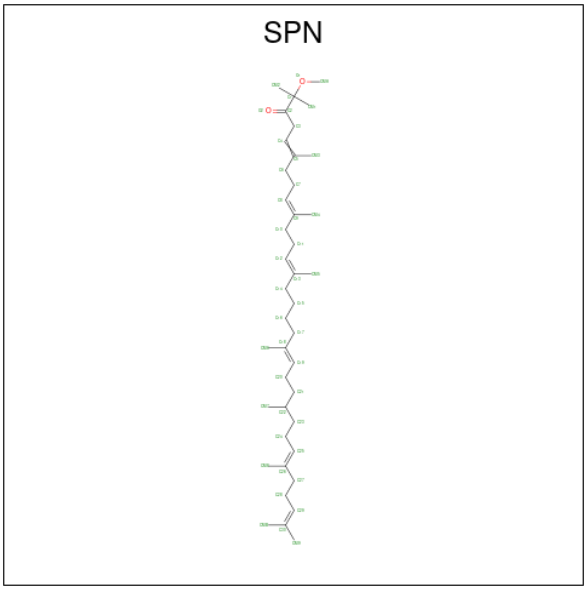


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
11	M	1	63	59	4		0	0

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

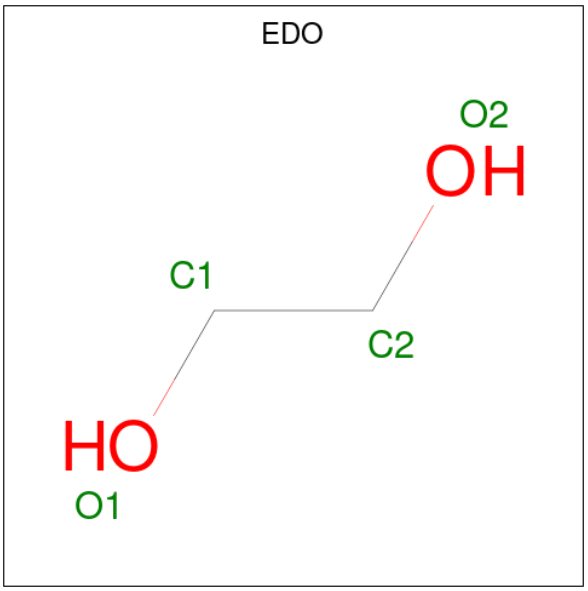
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
12	M	1	1	1	0	0

- Molecule 13 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



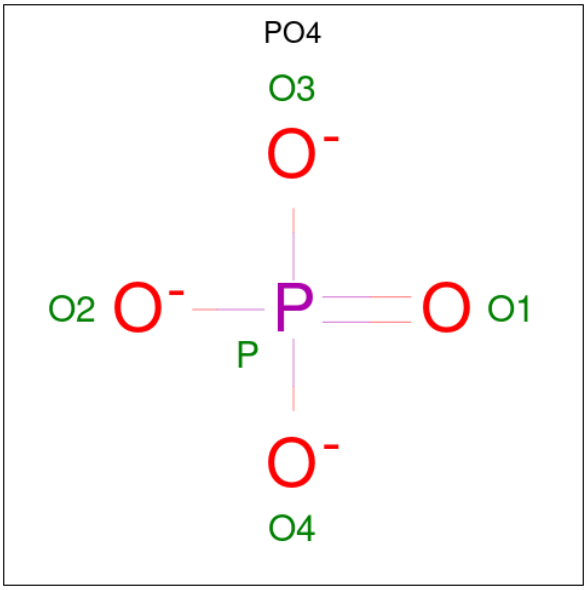
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	M	1	43	41	2	0	0

- Molecule 14 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	M	1	4	2	2	0	0

- Molecule 15 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
15	M	1	5	4	1	0	0

- Molecule 16 is water.

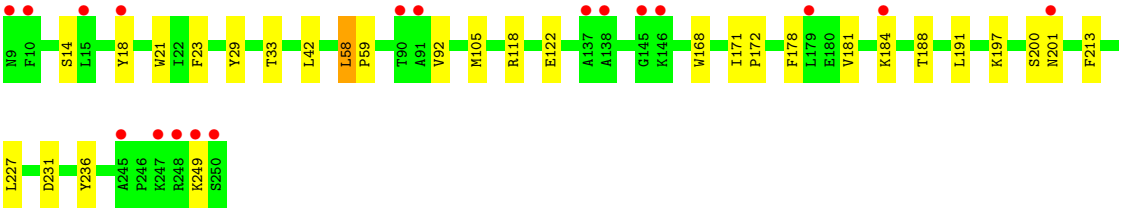
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	H	72	72	72	0	0
			Total	O		
16	L	53	53	53	0	0
			Total	O		
16	M	54	54	54	0	0

3 Residue-property plots (i)

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

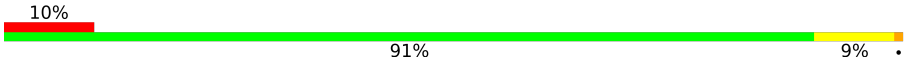
• Molecule 1: Reaction center protein H chain

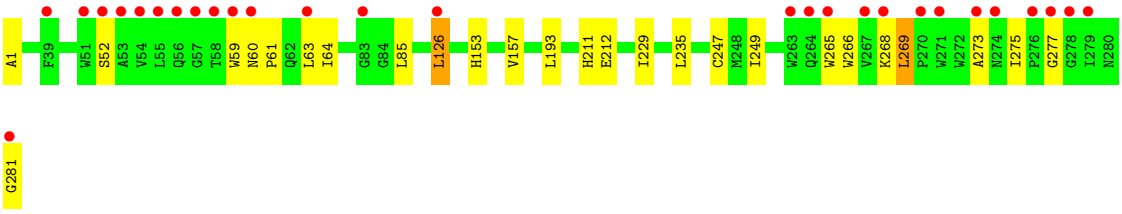
Chain H:



• Molecule 2: Reaction center protein L chain

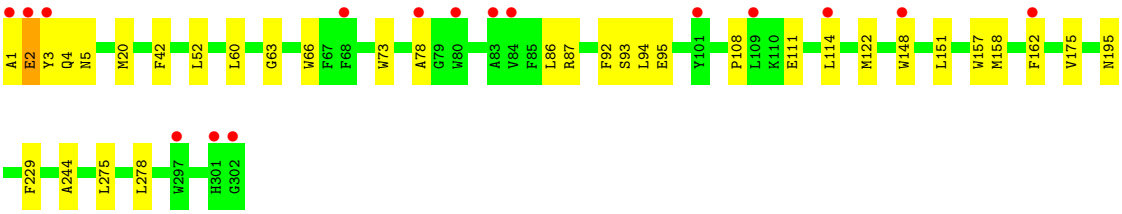
Chain L:





• Molecule 3: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.50Å 102.50Å 237.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.14 47.05 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.05-2.14) 88.0 (47.05-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.56 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.179 , 0.213 0.182 , 0.219	Depositor DCC
R_{free} test set	3550 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 75.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, U10, BCL, OLC, EDO, NKP, SPN, PO4, LDA, D12, MYS, BPH

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	H	0.34	0/1927	0.50	0/2620
2	L	0.29	0/2531	0.42	0/3468
3	M	0.32	0/2556	0.48	0/3488
All	All	0.31	0/7014	0.46	0/9576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1875	0	1876	17	0
2	L	2430	0	2366	17	0
3	M	2464	0	2381	24	0
4	H	16	0	31	1	0
4	M	64	0	124	3	0
5	L	132	0	148	0	0
5	M	132	0	148	4	0
6	L	65	0	76	1	0
6	M	65	0	76	3	0
7	L	12	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	12	0	26	0	0
8	L	15	0	32	0	0
9	L	25	0	40	1	0
10	M	58	0	78	3	0
11	M	63	0	90	2	0
12	M	1	0	0	0	0
13	M	43	0	70	8	0
14	M	4	0	6	0	0
15	M	5	0	0	0	0
16	H	72	0	0	0	0
16	L	53	0	0	0	0
16	M	54	0	0	0	0
All	All	7660	0	7594	63	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 4.

All (63) 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:M:108:PRO:HG2	3:M:111:GLU:HB2	1.65	0.79
1:H:197:LYS:HZ1	3:M:1:ALA:C	2.02	0.68
3:M:2:GLU:O	3:M:4:GLN:NE2	2.24	0.66
3:M:60:LEU:HD23	6:M:407:BPH:H4C1	1.84	0.59
1:H:197:LYS:NZ	3:M:1:ALA:C	2.61	0.58
2:L:229:ILE:HB	9:L:306:OLC:H21	1.87	0.57
5:M:405:BCL:H13	13:M:409:SPN:H101	1.87	0.57
2:L:61:PRO:HA	2:L:64:ILE:HD12	1.87	0.57
3:M:63:GLY:HA3	6:M:407:BPH:H5C1	1.90	0.53
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.90	0.53
6:M:407:BPH:HHD	6:M:407:BPH:HBC3	1.91	0.53
2:L:59:TRP:H	2:L:59:TRP:CD1	2.28	0.51
4:H:301:LDA:H121	4:M:410:LDA:H82	1.92	0.50
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.44	0.50
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.76	0.49
1:H:21:TRP:HZ2	4:M:410:LDA:HM13	1.78	0.48
3:M:151[A]:LEU:HD11	10:M:402:NKP:HAYA	1.96	0.48
3:M:157:TRP:CE2	13:M:409:SPN:HM73	2.48	0.48
2:L:275[A]:ILE:O	2:L:281[A]:GLY:HA3	2.15	0.47
2:L:60:ASN:HB3	2:L:63:LEU:HD12	1.97	0.47
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.97	0.47
2:L:268[A]:LYS:HD2	2:L:273[A]:ALA:HB1	1.97	0.46
1:H:29:TYR:O	1:H:33:THR:HG23	2.16	0.46
3:M:157:TRP:CZ2	13:M:409:SPN:HM73	2.51	0.46
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.99	0.45
2:L:153:HIS:O	2:L:157:VAL:HG23	2.16	0.45
1:H:201:ASN:OD1	1:H:201:ASN:N	2.50	0.44
1:H:58:LEU:HD22	1:H:59:PRO:HD2	2.00	0.44
1:H:42:LEU:HB3	2:L:1:ALA:HB1	1.99	0.44
5:M:405:BCL:CAB	13:M:409:SPN:H162	2.48	0.44
3:M:94:LEU:HD11	3:M:114[A]:LEU:HB3	2.00	0.43
5:M:405:BCL:H202	13:M:409:SPN:H61	1.99	0.43
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.53	0.43
3:M:175:VAL:HB	13:M:409:SPN:HM62	1.99	0.43
4:M:403:LDA:H72	4:M:403:LDA:H102	1.70	0.43
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.99	0.43
1:H:23:PHE:HA	10:M:401:NKP:HAV	2.00	0.43
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.01	0.43
1:H:105[A]:MET:HE3	1:H:236:TYR:CE1	2.54	0.43
2:L:126[A]:LEU:HD12	2:L:126[A]:LEU:HA	1.90	0.42
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.54	0.42
3:M:148:TRP:HE3	10:M:402:NKP:HAQA	1.84	0.42
2:L:85:LEU:HD23	2:L:85:LEU:HA	1.91	0.41
2:L:193:LEU:HD21	2:L:212:GLU:HB3	2.01	0.41
3:M:93:SER:OG	3:M:95:GLU:OE2	2.35	0.41
3:M:162:PHE:HB2	13:M:409:SPN:H242	2.02	0.41
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.55	0.41
6:L:303:BPH:HHC	6:L:303:BPH:OBB	2.20	0.41
5:M:406:BCL:OBB	5:M:406:BCL:HHC	2.20	0.41
11:M:404:U10:H28	11:M:404:U10:H322	1.78	0.41
1:H:181:VAL:O	1:H:188:THR:HA	2.21	0.41
3:M:73:TRP:HB2	3:M:114[A]:LEU:HD23	2.03	0.41
3:M:158:MET:HE3	3:M:158:MET:HB3	1.97	0.41
11:M:404:U10:H412	11:M:404:U10:H371	1.85	0.41
13:M:409:SPN:H111	13:M:409:SPN:HM41	1.80	0.40
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.02	0.40
1:H:171:ILE:HB	1:H:172:PRO:HD3	2.02	0.40
2:L:235:LEU:HD22	3:M:42:PHE:CE1	2.57	0.40
2:L:249:ILE:HD12	2:L:249:ILE:HA	1.99	0.40
1:H:14:SER:O	1:H:18:TYR:HD1	2.04	0.40
1:H:249:LYS:HA	1:H:249:LYS:HD3	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:266[B]:TRP:HA	2:L:269[B]:LEU:HD23	2.02	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	H	244/242 (101%)	242 (99%)	2 (1%)	0	100	100
2	L	300/281 (107%)	286 (95%)	14 (5%)	0	100	100
3	M	307/302 (102%)	296 (96%)	9 (3%)	2 (1%)	18	13
All	All	851/825 (103%)	824 (97%)	25 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	2	GLU
3	M	195	ASN

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	H	200/197 (102%)	193 (96%)	7 (4%)	32	31
2	L	238/220 (108%)	231 (97%)	7 (3%)	37	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	242/236 (102%)	239 (99%)	3 (1%)	63	69
All	All	680/653 (104%)	663 (98%)	17 (2%)	51	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	58	LEU
1	H	92	VAL
1	H	118[A]	ARG
1	H	118[B]	ARG
1	H	184	LYS
1	H	200	SER
1	H	231	ASP
2	L	126[A]	LEU
2	L	126[B]	LEU
2	L	247	CYS
2	L	265[A]	TRP
2	L	265[B]	TRP
2	L	269[A]	LEU
2	L	269[B]	LEU
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	86	LEU

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

Mol	Chain	Res	Type
2	L	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	NKP	M	402	-	28,28,28	0.35	0	31,32,32	0.43	0
7	D12	L	304	-	11,11,11	0.30	0	10,10,10	0.45	0
4	LDA	H	301	-	12,15,15	1.93	1 (8%)	14,17,17	0.65	0
15	PO4	M	415	-	4,4,4	0.88	0	6,6,6	0.37	0
8	MYS	L	305	-	14,14,14	0.29	0	13,13,13	0.50	0
5	BCL	M	405	3	69,74,74	1.16	5 (7%)	83,115,115	1.56	15 (18%)
4	LDA	M	411	-	12,15,15	2.06	1 (8%)	14,17,17	0.50	0
5	BCL	L	301	2	69,74,74	1.35	5 (7%)	83,115,115	1.43	13 (15%)
6	BPH	M	407	-	59,70,70	1.19	4 (6%)	61,101,101	2.23	11 (18%)
4	LDA	M	403	-	12,15,15	2.06	1 (8%)	14,17,17	0.69	0
4	LDA	M	410	-	12,15,15	2.02	1 (8%)	14,17,17	0.41	0
11	U10	M	404	-	63,63,63	2.64	17 (26%)	76,79,79	1.78	19 (25%)
10	NKP	M	401	-	28,28,28	0.37	0	31,32,32	0.52	0
13	SPN	M	409	-	40,42,42	0.54	0	50,52,52	1.60	10 (20%)
5	BCL	L	302	2	69,74,74	1.16	5 (7%)	83,115,115	1.40	8 (9%)
4	LDA	M	412	-	12,15,15	2.05	1 (8%)	14,17,17	0.61	0
5	BCL	M	406	3	69,74,74	1.30	6 (8%)	83,115,115	1.50	11 (13%)
7	D12	M	413	-	11,11,11	0.26	0	10,10,10	0.66	0
9	OLC	L	306	-	24,24,24	0.93	1 (4%)	25,25,25	0.87	0
14	EDO	M	414	-	3,3,3	0.41	0	2,2,2	0.80	0
6	BPH	L	303	-	59,70,70	1.11	6 (10%)	61,101,101	2.10	8 (13%)

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	NKP	M	402	-	-	8/28/28/28	-
7	D12	L	304	-	-	4/9/9/9	-
4	LDA	H	301	-	-	4/13/13/13	-
8	MYS	L	305	-	-	6/12/12/12	-
5	BCL	M	405	3	-	0/41/137/137	-
4	LDA	M	411	-	-	8/13/13/13	-
5	BCL	L	301	2	-	5/41/137/137	-
6	BPH	M	407	-	-	8/37/105/105	0/5/6/6
4	LDA	M	403	-	-	11/13/13/13	-
4	LDA	M	410	-	-	5/13/13/13	-
11	U10	M	404	-	-	16/63/87/87	0/1/1/1
10	NKP	M	401	-	-	9/28/28/28	-
13	SPN	M	409	-	-	18/50/51/51	-
5	BCL	L	302	2	-	2/41/137/137	-
4	LDA	M	412	-	-	7/13/13/13	-
5	BCL	M	406	3	-	0/41/137/137	-
7	D12	M	413	-	-	2/9/9/9	-
9	OLC	L	306	-	-	8/24/24/24	-
14	EDO	M	414	-	-	1/1/1/1	-
6	BPH	L	303	-	-	4/37/105/105	0/5/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	403	LDA	O1-N1	-7.06	1.25	1.42
4	M	411	LDA	O1-N1	-7.04	1.25	1.42
4	M	412	LDA	O1-N1	-7.03	1.25	1.42
4	M	410	LDA	O1-N1	-6.88	1.26	1.42
4	H	301	LDA	O1-N1	-6.63	1.26	1.42
11	M	404	U10	C33-C34	6.23	1.47	1.33
11	M	404	U10	C43-C44	6.07	1.47	1.33
11	M	404	U10	C48-C49	6.05	1.47	1.33
11	M	404	U10	C8-C9	6.04	1.47	1.33
11	M	404	U10	C28-C29	5.97	1.47	1.33
11	M	404	U10	C38-C39	5.92	1.47	1.33
5	L	301	BCL	MG-NA	5.87	2.20	2.06
11	M	404	U10	C18-C19	5.80	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	404	U10	C13-C14	5.66	1.46	1.33
11	M	404	U10	C23-C24	5.57	1.46	1.33
11	M	404	U10	C53-C54	5.46	1.48	1.32
5	M	406	BCL	MG-NA	5.40	2.19	2.06
11	M	404	U10	O3-C3	-4.72	1.25	1.36
5	L	302	BCL	MG-NA	4.71	2.17	2.06
11	M	404	U10	O4-C4	-4.66	1.25	1.36
5	M	405	BCL	MG-NA	4.44	2.16	2.06
9	L	306	OLC	O20-C1	4.21	1.45	1.33
5	L	301	BCL	MG-NC	3.96	2.15	2.06
6	M	407	BPH	CBD-CGD	-3.92	1.47	1.52
5	M	406	BCL	MG-NC	3.62	2.14	2.06
5	L	301	BCL	C1D-ND	3.19	1.41	1.37
5	M	406	BCL	C3B-C4B	3.18	1.47	1.41
5	M	405	BCL	MG-NC	3.18	2.13	2.06
5	L	301	BCL	C3B-C4B	3.17	1.47	1.41
6	M	407	BPH	CHA-CBD	3.16	1.55	1.51
11	M	404	U10	C3-C2	-3.13	1.39	1.48
11	M	404	U10	C4-C5	-3.08	1.40	1.48
6	L	303	BPH	C3D-CAD	-3.02	1.41	1.47
5	M	405	BCL	C3B-C4B	2.98	1.46	1.41
5	M	406	BCL	C1D-ND	2.92	1.41	1.37
6	M	407	BPH	OBD-CAD	2.90	1.26	1.22
5	L	302	BCL	MG-NC	2.90	2.13	2.06
11	M	404	U10	C6-C1	2.80	1.40	1.35
5	L	302	BCL	CHD-C1D	2.75	1.43	1.38
6	M	407	BPH	C3D-CAD	-2.72	1.41	1.47
5	M	406	BCL	CHD-C1D	2.60	1.43	1.38
6	L	303	BPH	CBD-CGD	-2.56	1.49	1.52
5	L	302	BCL	C1D-ND	2.56	1.40	1.37
6	L	303	BPH	CHA-CBD	2.48	1.54	1.51
5	L	302	BCL	C3B-C4B	2.44	1.45	1.41
6	L	303	BPH	C1D-C2D	2.41	1.42	1.39
5	L	301	BCL	CHD-C1D	2.39	1.43	1.38
11	M	404	U10	C6-C5	-2.30	1.40	1.46
5	M	405	BCL	CHD-C1D	2.23	1.42	1.38
6	L	303	BPH	O1A-CGA	-2.12	1.16	1.22
6	L	303	BPH	C3B-C4B	2.07	1.45	1.41
11	M	404	U10	C1-C2	-2.06	1.39	1.47
5	M	406	BCL	CBD-CGD	-2.05	1.46	1.52
5	M	405	BCL	CHC-C1C	2.01	1.42	1.37

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	407	BPH	C4D-CHA-CBD	-12.82	102.72	108.52
6	L	303	BPH	C4D-CHA-CBD	-12.42	102.90	108.52
5	L	302	BCL	CHD-C1D-ND	-5.66	119.25	124.45
5	M	406	BCL	C4D-CHA-C1A	5.48	127.92	121.25
5	L	302	BCL	C4D-CHA-C1A	5.39	127.81	121.25
5	M	405	BCL	CHD-C1D-ND	-5.39	119.50	124.45
6	L	303	BPH	C4D-ND-C1D	-4.99	103.75	108.83
5	L	301	BCL	CHD-C1D-ND	-4.84	120.01	124.45
6	M	407	BPH	C4D-ND-C1D	-4.83	103.92	108.83
5	M	405	BCL	C4D-CHA-C1A	4.74	127.01	121.25
5	M	406	BCL	CHD-C1D-ND	-4.72	120.12	124.45
5	L	301	BCL	C4D-CHA-C1A	4.68	126.94	121.25
5	M	406	BCL	C4A-NA-C1A	4.27	108.62	106.71
11	M	404	U10	C22-C23-C24	-4.09	117.81	127.66
13	M	409	SPN	CM5-C13-C14	4.08	122.14	115.27
5	M	405	BCL	C1-C2-C3	-4.08	118.98	126.04
5	L	302	BCL	C1D-ND-C4D	-4.05	103.45	106.33
6	M	407	BPH	C17-C16-C15	4.02	131.72	113.24
11	M	404	U10	C12-C13-C14	-3.81	118.47	127.66
5	M	405	BCL	C1D-ND-C4D	-3.81	103.63	106.33
11	M	404	U10	C32-C33-C34	-3.59	119.02	127.66
13	M	409	SPN	CM6-C18-C17	3.57	121.28	115.27
6	M	407	BPH	O2D-CGD-CBD	3.57	115.52	111.00
5	L	301	BCL	C1D-ND-C4D	-3.49	103.86	106.33
11	M	404	U10	C37-C38-C39	-3.46	119.34	127.66
11	M	404	U10	C47-C48-C49	-3.35	119.59	127.66
11	M	404	U10	C50-C49-C51	3.33	120.88	115.27
5	M	406	BCL	CHA-C1A-NA	-3.29	118.86	126.40
11	M	404	U10	C45-C44-C46	3.28	120.79	115.27
11	M	404	U10	C42-C43-C44	-3.23	119.88	127.66
11	M	404	U10	C30-C29-C31	3.21	120.67	115.27
5	M	406	BCL	C1D-ND-C4D	-3.16	104.09	106.33
6	L	303	BPH	OBD-CAD-CBD	-3.15	121.20	125.82
5	M	405	BCL	CHA-C1A-NA	-3.14	119.20	126.40
5	L	302	BCL	CHA-C1A-NA	-3.06	119.39	126.40
11	M	404	U10	C40-C39-C41	3.06	120.42	115.27
6	L	303	BPH	C3D-C4D-ND	3.05	111.88	107.72
5	M	406	BCL	C2A-C1A-CHA	3.02	129.14	123.86
6	M	407	BPH	C3D-C4D-ND	2.99	111.80	107.72
13	M	409	SPN	CM4-C9-C10	2.99	120.30	115.27
6	L	303	BPH	CMB-C2B-C3B	2.94	130.18	124.68
11	M	404	U10	C17-C18-C19	-2.94	120.58	127.66
13	M	409	SPN	CM3-C5-C6	2.94	120.21	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	404	U10	C25-C24-C26	2.91	120.17	115.27
5	M	406	BCL	CAB-C3B-C2B	2.90	132.68	128.34
13	M	409	SPN	C20-C19-C18	-2.88	120.72	127.66
13	M	409	SPN	C7-C8-C9	-2.86	120.78	127.66
11	M	404	U10	C27-C28-C29	-2.85	120.80	127.66
11	M	404	U10	C20-C19-C21	2.83	120.02	115.27
5	L	301	BCL	C2A-C1A-CHA	2.82	128.79	123.86
5	L	301	BCL	CHA-C1A-NA	-2.79	120.02	126.40
6	M	407	BPH	OBD-CAD-CBD	-2.74	121.81	125.82
13	M	409	SPN	CM8-C26-C27	2.71	119.83	115.27
11	M	404	U10	C15-C14-C16	2.69	119.80	115.27
6	M	407	BPH	CMB-C2B-C3B	2.67	129.67	124.68
6	L	303	BPH	C2D-C1D-ND	2.64	111.35	109.53
5	M	406	BCL	CHC-C4B-NB	-2.63	121.48	124.26
5	L	301	BCL	C1-C2-C3	-2.61	121.53	126.04
6	M	407	BPH	CAC-C3C-C2C	-2.57	107.84	114.26
5	M	405	BCL	C6-C7-C8	2.55	124.18	115.92
5	L	301	BCL	O2D-CGD-O1D	-2.53	118.88	123.84
5	L	301	BCL	C4A-NA-C1A	2.53	107.84	106.71
5	M	405	BCL	C1-O2A-CGA	2.49	122.98	116.44
11	M	404	U10	C35-C34-C36	2.47	119.42	115.27
5	M	405	BCL	CMB-C2B-C1B	-2.46	121.63	125.37
5	M	405	BCL	C2A-C1A-CHA	2.45	128.14	123.86
11	M	404	U10	C10-C9-C11	2.43	119.36	115.27
5	M	405	BCL	C11-C10-C8	-2.42	108.11	115.92
13	M	409	SPN	C23-C24-C25	-2.41	105.88	112.23
13	M	409	SPN	CMB-C30-CM9	2.38	119.87	114.60
6	L	303	BPH	O2D-CGD-CBD	2.33	113.95	111.00
6	M	407	BPH	C1-C2-C3	-2.33	122.02	126.04
6	M	407	BPH	C11-C10-C8	2.31	123.38	115.92
5	L	302	BCL	C2A-C1A-CHA	2.29	127.87	123.86
5	M	405	BCL	C4A-NA-C1A	2.26	107.72	106.71
11	M	404	U10	C4M-O4-C4	2.25	124.46	116.47
5	M	405	BCL	C2D-C1D-ND	2.24	111.75	110.10
6	L	303	BPH	CMD-C2D-C3D	2.24	128.86	124.68
6	M	407	BPH	C2D-C1D-ND	2.21	111.05	109.53
5	M	405	BCL	OBB-CAB-CBB	-2.20	114.86	119.73
5	M	406	BCL	CED-O2D-CGD	2.19	120.90	115.94
5	L	301	BCL	CHC-C4B-NB	-2.18	121.95	124.26
13	M	409	SPN	C3-C4-C5	-2.14	123.23	126.79
5	M	405	BCL	CHC-C4B-NB	-2.14	122.00	124.26
11	M	404	U10	C56-C54-C55	2.13	119.31	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	302	BCL	CHC-C4B-NB	-2.13	122.00	124.26
5	M	406	BCL	CMB-C2B-C1B	-2.11	122.16	125.37
5	M	405	BCL	C4B-C3B-C2B	-2.08	105.01	108.36
5	L	302	BCL	C2D-C1D-ND	2.08	111.63	110.10
5	L	301	BCL	OBB-CAB-CBB	-2.06	115.17	119.73
5	M	406	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
5	L	301	BCL	O2D-CGD-CBD	2.05	114.91	111.27
5	L	301	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
5	L	302	BCL	CAB-C3B-C2B	2.01	131.35	128.34
5	L	301	BCL	C2D-C1D-ND	2.01	111.58	110.10

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	403	LDA	C2-C1-N1-O1
4	M	403	LDA	C2-C1-N1-CM2
4	M	410	LDA	C2-C1-N1-CM2
4	M	411	LDA	C2-C1-N1-O1
4	M	411	LDA	C2-C1-N1-CM1
4	M	411	LDA	C2-C1-N1-CM2
4	M	412	LDA	C2-C1-N1-O1
4	M	412	LDA	C2-C1-N1-CM1
4	M	412	LDA	C2-C1-N1-CM2
9	L	306	OLC	O20-C21-C22-O23
10	M	402	NKP	CAH-CAG-OAF-PAC
11	M	404	U10	C32-C33-C34-C35
11	M	404	U10	C32-C33-C34-C36
11	M	404	U10	C42-C43-C44-C45
11	M	404	U10	C42-C43-C44-C46
13	M	409	SPN	CM1-C1-O1-CMA
13	M	409	SPN	C2-C1-O1-CMA
10	M	401	NKP	OAE-CAK-OAJ-CAI
11	M	404	U10	C52-C53-C54-C55
11	M	404	U10	C52-C53-C54-C56
10	M	401	NKP	CAL-CAK-OAJ-CAI
13	M	409	SPN	CM5-C13-C14-C15
4	M	403	LDA	C7-C8-C9-C10
13	M	409	SPN	C11-C10-C9-CM4
13	M	409	SPN	C16-C17-C18-CM6
13	M	409	SPN	C11-C10-C9-C8
13	M	409	SPN	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	M	409	SPN	C16-C17-C18-C19
11	M	404	U10	C29-C31-C32-C33
13	M	409	SPN	C26-C27-C28-C29
10	M	401	NKP	OBC-CAH-CAI-OAJ
6	M	407	BPH	C5-C6-C7-C8
6	M	407	BPH	C10-C11-C12-C13
10	M	402	NKP	CAW-CAX-CAY-CAZ
4	M	403	LDA	C1-C2-C3-C4
11	M	404	U10	C24-C26-C27-C28
13	M	409	SPN	C9-C10-C11-C12
9	L	306	OLC	C1-C2-C3-C4
11	M	404	U10	C37-C38-C39-C41
13	M	409	SPN	C14-C15-C16-C17
4	M	411	LDA	C4-C5-C6-C7
9	L	306	OLC	O20-C21-C22-C24
7	L	304	D12	C5-C6-C7-C8
7	M	413	D12	C2-C3-C4-C5
9	L	306	OLC	C11-C12-C13-C14
13	M	409	SPN	CM2-C1-O1-CMA
6	M	407	BPH	C4-C3-C5-C6
4	M	412	LDA	C7-C8-C9-C10
8	L	305	MYS	C9-C10-C11-C12
6	M	407	BPH	C2-C3-C5-C6
4	M	411	LDA	C1-C2-C3-C4
4	M	410	LDA	C1-C2-C3-C4
7	L	304	D12	C4-C5-C6-C7
9	L	306	OLC	C5-C6-C7-C8
6	L	303	BPH	C4-C3-C5-C6
13	M	409	SPN	CM3-C5-C6-C7
6	L	303	BPH	C2-C3-C5-C6
4	M	412	LDA	C1-C2-C3-C4
4	M	411	LDA	C11-C10-C9-C8
4	M	403	LDA	C9-C10-C11-C12
13	M	409	SPN	C4-C5-C6-C7
11	M	404	U10	C37-C38-C39-C40
10	M	401	NKP	CAW-CAX-CAY-CAZ
6	M	407	BPH	C8-C10-C11-C12
7	L	304	D12	C9-C10-C11-C12
4	H	301	LDA	C9-C10-C11-C12
11	M	404	U10	C14-C16-C17-C18
4	H	301	LDA	C1-C2-C3-C4
9	L	306	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
10	M	401	NKP	CAG-CAH-CAI-OAJ
8	L	305	MYS	C10-C11-C12-C13
10	M	402	NKP	OAJ-CAK-CAL-CAM
4	M	403	LDA	N1-C1-C2-C3
13	M	409	SPN	CM2-C1-C2-O2
13	M	409	SPN	CM2-C1-C2-C3
9	L	306	OLC	C4-C5-C6-C7
10	M	402	NKP	CAL-CAM-CAN-CAO
4	M	403	LDA	C11-C10-C9-C8
4	M	412	LDA	C5-C6-C7-C8
10	M	402	NKP	CAN-CAO-CAP-CAQ
4	M	411	LDA	C7-C8-C9-C10
6	L	303	BPH	CAD-CBD-CGD-O2D
4	M	403	LDA	C2-C1-N1-CM1
4	M	410	LDA	C2-C1-N1-CM1
4	M	411	LDA	C9-C10-C11-C12
13	M	409	SPN	O1-C1-C2-O2
7	L	304	D12	C7-C8-C9-C10
5	L	301	BCL	C12-C13-C15-C16
5	L	302	BCL	C14-C13-C15-C16
11	M	404	U10	C39-C41-C42-C43
5	L	302	BCL	C12-C13-C15-C16
5	L	301	BCL	C14-C13-C15-C16
4	H	301	LDA	C5-C6-C7-C8
10	M	401	NKP	CAH-CAG-OAF-PAC
10	M	401	NKP	CAV-CAW-CAX-CAY
4	M	410	LDA	C9-C10-C11-C12
14	M	414	EDO	O1-C1-C2-O2
6	M	407	BPH	O2A-C1-C2-C3
4	M	403	LDA	C2-C3-C4-C5
13	M	409	SPN	C21-C22-C23-C24
9	L	306	OLC	O20-C1-C2-C3
7	M	413	D12	C11-C10-C9-C8
8	L	305	MYS	C11-C10-C9-C8
8	L	305	MYS	C11-C12-C13-C14
6	M	407	BPH	C16-C17-C18-C19
11	M	404	U10	C25-C24-C26-C27
4	H	301	LDA	C7-C8-C9-C10
8	L	305	MYS	C7-C8-C9-C10
10	M	402	NKP	OAE-CAK-CAL-CAM
10	M	401	NKP	CAQ-CAR-CAS-CAT
11	M	404	U10	C50-C49-C51-C52

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Mol	Chain	Res	Type	Atoms
10	M	401	NKP	CAR-CAS-CAT-CAU
5	L	301	BCL	CAD-CBD-CGD-O2D
6	M	407	BPH	CAD-CBD-CGD-O2D
8	L	305	MYS	C3-C4-C5-C6
6	L	303	BPH	O2A-C1-C2-C3
4	M	403	LDA	C4-C5-C6-C7
11	M	404	U10	C3-C4-O4-C4M
11	M	404	U10	C5-C4-O4-C4M
4	M	403	LDA	C5-C6-C7-C8
10	M	402	NKP	CAS-CAT-CAU-CAV
4	M	410	LDA	C7-C8-C9-C10
5	L	301	BCL	C2A-CAA-CBA-CGA
10	M	402	NKP	OAF-CAG-CAH-OBC
5	L	301	BCL	C15-C16-C17-C18
4	M	412	LDA	C9-C10-C11-C12

There are no ring outliers.

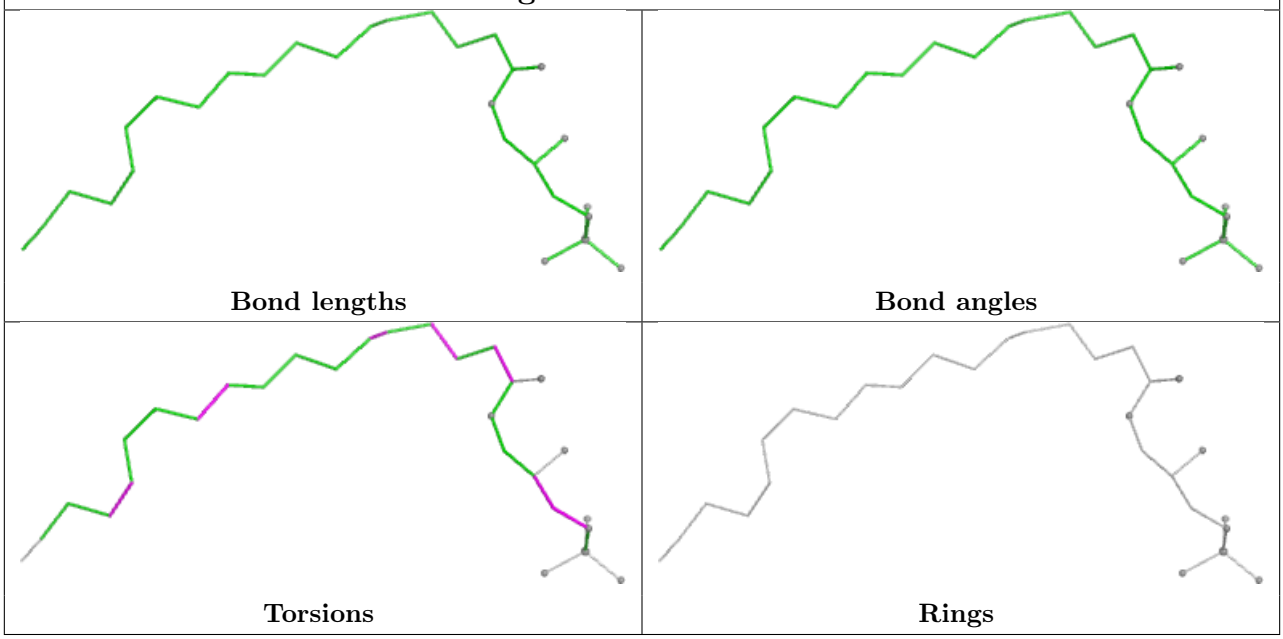
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	402	NKP	2	0
4	H	301	LDA	1	0
5	M	405	BCL	3	0
6	M	407	BPH	3	0
4	M	403	LDA	1	0
4	M	410	LDA	2	0
11	M	404	U10	2	0
10	M	401	NKP	1	0
13	M	409	SPN	8	0
5	M	406	BCL	1	0
9	L	306	OLC	1	0
6	L	303	BPH	1	0

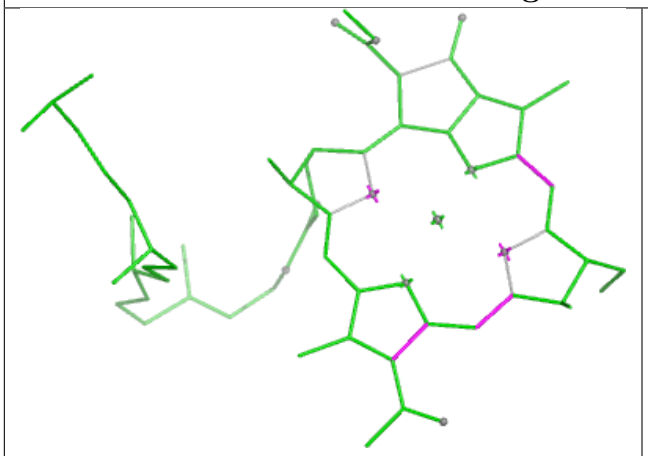
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

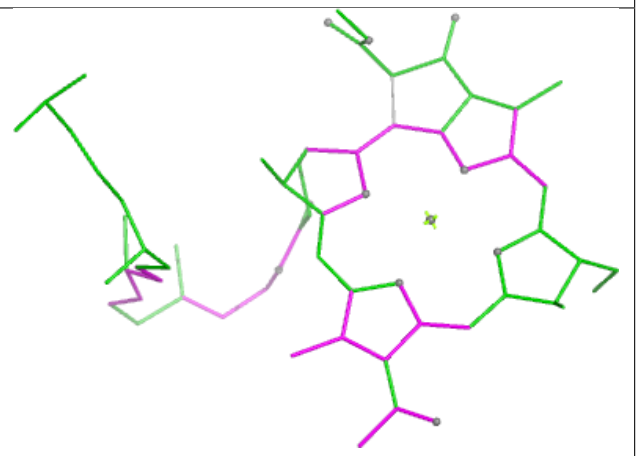
Ligand NKP M 402



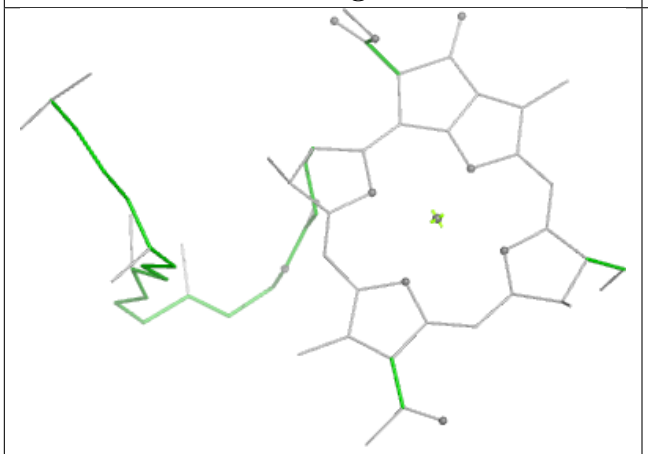
Ligand BCL M 405



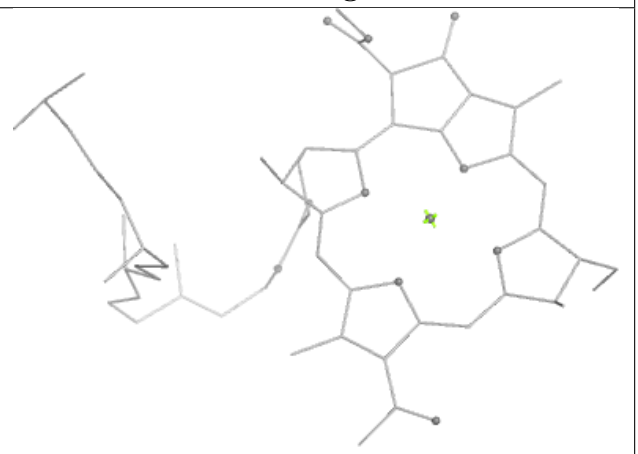
Bond lengths



Bond angles

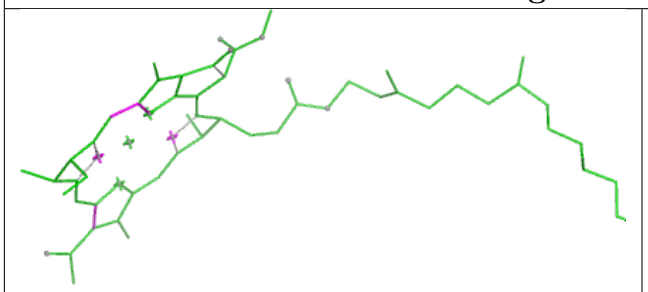


Torsions

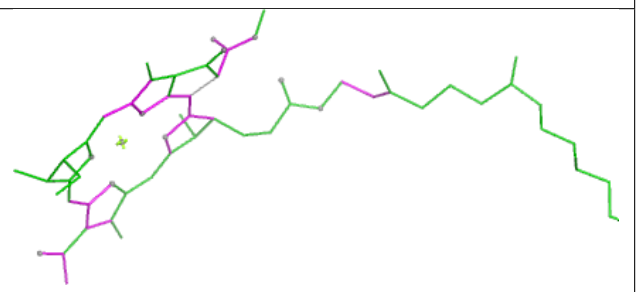


Rings

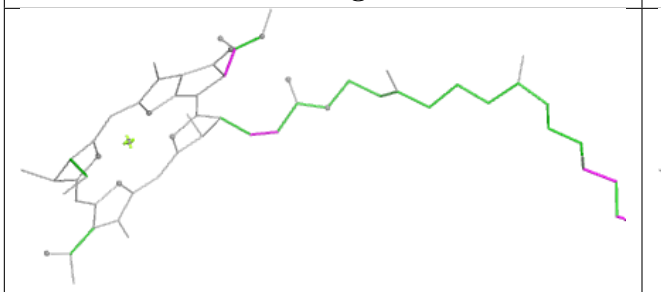
Ligand BCL L 301



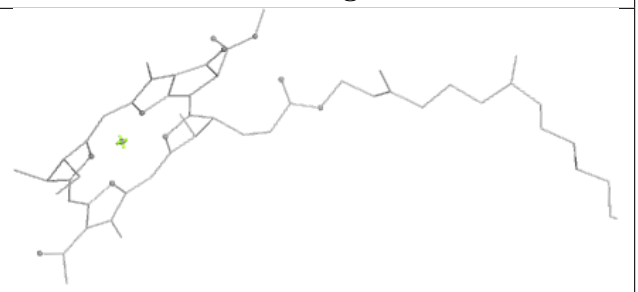
Bond lengths



Bond angles

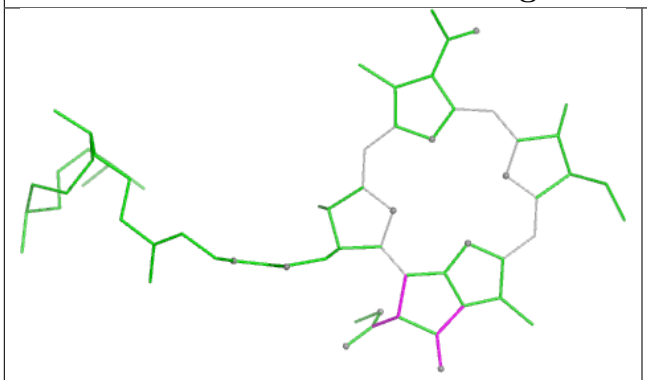


Torsions

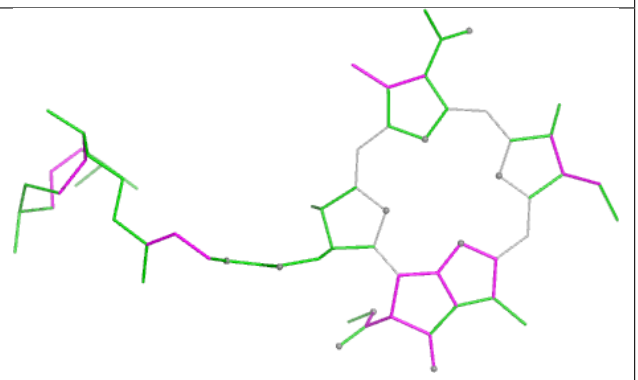


Rings

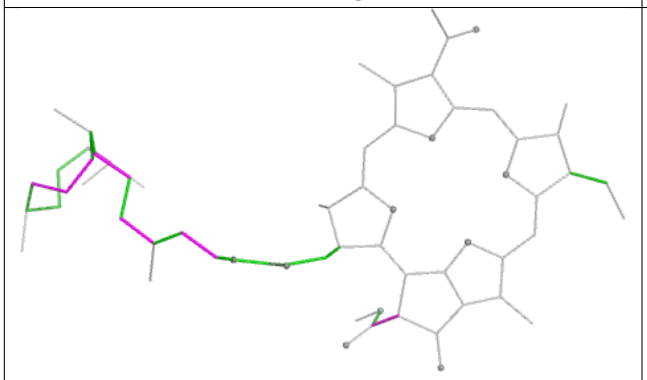
Ligand BPH M 407



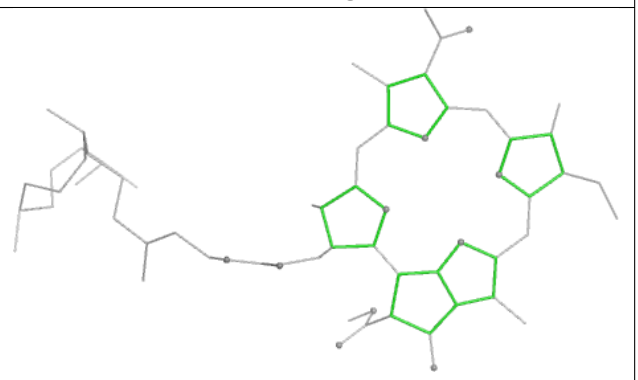
Bond lengths



Bond angles

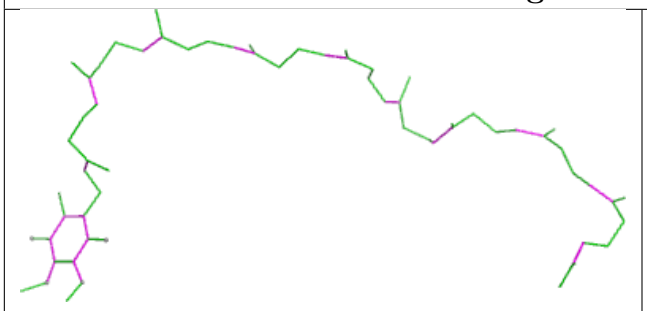


Torsions

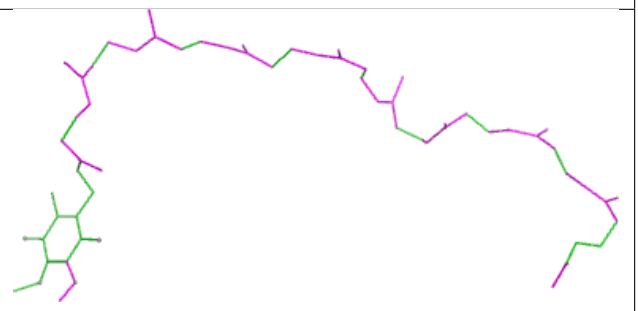


Rings

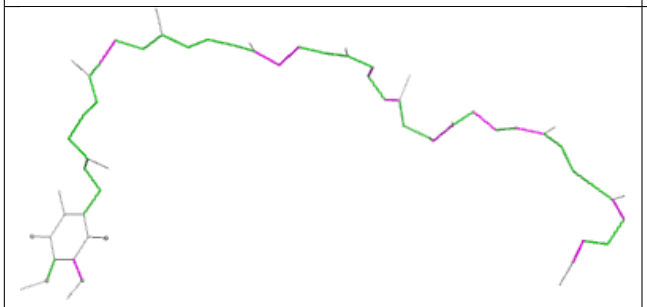
Ligand U10 M 404



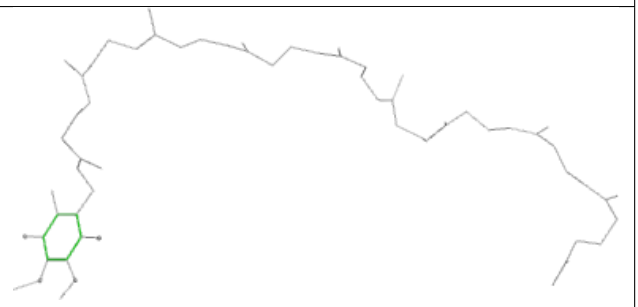
Bond lengths



Bond angles

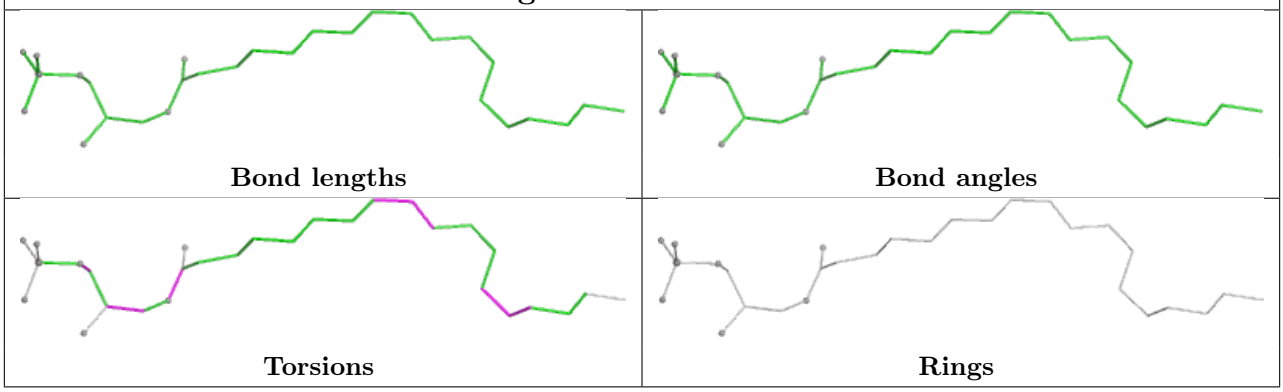


Torsions

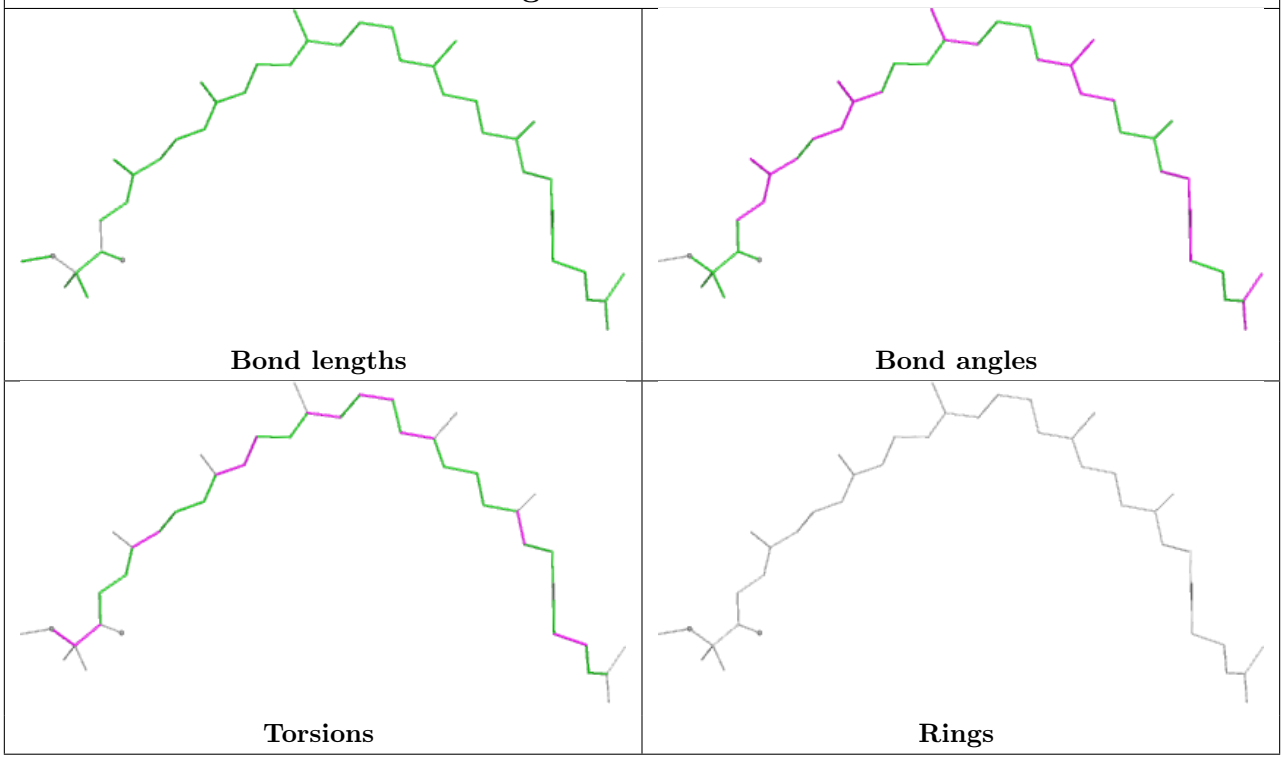


Rings

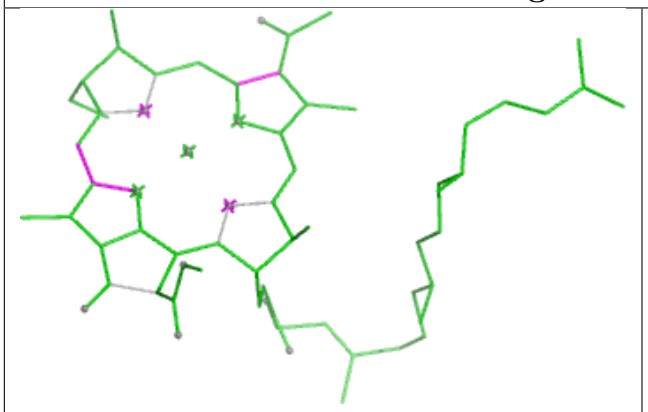
Ligand NKP M 401



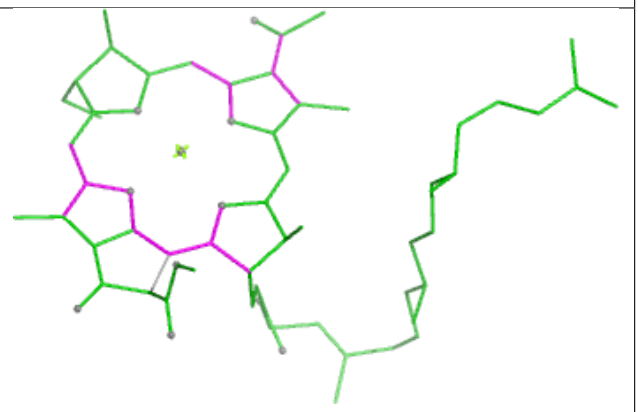
Ligand SPN M 409



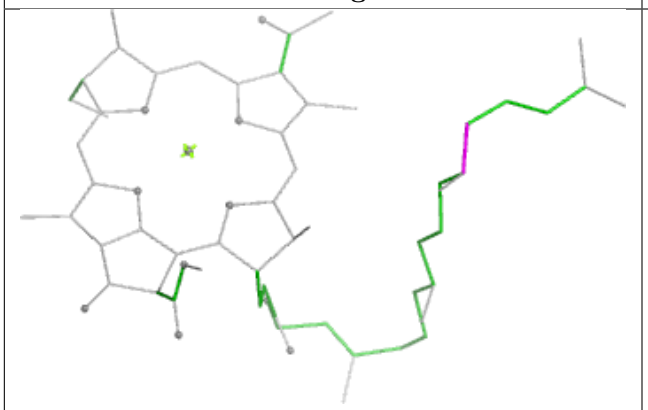
Ligand BCL L 302



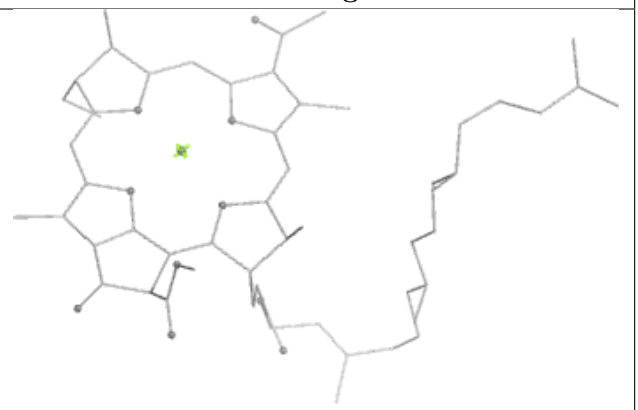
Bond lengths



Bond angles

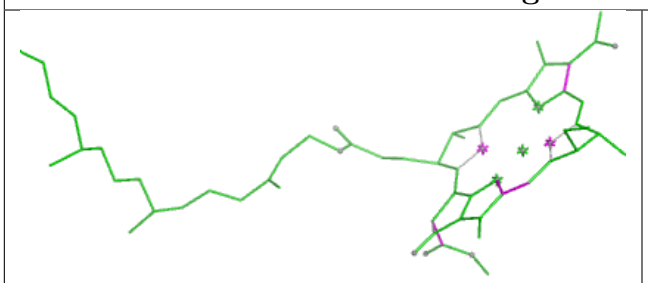


Torsions

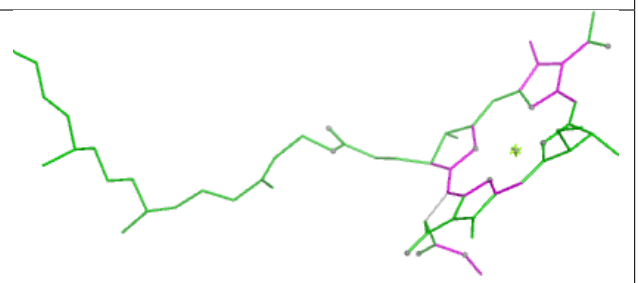


Rings

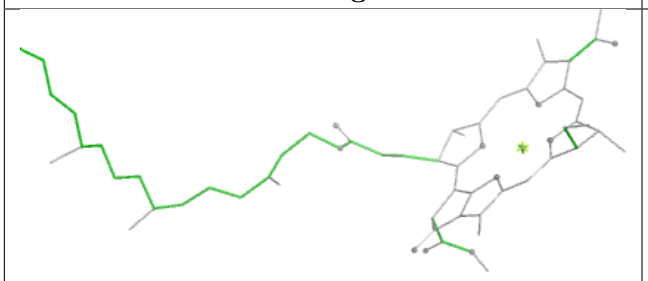
Ligand BCL M 406



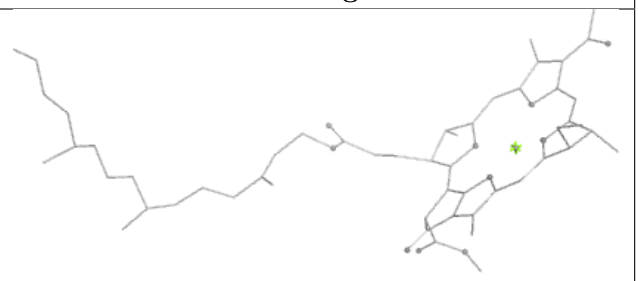
Bond lengths



Bond angles

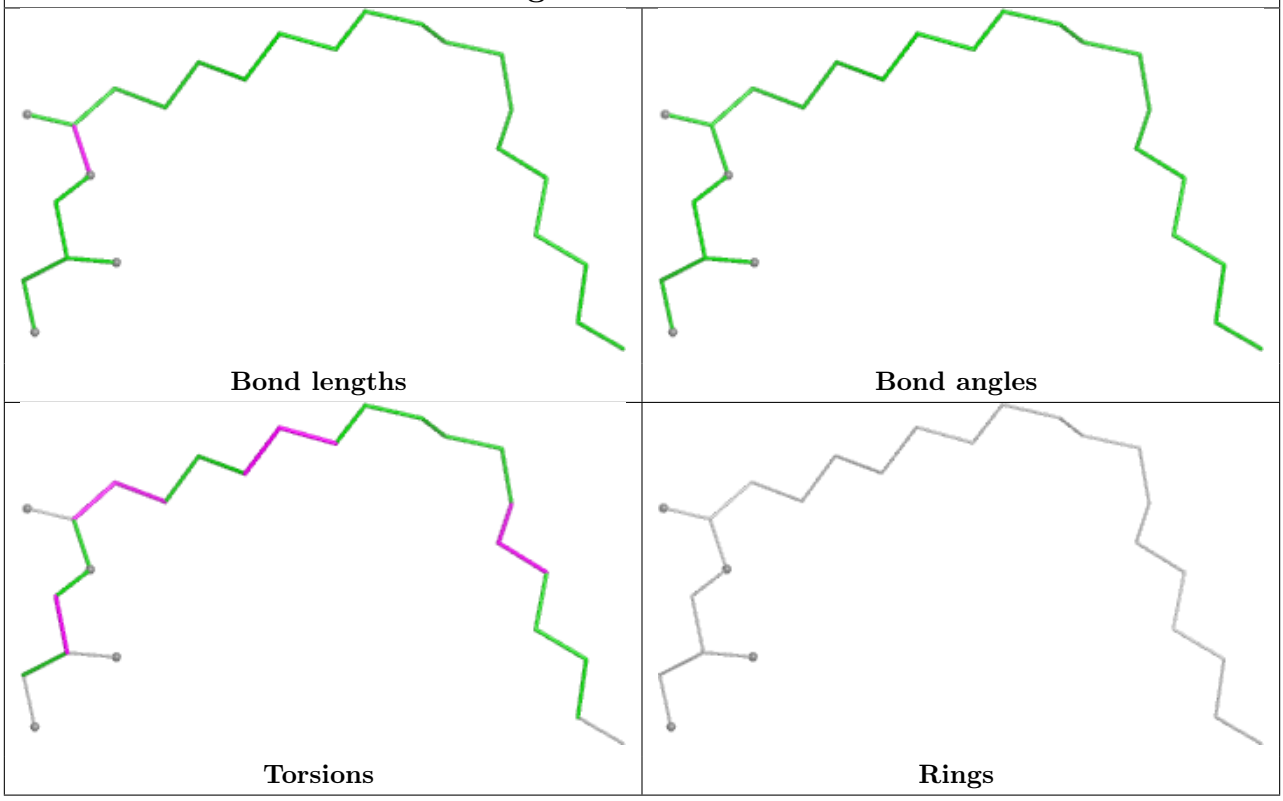


Torsions

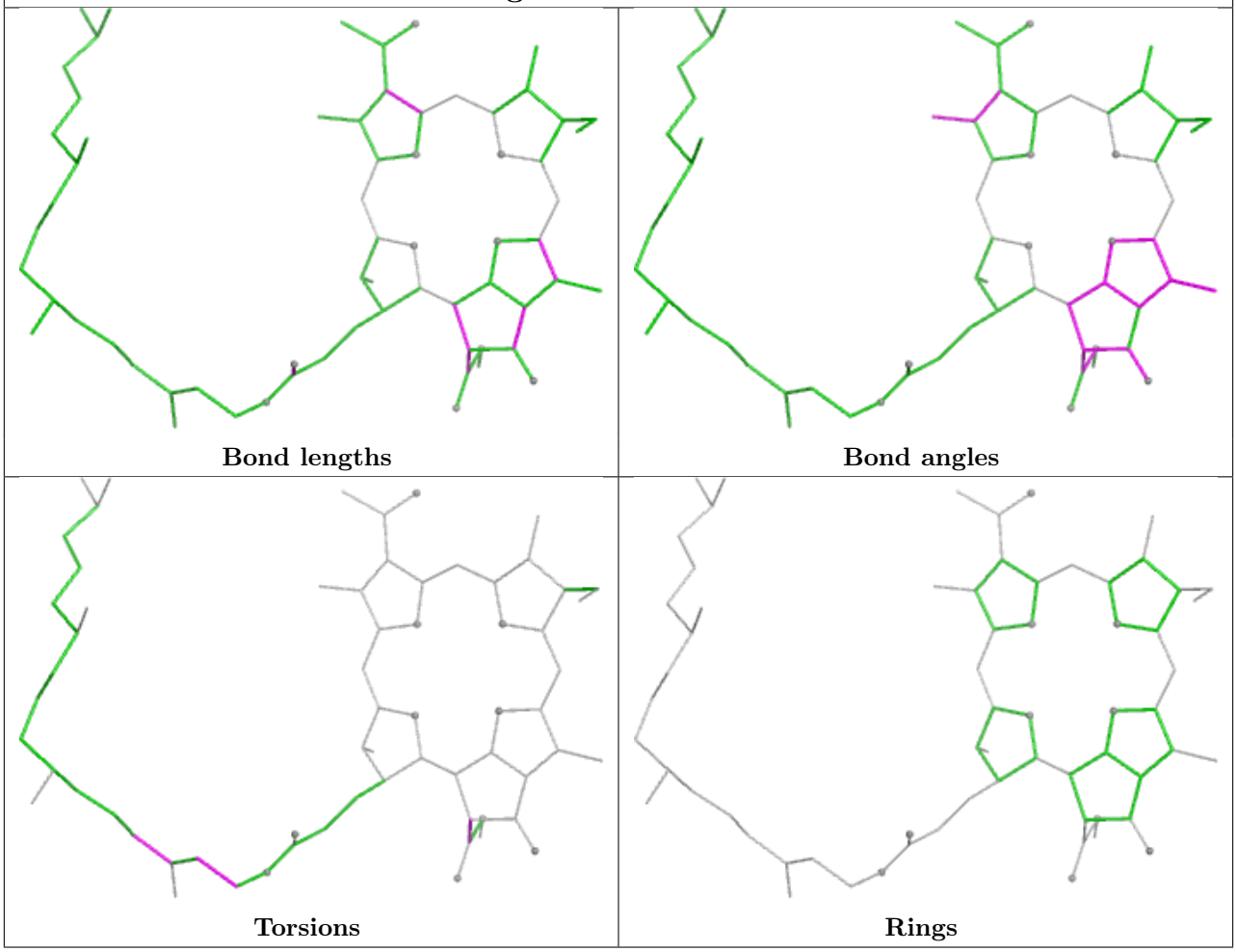


Rings

Ligand OLC L 306



Ligand BPH L 303



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	H	242/242 (100%)	0.43	18 (7%)	20	24	16, 40, 63, 114	4 (1%)
2	L	281/281 (100%)	0.35	28 (9%)	12	14	18, 35, 57, 117	22 (7%)
3	M	302/302 (100%)	0.23	16 (5%)	32	36	13, 35, 63, 111	7 (2%)
All	All	825/825 (100%)	0.33	62 (7%)	20	23	13, 37, 63, 117	33 (4%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	6.8
3	M	1	ALA	6.4
1	H	9	ASN	5.8
2	L	270[A]	PRO	5.0
3	M	302	GLY	4.9
1	H	10	PHE	4.7
1	H	249	LYS	4.6
2	L	277[A]	GLY	4.5
2	L	273[A]	ALA	4.5
2	L	265[A]	TRP	4.1
3	M	148	TRP	4.0
2	L	63	LEU	3.8
2	L	51	TRP	3.7
2	L	281[A]	GLY	3.6
3	M	3	TYR	3.5
3	M	301	HIS	3.5
1	H	90	THR	3.5
1	H	250	SER	3.4
3	M	68	PHE	3.4
1	H	248	ARG	3.4
1	H	247	LYS	3.4
2	L	264[A]	GLN	3.4
3	M	109	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	M	297	TRP	3.2
2	L	58	THR	3.1
1	H	245	ALA	3.0
2	L	278[A]	GLY	2.9
2	L	57	GLY	2.9
2	L	55	LEU	2.9
2	L	126[A]	LEU	2.8
2	L	274[A]	ASN	2.7
3	M	2	GLU	2.6
2	L	52	SER	2.6
2	L	39	PHE	2.5
2	L	276[A]	PRO	2.5
1	H	201	ASN	2.5
2	L	268[A]	LYS	2.5
3	M	80	TRP	2.5
2	L	267[A]	VAL	2.4
2	L	53	ALA	2.4
1	H	15	LEU	2.4
1	H	138	ALA	2.4
1	H	145	GLY	2.4
2	L	56	GLN	2.3
1	H	18	TYR	2.3
1	H	179	LEU	2.3
3	M	162	PHE	2.3
1	H	137	ALA	2.3
1	H	146	LYS	2.3
1	H	91	ALA	2.3
2	L	83	GLY	2.3
2	L	60	ASN	2.2
1	H	184	LYS	2.2
2	L	271[A]	TRP	2.2
3	M	78	ALA	2.1
3	M	101	TYR	2.1
3	M	83	ALA	2.1
3	M	114[A]	LEU	2.1
2	L	279[A]	ILE	2.1
2	L	263[A]	TRP	2.1
3	M	84	VAL	2.1
2	L	54	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

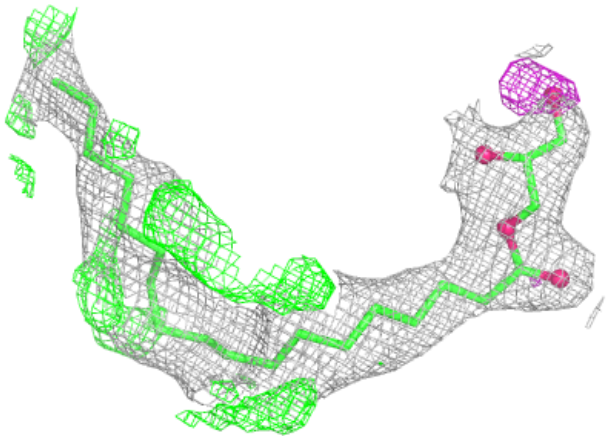
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

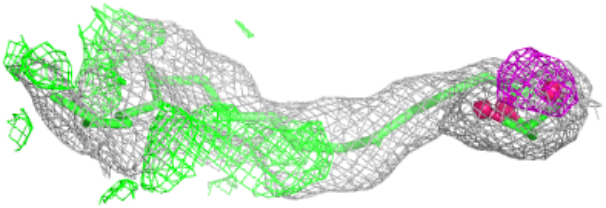
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	M	411	16/16	0.68	0.28	66,74,88,89	0
4	LDA	M	403	16/16	0.70	0.21	58,71,83,84	0
9	OLC	L	306	25/25	0.72	0.23	32,55,74,82	0
10	NKP	M	402	29/29	0.72	0.23	45,62,79,87	0
8	MYS	L	305	15/15	0.74	0.22	49,66,77,82	0
4	LDA	M	412	16/16	0.75	0.24	66,78,108,108	0
4	LDA	M	410	16/16	0.77	0.19	47,63,77,79	0
13	SPN	M	409	43/43	0.79	0.20	36,57,78,82	0
14	EDO	M	414	4/4	0.82	0.20	48,55,61,68	0
10	NKP	M	401	29/29	0.83	0.20	37,69,84,88	0
7	D12	L	304	12/12	0.83	0.17	50,57,62,63	0
15	PO4	M	415	5/5	0.83	0.11	58,73,86,90	0
7	D12	M	413	12/12	0.86	0.14	47,64,80,83	0
4	LDA	H	301	16/16	0.89	0.12	36,43,65,77	0
11	U10	M	404	63/63	0.90	0.15	22,52,77,82	0
5	BCL	M	405	66/66	0.94	0.11	26,35,82,89	0
6	BPH	M	407	65/65	0.94	0.11	24,32,102,108	0
6	BPH	L	303	65/65	0.95	0.08	21,29,44,47	0
5	BCL	L	302	66/66	0.95	0.08	22,33,58,68	0
5	BCL	L	301	66/66	0.95	0.08	23,33,46,67	0
5	BCL	M	406	66/66	0.95	0.09	17,32,55,91	0
12	FE	M	408	1/1	1.00	0.01	24,24,24,24	0

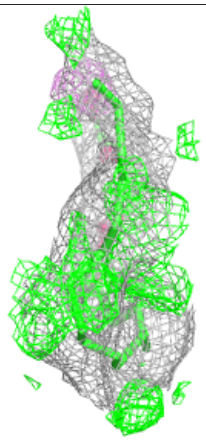
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC L 306:

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

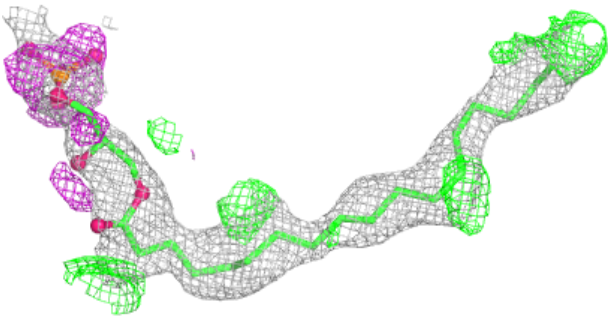


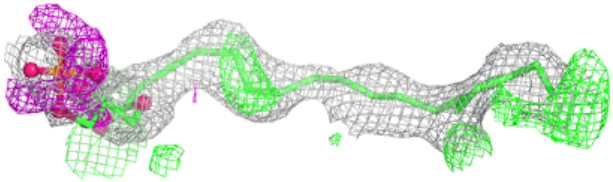




Electron density around NKP M 402:

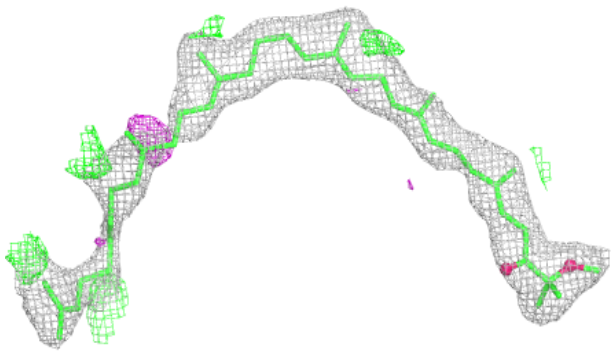
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

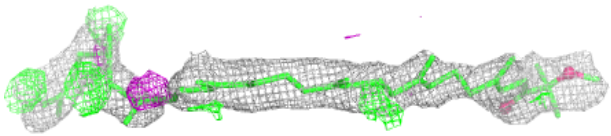


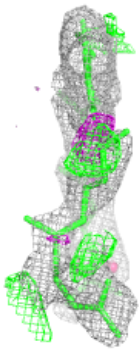


Electron density around SPN M 409:

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

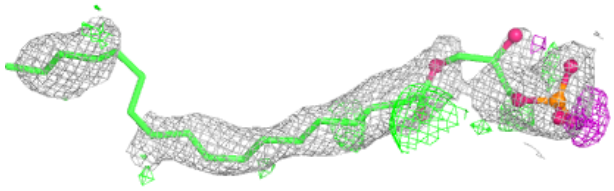


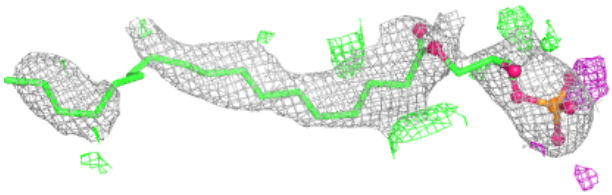


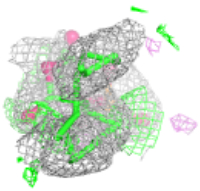


Electron density around NKP M 401:

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

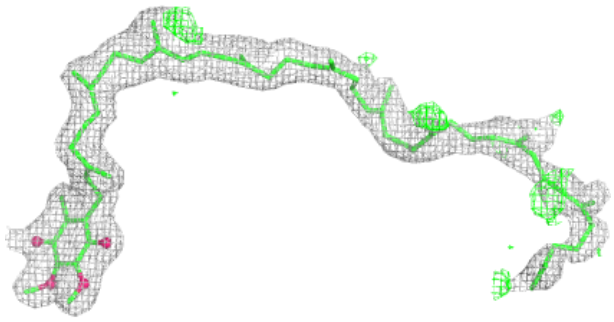


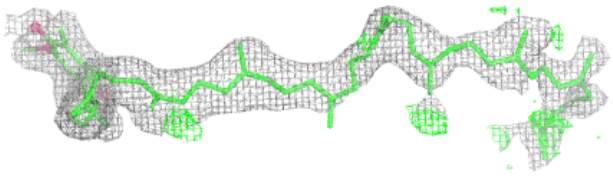


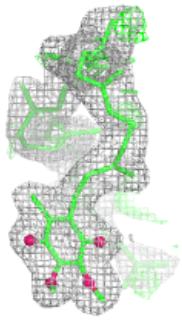


Electron density around U10 M 404:

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

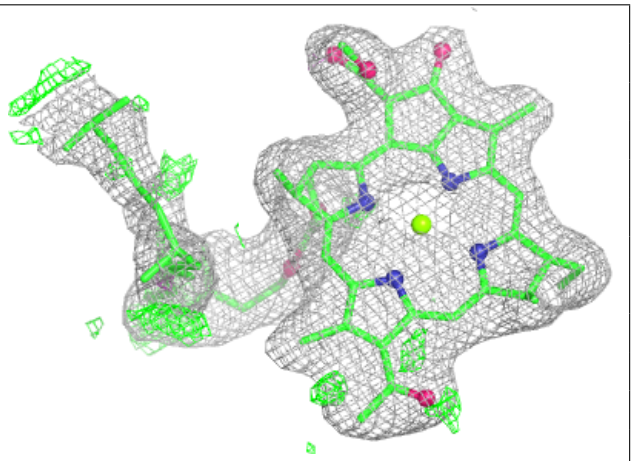


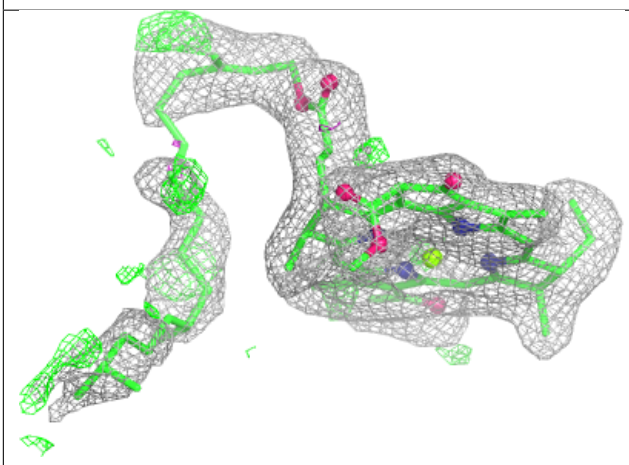




Electron density around BCL M 405:

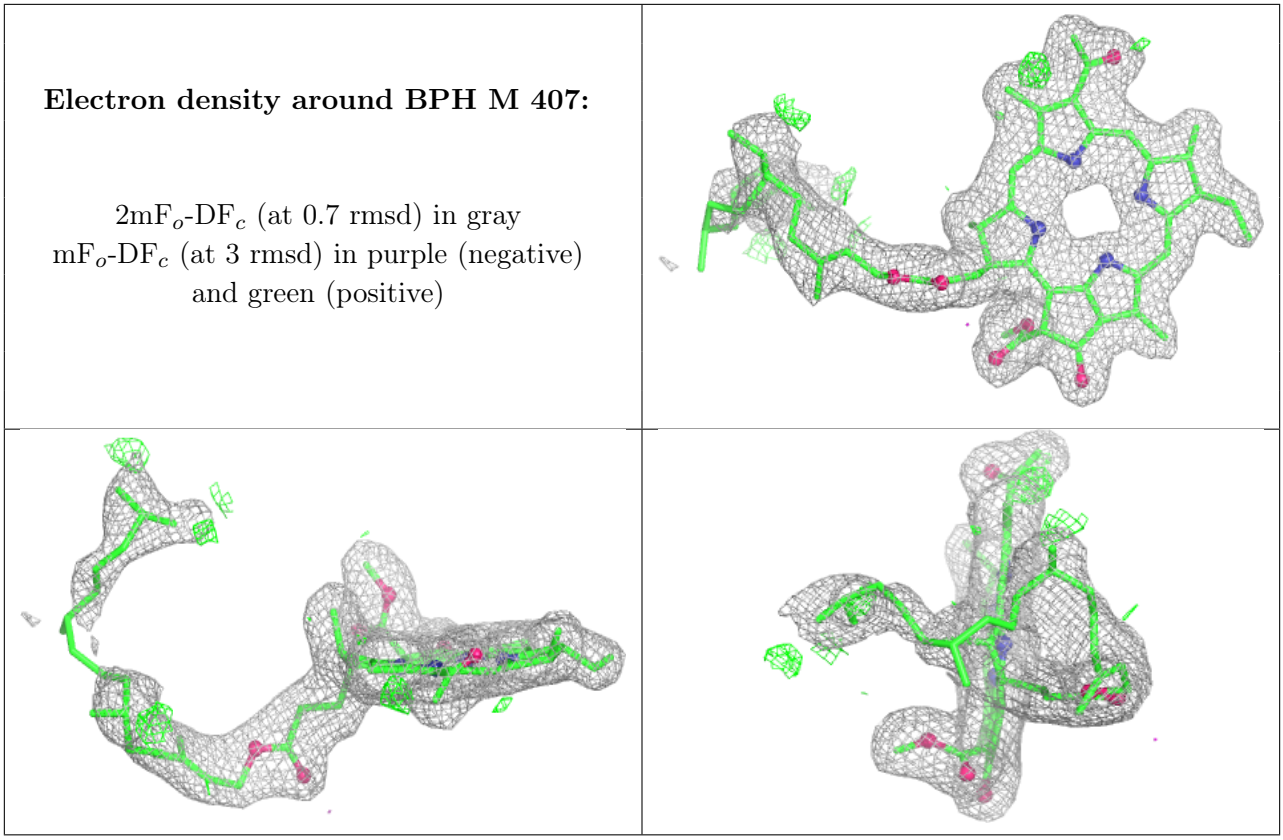
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





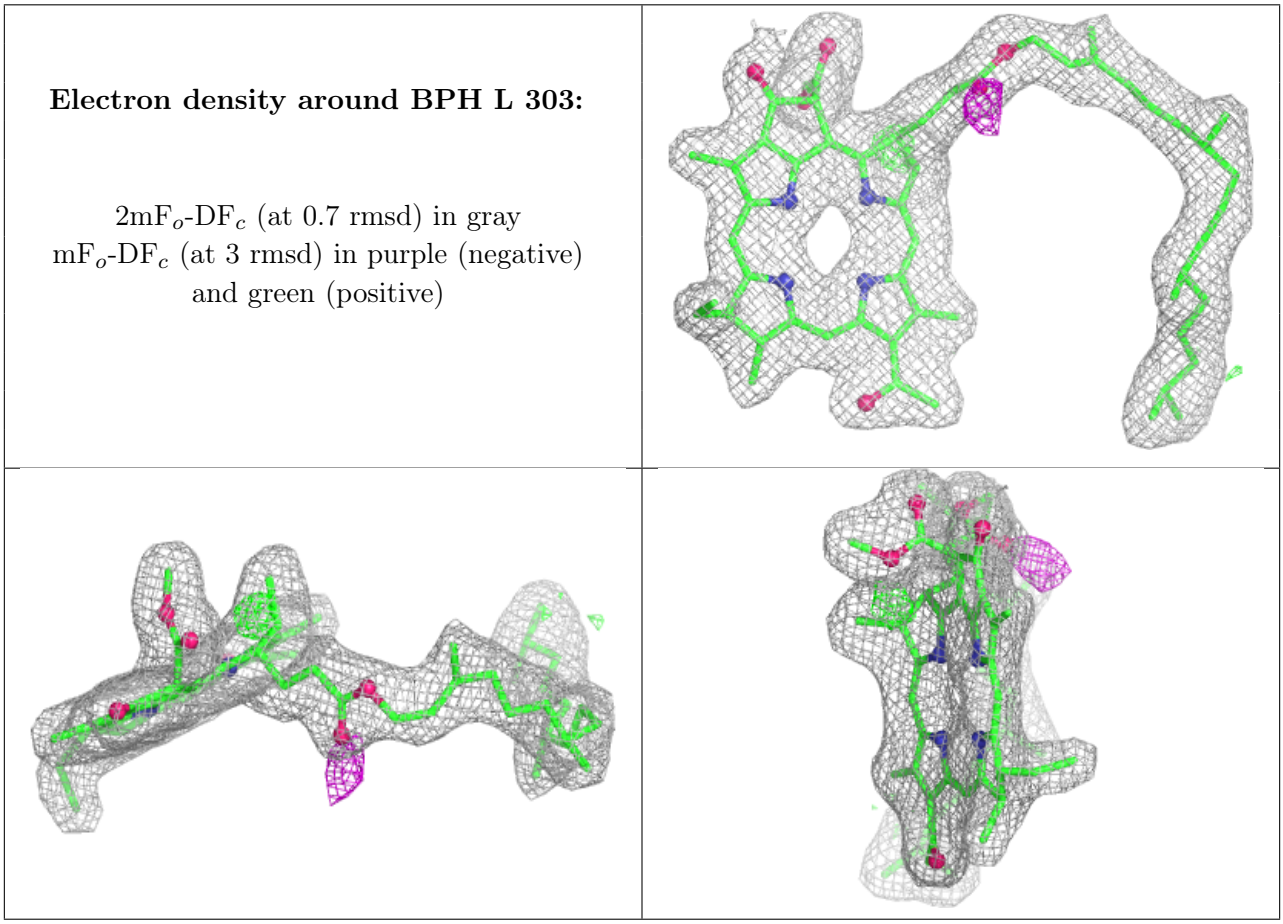
Electron density around BPH M 407:

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



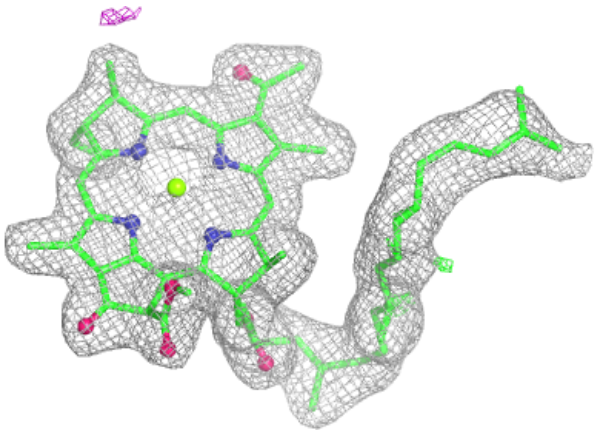
Electron density around BPH L 303:

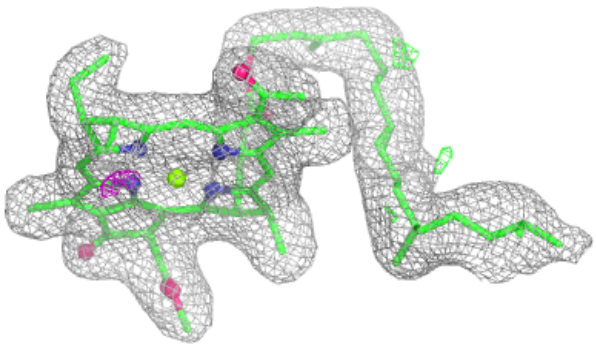
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

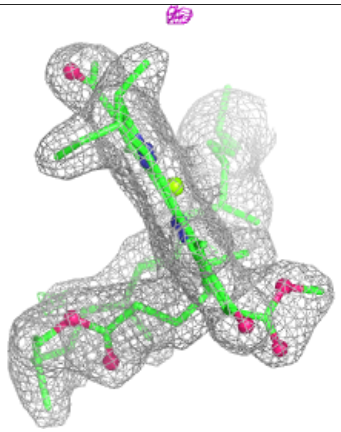


Electron density around BCL L 302:

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

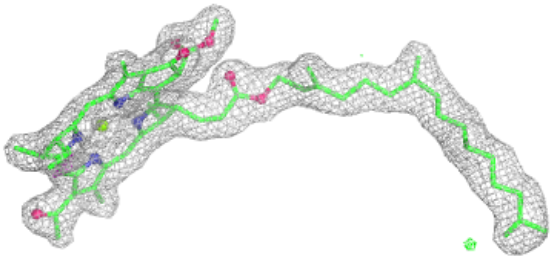


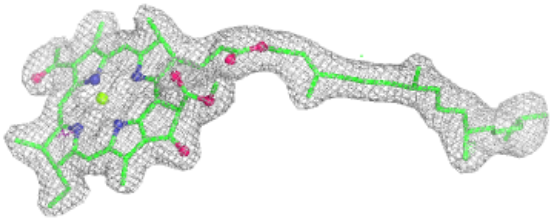


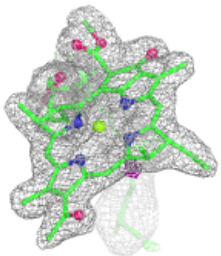


Electron density around BCL L 301:

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

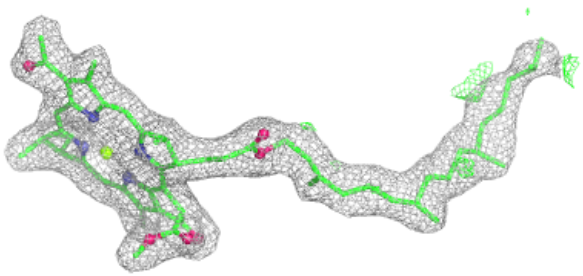


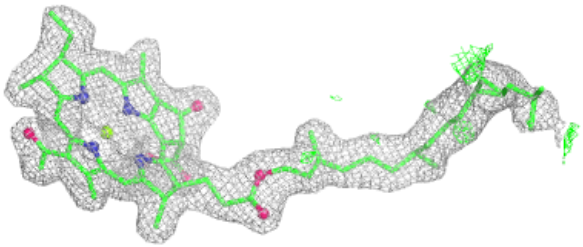


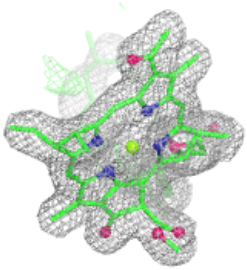


Electron density around BCL M 406:

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

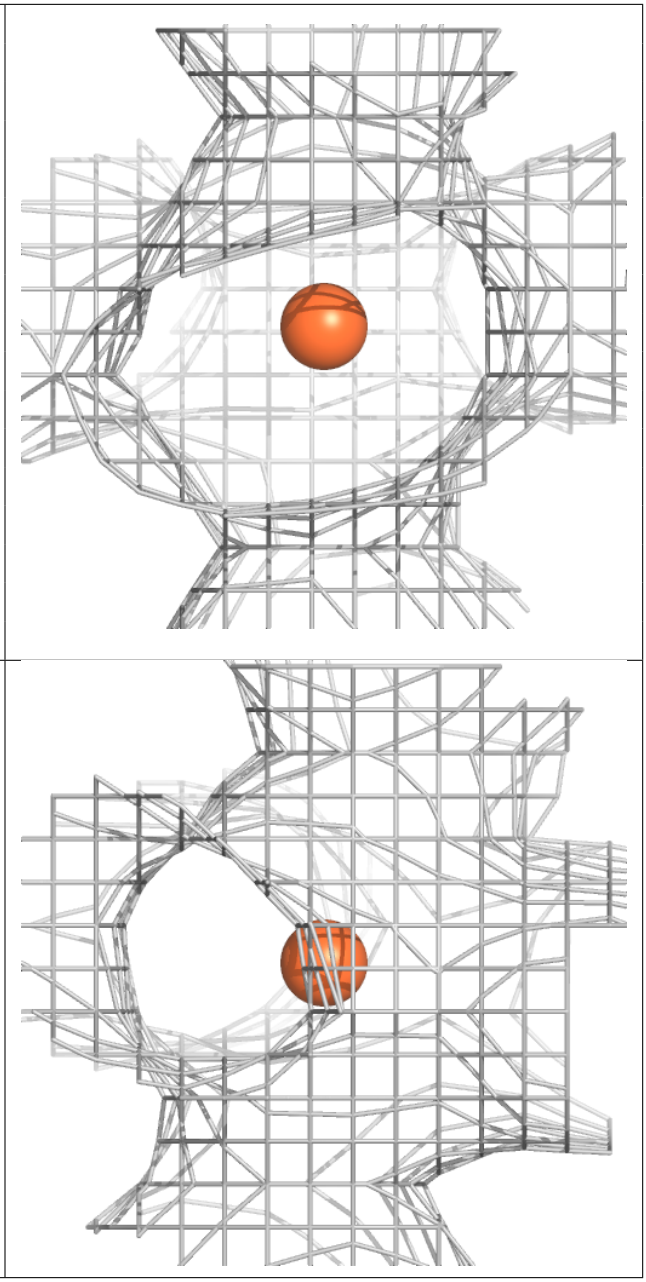






Electron density around FE M 408:

$2mF_o$-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.