



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 02:45 PM EDT

PDB ID : 5MDX
EMDB ID: : EMD-3491
Title : Cryo-EM structure of the PSII supercomplex from Arabidopsis thaliana
Authors : van Bezouwen, L.S.; Caffarri, S.; Kale, R.S.; Kouril, R.; Thunnissen, A.M.W.H.; Oostergetel, G.T.; Boekema, E.J.
Deposited on : unknown
Resolution : 5.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

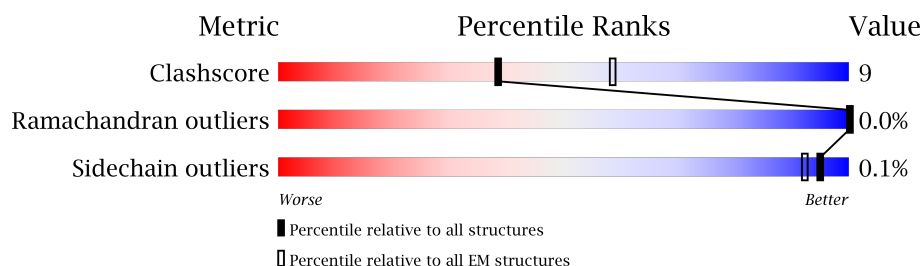
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 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.









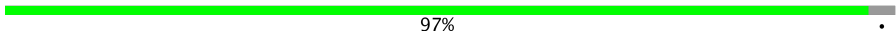

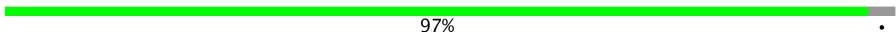













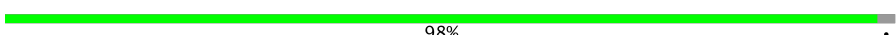


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	343	68% 22% 10%
1	a	343	96% .
2	B	507	65% 29% 6%
2	b	507	94% 6%
3	C	459	65% 29% 6%
3	c	459	94% 6%
4	D	352	68% 28% 5%
4	d	352	95% . 5%
5	E	83	70% 17% 13%

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Mol	Chain	Length	Quality of chain
5	e	83	
6	F	39	
6	f	39	
7	H	72	
7	h	72	
8	I	36	
8	i	36	
9	K	37	
9	k	37	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	O	247	
12	o	247	
13	T	33	
13	t	33	
14	W	54	
14	w	54	
15	X	116	
15	x	116	
16	Z	62	
16	z	62	
17	R	250	
17	r	250	

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Mol	Chain	Length	Quality of chain
18	S	232	
18	s	232	
19	1	224	
19	2	224	
19	3	224	
19	5	224	
19	6	224	
19	7	224	
19	G	224	
19	N	224	
19	Y	224	
19	g	224	
19	n	224	
19	y	224	
20	4	210	
20	8	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	314	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	N	614	X	-	-	-
22	CLA	R	301	X	-	-	-
22	CLA	R	302	X	-	X	-
22	CLA	R	303	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	R	312	X	-	X	-
22	CLA	S	301	X	-	X	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	S	314	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	a	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	n	614	X	-	-	-
22	CLA	r	301	X	-	-	-
22	CLA	r	302	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	307	X	-	-	-
22	CLA	r	308	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-
22	CLA	s	313	X	-	-	-
22	CLA	s	314	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	-	-
22	CLA	y	613	X	-	-	-
22	CLA	y	614	X	-	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 78324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2388	1558	392	426	12		
1	a	330	Total	C	N	O	S	0	0
			2584	1688	426	457	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		
2	b	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
3	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		
4	d	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	72	Total	C	N	O	0	0
			586	386	93	107		
5	e	72	Total	C	N	O	0	0
			586	386	93	107		

- Molecule 6 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
6	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	52	Total	C	N	O	S	0	0
			389	257	61	69	2		
7	h	52	Total	C	N	O	S	0	0
			389	257	61	69	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
8	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	36	Total	C	N	O	S	0	0
			290	205	40	44	1		
9	k	36	Total	C	N	O	S	0	0
			290	205	40	44	1		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			302	200	47	55		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	36	Total	C	N	O	0	0
			302	200	47	55		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	29	Total	C	N	O	0	0
			226	158	32	36		
11	m	29	Total	C	N	O	0	0
			226	158	32	36		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	193	Total	C	N	O	S	0	0
			1487	951	235	297	4		
12	o	193	Total	C	N	O	S	0	0
			1487	951	235	297	4		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
13	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 14 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	46	Total	C	N	O	S	0	0
			372	247	53	71	1		
14	w	46	Total	C	N	O	S	0	0
			372	247	53	71	1		

- Molecule 15 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	32	Total	C	N	O	0	0
			226	149	35	42		
15	x	32	Total	C	N	O	0	0
			226	149	35	42		

- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
16	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		
17	r	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	Y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	1	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	2	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	3	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	6	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	7	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

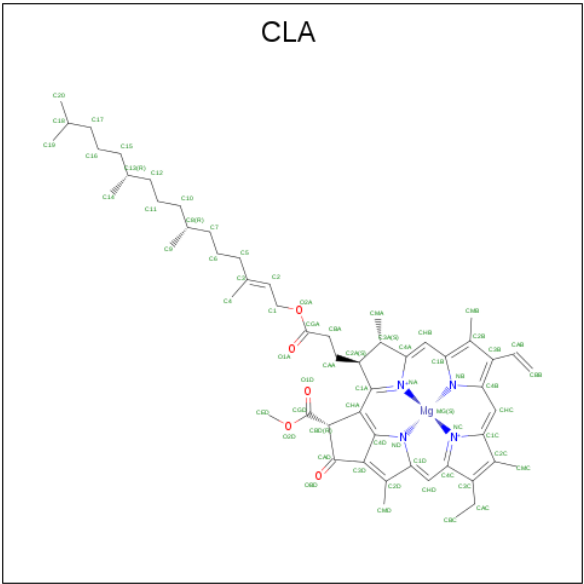
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
20	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Fe	0
			1	1	
21	a	1	Total	Fe	0
			1	1	

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0

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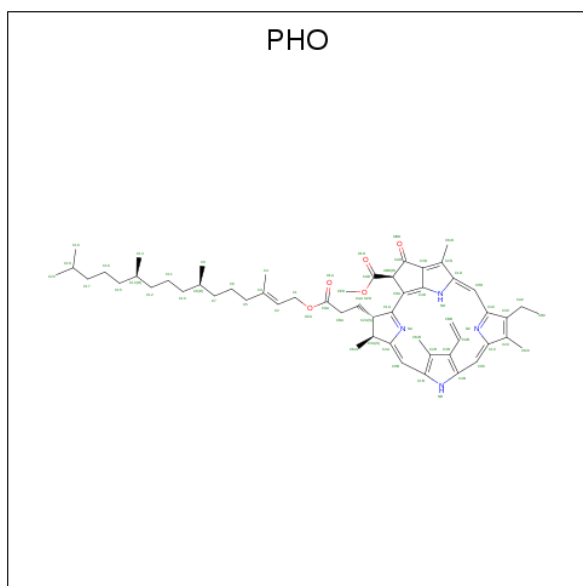
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0

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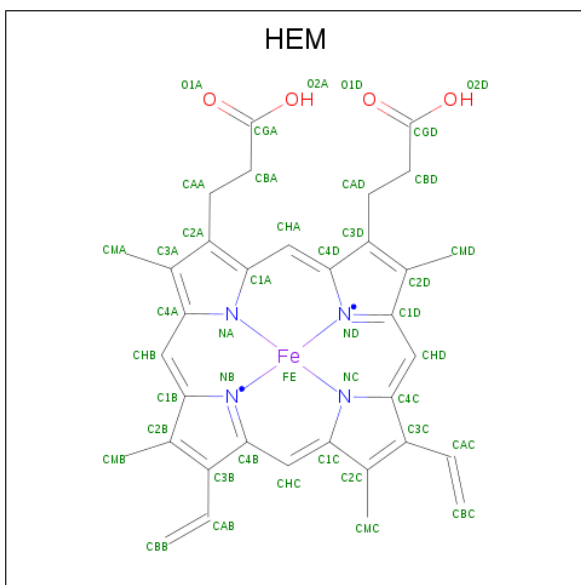
Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			225	175	5	20	25	

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



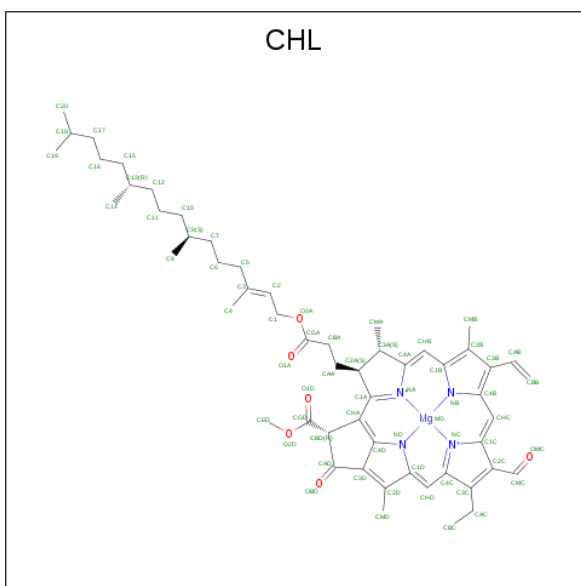
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	N	O	0
			44	35	4	5	
23	D	1	Total	C	N	O	0
			44	35	4	5	
23	a	1	Total	C	N	O	0
			44	35	4	5	
23	d	1	Total	C	N	O	0
			44	35	4	5	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
24	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total 138	C 105	Mg 3	N 12	O 18	0
25	R	1	Total 138	C 105	Mg 3	N 12	O 18	0

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	

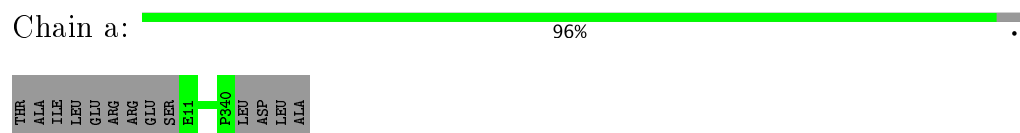
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

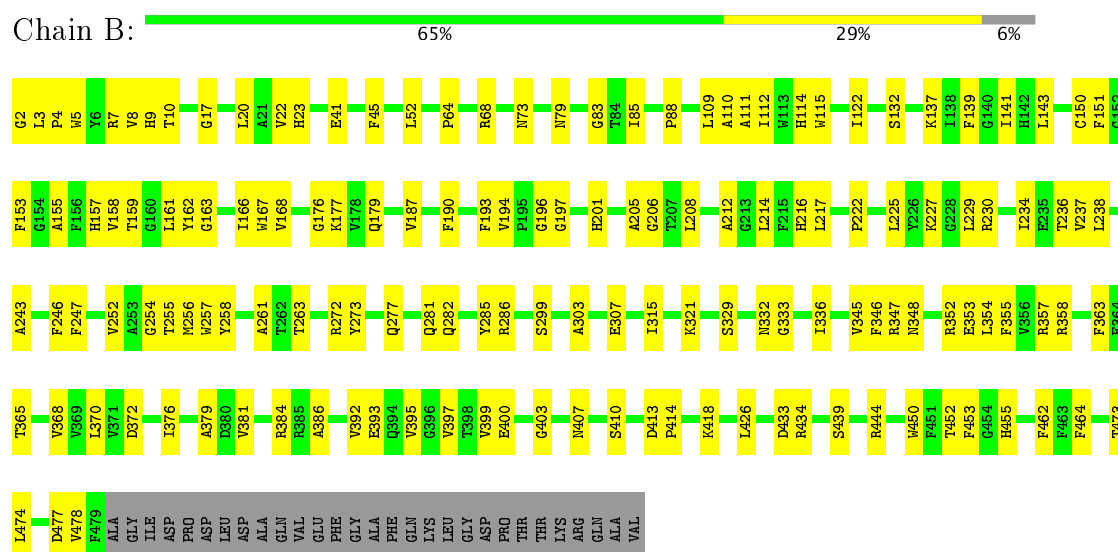
- Molecule 1: Photosystem II protein D1



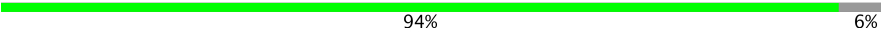
- Molecule 1: Photosystem II protein D1

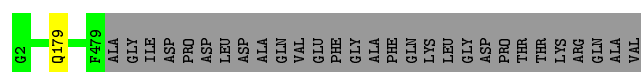


- Molecule 2: Photosystem II CP47 reaction center protein



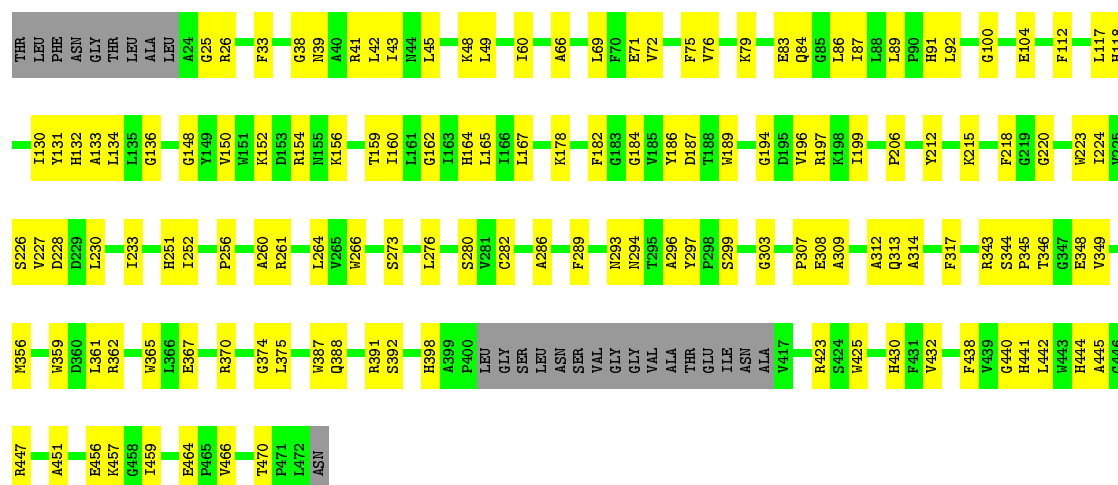
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  94% 6%



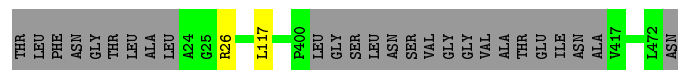
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  65% 29% 6%



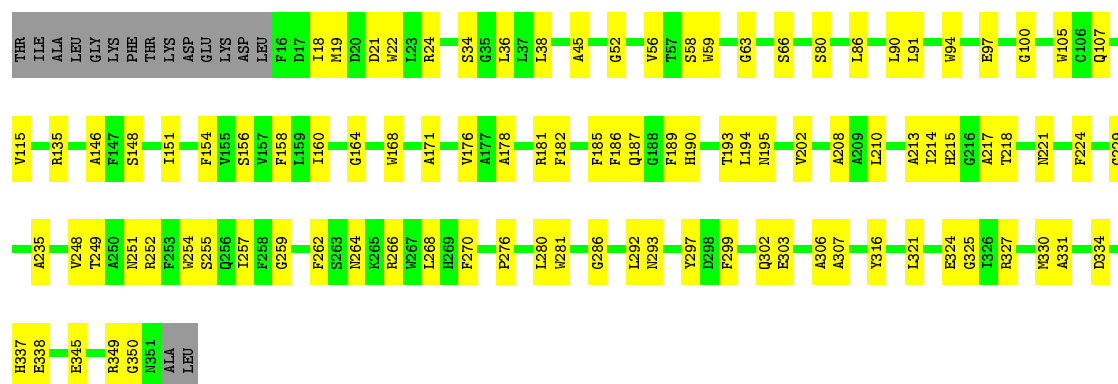
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  94% 6%



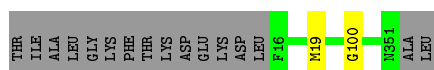
- Molecule 4: Photosystem II D2 protein

Chain D:  68% 28% 5%



- Molecule 4: Photosystem II D2 protein

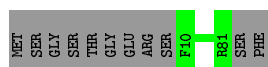
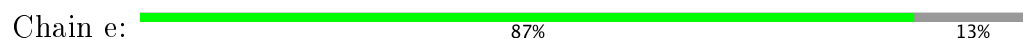
Chain d:  95% 5%



- Molecule 5: Cytochrome b559 subunit alpha



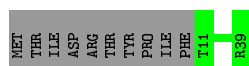
- Molecule 5: Cytochrome b559 subunit alpha



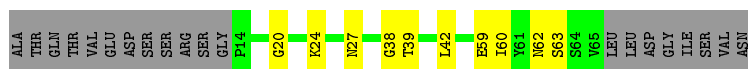
- Molecule 6: Cytochrome b559 subunit beta (PsbF)



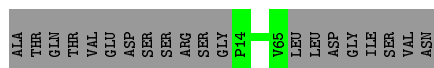
- Molecule 6: Cytochrome b559 subunit beta (PsbF)



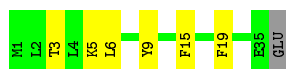
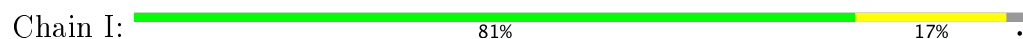
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  97%



- Molecule 9: Photosystem II reaction center protein K

Chain K:  68% 30%



- Molecule 9: Photosystem II reaction center protein K

Chain k:  97%




- Molecule 10: Photosystem II reaction center protein L

Chain L:  61% 32% 5%



- Molecule 10: Photosystem II reaction center protein L

Chain l:  92% 5%




- Molecule 11: Photosystem II reaction center protein M

Chain M:  56% 29% 15%



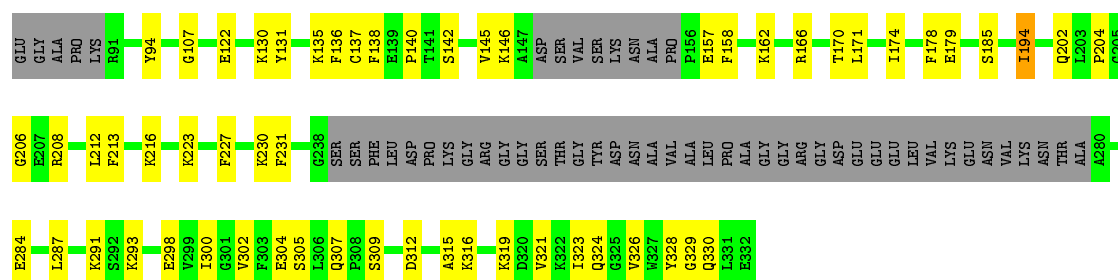
- Molecule 11: Photosystem II reaction center protein M

Chain m:  82% 15%



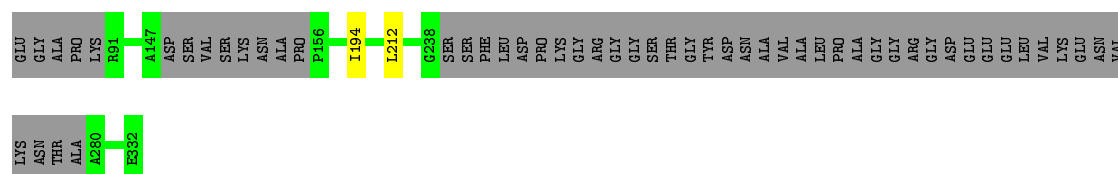
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:  55% 23% 22%



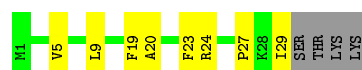
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplasic

Chain o: 77% 22%



- Molecule 13: Photosystem II reaction center protein T

Chain T: 64% 24% 12%



- Molecule 13: Photosystem II reaction center protein T

Chain t: 88% 12%



- Molecule 14: Photosystem II reaction center W protein, chloroplasic

Chain W: 63% 22% 15%



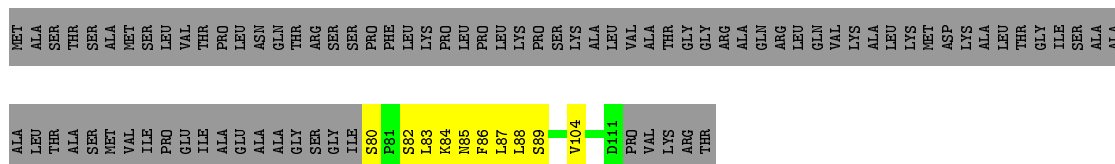
- Molecule 14: Photosystem II reaction center W protein, chloroplasic

Chain w: 85% 15%

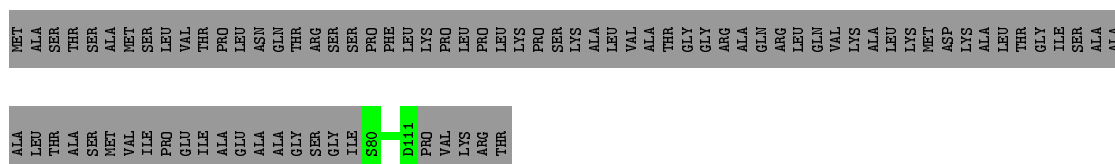


- Molecule 15: Photosystem II reaction center protein X

Chain X: 19% 9% 72%



- Molecule 15: Photosystem II reaction center protein X



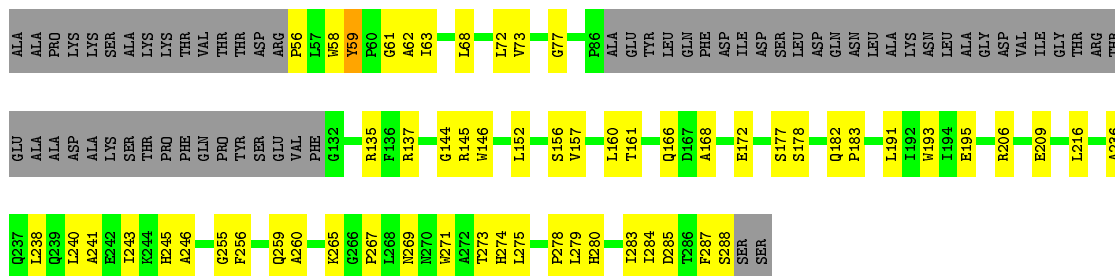
- Molecule 16: Photosystem II reaction center protein Z



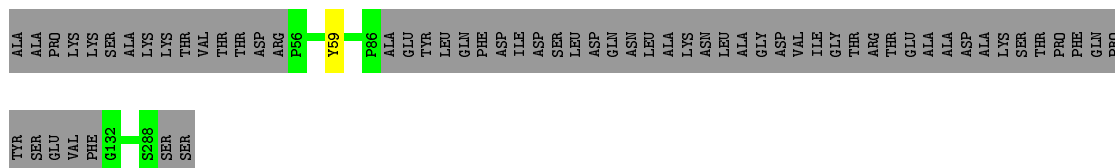
- Molecule 16: Photosystem II reaction center protein Z



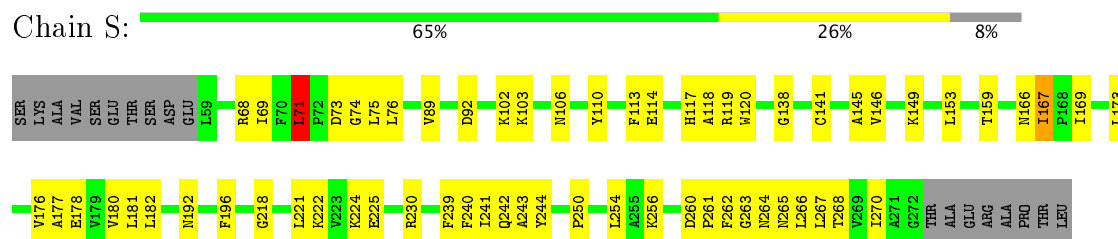
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



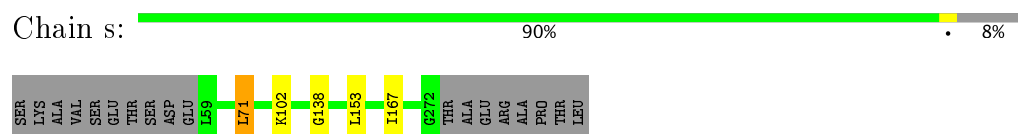
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



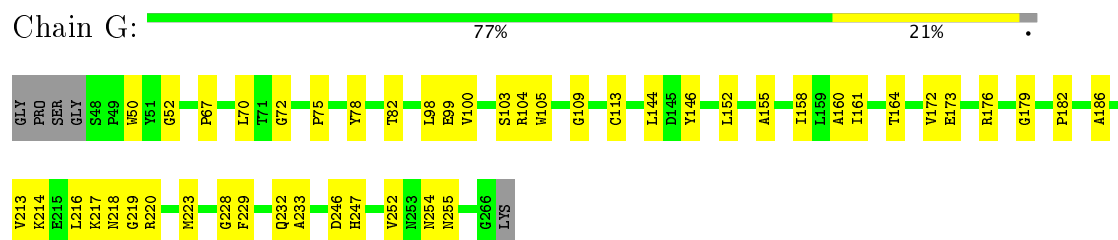
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



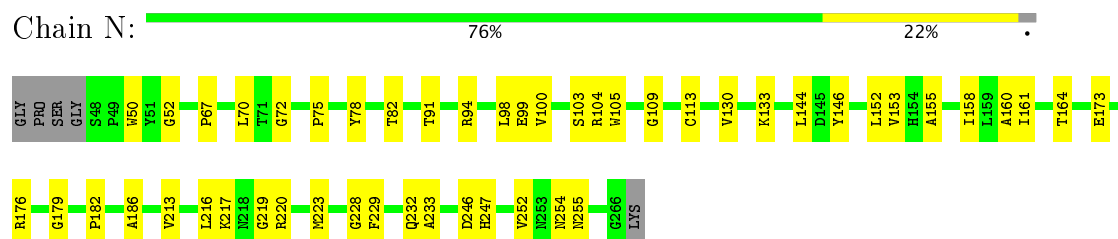
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



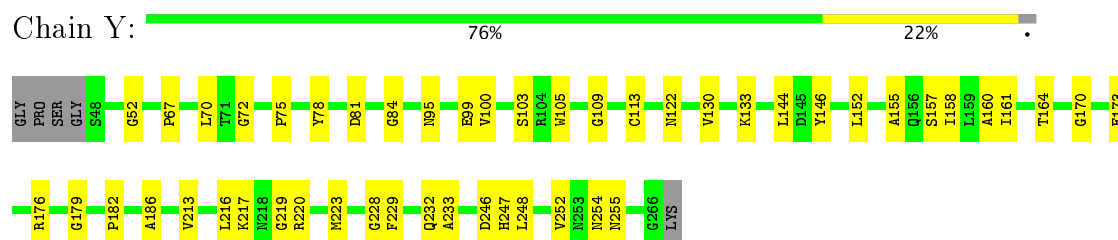
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



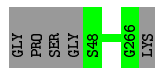
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic





- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain n: 98%



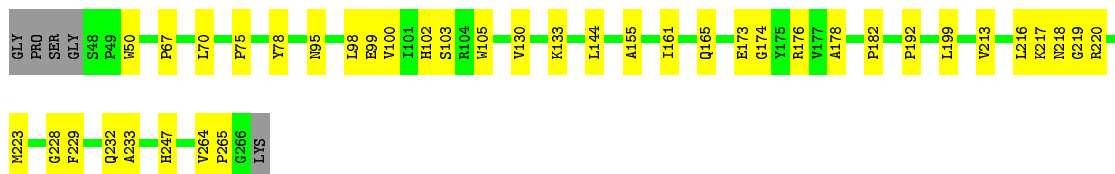
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 98%



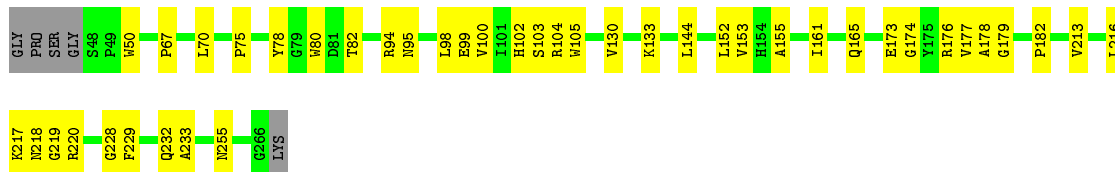
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 1: 80%



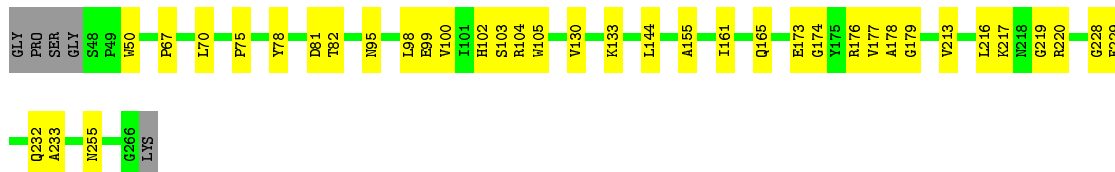
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 2: 79%



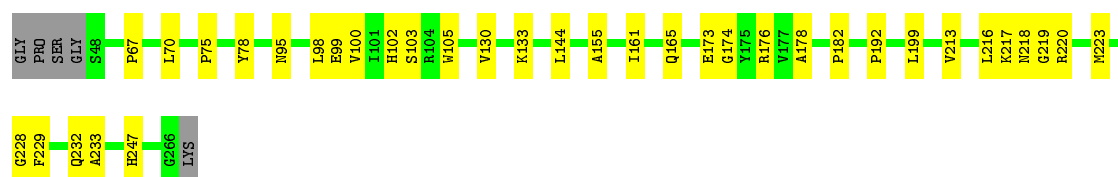
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 3: 81%



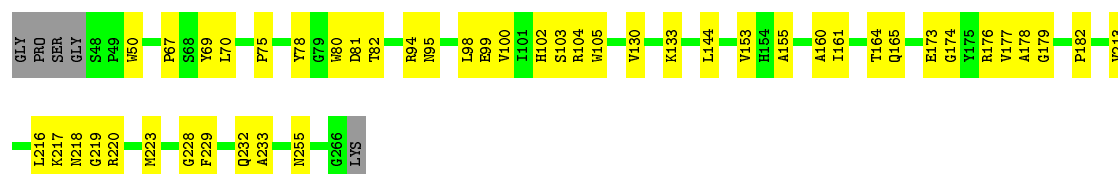
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 5: 82%



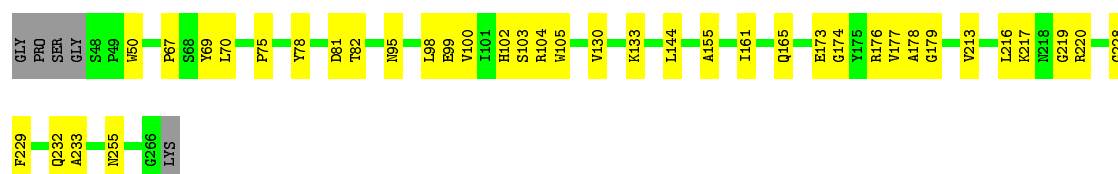
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 6: 77% 21% .



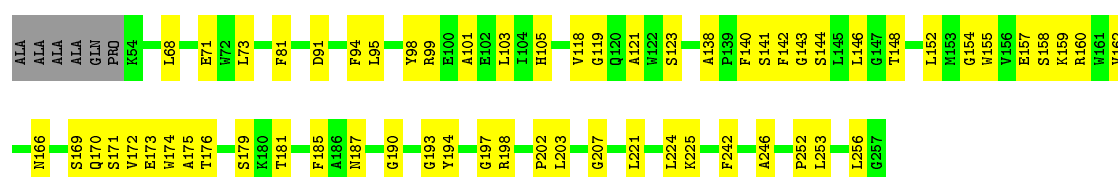
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 7: 81% 17% .



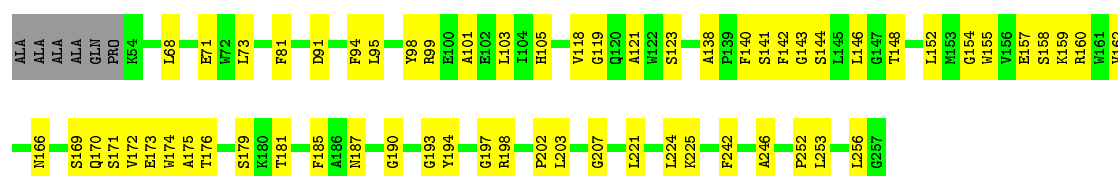
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 68% 29% .



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 68% 29% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, HEM, PHO, CLA, FE2

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 >2	RMSZ	# Z >2
1	A	0.36	0/2458	0.58	0/3348
1	a	0.36	0/2665	0.58	0/3634
10	L	0.41	0/310	0.77	1/421 (0.2%)
10	l	0.41	0/310	0.77	1/421 (0.2%)
11	M	0.42	0/230	0.65	0/315
11	m	0.42	0/230	0.65	0/315
12	O	0.35	0/1518	0.68	1/2049 (0.0%)
12	o	0.35	0/1518	0.68	1/2049 (0.0%)
13	T	0.39	0/246	0.61	0/333
13	t	0.39	0/246	0.61	0/333
14	W	0.37	0/383	0.65	0/519
14	w	0.37	0/383	0.66	0/519
15	X	0.37	0/228	0.46	0/310
15	x	0.37	0/228	0.46	0/310
16	Z	0.31	0/468	0.50	0/641
16	z	0.32	0/468	0.50	0/641
17	R	0.35	0/1502	0.52	0/2047
17	r	0.35	0/1502	0.52	0/2047
18	S	0.37	0/1698	0.78	4/2305 (0.2%)
18	s	0.37	0/1698	0.78	4/2305 (0.2%)
19	1	0.31	0/1716	0.53	0/2336
19	2	0.31	0/1716	0.53	0/2336
19	3	0.31	0/1716	0.53	0/2336
19	5	0.31	0/1716	0.53	0/2336
19	6	0.31	0/1716	0.53	0/2336
19	7	0.31	0/1716	0.53	0/2336
19	G	0.36	0/1716	0.57	0/2336
19	N	0.36	0/1716	0.56	0/2336
19	Y	0.36	0/1716	0.57	0/2336
19	g	0.36	0/1716	0.57	0/2336
19	n	0.36	0/1716	0.56	0/2336
19	y	0.36	0/1716	0.57	0/2336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	B	0.35	0/3881	0.58	0/5286
2	b	0.35	0/3881	0.58	0/5286
20	4	0.36	0/1652	0.97	3/2242 (0.1%)
20	8	0.36	0/1652	0.97	3/2242 (0.1%)
3	C	0.37	0/3487	0.60	1/4750 (0.0%)
3	c	0.37	0/3487	0.60	1/4750 (0.0%)
4	D	0.38	0/2768	0.60	1/3774 (0.0%)
4	d	0.38	0/2768	0.60	1/3774 (0.0%)
5	E	0.37	0/603	0.65	0/819
5	e	0.37	0/603	0.65	0/819
6	F	0.36	0/229	0.62	0/311
6	f	0.36	0/229	0.62	0/311
7	H	0.34	0/398	0.55	0/541
7	h	0.34	0/398	0.56	0/541
8	I	0.46	0/294	0.69	0/397
8	i	0.46	0/294	0.69	0/397
9	K	0.40	0/301	0.66	0/414
9	k	0.40	0/301	0.66	0/414
All	All	0.36	0/66107	0.62	22/89962 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	R	0	1
17	r	0	1
18	S	0	1
18	s	0	1
2	B	0	1
2	b	0	1
20	4	0	1
20	8	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	CA-C-N	-23.99	64.42	117.20
20	8	207	GLY	CA-C-N	-23.99	64.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
20	4	207	GLY	O-C-N	-21.84	87.76	122.70
20	8	207	GLY	O-C-N	-21.84	87.76	122.70
20	4	207	GLY	CA-C-O	17.55	152.19	120.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	179	GLN	Peptide
17	R	59	TYR	Peptide
18	S	71	LEU	Peptide
2	b	179	GLN	Peptide
17	r	59	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2309	70	0
1	a	2584	0	2490	0	0
2	B	3752	0	3636	152	0
2	b	3752	0	3636	0	0
3	C	3373	0	3302	143	0
3	c	3373	0	3302	0	0
4	D	2675	0	2565	99	0
4	d	2675	0	2565	0	0
5	E	586	0	566	17	0
5	e	586	0	566	0	0
6	F	224	0	233	6	0
6	f	224	0	233	0	0
7	H	389	0	411	11	0
7	h	389	0	411	0	0
8	I	286	0	295	5	0
8	i	286	0	295	0	0
9	K	290	0	300	7	0
9	k	290	0	300	0	0
10	L	302	0	291	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	l	302	0	291	0	0
11	M	226	0	252	10	0
11	m	226	0	252	0	0
12	O	1487	0	1462	39	0
12	o	1487	0	1462	0	0
13	T	239	0	255	8	0
13	t	239	0	255	0	0
14	W	372	0	346	8	0
14	w	372	0	346	0	0
15	X	226	0	244	8	0
15	x	226	0	244	0	0
16	Z	458	0	490	39	0
16	z	458	0	489	0	0
17	R	1459	0	1428	223	0
17	r	1459	0	1428	0	0
18	S	1653	0	1639	110	0
18	s	1653	0	1639	0	0
19	1	1666	0	1593	33	0
19	2	1666	0	1593	35	0
19	3	1666	0	1593	29	0
19	5	1666	0	1593	31	0
19	6	1666	0	1593	39	0
19	7	1666	0	1593	31	0
19	G	1666	0	1593	35	0
19	N	1666	0	1593	37	0
19	Y	1666	0	1593	37	0
19	g	1666	0	1593	0	0
19	n	1666	0	1593	0	0
19	y	1666	0	1593	0	0
20	4	1597	0	1526	155	0
20	8	1597	0	1526	157	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	1	360	0	264	4	0
22	2	360	0	264	21	0
22	3	360	0	264	2	0
22	4	225	0	165	7	0
22	5	360	0	264	4	0
22	6	360	0	264	21	0
22	7	360	0	264	2	0
22	8	225	0	165	8	0
22	A	135	0	99	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	720	0	528	39	0
22	C	540	0	396	23	0
22	D	135	0	99	4	0
22	G	360	0	264	12	0
22	N	360	0	264	5	0
22	R	405	0	295	101	0
22	S	450	0	330	32	0
22	Y	360	0	264	10	0
22	a	135	0	99	0	0
22	b	720	0	528	0	0
22	c	540	0	396	0	0
22	d	135	0	99	0	0
22	g	360	0	264	0	0
22	n	360	0	264	0	0
22	r	405	0	295	0	0
22	s	450	0	330	0	0
22	y	360	0	264	0	0
23	A	44	0	35	3	0
23	D	44	0	35	2	0
23	a	44	0	35	0	0
23	d	44	0	35	0	0
24	E	43	0	30	4	0
24	e	43	0	30	0	0
25	1	318	0	213	12	0
25	2	226	0	151	15	0
25	3	272	0	182	9	0
25	4	230	0	155	13	0
25	5	318	0	213	10	0
25	6	226	0	151	15	0
25	7	272	0	182	10	0
25	8	230	0	155	16	0
25	G	272	0	182	13	0
25	N	272	0	182	10	0
25	R	138	0	93	5	0
25	S	184	0	124	4	0
25	Y	272	0	182	13	0
25	g	272	0	182	0	0
25	n	272	0	182	0	0
25	r	138	0	93	0	0
25	s	184	0	124	0	0
25	y	272	0	182	0	0
All	All	78324	0	72516	1364	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 9.

The worst 5 of 1364 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:C:182:PHE:CZ	18:S:261:PRO:HG2	1.17	1.70
16:Z:59:SER:CB	18:S:267:LEU:CD2	1.74	1.58
17:R:280:HIS:HA	20:4:141:SER:N	167.28	1.48
16:Z:59:SER:CB	18:S:267:LEU:HD23	1.02	1.47
2:B:214:LEU:HD22	22:R:302:CLA:CED	105.31	1.47

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/343 (88%)	282 (93%)	21 (7%)	0	100	100
1	a	328/343 (96%)	306 (93%)	22 (7%)	0	100	100
2	B	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
2	b	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
3	C	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
3	c	429/459 (94%)	402 (94%)	27 (6%)	0	100	100
4	D	334/352 (95%)	308 (92%)	26 (8%)	0	100	100
4	d	334/352 (95%)	307 (92%)	27 (8%)	0	100	100
5	E	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
5	e	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
7	h	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
9	K	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	k	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	L	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
10	l	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
11	M	27/34 (79%)	27 (100%)	0	0	100	100
11	m	27/34 (79%)	27 (100%)	0	0	100	100
12	O	187/247 (76%)	162 (87%)	24 (13%)	1 (0%)	32	74
12	o	187/247 (76%)	163 (87%)	23 (12%)	1 (0%)	32	74
13	T	27/33 (82%)	27 (100%)	0	0	100	100
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	W	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
14	w	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
15	X	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
15	x	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	R	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
17	r	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
18	S	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
18	s	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
19	1	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	2	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	3	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	5	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	6	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	7	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	G	217/224 (97%)	203 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	N	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	Y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	g	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	n	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
20	4	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
20	8	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
All	All	8149/9096 (90%)	7521 (92%)	626 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	O	194	ILE
12	o	194	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/278 (89%)	247 (100%)	0	100	100
1	a	267/278 (96%)	267 (100%)	0	100	100
2	B	379/401 (94%)	379 (100%)	0	100	100
2	b	379/401 (94%)	379 (100%)	0	100	100
3	C	340/359 (95%)	339 (100%)	1 (0%)	94	96
3	c	340/359 (95%)	339 (100%)	1 (0%)	94	96
4	D	269/282 (95%)	268 (100%)	1 (0%)	93	95
4	d	269/282 (95%)	268 (100%)	1 (0%)	93	95
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	24/34 (71%)	24 (100%)	0	100	100
7	H	43/60 (72%)	43 (100%)	0	100	100
7	h	43/60 (72%)	43 (100%)	0	100	100
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	K	31/32 (97%)	31 (100%)	0	100	100
9	k	31/32 (97%)	31 (100%)	0	100	100
10	L	34/36 (94%)	34 (100%)	0	100	100
10	l	34/36 (94%)	34 (100%)	0	100	100
11	M	25/30 (83%)	25 (100%)	0	100	100
11	m	25/30 (83%)	24 (96%)	1 (4%)	36	65
12	O	164/204 (80%)	164 (100%)	0	100	100
12	o	164/204 (80%)	164 (100%)	0	100	100
13	T	26/30 (87%)	26 (100%)	0	100	100
13	t	26/30 (87%)	26 (100%)	0	100	100
14	W	40/47 (85%)	40 (100%)	0	100	100
14	w	40/47 (85%)	40 (100%)	0	100	100
15	X	27/92 (29%)	27 (100%)	0	100	100
15	x	27/92 (29%)	27 (100%)	0	100	100
16	Z	53/54 (98%)	53 (100%)	0	100	100
16	z	53/54 (98%)	53 (100%)	0	100	100
17	R	150/201 (75%)	150 (100%)	0	100	100
17	r	150/201 (75%)	150 (100%)	0	100	100
18	S	165/180 (92%)	164 (99%)	1 (1%)	89	94
18	s	165/180 (92%)	164 (99%)	1 (1%)	89	94
19	1	167/170 (98%)	167 (100%)	0	100	100
19	2	167/170 (98%)	167 (100%)	0	100	100
19	3	167/170 (98%)	167 (100%)	0	100	100
19	5	167/170 (98%)	167 (100%)	0	100	100
19	6	167/170 (98%)	167 (100%)	0	100	100
19	7	167/170 (98%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	G	167/170 (98%)	167 (100%)	0	100	100
19	N	167/170 (98%)	167 (100%)	0	100	100
19	Y	167/170 (98%)	167 (100%)	0	100	100
19	g	167/170 (98%)	167 (100%)	0	100	100
19	n	167/170 (98%)	167 (100%)	0	100	100
19	y	167/170 (98%)	167 (100%)	0	100	100
20	4	156/158 (99%)	156 (100%)	0	100	100
20	8	156/158 (99%)	156 (100%)	0	100	100
All	All	6560/7208 (91%)	6553 (100%)	7 (0%)	95	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	m	16	LEU
18	s	102	LYS
3	c	26	ARG
4	D	19	MET
18	S	102	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
19	G	122	ASN
17	r	182	GLN
19	6	95	ASN
19	G	156	GLN
19	N	156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 316 ligands modelled in this entry, 2 are monoatomic - leaving 314 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$
25	CHL	1	601	19	41,54,74	5.27	24 (58%)	24,90,114	3.64	14 (58%)
22	CLA	1	602	19	33,53,73	2.18	10 (30%)	37,89,113	3.41	18 (48%)
22	CLA	1	603	-	33,53,73	2.21	10 (30%)	37,89,113	3.37	19 (51%)
22	CLA	1	604	-	33,53,73	2.16	9 (27%)	37,89,113	3.39	17 (45%)
25	CHL	1	605	19	40,50,74	5.42	23 (57%)	25,85,114	3.43	15 (60%)
25	CHL	1	606	-	41,54,74	5.34	24 (58%)	24,90,114	3.65	14 (58%)
25	CHL	1	607	-	41,54,74	5.33	24 (58%)	24,90,114	3.76	16 (66%)
25	CHL	1	608	-	41,54,74	5.31	24 (58%)	24,90,114	3.55	14 (58%)
25	CHL	1	609	19	41,54,74	5.36	24 (58%)	24,90,114	3.63	13 (54%)
22	CLA	1	610	19	33,53,73	2.25	8 (24%)	37,89,113	3.39	16 (43%)
22	CLA	1	611	-	33,53,73	2.20	9 (27%)	37,89,113	3.42	17 (45%)
22	CLA	1	612	19	33,53,73	2.17	9 (27%)	37,89,113	3.29	20 (54%)
22	CLA	1	613	19	33,53,73	2.19	9 (27%)	37,89,113	3.35	17 (45%)
22	CLA	1	614	-	33,53,73	2.21	11 (33%)	37,89,113	3.53	19 (51%)
25	CHL	1	615	-	41,54,74	5.31	24 (58%)	24,90,114	3.64	15 (62%)
25	CHL	2	601	19	41,54,74	5.32	24 (58%)	24,90,114	3.64	13 (54%)
22	CLA	2	602	19	33,53,73	2.17	11 (33%)	37,89,113	3.39	17 (45%)
22	CLA	2	603	-	33,53,73	2.19	9 (27%)	37,89,113	3.31	17 (45%)
22	CLA	2	604	-	33,53,73	2.19	10 (30%)	37,89,113	3.37	19 (51%)
25	CHL	2	605	19	40,50,74	5.34	23 (57%)	25,85,114	3.39	14 (56%)
25	CHL	2	606	-	41,54,74	5.36	24 (58%)	24,90,114	3.68	16 (66%)
25	CHL	2	607	-	41,54,74	5.26	24 (58%)	24,90,114	3.60	14 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	2	608	19	41,54,74	5.40	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	2	609	19	33,53,73	2.26	9 (27%)	37,89,113	3.31	18 (48%)
22	CLA	2	610	-	33,53,73	2.23	10 (30%)	37,89,113	3.35	18 (48%)
22	CLA	2	611	19	33,53,73	2.21	9 (27%)	37,89,113	3.25	16 (43%)
22	CLA	2	612	19	33,53,73	2.18	10 (30%)	37,89,113	3.49	16 (43%)
22	CLA	2	613	-	33,53,73	2.28	11 (33%)	37,89,113	3.24	16 (43%)
25	CHL	3	301	-	41,54,74	5.32	24 (58%)	24,90,114	3.59	15 (62%)
25	CHL	3	302	19	41,54,74	5.32	25 (60%)	24,90,114	3.67	13 (54%)
22	CLA	3	303	19	33,53,73	2.19	10 (30%)	37,89,113	3.37	18 (48%)
22	CLA	3	304	-	33,53,73	2.18	11 (33%)	37,89,113	3.32	19 (51%)
22	CLA	3	305	-	33,53,73	2.19	11 (33%)	37,89,113	3.36	19 (51%)
25	CHL	3	306	19	40,50,74	5.32	23 (57%)	25,85,114	3.38	13 (52%)
25	CHL	3	307	-	41,54,74	5.27	24 (58%)	24,90,114	3.69	14 (58%)
25	CHL	3	308	-	41,54,74	5.31	24 (58%)	24,90,114	3.56	12 (50%)
25	CHL	3	309	19	41,54,74	5.37	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	3	310	19	33,53,73	2.30	10 (30%)	37,89,113	3.35	17 (45%)
22	CLA	3	311	-	33,53,73	2.23	11 (33%)	37,89,113	3.36	18 (48%)
22	CLA	3	312	19	33,53,73	2.22	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	3	313	19	33,53,73	2.22	10 (30%)	37,89,113	3.40	17 (45%)
22	CLA	3	314	-	33,53,73	2.26	11 (33%)	37,89,113	3.13	16 (43%)
25	CHL	4	301	-	41,54,74	5.36	24 (58%)	24,90,114	3.52	15 (62%)
22	CLA	4	302	20	33,53,73	2.21	10 (30%)	37,89,113	3.72	19 (51%)
22	CLA	4	303	-	33,53,73	2.23	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	4	304	-	33,53,73	2.19	11 (33%)	37,89,113	3.39	18 (48%)
25	CHL	4	305	20	41,54,74	5.32	24 (58%)	24,90,114	3.84	14 (58%)
25	CHL	4	306	-	41,54,74	5.33	24 (58%)	24,90,114	3.68	14 (58%)
25	CHL	4	307	-	41,54,74	5.35	24 (58%)	24,90,114	8.23	16 (66%)
25	CHL	4	308	20	41,54,74	5.36	24 (58%)	24,90,114	3.59	14 (58%)
22	CLA	4	309	20	33,53,73	2.23	10 (30%)	37,89,113	3.26	19 (51%)
22	CLA	4	310	-	33,53,73	2.24	11 (33%)	37,89,113	3.26	19 (51%)
25	CHL	5	601	19	41,54,74	5.27	24 (58%)	24,90,114	3.64	14 (58%)
22	CLA	5	602	19	33,53,73	2.18	10 (30%)	37,89,113	3.41	18 (48%)
22	CLA	5	603	-	33,53,73	2.21	10 (30%)	37,89,113	3.37	19 (51%)
22	CLA	5	604	-	33,53,73	2.16	9 (27%)	37,89,113	3.39	17 (45%)
25	CHL	5	605	19	40,50,74	5.42	23 (57%)	25,85,114	3.43	15 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	5	606	-	41,54,74	5.34	24 (58%)	24,90,114	3.65	14 (58%)
25	CHL	5	607	-	41,54,74	5.33	24 (58%)	24,90,114	3.76	16 (66%)
25	CHL	5	608	-	41,54,74	5.31	24 (58%)	24,90,114	3.55	14 (58%)
25	CHL	5	609	19	41,54,74	5.36	24 (58%)	24,90,114	3.63	13 (54%)
22	CLA	5	610	19	33,53,73	2.25	8 (24%)	37,89,113	3.39	16 (43%)
22	CLA	5	611	-	33,53,73	2.20	9 (27%)	37,89,113	3.42	17 (45%)
22	CLA	5	612	19	33,53,73	2.17	9 (27%)	37,89,113	3.29	20 (54%)
22	CLA	5	613	19	33,53,73	2.19	9 (27%)	37,89,113	3.35	17 (45%)
22	CLA	5	614	-	33,53,73	2.21	11 (33%)	37,89,113	3.53	19 (51%)
25	CHL	5	615	-	41,54,74	5.31	24 (58%)	24,90,114	3.64	15 (62%)
25	CHL	6	601	19	41,54,74	5.32	24 (58%)	24,90,114	3.64	13 (54%)
22	CLA	6	602	19	33,53,73	2.17	11 (33%)	37,89,113	3.39	17 (45%)
22	CLA	6	603	-	33,53,73	2.19	9 (27%)	37,89,113	3.31	17 (45%)
22	CLA	6	604	-	33,53,73	2.19	10 (30%)	37,89,113	3.37	19 (51%)
25	CHL	6	605	19	40,50,74	5.34	23 (57%)	25,85,114	3.39	14 (56%)
25	CHL	6	606	-	41,54,74	5.36	24 (58%)	24,90,114	3.68	16 (66%)
25	CHL	6	607	-	41,54,74	5.26	24 (58%)	24,90,114	3.60	14 (58%)
25	CHL	6	608	19	41,54,74	5.40	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	6	609	19	33,53,73	2.26	9 (27%)	37,89,113	3.31	18 (48%)
22	CLA	6	610	-	33,53,73	2.23	10 (30%)	37,89,113	3.35	18 (48%)
22	CLA	6	611	19	33,53,73	2.21	9 (27%)	37,89,113	3.25	16 (43%)
22	CLA	6	612	19	33,53,73	2.18	10 (30%)	37,89,113	3.49	16 (43%)
22	CLA	6	613	-	33,53,73	2.28	11 (33%)	37,89,113	3.24	16 (43%)
25	CHL	7	301	-	41,54,74	5.32	24 (58%)	24,90,114	3.59	15 (62%)
25	CHL	7	302	19	41,54,74	5.32	25 (60%)	24,90,114	3.67	13 (54%)
22	CLA	7	303	19	33,53,73	2.19	10 (30%)	37,89,113	3.37	18 (48%)
22	CLA	7	304	-	33,53,73	2.18	11 (33%)	37,89,113	3.32	19 (51%)
22	CLA	7	305	-	33,53,73	2.19	11 (33%)	37,89,113	3.36	19 (51%)
25	CHL	7	306	19	40,50,74	5.32	23 (57%)	25,85,114	3.38	13 (52%)
25	CHL	7	307	-	41,54,74	5.27	24 (58%)	24,90,114	3.69	14 (58%)
25	CHL	7	308	-	41,54,74	5.31	24 (58%)	24,90,114	3.56	12 (50%)
25	CHL	7	309	19	41,54,74	5.37	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	7	310	19	33,53,73	2.30	10 (30%)	37,89,113	3.35	17 (45%)
22	CLA	7	311	-	33,53,73	2.23	11 (33%)	37,89,113	3.36	18 (48%)
22	CLA	7	312	19	33,53,73	2.22	9 (27%)	37,89,113	3.41	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	313	19	33,53,73	2.22	10 (30%)	37,89,113	3.40	17 (45%)
22	CLA	7	314	-	33,53,73	2.26	11 (33%)	37,89,113	3.13	16 (43%)
25	CHL	8	301	-	41,54,74	5.36	24 (58%)	24,90,114	3.52	15 (62%)
22	CLA	8	302	20	33,53,73	2.21	10 (30%)	37,89,113	3.72	19 (51%)
22	CLA	8	303	-	33,53,73	2.23	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	8	304	-	33,53,73	2.19	11 (33%)	37,89,113	3.39	18 (48%)
25	CHL	8	305	20	41,54,74	5.32	24 (58%)	24,90,114	3.84	14 (58%)
25	CHL	8	306	-	41,54,74	5.33	24 (58%)	24,90,114	3.68	14 (58%)
25	CHL	8	307	-	41,54,74	5.35	24 (58%)	24,90,114	8.23	16 (66%)
25	CHL	8	308	20	41,54,74	5.36	24 (58%)	24,90,114	3.59	14 (58%)
22	CLA	8	309	20	33,53,73	2.23	10 (30%)	37,89,113	3.26	19 (51%)
22	CLA	8	310	-	33,53,73	2.24	11 (33%)	37,89,113	3.26	19 (51%)
22	CLA	A	402	-	33,53,73	2.11	7 (21%)	37,89,113	3.55	19 (51%)
22	CLA	A	403	-	33,53,73	2.15	9 (27%)	37,89,113	3.37	19 (51%)
23	PHO	A	404	-	44,49,69	2.02	13 (29%)	59,75,99	2.27	16 (27%)
22	CLA	A	405	-	33,53,73	2.10	8 (24%)	37,89,113	3.51	18 (48%)
22	CLA	B	601	-	33,53,73	2.14	8 (24%)	37,89,113	3.20	16 (43%)
22	CLA	B	602	-	33,53,73	2.16	8 (24%)	37,89,113	3.51	18 (48%)
22	CLA	B	603	-	33,53,73	2.06	7 (21%)	37,89,113	3.51	20 (54%)
22	CLA	B	604	-	33,53,73	1.98	8 (24%)	37,89,113	3.70	19 (51%)
22	CLA	B	605	-	33,53,73	2.03	9 (27%)	37,89,113	3.45	19 (51%)
22	CLA	B	606	-	33,53,73	2.03	7 (21%)	37,89,113	3.34	18 (48%)
22	CLA	B	607	-	33,53,73	2.06	9 (27%)	37,89,113	3.49	19 (51%)
22	CLA	B	608	-	33,53,73	2.11	9 (27%)	37,89,113	3.70	18 (48%)
22	CLA	B	609	-	33,53,73	2.09	9 (27%)	37,89,113	3.59	20 (54%)
22	CLA	B	610	-	33,53,73	2.11	8 (24%)	37,89,113	3.35	18 (48%)
22	CLA	B	611	-	33,53,73	2.13	9 (27%)	37,89,113	3.34	19 (51%)
22	CLA	B	612	-	33,53,73	2.17	8 (24%)	37,89,113	3.62	18 (48%)
22	CLA	B	613	-	33,53,73	2.12	9 (27%)	37,89,113	3.38	21 (56%)
22	CLA	B	614	-	33,53,73	2.19	8 (24%)	37,89,113	3.45	19 (51%)
22	CLA	B	615	-	33,53,73	2.10	8 (24%)	37,89,113	3.82	20 (54%)
22	CLA	B	616	-	33,53,73	2.26	9 (27%)	37,89,113	3.61	21 (56%)
22	CLA	C	501	-	33,53,73	2.08	8 (24%)	37,89,113	3.53	23 (62%)
22	CLA	C	502	-	33,53,73	2.07	8 (24%)	37,89,113	3.09	19 (51%)
22	CLA	C	503	-	33,53,73	2.04	7 (21%)	37,89,113	3.34	20 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	504	-	33,53,73	2.12	9 (27%)	37,89,113	3.48	18 (48%)
22	CLA	C	505	-	33,53,73	2.02	8 (24%)	37,89,113	3.43	19 (51%)
22	CLA	C	506	-	33,53,73	2.07	9 (27%)	37,89,113	3.73	18 (48%)
22	CLA	C	507	-	33,53,73	2.04	8 (24%)	37,89,113	3.50	18 (48%)
22	CLA	C	508	-	33,53,73	2.06	9 (27%)	37,89,113	3.74	20 (54%)
22	CLA	C	509	-	33,53,73	2.16	9 (27%)	37,89,113	3.35	20 (54%)
22	CLA	C	510	-	33,53,73	2.09	8 (24%)	37,89,113	3.67	20 (54%)
22	CLA	C	511	3	33,53,73	2.11	10 (30%)	37,89,113	3.44	20 (54%)
22	CLA	C	512	-	33,53,73	2.16	10 (30%)	37,89,113	3.23	19 (51%)
22	CLA	D	401	-	33,53,73	2.03	8 (24%)	37,89,113	3.43	19 (51%)
23	PHO	D	402	-	44,49,69	2.01	11 (25%)	59,75,99	2.27	18 (30%)
22	CLA	D	403	-	33,53,73	2.13	8 (24%)	37,89,113	3.63	21 (56%)
22	CLA	D	404	-	33,53,73	2.13	9 (27%)	37,89,113	3.42	17 (45%)
24	HEM	E	101	5,6	28,50,50	2.06	4 (14%)	17,82,82	1.28	1 (5%)
25	CHL	G	601	19	41,54,74	5.45	26 (63%)	24,90,114	3.60	15 (62%)
22	CLA	G	602	19	33,53,73	2.09	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	G	603	-	33,53,73	2.07	9 (27%)	37,89,113	3.35	19 (51%)
22	CLA	G	604	-	33,53,73	2.07	9 (27%)	37,89,113	3.45	19 (51%)
25	CHL	G	605	19	40,50,74	5.37	23 (57%)	25,85,114	3.38	15 (60%)
25	CHL	G	606	-	41,54,74	5.49	24 (58%)	24,90,114	3.65	16 (66%)
25	CHL	G	607	-	41,54,74	5.39	24 (58%)	24,90,114	3.64	16 (66%)
25	CHL	G	608	-	41,54,74	5.52	24 (58%)	24,90,114	3.57	14 (58%)
25	CHL	G	609	19	41,54,74	5.54	25 (60%)	24,90,114	3.58	12 (50%)
22	CLA	G	610	19	33,53,73	2.19	7 (21%)	37,89,113	3.33	18 (48%)
22	CLA	G	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.44	20 (54%)
22	CLA	G	612	19	33,53,73	2.10	8 (24%)	37,89,113	3.35	20 (54%)
22	CLA	G	613	19	33,53,73	2.06	8 (24%)	37,89,113	3.44	18 (48%)
22	CLA	G	614	-	33,53,73	2.18	10 (30%)	37,89,113	3.29	20 (54%)
25	CHL	N	601	19	41,54,74	5.49	24 (58%)	24,90,114	3.59	15 (62%)
22	CLA	N	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.44	17 (45%)
22	CLA	N	603	-	33,53,73	2.01	8 (24%)	37,89,113	3.37	19 (51%)
22	CLA	N	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.38	18 (48%)
25	CHL	N	605	19	40,50,74	5.54	24 (60%)	25,85,114	3.43	16 (64%)
25	CHL	N	606	-	41,54,74	5.55	23 (56%)	24,90,114	3.67	15 (62%)
25	CHL	N	607	-	41,54,74	5.57	25 (60%)	24,90,114	3.69	17 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	N	608	-	41,54,74	5.54	24 (58%)	24,90,114	3.54	15 (62%)
25	CHL	N	609	19	41,54,74	5.64	25 (60%)	24,90,114	3.52	14 (58%)
22	CLA	N	610	19	33,53,73	2.15	8 (24%)	37,89,113	3.34	17 (45%)
22	CLA	N	611	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	21 (56%)
22	CLA	N	612	19	33,53,73	2.09	8 (24%)	37,89,113	3.36	18 (48%)
22	CLA	N	613	19	33,53,73	2.04	9 (27%)	37,89,113	3.47	17 (45%)
22	CLA	N	614	-	33,53,73	2.24	11 (33%)	37,89,113	3.25	17 (45%)
22	CLA	R	301	17	33,53,73	2.14	8 (24%)	37,89,113	3.42	19 (51%)
22	CLA	R	302	-	33,53,73	2.19	8 (24%)	37,89,113	3.35	16 (43%)
22	CLA	R	303	-	33,53,73	2.07	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	R	304	-	41,54,74	5.47	24 (58%)	24,90,114	3.79	16 (66%)
25	CHL	R	305	-	41,54,74	5.48	24 (58%)	24,90,114	3.78	16 (66%)
25	CHL	R	306	-	41,54,74	5.40	25 (60%)	24,90,114	3.62	15 (62%)
22	CLA	R	307	17	33,53,73	2.12	9 (27%)	37,89,113	3.39	17 (45%)
22	CLA	R	308	17	33,53,73	2.19	9 (27%)	37,89,113	3.30	19 (51%)
22	CLA	R	309	-	33,53,73	2.10	8 (24%)	37,89,113	3.41	19 (51%)
22	CLA	R	310	-	33,53,73	2.15	8 (24%)	37,89,113	3.30	17 (45%)
22	CLA	R	311	17	33,53,73	2.14	9 (27%)	37,89,113	3.50	17 (45%)
22	CLA	R	312	20,17	33,53,73	2.18	11 (33%)	37,89,113	3.36	20 (54%)
22	CLA	S	301	-	33,53,73	2.19	8 (24%)	37,89,113	3.53	18 (48%)
25	CHL	S	302	18	41,54,74	5.54	25 (60%)	24,90,114	3.58	14 (58%)
22	CLA	S	303	18	33,53,73	2.12	9 (27%)	37,89,113	3.41	19 (51%)
22	CLA	S	304	-	33,53,73	2.19	9 (27%)	37,89,113	3.09	17 (45%)
22	CLA	S	305	-	33,53,73	2.12	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	S	306	18	41,54,74	5.42	24 (58%)	24,90,114	3.79	15 (62%)
25	CHL	S	307	-	41,54,74	5.53	24 (58%)	24,90,114	8.30	17 (70%)
25	CHL	S	308	-	41,54,74	5.50	26 (63%)	24,90,114	3.52	15 (62%)
22	CLA	S	309	18	33,53,73	2.16	9 (27%)	37,89,113	3.32	19 (51%)
22	CLA	S	310	18	33,53,73	2.06	9 (27%)	37,89,113	3.37	19 (51%)
22	CLA	S	311	-	33,53,73	2.07	7 (21%)	37,89,113	3.43	19 (51%)
22	CLA	S	312	18	33,53,73	2.08	9 (27%)	37,89,113	3.44	20 (54%)
22	CLA	S	313	18	33,53,73	2.03	8 (24%)	37,89,113	3.42	21 (56%)
22	CLA	S	314	-	33,53,73	2.05	8 (24%)	37,89,113	3.53	19 (51%)
25	CHL	Y	601	19	41,54,74	5.46	25 (60%)	24,90,114	3.56	15 (62%)
22	CLA	Y	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.46	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Y	603	-	33,53,73	2.00	8 (24%)	37,89,113	3.45	20 (54%)
22	CLA	Y	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.66	19 (51%)
25	CHL	Y	605	19	40,50,74	5.68	24 (60%)	25,85,114	3.43	18 (72%)
25	CHL	Y	606	-	41,54,74	5.47	23 (56%)	24,90,114	3.83	14 (58%)
25	CHL	Y	607	-	41,54,74	5.53	25 (60%)	24,90,114	3.67	17 (70%)
25	CHL	Y	608	-	41,54,74	5.55	25 (60%)	24,90,114	3.53	15 (62%)
25	CHL	Y	609	19	41,54,74	5.67	24 (58%)	24,90,114	3.67	13 (54%)
22	CLA	Y	610	19	33,53,73	2.13	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	Y	611	-	33,53,73	2.05	8 (24%)	37,89,113	3.54	18 (48%)
22	CLA	Y	612	19	33,53,73	1.99	8 (24%)	37,89,113	3.29	20 (54%)
22	CLA	Y	613	19	33,53,73	2.02	9 (27%)	37,89,113	3.60	17 (45%)
22	CLA	Y	614	-	33,53,73	2.07	7 (21%)	37,89,113	3.46	21 (56%)
22	CLA	a	402	-	33,53,73	2.12	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	a	403	-	33,53,73	2.09	8 (24%)	37,89,113	3.52	19 (51%)
23	PHO	a	404	-	44,49,69	2.02	12 (27%)	59,75,99	2.19	17 (28%)
22	CLA	a	405	-	33,53,73	2.10	7 (21%)	37,89,113	3.62	20 (54%)
22	CLA	b	601	-	33,53,73	2.15	8 (24%)	37,89,113	3.25	18 (48%)
22	CLA	b	602	-	33,53,73	2.06	8 (24%)	37,89,113	3.44	16 (43%)
22	CLA	b	603	-	33,53,73	2.09	9 (27%)	37,89,113	3.37	20 (54%)
22	CLA	b	604	-	33,53,73	2.06	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	b	605	-	33,53,73	2.13	8 (24%)	37,89,113	3.29	18 (48%)
22	CLA	b	606	-	33,53,73	2.25	11 (33%)	37,89,113	2.98	18 (48%)
22	CLA	b	607	-	33,53,73	2.06	9 (27%)	37,89,113	3.44	19 (51%)
22	CLA	b	608	-	33,53,73	2.07	8 (24%)	37,89,113	3.28	20 (54%)
22	CLA	b	609	-	33,53,73	2.05	8 (24%)	37,89,113	3.63	20 (54%)
22	CLA	b	610	-	33,53,73	2.15	10 (30%)	37,89,113	3.48	19 (51%)
22	CLA	b	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.52	21 (56%)
22	CLA	b	612	-	33,53,73	2.24	10 (30%)	37,89,113	3.24	19 (51%)
22	CLA	b	613	-	33,53,73	2.13	9 (27%)	37,89,113	3.73	23 (62%)
22	CLA	b	614	-	33,53,73	2.08	9 (27%)	37,89,113	3.43	18 (48%)
22	CLA	b	615	-	33,53,73	2.11	8 (24%)	37,89,113	3.13	18 (48%)
22	CLA	b	616	-	33,53,73	2.00	9 (27%)	37,89,113	3.65	24 (64%)
22	CLA	c	501	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	20 (54%)
22	CLA	c	502	-	33,53,73	2.02	8 (24%)	37,89,113	3.42	20 (54%)
22	CLA	c	503	-	33,53,73	2.03	7 (21%)	37,89,113	3.51	19 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	504	-	33,53,73	2.14	9 (27%)	37,89,113	3.34	17 (45%)
22	CLA	c	505	-	33,53,73	2.03	7 (21%)	37,89,113	3.49	21 (56%)
22	CLA	c	506	-	33,53,73	2.09	9 (27%)	37,89,113	3.68	19 (51%)
22	CLA	c	507	-	33,53,73	1.99	7 (21%)	37,89,113	3.50	19 (51%)
22	CLA	c	508	-	33,53,73	2.06	9 (27%)	37,89,113	3.64	20 (54%)
22	CLA	c	509	-	33,53,73	2.16	8 (24%)	37,89,113	3.29	18 (48%)
22	CLA	c	510	-	33,53,73	2.18	8 (24%)	37,89,113	3.44	19 (51%)
22	CLA	c	511	3	33,53,73	2.08	9 (27%)	37,89,113	3.33	18 (48%)
22	CLA	c	512	-	33,53,73	2.10	9 (27%)	37,89,113	3.63	20 (54%)
22	CLA	d	401	-	33,53,73	2.07	8 (24%)	37,89,113	3.39	19 (51%)
23	PHO	d	402	-	44,49,69	2.04	11 (25%)	59,75,99	2.22	17 (28%)
22	CLA	d	403	-	33,53,73	2.15	8 (24%)	37,89,113	3.60	22 (59%)
22	CLA	d	404	-	33,53,73	2.15	9 (27%)	37,89,113	3.25	17 (45%)
24	HEM	e	101	5,6	28,50,50	2.12	4 (14%)	17,82,82	1.49	3 (17%)
25	CHL	g	601	19	41,54,74	5.45	26 (63%)	24,90,114	3.60	15 (62%)
22	CLA	g	602	19	33,53,73	2.09	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	g	603	-	33,53,73	2.07	9 (27%)	37,89,113	3.35	19 (51%)
22	CLA	g	604	-	33,53,73	2.07	9 (27%)	37,89,113	3.45	19 (51%)
25	CHL	g	605	19	40,50,74	5.37	23 (57%)	25,85,114	3.38	15 (60%)
25	CHL	g	606	-	41,54,74	5.49	24 (58%)	24,90,114	3.65	16 (66%)
25	CHL	g	607	-	41,54,74	5.39	24 (58%)	24,90,114	3.64	16 (66%)
25	CHL	g	608	-	41,54,74	5.52	24 (58%)	24,90,114	3.57	14 (58%)
25	CHL	g	609	19	41,54,74	5.54	25 (60%)	24,90,114	3.58	12 (50%)
22	CLA	g	610	19	33,53,73	2.19	7 (21%)	37,89,113	3.33	18 (48%)
22	CLA	g	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.44	20 (54%)
22	CLA	g	612	19	33,53,73	2.10	8 (24%)	37,89,113	3.35	20 (54%)
22	CLA	g	613	19	33,53,73	2.06	8 (24%)	37,89,113	3.44	18 (48%)
22	CLA	g	614	-	33,53,73	2.18	10 (30%)	37,89,113	3.29	20 (54%)
25	CHL	n	601	19	41,54,74	5.49	24 (58%)	24,90,114	3.59	15 (62%)
22	CLA	n	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.44	17 (45%)
22	CLA	n	603	-	33,53,73	2.01	8 (24%)	37,89,113	3.37	19 (51%)
22	CLA	n	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.38	18 (48%)
25	CHL	n	605	19	40,50,74	5.54	24 (60%)	25,85,114	3.43	16 (64%)
25	CHL	n	606	-	41,54,74	5.55	23 (56%)	24,90,114	3.67	15 (62%)
25	CHL	n	607	-	41,54,74	5.57	25 (60%)	24,90,114	3.69	17 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	n	608	-	41,54,74	5.54	24 (58%)	24,90,114	3.54	15 (62%)
25	CHL	n	609	19	41,54,74	5.64	25 (60%)	24,90,114	3.52	14 (58%)
22	CLA	n	610	19	33,53,73	2.15	8 (24%)	37,89,113	3.34	17 (45%)
22	CLA	n	611	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	21 (56%)
22	CLA	n	612	19	33,53,73	2.09	8 (24%)	37,89,113	3.36	18 (48%)
22	CLA	n	613	19	33,53,73	2.04	9 (27%)	37,89,113	3.47	17 (45%)
22	CLA	n	614	-	33,53,73	2.24	11 (33%)	37,89,113	3.25	17 (45%)
22	CLA	r	301	17	33,53,73	2.14	8 (24%)	37,89,113	3.42	19 (51%)
22	CLA	r	302	-	33,53,73	2.19	8 (24%)	37,89,113	3.35	16 (43%)
22	CLA	r	303	-	33,53,73	2.07	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	r	304	-	41,54,74	5.47	24 (58%)	24,90,114	3.79	16 (66%)
25	CHL	r	305	-	41,54,74	5.48	24 (58%)	24,90,114	3.78	16 (66%)
25	CHL	r	306	-	41,54,74	5.40	25 (60%)	24,90,114	3.62	15 (62%)
22	CLA	r	307	17	33,53,73	2.12	9 (27%)	37,89,113	3.39	17 (45%)
22	CLA	r	308	17	33,53,73	2.19	9 (27%)	37,89,113	3.30	19 (51%)
22	CLA	r	309	-	33,53,73	2.10	8 (24%)	37,89,113	3.41	19 (51%)
22	CLA	r	310	-	33,53,73	2.15	8 (24%)	37,89,113	3.30	17 (45%)
22	CLA	r	311	17	33,53,73	2.14	9 (27%)	37,89,113	3.50	17 (45%)
22	CLA	r	312	20,17	33,53,73	2.18	11 (33%)	37,89,113	3.36	20 (54%)
22	CLA	s	301	-	33,53,73	2.17	9 (27%)	37,89,113	3.22	19 (51%)
25	CHL	s	302	18	41,54,74	5.54	25 (60%)	24,90,114	3.58	14 (58%)
22	CLA	s	303	18	33,53,73	2.12	9 (27%)	37,89,113	3.41	19 (51%)
22	CLA	s	304	-	33,53,73	2.19	9 (27%)	37,89,113	3.09	17 (45%)
22	CLA	s	305	-	33,53,73	2.12	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	s	306	18	41,54,74	5.42	24 (58%)	24,90,114	3.79	15 (62%)
25	CHL	s	307	-	41,54,74	5.53	24 (58%)	24,90,114	8.30	17 (70%)
25	CHL	s	308	-	41,54,74	5.50	26 (63%)	24,90,114	3.52	15 (62%)
22	CLA	s	309	18	33,53,73	2.16	9 (27%)	37,89,113	3.32	19 (51%)
22	CLA	s	310	18	33,53,73	2.06	9 (27%)	37,89,113	3.37	19 (51%)
22	CLA	s	311	-	33,53,73	2.07	7 (21%)	37,89,113	3.43	19 (51%)
22	CLA	s	312	18	33,53,73	2.08	9 (27%)	37,89,113	3.44	20 (54%)
22	CLA	s	313	18	33,53,73	2.03	8 (24%)	37,89,113	3.42	21 (56%)
22	CLA	s	314	-	33,53,73	2.05	8 (24%)	37,89,113	3.53	19 (51%)
25	CHL	y	601	19	41,54,74	5.46	25 (60%)	24,90,114	3.56	15 (62%)
22	CLA	y	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.46	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	y	603	-	33,53,73	2.00	8 (24%)	37,89,113	3.45	20 (54%)
22	CLA	y	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.66	19 (51%)
25	CHL	y	605	19	40,50,74	5.68	24 (60%)	25,85,114	3.43	18 (72%)
25	CHL	y	606	-	41,54,74	5.47	23 (56%)	24,90,114	3.83	14 (58%)
25	CHL	y	607	-	41,54,74	5.53	25 (60%)	24,90,114	3.67	17 (70%)
25	CHL	y	608	-	41,54,74	5.55	25 (60%)	24,90,114	3.53	15 (62%)
25	CHL	y	609	19	41,54,74	5.67	24 (58%)	24,90,114	3.67	13 (54%)
22	CLA	y	610	19	33,53,73	2.13	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	y	611	-	33,53,73	2.05	8 (24%)	37,89,113	3.54	18 (48%)
22	CLA	y	612	19	33,53,73	1.99	8 (24%)	37,89,113	3.29	20 (54%)
22	CLA	y	613	19	33,53,73	2.02	9 (27%)	37,89,113	3.60	17 (45%)
22	CLA	y	614	-	33,53,73	2.07	7 (21%)	37,89,113	3.46	21 (56%)

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
25	CHL	1	601	19	-	0/15/153/177	0/0/9/9
22	CLA	1	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	1	605	19	-	0/12/148/177	0/0/9/9
25	CHL	1	606	-	-	1/15/153/177	0/0/9/9
25	CHL	1	607	-	-	0/15/153/177	0/0/9/9
25	CHL	1	608	-	-	0/15/153/177	0/0/9/9
25	CHL	1	609	19	-	0/15/153/177	0/0/9/9
22	CLA	1	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	1	615	-	-	0/15/153/177	0/0/9/9
25	CHL	2	601	19	-	0/15/153/177	0/0/9/9
22	CLA	2	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	603	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	2	605	19	-	0/12/148/177	0/0/9/9
25	CHL	2	606	-	-	1/15/153/177	0/0/9/9
25	CHL	2	607	-	-	0/15/153/177	0/0/9/9
25	CHL	2	608	19	-	0/15/153/177	0/0/9/9
22	CLA	2	609	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	611	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	613	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	3	301	-	-	0/15/153/177	0/0/9/9
25	CHL	3	302	19	-	0/15/153/177	0/0/9/9
22	CLA	3	303	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	3	306	19	-	0/12/148/177	0/0/9/9
25	CHL	3	307	-	-	1/15/153/177	0/0/9/9
25	CHL	3	308	-	-	0/15/153/177	0/0/9/9
25	CHL	3	309	19	-	0/15/153/177	0/0/9/9
22	CLA	3	310	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	312	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	313	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	4	301	-	-	0/15/153/177	0/0/9/9
22	CLA	4	302	20	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	4	303	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	4	304	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	4	305	20	-	0/15/153/177	0/0/9/9
25	CHL	4	306	-	-	0/15/153/177	0/0/9/9
25	CHL	4	307	-	-	0/15/153/177	0/0/9/9
25	CHL	4	308	20	-	0/15/153/177	0/0/9/9
22	CLA	4	309	20	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	4	310	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	5	601	19	-	0/15/153/177	0/0/9/9
22	CLA	5	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	603	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	5	605	19	-	0/12/148/177	0/0/9/9
25	CHL	5	606	-	-	1/15/153/177	0/0/9/9
25	CHL	5	607	-	-	0/15/153/177	0/0/9/9
25	CHL	5	608	-	-	0/15/153/177	0/0/9/9
25	CHL	5	609	19	-	0/15/153/177	0/0/9/9
22	CLA	5	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	5	615	-	-	0/15/153/177	0/0/9/9
25	CHL	6	601	19	-	0/15/153/177	0/0/9/9
22	CLA	6	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	6	605	19	-	0/12/148/177	0/0/9/9
25	CHL	6	606	-	-	1/15/153/177	0/0/9/9
25	CHL	6	607	-	-	0/15/153/177	0/0/9/9
25	CHL	6	608	19	-	0/15/153/177	0/0/9/9
22	CLA	6	609	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	611	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	613	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	7	301	-	-	0/15/153/177	0/0/9/9
25	CHL	7	302	19	-	0/15/153/177	0/0/9/9
22	CLA	7	303	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	7	306	19	-	0/12/148/177	0/0/9/9
25	CHL	7	307	-	-	1/15/153/177	0/0/9/9
25	CHL	7	308	-	-	0/15/153/177	0/0/9/9
25	CHL	7	309	19	-	0/15/153/177	0/0/9/9
22	CLA	7	310	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	312	19	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	313	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	8	301	-	-	0/15/153/177	0/0/9/9
22	CLA	8	302	20	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	8	303	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	8	304	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	8	305	20	-	0/15/153/177	0/0/9/9
25	CHL	8	306	-	-	0/15/153/177	0/0/9/9
25	CHL	8	307	-	-	0/15/153/177	0/0/9/9
25	CHL	8	308	20	-	0/15/153/177	0/0/9/9
22	CLA	8	309	20	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	8	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	A	402	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	A	403	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	A	404	-	-	0/27/79/103	0/1/6/6
22	CLA	A	405	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	601	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	602	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	603	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	604	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	605	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	606	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	607	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	608	-	1/1/16/25	0/11/111/135	0/0/9/9
22	CLA	B	609	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	612	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	613	-	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	B	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	615	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	616	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	501	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	502	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	503	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	504	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	505	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	C	506	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	507	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	508	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	509	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	510	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	511	3	1/1/16/25	1/11/111/135	0/0/9/9
22	CLA	C	512	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	D	401	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	D	402	-	-	0/27/79/103	0/1/6/6
22	CLA	D	403	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	D	404	-	3/3/16/25	0/11/111/135	0/0/9/9
24	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
25	CHL	G	601	19	-	0/15/153/177	0/0/9/9
22	CLA	G	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	G	605	19	-	0/12/148/177	0/0/9/9
25	CHL	G	606	-	-	1/15/153/177	0/0/9/9
25	CHL	G	607	-	-	0/15/153/177	0/0/9/9
25	CHL	G	608	-	-	0/15/153/177	0/0/9/9
25	CHL	G	609	19	-	0/15/153/177	0/0/9/9
22	CLA	G	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	N	601	19	-	0/15/153/177	0/0/9/9
22	CLA	N	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	N	605	19	-	0/12/148/177	0/0/9/9
25	CHL	N	606	-	-	1/15/153/177	0/0/9/9
25	CHL	N	607	-	-	0/15/153/177	0/0/9/9
25	CHL	N	608	-	-	0/15/153/177	0/0/9/9
25	CHL	N	609	19	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	N	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	301	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	302	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	303	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	R	304	-	-	0/15/153/177	0/0/9/9
25	CHL	R	305	-	-	1/15/153/177	0/0/9/9
25	CHL	R	306	-	-	0/15/153/177	0/0/9/9
22	CLA	R	307	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	308	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	309	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	311	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	312	20,17	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	301	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	S	302	18	-	0/15/153/177	0/0/9/9
22	CLA	S	303	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	S	306	18	-	0/15/153/177	0/0/9/9
25	CHL	S	307	-	-	0/15/153/177	0/0/9/9
25	CHL	S	308	-	-	0/15/153/177	0/0/9/9
22	CLA	S	309	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	310	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	312	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	313	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	Y	601	19	-	0/15/153/177	0/0/9/9
22	CLA	Y	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	Y	605	19	-	0/12/148/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	Y	606	-	-	1/15/153/177	0/0/9/9
25	CHL	Y	607	-	-	0/15/153/177	0/0/9/9
25	CHL	Y	608	-	-	0/15/153/177	0/0/9/9
25	CHL	Y	609	19	-	0/15/153/177	0/0/9/9
22	CLA	Y	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	a	402	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	a	403	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	a	404	-	-	0/27/79/103	0/1/6/6
22	CLA	a	405	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	601	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	602	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	603	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	604	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	605	-	1/1/16/25	0/11/111/135	0/0/9/9
22	CLA	b	606	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	607	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	608	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	609	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	611	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	612	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	613	-	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	b	614	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	615	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	616	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	501	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	502	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	503	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	504	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	505	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	506	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	508	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	509	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	510	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	511	3	1/1/16/25	1/11/111/135	0/0/9/9
22	CLA	c	512	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	d	401	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	d	402	-	-	0/27/79/103	0/1/6/6
22	CLA	d	403	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	d	404	-	3/3/16/25	0/11/111/135	0/0/9/9
24	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
25	CHL	g	601	19	-	0/15/153/177	0/0/9/9
22	CLA	g	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	g	605	19	-	0/12/148/177	0/0/9/9
25	CHL	g	606	-	-	1/15/153/177	0/0/9/9
25	CHL	g	607	-	-	0/15/153/177	0/0/9/9
25	CHL	g	608	-	-	0/15/153/177	0/0/9/9
25	CHL	g	609	19	-	0/15/153/177	0/0/9/9
22	CLA	g	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	n	601	19	-	0/15/153/177	0/0/9/9
22	CLA	n	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	n	605	19	-	0/12/148/177	0/0/9/9
25	CHL	n	606	-	-	1/15/153/177	0/0/9/9
25	CHL	n	607	-	-	0/15/153/177	0/0/9/9
25	CHL	n	608	-	-	0/15/153/177	0/0/9/9
25	CHL	n	609	19	-	0/15/153/177	0/0/9/9
22	CLA	n	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	612	19	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	n	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	301	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	302	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	303	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	r	304	-	-	0/15/153/177	0/0/9/9
25	CHL	r	305	-	-	1/15/153/177	0/0/9/9
25	CHL	r	306	-	-	0/15/153/177	0/0/9/9
22	CLA	r	307	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	308	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	309	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	311	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	312	20,17	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	301	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	s	302	18	-	0/15/153/177	0/0/9/9
22	CLA	s	303	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	s	306	18	-	0/15/153/177	0/0/9/9
25	CHL	s	307	-	-	0/15/153/177	0/0/9/9
25	CHL	s	308	-	-	0/15/153/177	0/0/9/9
22	CLA	s	309	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	310	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	312	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	313	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	y	601	19	-	0/15/153/177	0/0/9/9
22	CLA	y	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	y	605	19	-	0/12/148/177	0/0/9/9
25	CHL	y	606	-	-	1/15/153/177	0/0/9/9
25	CHL	y	607	-	-	0/15/153/177	0/0/9/9
25	CHL	y	608	-	-	0/15/153/177	0/0/9/9
25	CHL	y	609	19	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	y	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	614	-	3/3/16/25	0/11/111/135	0/0/9/9

The worst 5 of 4253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	608	CHL	C3B-C2B	-15.86	1.35	1.55
25	G	608	CHL	C3B-C2B	-15.86	1.35	1.55
25	g	606	CHL	C3B-C2B	-15.69	1.36	1.55
25	G	606	CHL	C3B-C2B	-15.69	1.36	1.55
25	y	608	CHL	C3B-C2B	-15.63	1.36	1.55

The worst 5 of 5412 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	307	CHL	O2D-CGD-O1D	-23.26	77.05	123.82
25	S	307	CHL	O2D-CGD-O1D	-23.26	77.05	123.82
25	4	307	CHL	O2D-CGD-O1D	-22.59	78.38	123.82
25	8	307	CHL	O2D-CGD-O1D	-22.59	78.38	123.82
25	4	307	CHL	O1D-CGD-CBD	-20.34	82.50	124.53

5 of 613 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	5	604	CLA	NA
22	5	604	CLA	NC
22	5	604	CLA	ND
22	s	309	CLA	NC
22	s	309	CLA	ND

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	2	606	CHL	CED-O2D-CGD-CBD
25	6	606	CHL	CED-O2D-CGD-CBD
22	2	613	CLA	CED-O2D-CGD-CBD
22	6	613	CLA	CED-O2D-CGD-CBD
22	R	312	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

154 monomers are involved in 438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	601	CHL	2	0
25	1	605	CHL	1	0
25	1	606	CHL	1	0
25	1	608	CHL	4	0
25	1	609	CHL	2	0
22	1	611	CLA	1	0
22	1	612	CLA	1	0
22	1	613	CLA	1	0
22	1	614	CLA	2	0
25	1	615	CHL	2	0
25	2	601	CHL	3	0
22	2	602	CLA	1	0
25	2	605	CHL	2	0
25	2	606	CHL	2	0
25	2	607	CHL	5	0
25	2	608	CHL	3	0
22	2	609	CLA	1	0
22	2	610	CLA	2	0
22	2	611	CLA	1	0
22	2	612	CLA	1	0
22	2	613	CLA	15	0
25	3	301	CHL	1	0
25	3	306	CHL	1	0
25	3	308	CHL	4	0
25	3	309	CHL	3	0
22	3	311	CLA	1	0
22	3	313	CLA	1	0
25	4	301	CHL	10	0
22	4	302	CLA	2	0
22	4	303	CLA	1	0
22	4	304	CLA	1	0
25	4	305	CHL	1	0
25	4	306	CHL	2	0
25	4	308	CHL	1	0
22	4	309	CLA	3	0
25	5	601	CHL	2	0
25	5	605	CHL	1	0
25	5	606	CHL	1	0
25	5	608	CHL	4	0
25	5	609	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	610	CLA	1	0
22	5	612	CLA	1	0
22	5	613	CLA	1	0
22	5	614	CLA	2	0
25	6	601	CHL	3	0
22	6	602	CLA	1	0
25	6	605	CHL	2	0
25	6	606	CHL	2	0
25	6	607	CHL	5	0
25	6	608	CHL	3	0
22	6	610	CLA	2	0
22	6	611	CLA	1	0
22	6	612	CLA	1	0
22	6	613	CLA	16	0
25	7	301	CHL	1	0
25	7	306	CHL	1	0
25	7	307	CHL	1	0
25	7	308	CHL	4	0
25	7	309	CHL	3	0
22	7	311	CLA	1	0
22	7	313	CLA	1	0
25	8	301	CHL	12	0
22	8	302	CLA	2	0
22	8	303	CLA	1	0
22	8	304	CLA	1	0
25	8	305	CHL	1	0
25	8	306	CHL	2	0
25	8	307	CHL	1	0
25	8	308	CHL	1	0
22	8	309	CLA	4	0
22	A	402	CLA	2	0
22	A	403	CLA	1	0
23	A	404	PHO	3	0
22	A	405	CLA	1	0
22	B	601	CLA	2	0
22	B	602	CLA	7	0
22	B	603	CLA	3	0
22	B	604	CLA	3	0
22	B	606	CLA	3	0
22	B	607	CLA	2	0
22	B	608	CLA	1	0
22	B	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	610	CLA	1	0
22	B	611	CLA	3	0
22	B	612	CLA	2	0
22	B	613	CLA	1	0
22	B	614	CLA	5	0
22	B	615	CLA	1	0
22	B	616	CLA	3	0
22	C	501	CLA	3	0
22	C	502	CLA	3	0
22	C	504	CLA	1	0
22	C	505	CLA	1	0
22	C	506	CLA	3	0
22	C	507	CLA	1	0
22	C	508	CLA	5	0
22	C	509	CLA	3	0
22	C	510	CLA	1	0
22	C	511	CLA	3	0
22	C	512	CLA	1	0
23	D	402	PHO	2	0
22	D	403	CLA	4	0
24	E	101	HEM	4	0
25	G	601	CHL	2	0
22	G	602	CLA	1	0
25	G	605	CHL	1	0
25	G	606	CHL	2	0
25	G	607	CHL	1	0
25	G	608	CHL	5	0
25	G	609	CHL	3	0
22	G	610	CLA	1	0
22	G	611	CLA	6	0
22	G	612	CLA	2	0
22	G	613	CLA	2	0
22	G	614	CLA	1	0
25	N	601	CHL	1	0
22	N	602	CLA	1	0
25	N	605	CHL	1	0
25	N	606	CHL	3	0
25	N	607	CHL	2	0
25	N	608	CHL	3	0
25	N	609	CHL	2	0
22	N	610	CLA	2	0
22	N	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	613	CLA	1	0
22	R	302	CLA	22	0
22	R	303	CLA	1	0
25	R	304	CHL	1	0
25	R	305	CHL	3	0
25	R	306	CHL	2	0
22	R	307	CLA	2	0
22	R	308	CLA	2	0
22	R	311	CLA	2	0
22	R	312	CLA	72	0
22	S	301	CLA	24	0
25	S	302	CHL	1	0
22	S	303	CLA	3	0
22	S	304	CLA	1	0
25	S	306	CHL	1	0
25	S	308	CHL	2	0
22	S	309	CLA	1	0
22	S	310	CLA	1	0
22	S	313	CLA	3	0
25	Y	601	CHL	2	0
22	Y	602	CLA	1	0
25	Y	605	CHL	3	0
25	Y	606	CHL	3	0
25	Y	607	CHL	1	0
25	Y	608	CHL	2	0
25	Y	609	CHL	3	0
22	Y	610	CLA	1	0
22	Y	611	CLA	1	0
22	Y	613	CLA	2	0
22	Y	614	CLA	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.