



## wwPDB EM Map/Model Validation Report ⓘ

Jun 2, 2016 – 09:45 AM EDT

PDB ID : 3JCU  
EMDB ID: : EMD-6617  
Title : Cryo-EM structure of spinach PSII-LHCII supercomplex at 3.2 Angstrom resolution  
Authors : Wei, X.P.; Zhang, X.Z.; Su, X.D.; Cao, P.; Liu, X.Y.; Li, M.; Chang, W.R.; Liu, Z.F.  
Deposited on : 2016-03-10  
Resolution : 3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

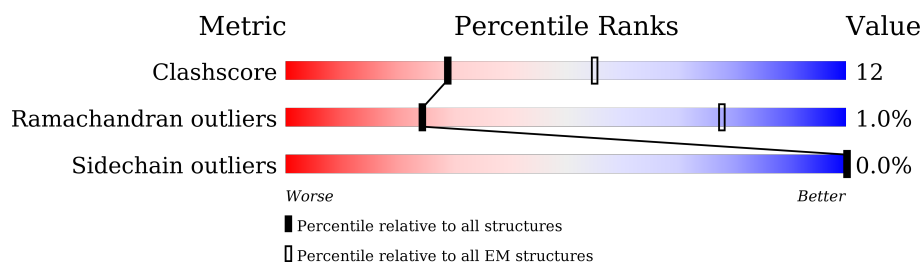
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.



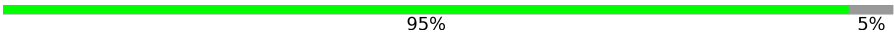









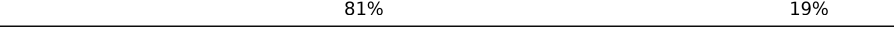
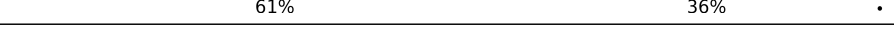
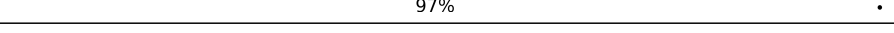


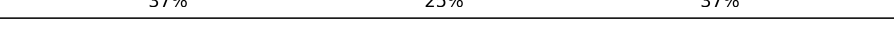


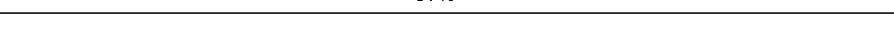






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	344	58% 39% .
1	a	344	97% .
2	B	508	54% 41% .
2	b	508	95% . .
3	C	473	54% 40% 5%
3	c	473	95% 5%
4	D	353	54% 42% .
4	d	353	96% .
5	E	83	66% 29% 5%

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Mol	Chain	Length	Quality of chain
5	e	83	 95% 5%
6	F	39	 64% 18% 18%
6	f	39	 82% 18%
7	G	267	 46% 35% 18%
7	N	267	 48% 34% 18%
7	Y	267	 52% 29% 18%
7	g	267	 81% 18%
7	n	267	 81% 18%
7	y	267	 81% 18%
8	H	73	 47% 34% 19%
8	h	73	 81% 19%
9	I	36	 61% 36% .
9	i	36	 97% .
10	J	40	 55% 30% 15%
10	j	40	 85% 15%
11	K	59	 37% 25% 37%
11	k	59	 63% 37%
12	L	38	 79% 18% .
12	l	38	 97% .
13	M	34	 65% 32% .
13	m	34	 97% .
14	O	332	 33% 39% . 27%
14	o	332	 72% . 27%
15	P	267	 33% 31% 36%
15	p	267	 64% . 36%

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Mol	Chain	Length	Quality of chain
16	Q	232	
16	q	232	
17	R	243	
17	r	243	
18	S	295	
18	s	295	
19	T	33	
19	t	33	
20	U	99	
20	u	99	
21	W	137	
21	w	137	
22	X	117	
22	x	117	
23	Z	62	
23	z	62	

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
27	CLA	A	405	X	-	-	-
27	CLA	A	406	X	-	-	-
27	CLA	A	407	X	-	-	-
27	CLA	A	410	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	616	X	-	-	-
27	CLA	B	617	X	-	-	-
27	CLA	C	501	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	403	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	G	612	X	-	-	-
27	CLA	G	613	X	-	-	-
27	CLA	G	614	X	-	-	-
27	CLA	N	602	X	-	-	-
27	CLA	N	603	X	-	-	-
27	CLA	N	604	X	-	-	-
27	CLA	N	610	X	-	-	-
27	CLA	N	611	X	-	-	-
27	CLA	N	612	X	-	-	-
27	CLA	N	613	X	-	-	-
27	CLA	N	614	X	-	-	-
27	CLA	R	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	R	602	X	-	-	-
27	CLA	R	603	X	-	-	-
27	CLA	R	604	X	-	-	-
27	CLA	R	609	X	-	-	-
27	CLA	R	610	X	-	-	-
27	CLA	R	611	X	-	-	-
27	CLA	R	612	X	-	-	-
27	CLA	R	613	X	-	-	-
27	CLA	R	616	X	-	-	-
27	CLA	S	602	X	-	-	-
27	CLA	S	603	X	-	-	-
27	CLA	S	604	X	-	-	-
27	CLA	S	609	X	-	-	-
27	CLA	S	610	X	-	-	-
27	CLA	S	611	X	-	-	-
27	CLA	S	612	X	-	-	-
27	CLA	S	613	X	-	-	-
27	CLA	S	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-
27	CLA	a	405	X	-	-	-
27	CLA	a	406	X	-	-	-
27	CLA	a	407	X	-	-	-
27	CLA	a	410	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	614	X	-	-	-
27	CLA	b	615	X	-	-	-
27	CLA	b	616	X	-	-	-
27	CLA	b	617	X	-	-	-
27	CLA	c	501	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	403	X	-	-	-
27	CLA	g	602	X	-	-	-
27	CLA	g	603	X	-	-	-
27	CLA	g	604	X	-	-	-
27	CLA	g	610	X	-	-	-
27	CLA	g	611	X	-	-	-
27	CLA	g	612	X	-	-	-
27	CLA	g	613	X	-	-	-
27	CLA	g	614	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	611	X	-	-	-
27	CLA	n	612	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	n	614	X	-	-	-
27	CLA	r	601	X	-	-	-
27	CLA	r	602	X	-	-	-
27	CLA	r	603	X	-	-	-
27	CLA	r	604	X	-	-	-
27	CLA	r	609	X	-	-	-
27	CLA	r	610	X	-	-	-
27	CLA	r	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	r	612	X	-	-	-
27	CLA	r	613	X	-	-	-
27	CLA	r	616	X	-	-	-
27	CLA	s	602	X	-	-	-
27	CLA	s	603	X	-	-	-
27	CLA	s	604	X	-	-	-
27	CLA	s	609	X	-	-	-
27	CLA	s	610	X	-	-	-
27	CLA	s	611	X	-	-	-
27	CLA	s	612	X	-	-	-
27	CLA	s	613	X	-	-	-
27	CLA	s	614	X	-	-	-
27	CLA	y	602	X	-	-	-
27	CLA	y	603	X	-	-	-
27	CLA	y	604	X	-	-	-
27	CLA	y	610	X	-	-	-
27	CLA	y	611	X	-	-	-
27	CLA	y	612	X	-	-	-
27	CLA	y	613	X	-	-	-
27	CLA	y	614	X	-	-	-
33	BCT	D	401	-	-	X	-



## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 75994 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	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		
1	a	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		
2	b	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		
3	c	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		
4	d	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total	C	N	O	0	0
			636	412	104	120		
5	e	79	Total	C	N	O	0	0
			636	412	104	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			257	174	43	39	1		
6	f	32	Total	C	N	O	S	0	0
			257	174	43	39	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	g	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	n	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			434	288	65	78	3		
8	h	59	Total	C	N	O	S	0	0
			434	288	65	78	3		

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	34	Total	C	N	O		0	0
			247	168	38	41			
10	j	34	Total	C	N	O		0	0
			247	168	38	41			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			307	217	43	46	1		
11	k	37	Total	C	N	O	S	0	0
			307	217	43	46	1		

- Molecule 12 is a protein called Protein Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	37	Total	C	N	O		0	0
			311	205	49	57			
12	l	37	Total	C	N	O		0	0
			311	205	49	57			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	33	Total	C	N	O		0	0
			258	176	37	45			
13	m	33	Total	C	N	O		0	0
			258	176	37	45			

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		
14	o	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		
15	p	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O		0	0
			1162	736	202	224			
16	q	148	Total	C	N	O		0	0
			1162	736	202	224			

- Molecule 17 is a protein called Chlorophyll A-B Binding protein 29 kD (CP29).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		
17	r	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		

- Molecule 18 is a protein called Chlorophyll A-B Binding protein 26 kD (CP26).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		
18	s	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		

- Molecule 19 is a protein called Photosystem II Reaction Center protein Tc.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			245	171	34	39	1		
19	t	30	Total	C	N	O	S	0	0
			245	171	34	39	1		

- Molecule 20 is a protein called Photosystem II Reaction Center Tn protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	276	61	81	1		
21	w	54	Total	C	N	O	S	0	0
			419	276	61	81	1		

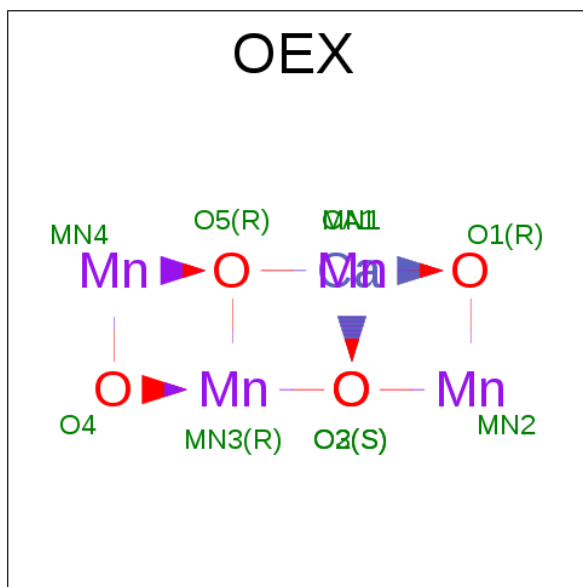
- Molecule 22 is a protein called Photosystem II Reaction Center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	35	Total	C	N	O	0	0
			246	163	38	45		
22	x	35	Total	C	N	O	0	0
			246	163	38	45		

- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	61	Total	C	N	O	0	0
			454	306	68	80		
23	z	61	Total	C	N	O	0	0
			454	306	68	80		

- Molecule 24 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
24	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

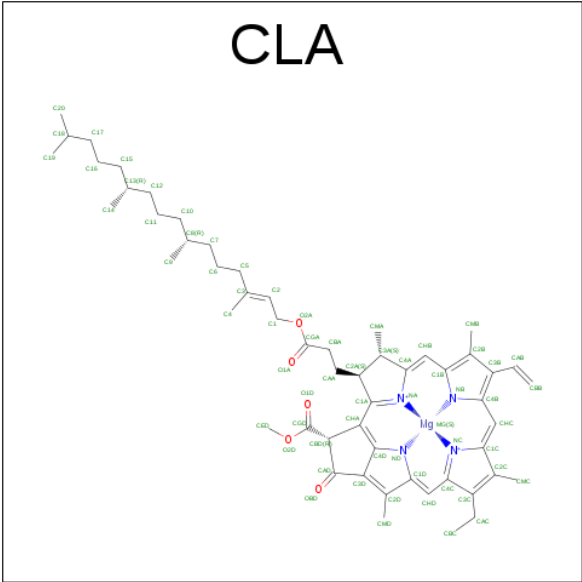
- Molecule 25 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Cl	0
			2	2	
26	a	2	Total	Cl	0
			2	2	

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0

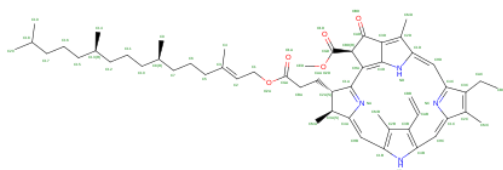
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Mol	Chain	Residues	Atoms					AltConf
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0

- Molecule 28 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).

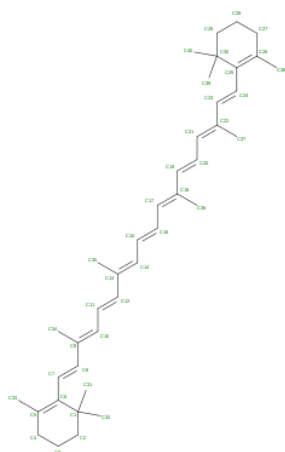
## PHO



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			128	110	8	10	
28	A	1	Total	C	N	O	0
			128	110	8	10	
28	a	1	Total	C	N	O	0
			128	110	8	10	
28	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).

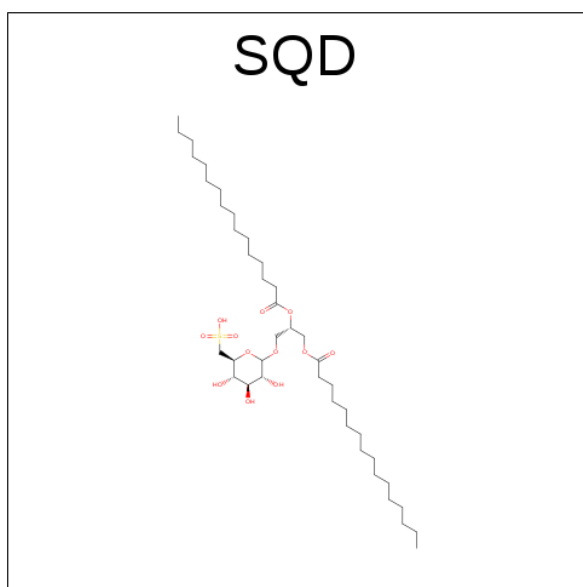
## BCR



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	D	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	d	1	Total C 40 40	0
29	h	1	Total C 40 40	0

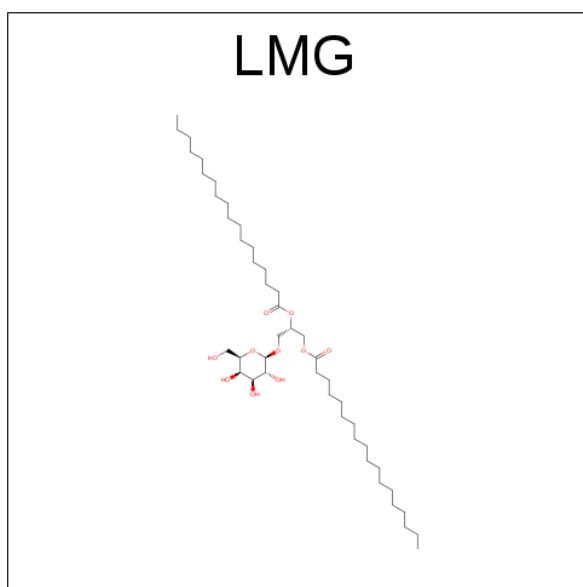
- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).





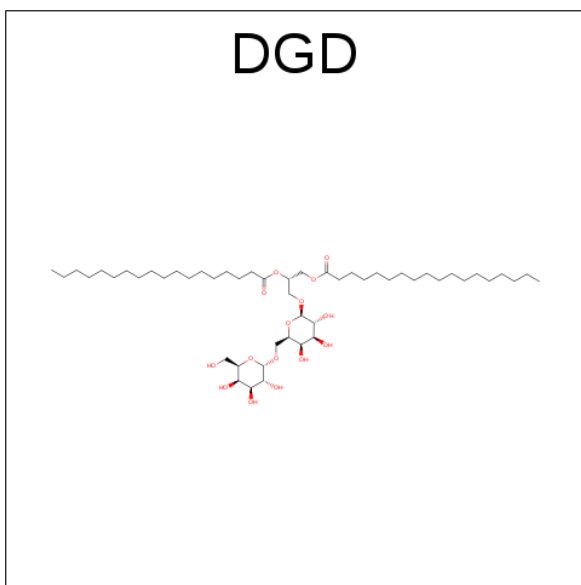
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



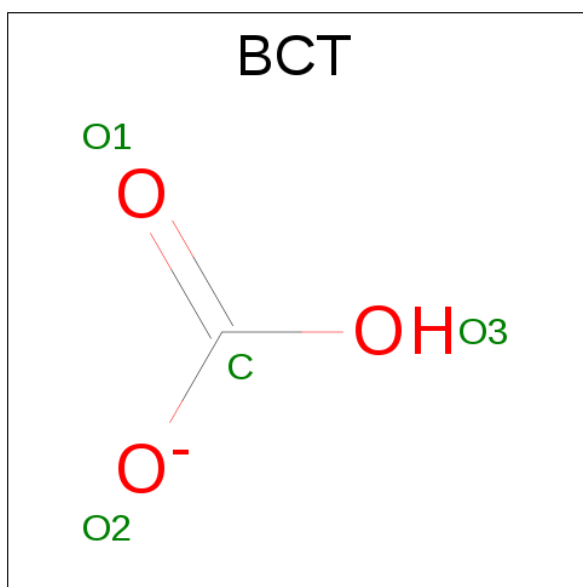
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			48	38	10	
31	B	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	D	1	Total	C	O	0
			46	36	10	
31	Z	1	Total	C	O	0
			51	41	10	
31	a	1	Total	C	O	0
			48	38	10	
31	b	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	d	1	Total	C	O	0
			46	36	10	
31	z	1	Total	C	O	0
			51	41	10	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



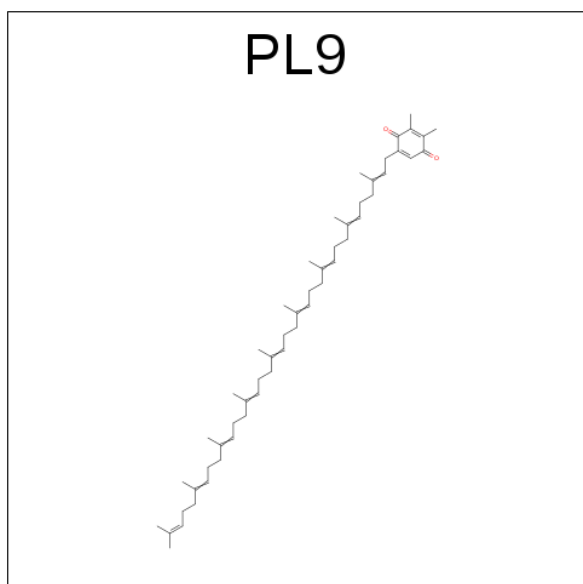
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			179	134	45	
32	C	1	Total	C	O	0
			179	134	45	
32	C	1	Total	C	O	0
			179	134	45	
32	H	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			179	134	45	
32	c	1	Total	C	O	0
			179	134	45	
32	c	1	Total	C	O	0
			179	134	45	
32	h	1	Total	C	O	0
			62	47	15	

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



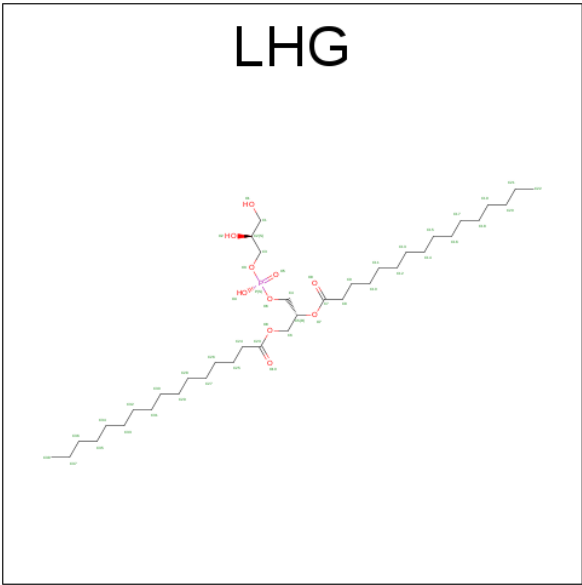
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			55	53	2	
34	d	1	Total	C	O	0
			55	53	2	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



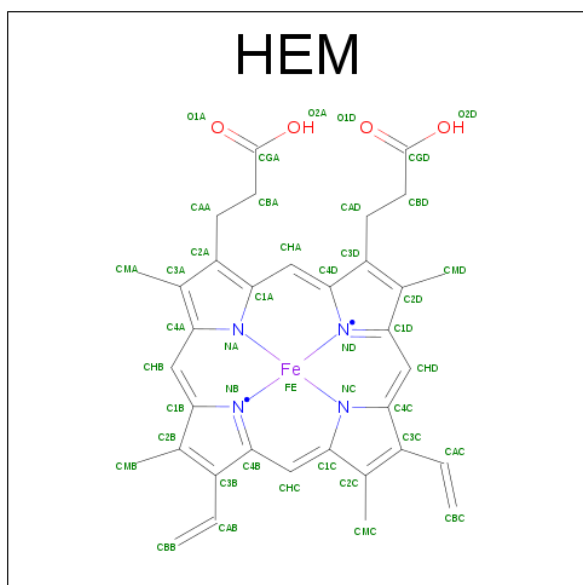
Mol	Chain	Residues	Atoms				AltConf
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			49	38	10	1	
35	R	1	Total	C	O	P	0
			49	38	10	1	
35	S	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	

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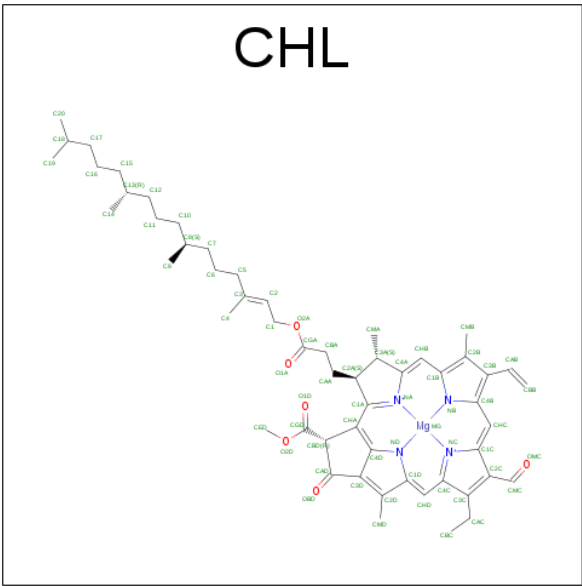
Mol	Chain	Residues	Atoms				AltConf
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	g	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			49	38	10	1	
35	r	1	Total	C	O	P	0
			49	38	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
36	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
37	G	1	Total	C	Mg	N	O	0
	G	1	314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
	G	1	314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
37	G	1	Total	C	Mg	N	O	0
	G	1	314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
	G	1	314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
37	N	1	Total	C	Mg	N	O	0
	N	1	314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
	N	1	314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
37	N	1	Total	C	Mg	N	O	0
	N	1	314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
	N	1	314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
37	R	1	Total	C	Mg	N	O	0
	R	1	150	117	3	12	18	

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Mol	Chain	Residues	Atoms					AltConf
37	R	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	R	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	

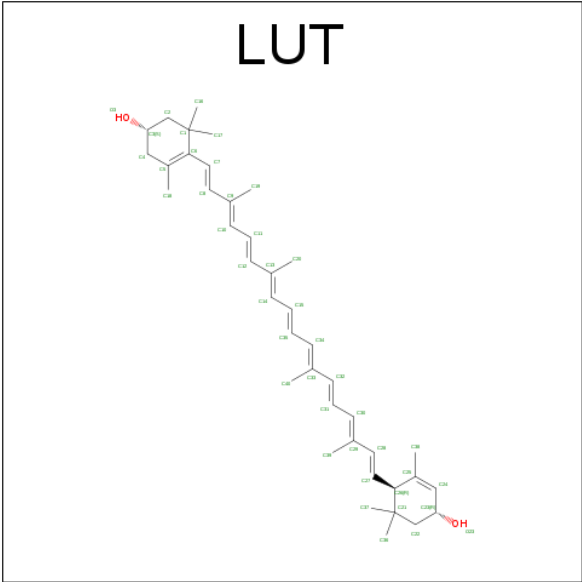
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Mol	Chain	Residues	Atoms					AltConf
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



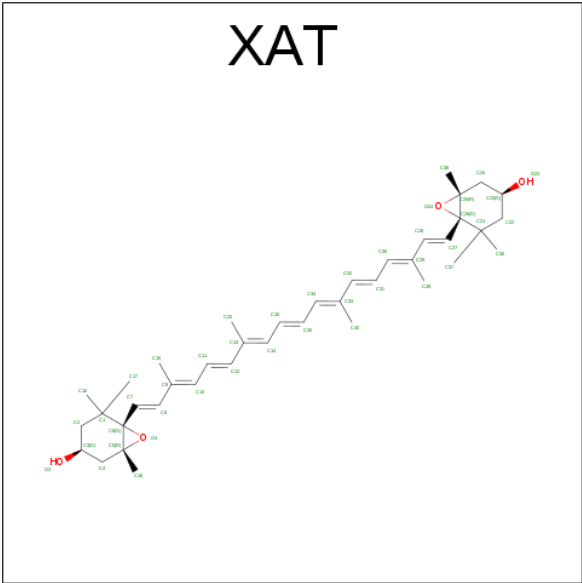
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			84	80	4	
38	G	1	Total	C	O	0
			84	80	4	
38	N	1	Total	C	O	0
			84	80	4	
38	N	1	Total	C	O	0
			84	80	4	
38	R	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			84	80	4	
38	S	1	Total	C	O	0
			84	80	4	
38	Y	1	Total	C	O	0
			84	80	4	
38	Y	1	Total	C	O	0
			84	80	4	
38	g	1	Total	C	O	0
			84	80	4	
38	g	1	Total	C	O	0
			84	80	4	
38	n	1	Total	C	O	0
			84	80	4	
38	n	1	Total	C	O	0
			84	80	4	
38	r	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
38	s	1	Total	C	O	0
			84	80	4	
38	s	1	Total	C	O	0
			84	80	4	
38	y	1	Total	C	O	0
			84	80	4	
38	y	1	Total	C	O	0
			84	80	4	

- Molecule 39 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



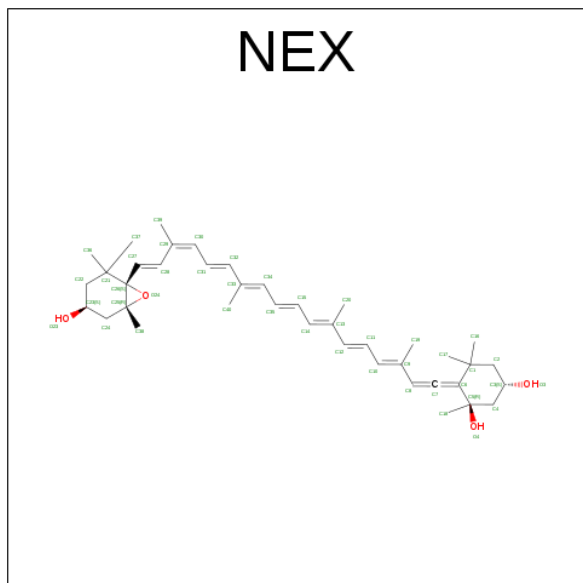
Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	R	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	g	1	Total	C	O	0
			44	40	4	
39	n	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
39	y	1	Total	C	O	0
			44	40	4	

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	R	1	Total	C	O	0
			44	40	4	
40	S	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	
40	s	1	Total	C	O	0
			44	40	4	

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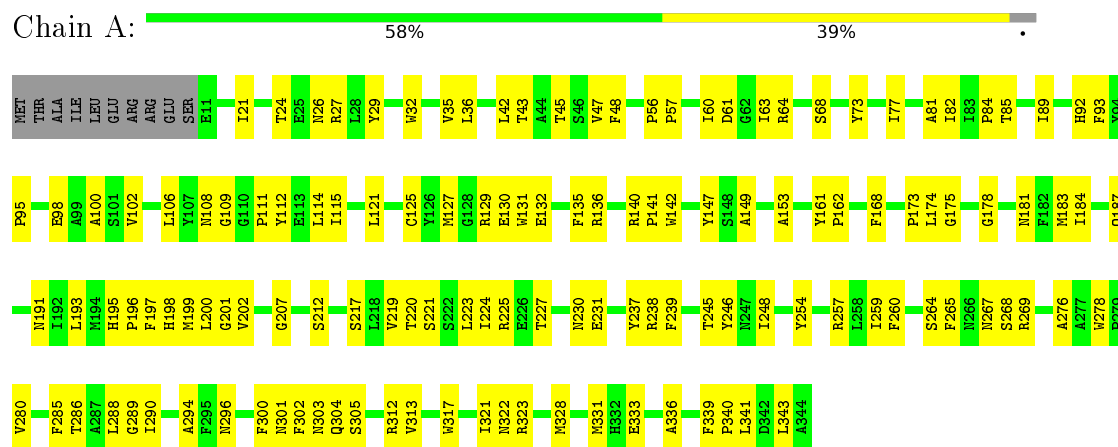
*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	y	1	44	40	4	0

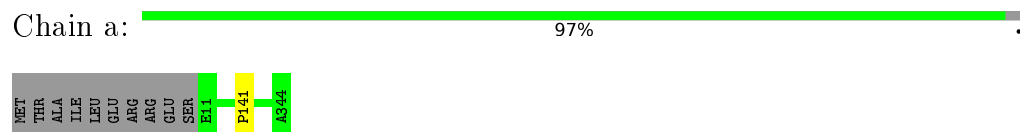
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

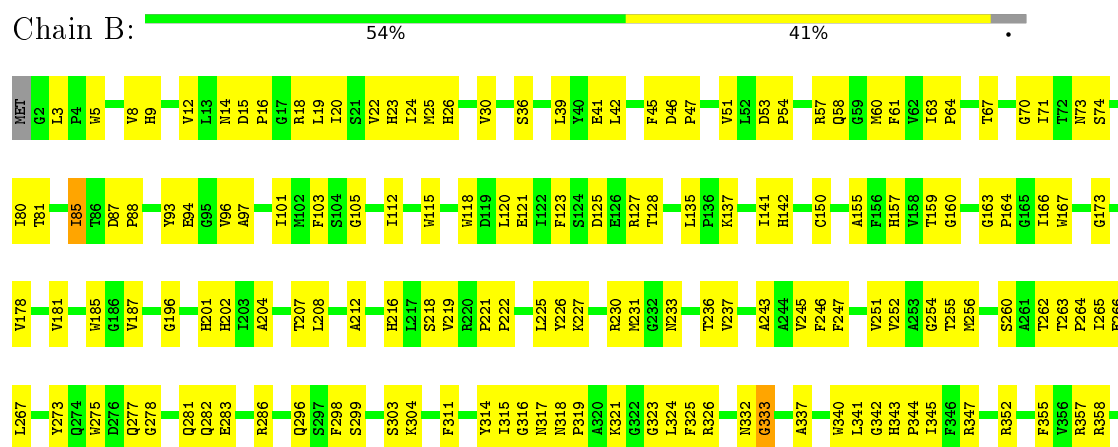
#### • Molecule 1: Photosystem II protein D1

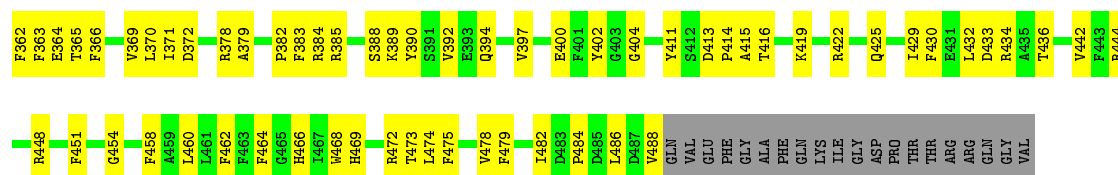


#### • Molecule 1: Photosystem II protein D1



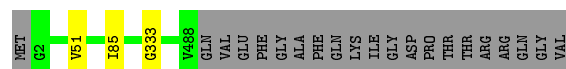
#### • Molecule 2: Photosystem II CP47 reaction center protein





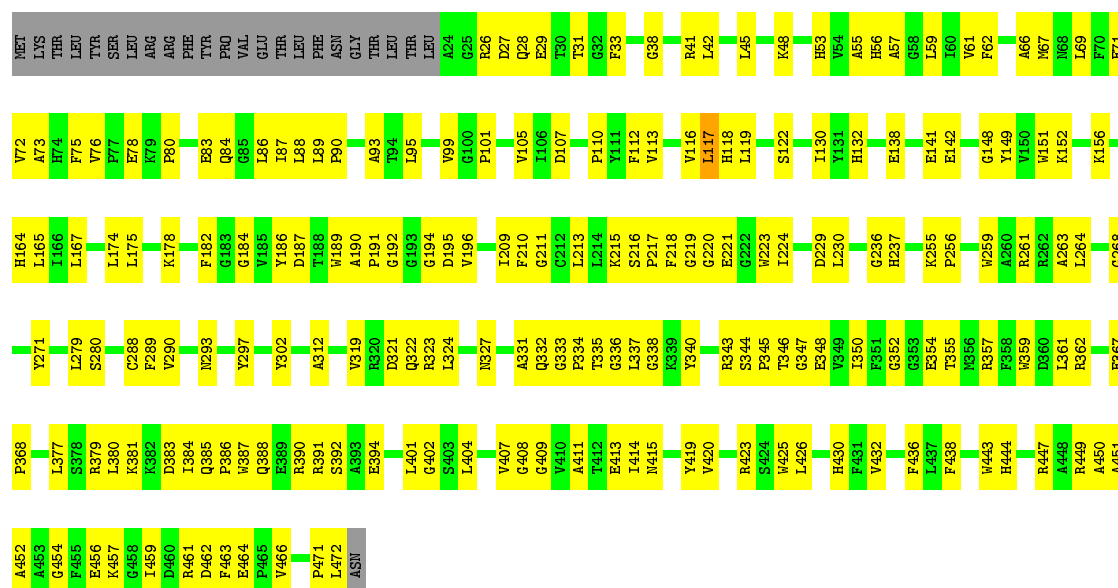
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  95%



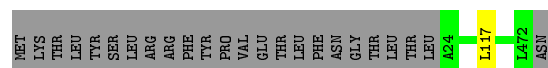
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  54% 40% 5%



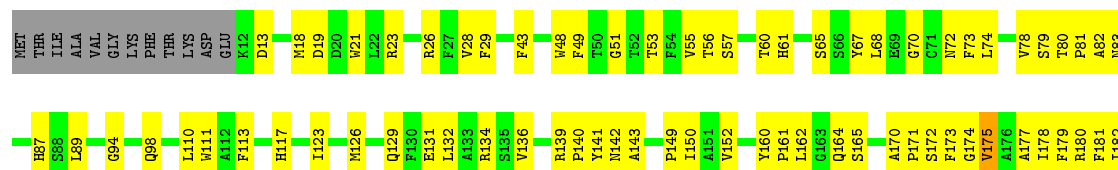
• Molecule 3: Photosystem II CP43 reaction center protein

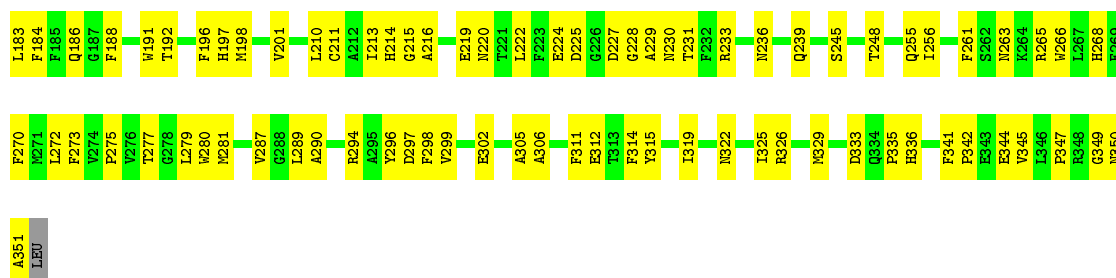
Chain c:  95% 5%



• Molecule 4: Photosystem II D2 protein

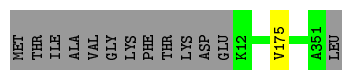
Chain D:  54% 42%





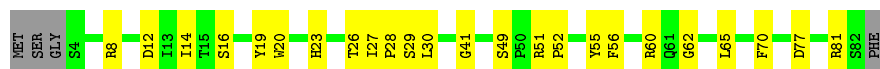
- Molecule 4: Photosystem II D2 protein

Chain d: 96%



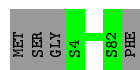
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 66%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 95%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 64%



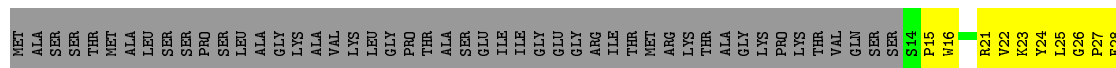
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 82%



- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

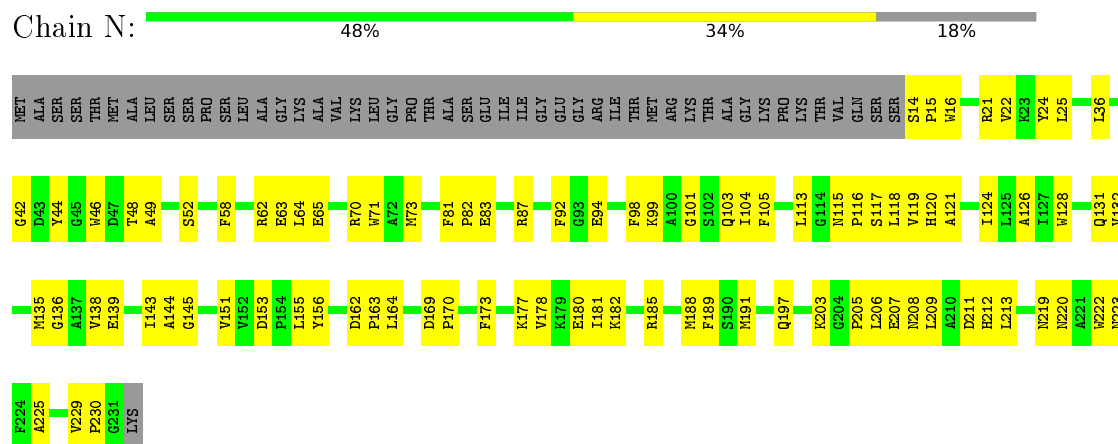
Chain G: 46%



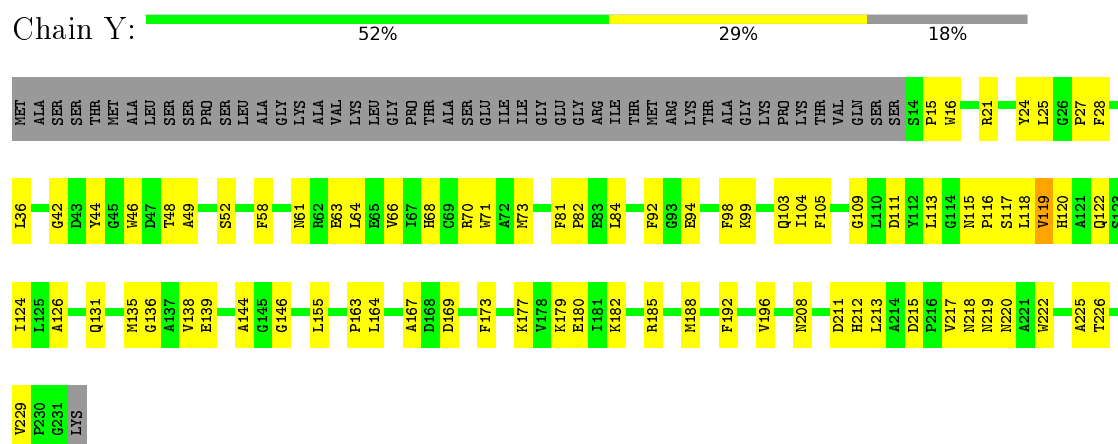




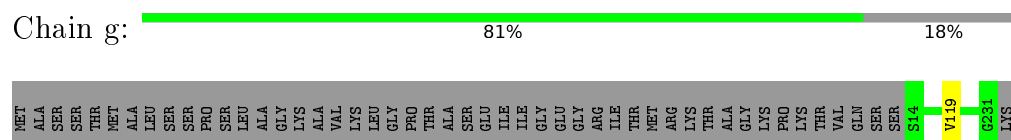
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



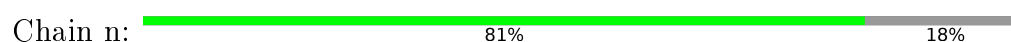
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

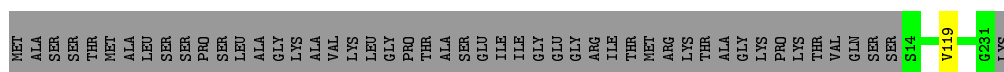


- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



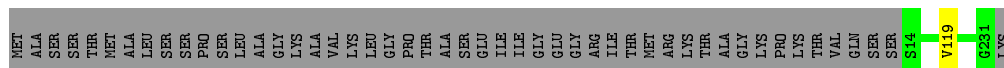
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic





- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain y: 81% 18%



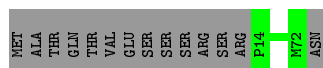
- Molecule 8: Photosystem II reaction center protein H

Chain H: 47% 34% 19%



- Molecule 8: Photosystem II reaction center protein H

Chain h: 81% 19%



- Molecule 9: Protein Photosystem II reaction center protein I

Chain I: 61% 36%



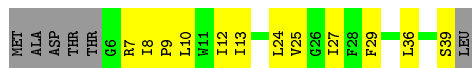
- Molecule 9: Protein Photosystem II reaction center protein I

Chain i: 97%



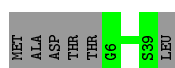
- Molecule 10: Photosystem II reaction center protein J

Chain J: 55% 30% 15%

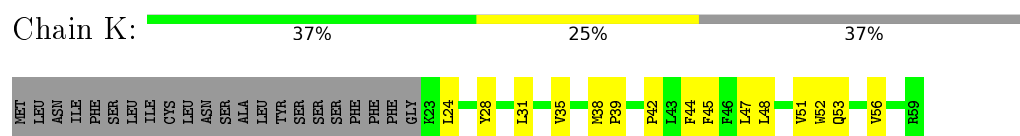


- Molecule 10: Photosystem II reaction center protein J

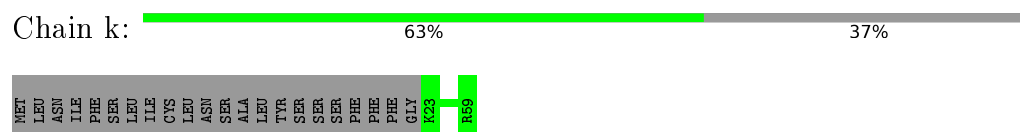
Chain j: 85% 15%



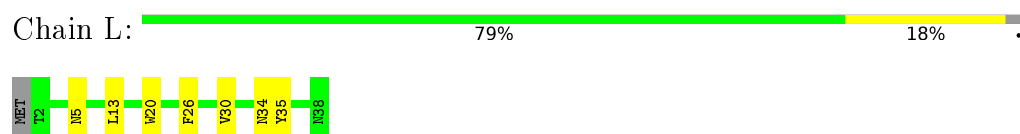
- Molecule 11: Photosystem II reaction center protein K



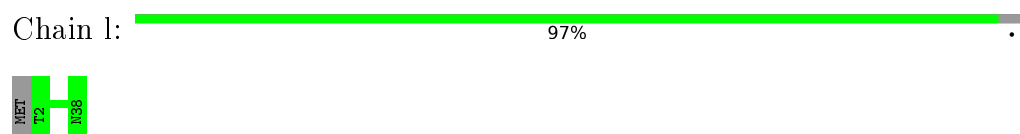
- Molecule 11: Photosystem II reaction center protein K



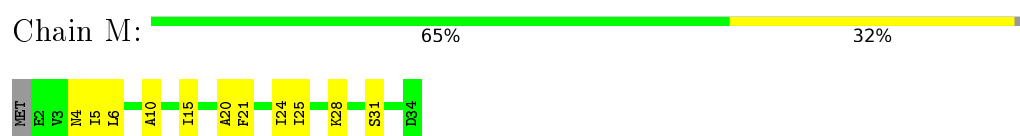
- Molecule 12: Protein Photosystem II reaction center protein L



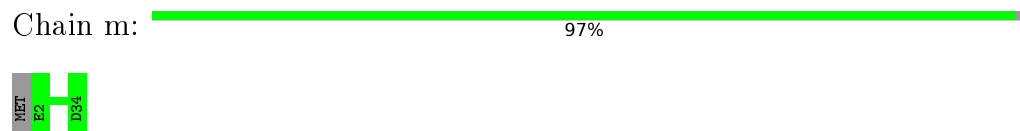
- Molecule 12: Protein Photosystem II reaction center protein L



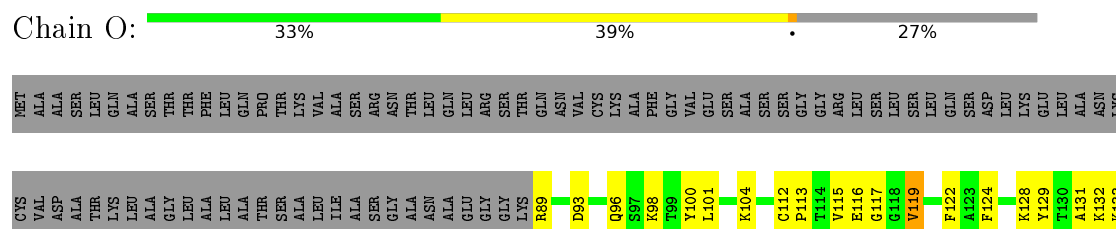
- Molecule 13: Photosystem II reaction center protein M

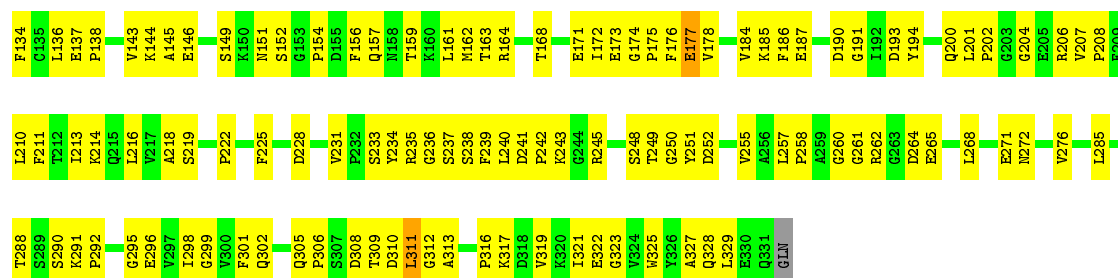


- Molecule 13: Photosystem II reaction center protein M



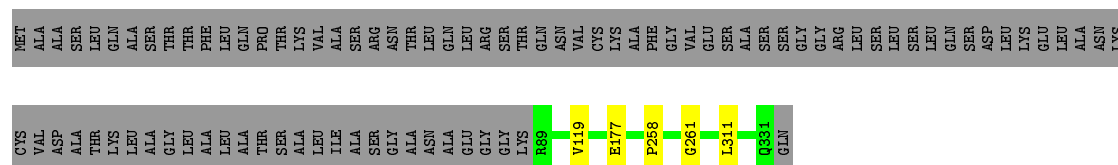
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic





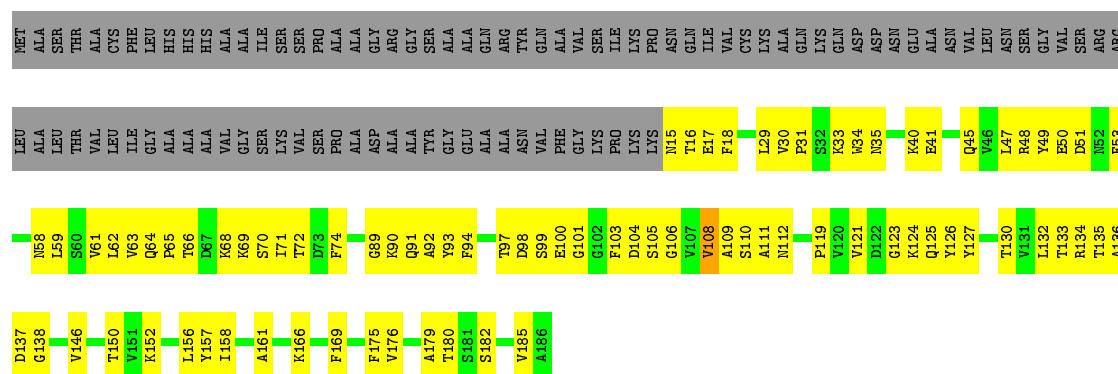
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 72% 27%



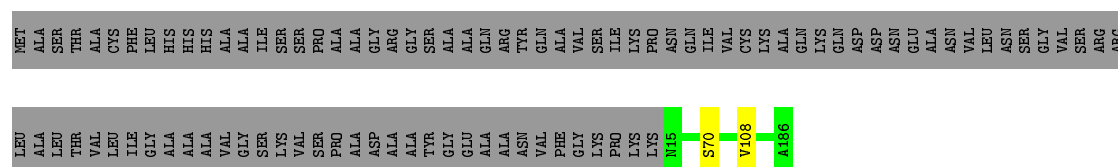
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P: 33% 31% 36%



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

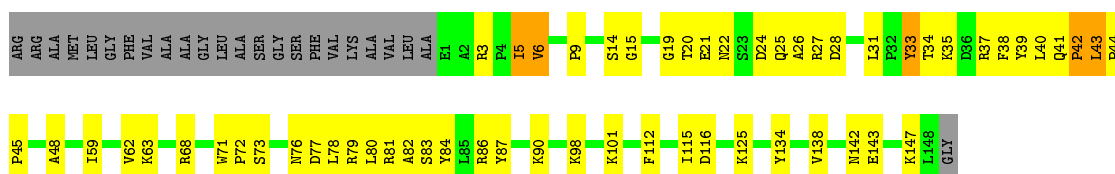
Chain p: 64% 36%



- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

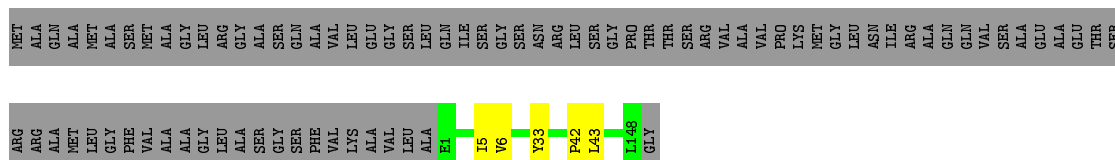
Chain Q: 38% 23% 36%





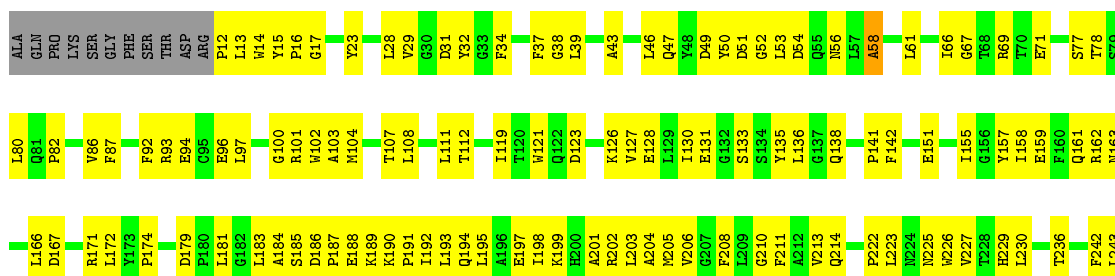
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain q: 62% 36%



- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

Chain R: 47% 48% 5%



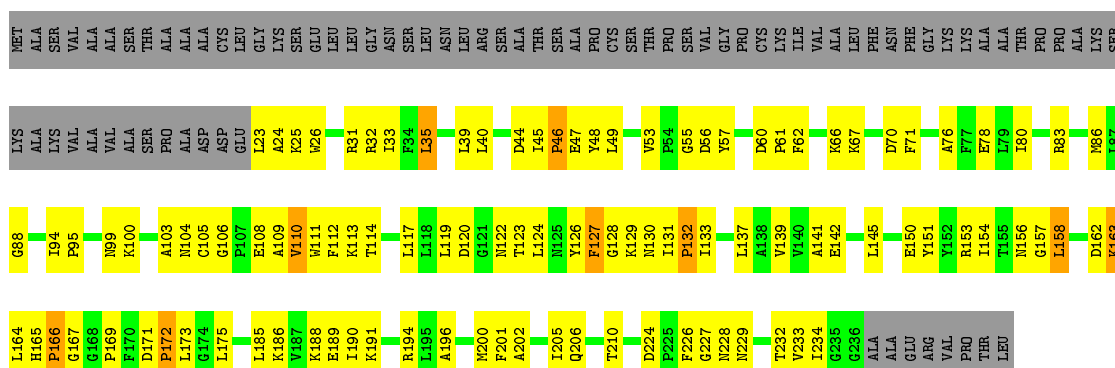
- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

Chain r: 92% 5%



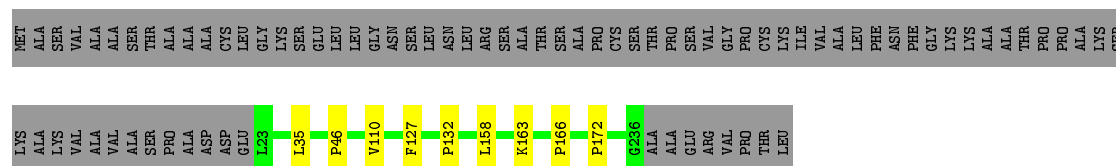
- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

Chain S: 36% 33% 27%



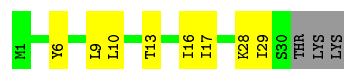
- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

Chain s:  69% . 27%



- Molecule 19: Photosystem II Reaction Center protein Tc

Chain T:  67% 24% 9%



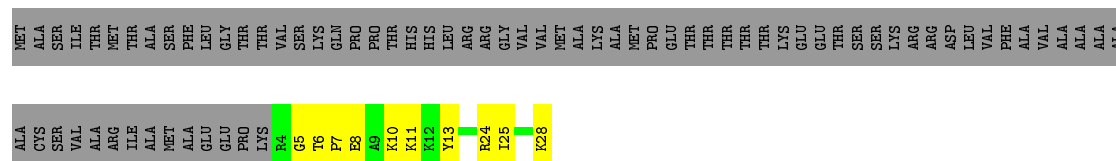
- Molecule 19: Photosystem II Reaction Center protein Tc

Chain t:  91% 9%



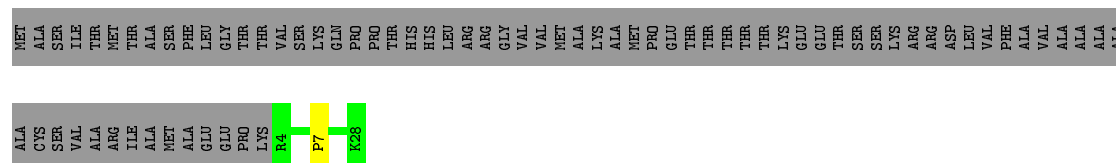
- Molecule 20: Photosystem II Reaction Center Tn protein

Chain U:  15% 10% 75%



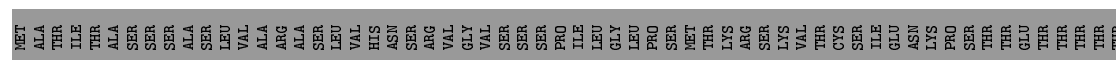
- Molecule 20: Photosystem II Reaction Center Tn protein

Chain u:  24% . 75%



- Molecule 21: Photosystem II reaction center W protein, chloroplatic

Chain W:  23% 17% 61%





## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	109042	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	OTHER	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, LUT, DGD, CL, CHL, XAT, CLA, PL9, FE2, NEX, HEM, BCT, PHO, SQD, BCR, LMG

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	0.60	0/2695	0.59	0/3674
1	a	0.60	0/2695	0.59	0/3674
10	J	0.28	0/253	0.45	0/343
10	j	0.29	0/253	0.45	0/343
11	K	0.49	0/320	0.49	0/436
11	k	0.49	0/320	0.49	0/436
12	L	0.60	0/319	0.49	0/434
12	l	0.60	0/319	0.49	0/434
13	M	0.52	0/262	0.55	0/359
13	m	0.52	0/262	0.55	0/359
14	O	0.39	0/1880	0.51	0/2541
14	o	0.39	0/1880	0.51	0/2541
15	P	0.28	0/1353	0.49	0/1828
15	p	0.28	0/1353	0.49	0/1828
16	Q	0.28	0/1186	0.57	2/1609 (0.1%)
16	q	0.28	0/1186	0.57	2/1609 (0.1%)
17	R	0.41	0/1853	0.55	0/2522
17	r	0.41	0/1853	0.55	0/2522
18	S	0.39	0/1700	0.62	0/2310
18	s	0.39	0/1700	0.62	0/2310
19	T	0.56	0/252	0.55	0/341
19	t	0.56	0/252	0.55	0/341
2	B	0.59	0/3951	0.55	0/5379
2	b	0.59	0/3951	0.55	0/5379
20	U	0.44	0/197	0.55	0/264
20	u	0.44	0/197	0.55	0/264
21	W	0.49	0/429	0.60	0/582
21	w	0.49	0/429	0.60	0/582
22	X	0.42	0/250	0.50	0/342
22	x	0.43	0/250	0.50	0/342
23	Z	0.38	0/464	0.53	0/636

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
23	z	0.38	0/464	0.53	0/636
3	C	0.56	0/3589	0.55	0/4891
3	c	0.56	0/3589	0.55	0/4891
4	D	0.62	0/2796	0.56	0/3811
4	d	0.62	0/2796	0.56	0/3811
5	E	0.42	0/654	0.48	0/889
5	e	0.42	0/654	0.48	0/889
6	F	0.42	0/265	0.48	0/358
6	f	0.43	0/265	0.48	0/358
7	G	0.42	0/1713	0.49	0/2333
7	N	0.42	0/1713	0.49	0/2333
7	Y	0.51	0/1713	0.51	0/2333
7	g	0.42	0/1713	0.49	0/2333
7	n	0.41	0/1713	0.49	0/2333
7	y	0.51	0/1713	0.51	0/2333
8	H	0.49	0/444	0.53	0/605
8	h	0.49	0/444	0.53	0/605
9	I	0.62	0/294	0.57	0/397
9	i	0.62	0/294	0.58	0/397
All	All	0.50	0/61090	0.54	4/83100 (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
1	A	0	1
1	a	0	1
18	S	0	1
18	s	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	42	PRO	CA-C-N	5.67	129.68	117.20
16	Q	42	PRO	CA-C-N	5.67	129.67	117.20
16	Q	42	PRO	C-N-CA	5.03	134.26	121.70
16	q	42	PRO	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
18	S	35	LEU	Peptide
1	a	141	PRO	Peptide
18	s	35	LEU	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	2614	0	2521	160	0
1	a	2614	0	2521	0	0
2	B	3820	0	3690	207	0
2	b	3820	0	3690	0	0
3	C	3475	0	3416	199	0
3	c	3475	0	3416	0	0
4	D	2703	0	2592	152	0
4	d	2703	0	2592	0	0
5	E	636	0	612	19	0
5	e	636	0	612	0	0
6	F	257	0	267	9	0
6	f	257	0	267	0	0
7	G	1661	0	1592	100	0
7	N	1661	0	1592	90	0
7	Y	1661	0	1592	79	0
7	g	1661	0	1592	0	0
7	n	1661	0	1592	0	0
7	y	1661	0	1592	0	0
8	H	434	0	459	24	0
8	h	434	0	459	0	0
9	I	286	0	295	12	0
9	i	286	0	295	0	0
10	J	247	0	258	9	0
10	j	247	0	258	0	0
11	K	307	0	310	18	0
11	k	307	0	310	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	311	0	299	10	0
12	l	311	0	299	0	0
13	M	258	0	277	10	0
13	m	258	0	277	0	0
14	O	1844	0	1812	122	0
14	o	1844	0	1812	0	0
15	P	1324	0	1283	76	0
15	p	1324	0	1283	0	0
16	Q	1162	0	1190	65	0
16	q	1162	0	1190	0	0
17	R	1806	0	1784	128	0
17	r	1806	0	1784	0	0
18	S	1653	0	1620	124	0
18	s	1653	0	1620	0	0
19	T	245	0	260	9	0
19	t	245	0	260	0	0
20	U	193	0	205	10	0
20	u	193	0	205	0	0
21	W	419	0	401	30	0
21	w	419	0	401	0	0
22	X	246	0	256	7	0
22	x	246	0	256	0	0
23	Z	454	0	479	20	0
23	z	454	0	479	0	0
24	A	10	0	0	2	0
24	a	10	0	0	0	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	A	2	0	0	1	0
26	a	2	0	0	0	0
27	A	239	0	242	34	0
27	B	1040	0	1152	109	0
27	C	829	0	903	73	0
27	D	130	0	144	16	0
27	G	424	0	378	44	0
27	N	424	0	378	31	0
27	R	522	0	456	59	0
27	S	441	0	351	39	0
27	Y	472	0	477	45	0
27	a	239	0	242	0	0
27	b	1040	0	1152	0	0
27	c	829	0	903	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	d	130	0	144	0	0
27	g	424	0	378	0	0
27	n	424	0	378	0	0
27	r	522	0	456	0	0
27	s	441	0	351	0	0
27	y	472	0	477	0	0
28	A	128	0	148	10	0
28	a	128	0	148	0	0
29	A	40	0	56	6	0
29	B	120	0	168	20	0
29	C	160	0	224	31	0
29	D	40	0	56	5	0
29	H	40	0	56	7	0
29	a	40	0	56	0	0
29	b	120	0	168	0	0
29	c	160	0	224	0	0
29	d	40	0	56	0	0
29	h	40	0	56	0	0
30	A	108	0	155	6	0
30	B	54	0	77	3	0
30	a	108	0	154	0	0
30	b	54	0	77	0	0
31	A	48	0	66	8	0
31	B	51	0	72	10	0
31	C	51	0	72	5	0
31	D	46	0	62	3	0
31	Z	51	0	72	6	0
31	a	48	0	66	0	0
31	b	51	0	72	0	0
31	c	51	0	72	0	0
31	d	46	0	62	0	0
31	z	51	0	72	0	0
32	C	179	0	232	31	0
32	H	62	0	82	10	0
32	c	179	0	232	0	0
32	h	62	0	82	0	0
33	D	4	0	0	5	0
33	d	4	0	0	0	0
34	D	55	0	80	9	0
34	d	55	0	80	0	0
35	D	129	0	177	14	0
35	G	49	0	74	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	49	0	74	7	0
35	N	49	0	74	7	0
35	R	49	0	74	3	0
35	S	49	0	74	3	0
35	Y	49	0	74	8	0
35	d	129	0	177	0	0
35	g	49	0	74	0	0
35	l	49	0	74	0	0
35	n	49	0	74	0	0
35	r	49	0	74	0	0
35	s	49	0	74	0	0
35	y	49	0	74	0	0
36	F	43	0	30	5	0
36	f	43	0	30	0	0
37	G	314	0	251	38	0
37	N	314	0	251	40	0
37	R	150	0	111	21	0
37	S	201	0	147	13	0
37	Y	330	0	284	30	0
37	g	314	0	251	0	0
37	n	314	0	251	0	0
37	r	150	0	111	0	0
37	s	201	0	147	0	0
37	y	330	0	284	0	0
38	G	84	0	112	16	0
38	N	84	0	112	18	0
38	R	42	0	56	13	0
38	S	84	0	112	19	0
38	Y	84	0	112	17	0
38	g	84	0	112	0	0
38	n	84	0	112	0	0
38	r	42	0	56	0	0
38	s	84	0	112	0	0
38	y	84	0	112	0	0
39	G	44	0	56	8	0
39	N	44	0	56	8	0
39	R	44	0	56	8	0
39	Y	44	0	56	10	0
39	g	44	0	56	0	0
39	n	44	0	56	0	0
39	r	44	0	56	0	0
39	y	44	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	G	44	0	56	3	0
40	N	44	0	56	3	0
40	R	44	0	56	6	0
40	S	44	0	56	5	0
40	Y	44	0	56	5	0
40	g	44	0	56	0	0
40	n	44	0	56	0	0
40	r	44	0	56	0	0
40	s	44	0	56	0	0
40	y	44	0	56	0	0
All	All	75994	0	75847	1874	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 12.

The worst 5 of 1874 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)
27:G:611:CLA:NB	35:G:2630:LHG:O4	1.78	1.15
1:A:317:TRP:HE3	4:D:180:ARG:HD3	1.26	0.98
1:A:303:ASN:O	3:C:415:ASN:ND2	2.05	0.90
17:R:158:ILE:HD11	40:R:623:NEX:H34	1.53	0.90
2:B:277:GLN:HB3	20:U:24:ARG:HG3	1.55	0.89

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	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	30	75
2	b	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	30	75
3	C	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
3	c	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
4	D	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	46	85
4	d	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	46	85
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	30/39 (77%)	30 (100%)	0	0	100	100
6	f	30/39 (77%)	30 (100%)	0	0	100	100
7	G	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	34	78
7	N	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	34	78
7	Y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	34	78
7	g	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	34	78
7	n	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	34	78
7	y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	34	78
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
9	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
9	i	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
10	J	32/40 (80%)	32 (100%)	0	0	100	100
10	j	32/40 (80%)	32 (100%)	0	0	100	100
11	K	35/59 (59%)	35 (100%)	0	0	100	100
11	k	35/59 (59%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
13	m	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
14	O	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	9	46
14	o	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	9	46
15	P	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	16	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	p	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	16	60
16	Q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	6	39
16	q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	6	39
17	R	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	4	28
17	r	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	4	28
18	S	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	4	28
18	s	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	4	28
19	T	28/33 (85%)	28 (100%)	0	0	100	100
19	t	28/33 (85%)	28 (100%)	0	0	100	100
20	U	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	3	25
20	u	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	3	25
21	W	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	10	50
21	w	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	10	50
22	X	33/117 (28%)	33 (100%)	0	0	100	100
22	x	33/117 (28%)	33 (100%)	0	0	100	100
23	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
23	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
All	All	7548/9396 (80%)	7100 (94%)	374 (5%)	74 (1%)	24	65

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
14	O	258	PRO
14	O	311	LEU
15	P	108	VAL
18	S	110	VAL

### 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	270/279 (97%)	270 (100%)	0	100	100
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	389/406 (96%)	389 (100%)	0	100	100
2	b	389/406 (96%)	389 (100%)	0	100	100
3	C	351/374 (94%)	350 (100%)	1 (0%)	94	98
3	c	351/374 (94%)	350 (100%)	1 (0%)	94	98
4	D	272/283 (96%)	272 (100%)	0	100	100
4	d	272/283 (96%)	272 (100%)	0	100	100
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/34 (79%)	27 (100%)	0	100	100
6	f	27/34 (79%)	27 (100%)	0	100	100
7	G	168/206 (82%)	168 (100%)	0	100	100
7	N	168/206 (82%)	168 (100%)	0	100	100
7	Y	168/206 (82%)	168 (100%)	0	100	100
7	g	168/206 (82%)	168 (100%)	0	100	100
7	n	168/206 (82%)	168 (100%)	0	100	100
7	y	168/206 (82%)	168 (100%)	0	100	100
8	H	48/61 (79%)	48 (100%)	0	100	100
8	h	48/61 (79%)	48 (100%)	0	100	100
9	I	32/33 (97%)	32 (100%)	0	100	100
9	i	32/33 (97%)	32 (100%)	0	100	100
10	J	25/30 (83%)	25 (100%)	0	100	100
10	j	25/30 (83%)	25 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	35 (100%)	0	100	100
13	M	29/30 (97%)	29 (100%)	0	100	100
13	m	29/30 (97%)	29 (100%)	0	100	100
14	O	202/269 (75%)	202 (100%)	0	100	100
14	o	202/269 (75%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	144/212 (68%)	144 (100%)	0	100	100
15	p	144/212 (68%)	144 (100%)	0	100	100
16	Q	129/187 (69%)	129 (100%)	0	100	100
16	q	129/187 (69%)	129 (100%)	0	100	100
17	R	189/198 (96%)	189 (100%)	0	100	100
17	r	189/198 (96%)	189 (100%)	0	100	100
18	S	167/226 (74%)	167 (100%)	0	100	100
18	s	167/226 (74%)	167 (100%)	0	100	100
19	T	27/30 (90%)	27 (100%)	0	100	100
19	t	27/30 (90%)	27 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/110 (40%)	44 (100%)	0	100	100
21	w	44/110 (40%)	44 (100%)	0	100	100
22	X	26/90 (29%)	26 (100%)	0	100	100
22	x	26/90 (29%)	26 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
23	z	52/53 (98%)	52 (100%)	0	100	100
All	All	6170/7528 (82%)	6168 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	117	LEU
3	c	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	104	ASN
2	b	296	GLN
17	r	235	HIS
7	Y	103	GLN
1	a	304	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 322 ligands modelled in this entry, 6 are monoatomic - leaving 316 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	$\# Z  > 2$
24	OEX	A	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
27	CLA	A	405	-	57,73,73	1.24	7 (12%)	61,113,113	1.24	6 (9%)
27	CLA	A	406	-	57,73,73	1.19	7 (12%)	61,113,113	1.24	5 (8%)
27	CLA	A	407	-	41,57,73	1.36	7 (17%)	43,93,113	1.39	6 (13%)
28	PHO	A	408	-	67,69,69	1.20	10 (14%)	86,99,99	1.15	10 (11%)
28	PHO	A	409	-	67,69,69	1.20	10 (14%)	86,99,99	1.12	6 (6%)
27	CLA	A	410	-	52,68,73	1.25	8 (15%)	55,107,113	1.29	6 (10%)
29	BCR	A	411	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
30	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.72	10 (16%)
31	LMG	A	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
30	SQD	A	418	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	9 (14%)
27	CLA	B	602	-	57,73,73	1.15	8 (14%)	61,113,113	1.17	5 (8%)
27	CLA	B	603	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	9 (14%)
27	CLA	B	604	-	57,73,73	1.22	8 (14%)	61,113,113	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	B	605	-	57,73,73	1.20	7 (12%)	61,113,113	1.40	11 (18%)
27	CLA	B	606	-	57,73,73	1.21	8 (14%)	61,113,113	1.15	5 (8%)
27	CLA	B	607	-	57,73,73	1.18	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	B	608	-	57,73,73	1.14	8 (14%)	61,113,113	1.22	5 (8%)
27	CLA	B	609	-	57,73,73	1.14	7 (12%)	61,113,113	1.25	6 (9%)
27	CLA	B	610	-	57,73,73	1.15	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	B	611	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	7 (11%)
27	CLA	B	612	-	57,73,73	1.22	7 (12%)	61,113,113	1.35	8 (13%)
27	CLA	B	613	-	57,73,73	1.20	8 (14%)	61,113,113	1.33	9 (14%)
27	CLA	B	614	-	57,73,73	1.19	8 (14%)	61,113,113	1.16	5 (8%)
27	CLA	B	615	-	57,73,73	1.20	8 (14%)	61,113,113	1.17	8 (13%)
27	CLA	B	616	-	57,73,73	1.19	7 (12%)	61,113,113	1.18	6 (9%)
27	CLA	B	617	-	57,73,73	1.19	7 (12%)	61,113,113	1.23	6 (9%)
29	BCR	B	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.21	18 (32%)
29	BCR	B	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
29	BCR	B	620	-	41,41,41	0.96	2 (4%)	56,56,56	2.13	17 (30%)
30	SQD	B	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.96	9 (14%)
31	LMG	B	622	-	51,51,55	0.78	2 (3%)	59,59,63	1.45	8 (13%)
27	CLA	C	501	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	8 (13%)
27	CLA	C	502	-	57,73,73	1.16	7 (12%)	61,113,113	1.26	5 (8%)
27	CLA	C	503	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	10 (16%)
27	CLA	C	504	-	57,73,73	1.17	7 (12%)	61,113,113	1.20	5 (8%)
27	CLA	C	505	-	57,73,73	1.20	7 (12%)	61,113,113	1.35	7 (11%)
27	CLA	C	506	-	57,73,73	1.17	8 (14%)	61,113,113	1.30	7 (11%)
27	CLA	C	507	-	57,73,73	1.22	8 (14%)	61,113,113	1.15	6 (9%)
27	CLA	C	508	-	57,73,73	1.25	8 (14%)	61,113,113	1.34	9 (14%)
27	CLA	C	509	-	57,73,73	1.21	8 (14%)	61,113,113	1.34	10 (16%)
27	CLA	C	510	-	57,73,73	1.17	7 (12%)	61,113,113	1.29	6 (9%)
27	CLA	C	511	3	57,73,73	1.17	7 (12%)	61,113,113	1.28	6 (9%)
27	CLA	C	512	-	57,73,73	1.15	7 (12%)	61,113,113	1.23	8 (13%)
27	CLA	C	513	-	41,57,73	1.37	7 (17%)	43,93,113	1.44	7 (16%)
29	BCR	C	514	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	19 (33%)
29	BCR	C	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	19 (33%)
29	BCR	C	516	-	41,41,41	0.79	0	56,56,56	2.30	18 (32%)
29	BCR	C	517	-	41,41,41	0.96	2 (4%)	56,56,56	2.32	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	DGD	C	518	-	56,56,67	1.13	8 (14%)	70,70,81	1.72	16 (22%)
32	DGD	C	519	-	63,63,67	0.97	4 (6%)	77,77,81	1.53	14 (18%)
32	DGD	C	520	-	63,63,67	0.96	4 (6%)	77,77,81	1.53	12 (15%)
31	LMG	C	521	-	51,51,55	0.73	0	59,59,63	1.39	8 (13%)
33	BCT	D	401	-	0,3,3	0.00	-	0,3,3	0.00	-
27	CLA	D	402	-	57,73,73	1.25	7 (12%)	61,113,113	1.28	7 (11%)
27	CLA	D	403	-	57,73,73	1.14	6 (10%)	61,113,113	1.30	7 (11%)
29	BCR	D	404	-	41,41,41	0.80	0	56,56,56	2.19	14 (25%)
34	PL9	D	405	-	54,55,55	1.60	9 (16%)	68,69,69	1.57	15 (22%)
35	LHG	D	408	-	42,42,48	0.76	1 (2%)	43,48,54	1.29	5 (11%)
35	LHG	D	409	-	48,48,48	0.74	1 (2%)	49,54,54	1.37	8 (16%)
35	LHG	D	410	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
31	LMG	D	411	-	46,46,55	0.83	4 (8%)	54,54,63	1.42	6 (11%)
36	HEM	F	101	5,6	24,50,50	2.33	6 (25%)	16,82,82	1.42	3 (18%)
38	LUT	G	1620	-	42,43,43	1.00	2 (4%)	49,60,60	1.91	15 (30%)
38	LUT	G	1621	-	42,43,43	1.04	2 (4%)	49,60,60	1.86	17 (34%)
39	XAT	G	1622	-	47,47,47	1.38	3 (6%)	40,74,74	1.82	8 (20%)
40	NEX	G	1623	-	42,46,46	1.25	2 (4%)	40,70,70	1.96	11 (27%)
35	LHG	G	2630	27	48,48,48	0.61	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	G	601	7	64,74,74	4.13	26 (40%)	47,114,114	2.08	16 (34%)
27	CLA	G	602	7	57,73,73	1.18	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	G	603	-	41,57,73	1.33	7 (17%)	43,93,113	1.37	6 (13%)
27	CLA	G	604	-	41,57,73	1.34	7 (17%)	43,93,113	1.32	7 (16%)
37	CHL	G	605	7	46,56,74	4.71	26 (56%)	28,92,114	2.52	15 (53%)
37	CHL	G	606	-	48,58,74	4.72	26 (54%)	29,94,114	2.51	14 (48%)
37	CHL	G	607	-	48,58,74	4.69	26 (54%)	29,94,114	2.31	12 (41%)
37	CHL	G	608	-	48,58,74	4.68	25 (52%)	29,94,114	2.35	13 (44%)
37	CHL	G	609	7	48,58,74	4.72	27 (56%)	29,94,114	2.36	12 (41%)
27	CLA	G	610	7	57,73,73	1.14	6 (10%)	61,113,113	1.23	5 (8%)
27	CLA	G	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.34	6 (13%)
27	CLA	G	612	7	41,57,73	1.35	7 (17%)	43,93,113	1.32	6 (13%)
27	CLA	G	613	7	41,57,73	1.32	7 (17%)	43,93,113	1.41	8 (18%)
27	CLA	G	614	-	41,57,73	1.32	5 (12%)	43,93,113	1.31	5 (11%)
29	BCR	H	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.00	19 (33%)
32	DGD	H	102	-	63,63,67	0.98	3 (4%)	77,77,81	1.49	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LHG	L	101	-	48,48,48	0.71	1 (2%)	49,54,54	1.32	7 (14%)
38	LUT	N	1620	-	42,43,43	0.98	3 (7%)	49,60,60	2.01	16 (32%)
38	LUT	N	1621	-	42,43,43	1.02	3 (7%)	49,60,60	1.82	13 (26%)
39	XAT	N	1622	-	47,47,47	1.38	3 (6%)	40,74,74	2.25	14 (35%)
40	NEX	N	1623	-	42,46,46	1.26	2 (4%)	40,70,70	1.99	9 (22%)
35	LHG	N	2630	27	48,48,48	0.60	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	N	601	7	48,58,74	4.68	24 (50%)	29,94,114	2.48	14 (48%)
27	CLA	N	602	7	57,73,73	1.17	7 (12%)	61,113,113	1.16	5 (8%)
27	CLA	N	603	-	41,57,73	1.35	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	N	604	-	41,57,73	1.33	7 (17%)	43,93,113	1.38	6 (13%)
37	CHL	N	605	7	46,56,74	4.84	26 (56%)	28,92,114	2.60	15 (53%)
37	CHL	N	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	N	607	-	64,74,74	4.13	26 (40%)	47,114,114	1.96	15 (31%)
37	CHL	N	608	-	48,58,74	4.74	26 (54%)	29,94,114	2.39	12 (41%)
37	CHL	N	609	7	48,58,74	4.81	26 (54%)	29,94,114	2.44	13 (44%)
27	CLA	N	610	7	57,73,73	1.16	6 (10%)	61,113,113	1.22	7 (11%)
27	CLA	N	611	35	41,57,73	1.29	6 (14%)	43,93,113	1.38	8 (18%)
27	CLA	N	612	7	41,57,73	1.34	7 (17%)	43,93,113	1.36	7 (16%)
27	CLA	N	613	7	41,57,73	1.33	7 (17%)	43,93,113	1.35	5 (11%)
27	CLA	N	614	-	41,57,73	1.27	4 (9%)	43,93,113	1.35	7 (16%)
35	LHG	R	2630	27	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
27	CLA	R	601	17	41,57,73	1.29	5 (12%)	43,93,113	1.45	8 (18%)
27	CLA	R	602	17	57,73,73	1.17	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	R	603	-	41,57,73	1.33	7 (17%)	43,93,113	1.33	7 (16%)
27	CLA	R	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.46	6 (13%)
37	CHL	R	606	-	48,58,74	4.71	26 (54%)	29,94,114	2.42	12 (41%)
37	CHL	R	607	-	48,58,74	4.72	25 (52%)	29,94,114	2.38	13 (44%)
37	CHL	R	608	-	48,58,74	4.73	26 (54%)	29,94,114	2.30	12 (41%)
27	CLA	R	609	17	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	R	610	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	R	611	35	41,57,73	1.30	5 (12%)	43,93,113	1.29	6 (13%)
27	CLA	R	612	-	41,57,73	1.31	7 (17%)	43,93,113	1.28	5 (11%)
27	CLA	R	613	17	41,57,73	1.30	5 (12%)	43,93,113	1.34	5 (11%)
27	CLA	R	616	17	41,57,73	1.32	6 (14%)	43,93,113	1.32	6 (13%)
38	LUT	R	620	-	42,43,43	0.95	2 (4%)	49,60,60	1.70	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	XAT	R	622	-	47,47,47	1.37	2 (4%)	40,74,74	1.91	13 (32%)
40	NEX	R	623	-	42,46,46	1.30	2 (4%)	40,70,70	1.85	12 (30%)
38	LUT	S	1620	-	42,43,43	0.99	3 (7%)	49,60,60	2.07	16 (32%)
38	LUT	S	1621	-	42,43,43	0.97	3 (7%)	49,60,60	1.82	16 (32%)
40	NEX	S	1623	-	42,46,46	1.21	3 (7%)	40,70,70	1.89	9 (22%)
35	LHG	S	2630	27	48,48,48	0.64	1 (2%)	49,54,54	1.28	6 (12%)
37	CHL	S	601	18	50,60,74	4.63	25 (50%)	29,97,114	2.51	13 (44%)
27	CLA	S	602	18	41,57,73	1.38	6 (14%)	43,93,113	1.37	7 (16%)
27	CLA	S	603	-	41,57,73	1.30	5 (12%)	43,93,113	1.38	5 (11%)
27	CLA	S	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.40	8 (18%)
37	CHL	S	606	-	48,58,74	4.65	25 (52%)	29,94,114	2.33	12 (41%)
37	CHL	S	607	-	48,58,74	4.61	24 (50%)	29,94,114	2.66	13 (44%)
37	CHL	S	608	-	47,57,74	4.59	23 (48%)	28,93,114	2.58	12 (42%)
27	CLA	S	609	18	41,57,73	1.34	4 (9%)	43,93,113	1.29	4 (9%)
27	CLA	S	610	18	41,57,73	1.32	5 (12%)	43,93,113	1.38	6 (13%)
27	CLA	S	611	35	41,57,73	1.33	6 (14%)	43,93,113	1.36	5 (11%)
27	CLA	S	612	18	41,57,73	1.33	7 (17%)	43,93,113	1.34	7 (16%)
27	CLA	S	613	18	41,57,73	1.32	7 (17%)	43,93,113	1.41	6 (13%)
27	CLA	S	614	-	41,57,73	1.36	7 (17%)	43,93,113	1.32	6 (13%)
38	LUT	Y	1620	-	42,43,43	1.05	3 (7%)	49,60,60	1.90	17 (34%)
38	LUT	Y	1621	-	42,43,43	1.12	4 (9%)	49,60,60	1.89	17 (34%)
39	XAT	Y	1622	-	47,47,47	1.35	2 (4%)	40,74,74	1.99	11 (27%)
40	NEX	Y	1623	-	42,46,46	1.28	2 (4%)	40,70,70	2.00	10 (25%)
35	LHG	Y	2630	27	48,48,48	0.74	2 (4%)	49,54,54	1.31	7 (14%)
37	CHL	Y	601	7	64,74,74	4.11	27 (42%)	47,114,114	2.08	15 (31%)
27	CLA	Y	602	7	57,73,73	1.20	8 (14%)	61,113,113	1.28	8 (13%)
27	CLA	Y	603	-	41,57,73	1.36	7 (17%)	43,93,113	1.35	7 (16%)
27	CLA	Y	604	-	41,57,73	1.39	8 (19%)	43,93,113	1.38	6 (13%)
37	CHL	Y	605	7	46,56,74	4.80	26 (56%)	28,92,114	2.41	11 (39%)
37	CHL	Y	606	-	48,58,74	4.77	26 (54%)	29,94,114	2.50	12 (41%)
37	CHL	Y	607	-	48,58,74	4.78	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	Y	608	-	48,58,74	4.76	27 (56%)	29,94,114	2.30	11 (37%)
37	CHL	Y	609	7	64,74,74	4.14	26 (40%)	47,114,114	2.13	14 (29%)
27	CLA	Y	610	7	57,73,73	1.17	7 (12%)	61,113,113	1.25	7 (11%)
27	CLA	Y	611	35	57,73,73	1.15	7 (12%)	61,113,113	1.22	7 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	Y	612	7	57,73,73	1.17	8 (14%)	61,113,113	1.23	7 (11%)
27	CLA	Y	613	7	57,73,73	1.18	8 (14%)	61,113,113	1.20	6 (9%)
27	CLA	Y	614	-	41,57,73	1.35	7 (17%)	43,93,113	1.34	7 (16%)
31	LMG	Z	101	-	51,51,55	0.71	0	59,59,63	1.35	7 (11%)
24	OEX	a	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
27	CLA	a	405	-	57,73,73	1.24	7 (12%)	61,113,113	1.24	6 (9%)
27	CLA	a	406	-	57,73,73	1.19	7 (12%)	61,113,113	1.24	5 (8%)
27	CLA	a	407	-	41,57,73	1.36	7 (17%)	43,93,113	1.39	6 (13%)
28	PHO	a	408	-	67,69,69	1.20	10 (14%)	86,99,99	1.15	10 (11%)
28	PHO	a	409	-	67,69,69	1.20	10 (14%)	86,99,99	1.12	6 (6%)
27	CLA	a	410	-	52,68,73	1.25	8 (15%)	55,107,113	1.29	6 (10%)
29	BCR	a	411	-	41,41,41	0.91	3 (7%)	56,56,56	2.08	16 (28%)
30	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	10 (16%)
31	LMG	a	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
30	SQD	a	418	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	10 (16%)
27	CLA	b	602	-	57,73,73	1.15	8 (14%)	61,113,113	1.17	5 (8%)
27	CLA	b	603	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	9 (14%)
27	CLA	b	604	-	57,73,73	1.22	8 (14%)	61,113,113	1.25	6 (9%)
27	CLA	b	605	-	57,73,73	1.20	7 (12%)	61,113,113	1.40	11 (18%)
27	CLA	b	606	-	57,73,73	1.21	8 (14%)	61,113,113	1.15	5 (8%)
27	CLA	b	607	-	57,73,73	1.18	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	b	608	-	57,73,73	1.14	8 (14%)	61,113,113	1.22	5 (8%)
27	CLA	b	609	-	57,73,73	1.14	7 (12%)	61,113,113	1.25	6 (9%)
27	CLA	b	610	-	57,73,73	1.16	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	b	611	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	7 (11%)
27	CLA	b	612	-	57,73,73	1.22	7 (12%)	61,113,113	1.34	8 (13%)
27	CLA	b	613	-	57,73,73	1.20	8 (14%)	61,113,113	1.33	9 (14%)
27	CLA	b	614	-	57,73,73	1.19	8 (14%)	61,113,113	1.16	5 (8%)
27	CLA	b	615	-	57,73,73	1.20	8 (14%)	61,113,113	1.17	8 (13%)
27	CLA	b	616	-	57,73,73	1.19	7 (12%)	61,113,113	1.18	7 (11%)
27	CLA	b	617	-	57,73,73	1.18	7 (12%)	61,113,113	1.23	6 (9%)
29	BCR	b	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.21	18 (32%)
29	BCR	b	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
29	BCR	b	620	-	41,41,41	0.96	3 (7%)	56,56,56	2.13	17 (30%)
30	SQD	b	621	-	53,54,54	0.94	5 (9%)	62,65,65	1.96	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMG	b	622	-	51,51,55	0.78	2 (3%)	59,59,63	1.45	7 (11%)
27	CLA	c	501	-	57,73,73	1.18	7 (12%)	61,113,113	1.25	8 (13%)
27	CLA	c	502	-	57,73,73	1.16	7 (12%)	61,113,113	1.26	6 (9%)
27	CLA	c	503	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	10 (16%)
27	CLA	c	504	-	57,73,73	1.17	6 (10%)	61,113,113	1.20	5 (8%)
27	CLA	c	505	-	57,73,73	1.20	7 (12%)	61,113,113	1.35	6 (9%)
27	CLA	c	506	-	57,73,73	1.17	8 (14%)	61,113,113	1.30	7 (11%)
27	CLA	c	507	-	57,73,73	1.22	8 (14%)	61,113,113	1.15	5 (8%)
27	CLA	c	508	-	57,73,73	1.24	8 (14%)	61,113,113	1.35	9 (14%)
27	CLA	c	509	-	57,73,73	1.21	8 (14%)	61,113,113	1.34	9 (14%)
27	CLA	c	510	-	57,73,73	1.17	7 (12%)	61,113,113	1.29	6 (9%)
27	CLA	c	511	3	57,73,73	1.17	7 (12%)	61,113,113	1.28	6 (9%)
27	CLA	c	512	-	57,73,73	1.15	7 (12%)	61,113,113	1.23	8 (13%)
27	CLA	c	513	-	41,57,73	1.37	8 (19%)	43,93,113	1.45	7 (16%)
29	BCR	c	514	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)
29	BCR	c	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	19 (33%)
29	BCR	c	516	-	41,41,41	0.78	0	56,56,56	2.29	18 (32%)
29	BCR	c	517	-	41,41,41	0.96	2 (4%)	56,56,56	2.32	16 (28%)
32	DGD	c	518	-	56,56,67	1.13	8 (14%)	70,70,81	1.73	16 (22%)
32	DGD	c	519	-	63,63,67	0.96	4 (6%)	77,77,81	1.54	14 (18%)
32	DGD	c	520	-	63,63,67	0.96	4 (6%)	77,77,81	1.53	11 (14%)
31	LMG	c	521	-	51,51,55	0.73	0	59,59,63	1.39	8 (13%)
33	BCT	d	401	-	0,3,3	0.00	-	0,3,3	0.00	-
27	CLA	d	402	-	57,73,73	1.25	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	d	403	-	57,73,73	1.14	6 (10%)	61,113,113	1.30	7 (11%)
29	BCR	d	404	-	41,41,41	0.81	0	56,56,56	2.19	14 (25%)
34	PL9	d	405	-	54,55,55	1.60	9 (16%)	68,69,69	1.57	15 (22%)
35	LHG	d	408	-	42,42,48	0.76	1 (2%)	43,48,54	1.29	5 (11%)
35	LHG	d	409	-	48,48,48	0.74	1 (2%)	49,54,54	1.37	8 (16%)
35	LHG	d	410	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
31	LMG	d	411	-	46,46,55	0.83	4 (8%)	54,54,63	1.42	6 (11%)
36	HEM	f	101	5,6	24,50,50	2.32	6 (25%)	16,82,82	1.42	3 (18%)
38	LUT	g	1620	-	42,43,43	0.99	2 (4%)	49,60,60	1.92	15 (30%)
38	LUT	g	1621	-	42,43,43	1.03	2 (4%)	49,60,60	1.87	17 (34%)
39	XAT	g	1622	-	47,47,47	1.38	3 (6%)	40,74,74	1.82	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	NEX	g	1623	-	42,46,46	1.26	3 (7%)	40,70,70	1.96	10 (25%)
35	LHG	g	2630	27	48,48,48	0.60	0	49,54,54	1.29	7 (14%)
37	CHL	g	601	7	64,74,74	4.13	26 (40%)	47,114,114	2.08	16 (34%)
27	CLA	g	602	7	57,73,73	1.18	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	g	603	-	41,57,73	1.33	6 (14%)	43,93,113	1.37	6 (13%)
27	CLA	g	604	-	41,57,73	1.34	6 (14%)	43,93,113	1.32	7 (16%)
37	CHL	g	605	7	46,56,74	4.70	26 (56%)	28,92,114	2.52	15 (53%)
37	CHL	g	606	-	48,58,74	4.71	26 (54%)	29,94,114	2.51	14 (48%)
37	CHL	g	607	-	48,58,74	4.68	26 (54%)	29,94,114	2.31	12 (41%)
37	CHL	g	608	-	48,58,74	4.69	25 (52%)	29,94,114	2.35	13 (44%)
37	CHL	g	609	7	48,58,74	4.71	26 (54%)	29,94,114	2.36	12 (41%)
27	CLA	g	610	7	57,73,73	1.14	6 (10%)	61,113,113	1.22	5 (8%)
27	CLA	g	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	g	612	7	41,57,73	1.35	7 (17%)	43,93,113	1.32	6 (13%)
27	CLA	g	613	7	41,57,73	1.32	8 (19%)	43,93,113	1.41	8 (18%)
27	CLA	g	614	-	41,57,73	1.32	5 (12%)	43,93,113	1.31	5 (11%)
29	BCR	h	101	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	19 (33%)
32	DGD	h	102	-	63,63,67	0.97	3 (4%)	77,77,81	1.49	10 (12%)
35	LHG	l	101	-	48,48,48	0.71	1 (2%)	49,54,54	1.32	7 (14%)
38	LUT	n	1620	-	42,43,43	0.97	2 (4%)	49,60,60	2.01	16 (32%)
38	LUT	n	1621	-	42,43,43	1.01	3 (7%)	49,60,60	1.82	13 (26%)
39	XAT	n	1622	-	47,47,47	1.38	3 (6%)	40,74,74	2.24	14 (35%)
40	NEX	n	1623	-	42,46,46	1.26	2 (4%)	40,70,70	1.99	9 (22%)
35	LHG	n	2630	27	48,48,48	0.60	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	n	601	7	48,58,74	4.68	24 (50%)	29,94,114	2.48	14 (48%)
27	CLA	n	602	7	57,73,73	1.17	7 (12%)	61,113,113	1.16	5 (8%)
27	CLA	n	603	-	41,57,73	1.35	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	n	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.38	6 (13%)
37	CHL	n	605	7	46,56,74	4.85	26 (56%)	28,92,114	2.60	15 (53%)
37	CHL	n	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	n	607	-	64,74,74	4.12	26 (40%)	47,114,114	1.96	15 (31%)
37	CHL	n	608	-	48,58,74	4.74	26 (54%)	29,94,114	2.39	12 (41%)
37	CHL	n	609	7	48,58,74	4.81	26 (54%)	29,94,114	2.44	13 (44%)
27	CLA	n	610	7	57,73,73	1.16	7 (12%)	61,113,113	1.22	7 (11%)
27	CLA	n	611	35	41,57,73	1.29	6 (14%)	43,93,113	1.39	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	n	612	7	41,57,73	1.34	6 (14%)	43,93,113	1.35	7 (16%)
27	CLA	n	613	7	41,57,73	1.32	7 (17%)	43,93,113	1.35	5 (11%)
27	CLA	n	614	-	41,57,73	1.27	4 (9%)	43,93,113	1.35	7 (16%)
35	LHG	r	2630	27	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
27	CLA	r	601	17	41,57,73	1.29	5 (12%)	43,93,113	1.45	8 (18%)
27	CLA	r	602	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	r	603	-	41,57,73	1.34	7 (17%)	43,93,113	1.33	6 (13%)
27	CLA	r	604	-	41,57,73	1.31	5 (12%)	43,93,113	1.45	6 (13%)
37	CHL	r	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.42	12 (41%)
37	CHL	r	607	-	48,58,74	4.72	25 (52%)	29,94,114	2.38	12 (41%)
37	CHL	r	608	-	48,58,74	4.73	26 (54%)	29,94,114	2.30	12 (41%)
27	CLA	r	609	17	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	r	610	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	r	611	35	41,57,73	1.30	5 (12%)	43,93,113	1.29	6 (13%)
27	CLA	r	612	-	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	r	613	17	41,57,73	1.30	5 (12%)	43,93,113	1.35	5 (11%)
27	CLA	r	616	17	41,57,73	1.32	5 (12%)	43,93,113	1.31	6 (13%)
38	LUT	r	620	-	42,43,43	0.94	2 (4%)	49,60,60	1.70	15 (30%)
39	XAT	r	622	-	47,47,47	1.37	3 (6%)	40,74,74	1.91	13 (32%)
40	NEX	r	623	-	42,46,46	1.30	2 (4%)	40,70,70	1.85	13 (32%)
38	LUT	s	1620	-	42,43,43	0.98	3 (7%)	49,60,60	2.06	16 (32%)
38	LUT	s	1621	-	42,43,43	0.98	3 (7%)	49,60,60	1.81	15 (30%)
40	NEX	s	1623	-	42,46,46	1.21	3 (7%)	40,70,70	1.89	9 (22%)
35	LHG	s	2630	27	48,48,48	0.63	1 (2%)	49,54,54	1.28	6 (12%)
37	CHL	s	601	18	50,60,74	4.62	25 (50%)	29,97,114	2.51	13 (44%)
27	CLA	s	602	18	41,57,73	1.37	6 (14%)	43,93,113	1.37	7 (16%)
27	CLA	s	603	-	41,57,73	1.30	5 (12%)	43,93,113	1.37	6 (13%)
27	CLA	s	604	-	41,57,73	1.32	7 (17%)	43,93,113	1.40	8 (18%)
37	CHL	s	606	-	48,58,74	4.64	25 (52%)	29,94,114	2.32	12 (41%)
37	CHL	s	607	-	48,58,74	4.61	24 (50%)	29,94,114	2.65	13 (44%)
37	CHL	s	608	-	47,57,74	4.59	23 (48%)	28,93,114	2.58	12 (42%)
27	CLA	s	609	18	41,57,73	1.33	5 (12%)	43,93,113	1.29	4 (9%)
27	CLA	s	610	18	41,57,73	1.32	5 (12%)	43,93,113	1.39	6 (13%)
27	CLA	s	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.36	5 (11%)
27	CLA	s	612	18	41,57,73	1.33	7 (17%)	43,93,113	1.34	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	s	613	18	41,57,73	1.32	7 (17%)	43,93,113	1.42	6 (13%)
27	CLA	s	614	-	41,57,73	1.37	7 (17%)	43,93,113	1.31	6 (13%)
38	LUT	y	1620	-	42,43,43	1.05	3 (7%)	49,60,60	1.90	17 (34%)
38	LUT	y	1621	-	42,43,43	1.12	4 (9%)	49,60,60	1.90	17 (34%)
39	XAT	y	1622	-	47,47,47	1.35	2 (4%)	40,74,74	1.98	11 (27%)
40	NEX	y	1623	-	42,46,46	1.28	2 (4%)	40,70,70	2.00	10 (25%)
35	LHG	y	2630	27	48,48,48	0.73	1 (2%)	49,54,54	1.31	7 (14%)
37	CHL	y	601	7	64,74,74	4.12	27 (42%)	47,114,114	2.08	15 (31%)
27	CLA	y	602	7	57,73,73	1.20	8 (14%)	61,113,113	1.28	8 (13%)
27	CLA	y	603	-	41,57,73	1.36	7 (17%)	43,93,113	1.35	7 (16%)
27	CLA	y	604	-	41,57,73	1.38	8 (19%)	43,93,113	1.38	6 (13%)
37	CHL	y	605	7	46,56,74	4.80	26 (56%)	28,92,114	2.41	11 (39%)
37	CHL	y	606	-	48,58,74	4.77	26 (54%)	29,94,114	2.50	13 (44%)
37	CHL	y	607	-	48,58,74	4.78	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	y	608	-	48,58,74	4.76	27 (56%)	29,94,114	2.30	11 (37%)
37	CHL	y	609	7	64,74,74	4.14	26 (40%)	47,114,114	2.12	14 (29%)
27	CLA	y	610	7	57,73,73	1.17	7 (12%)	61,113,113	1.25	7 (11%)
27	CLA	y	611	35	57,73,73	1.15	7 (12%)	61,113,113	1.22	7 (11%)
27	CLA	y	612	7	57,73,73	1.17	8 (14%)	61,113,113	1.23	7 (11%)
27	CLA	y	613	7	57,73,73	1.18	8 (14%)	61,113,113	1.20	7 (11%)
27	CLA	y	614	-	41,57,73	1.35	6 (14%)	43,93,113	1.33	7 (16%)
31	LMG	z	101	-	51,51,55	0.71	0	59,59,63	1.36	8 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OEX	A	401	1,3	-	0/0/68/68	0/0/6/6
27	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	A	406	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	A	407	-	3/3/16/25	0/18/116/135	0/0/9/9
28	PHO	A	408	-	-	0/53/103/103	0/1/6/6
28	PHO	A	409	-	-	0/53/103/103	0/1/6/6
27	CLA	A	410	-	3/3/19/25	0/31/129/135	0/0/9/9
29	BCR	A	411	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	A	412	-	-	0/49/69/69	0/1/1/1
31	LMG	A	413	-	-	0/43/63/70	0/1/1/1
30	SQD	A	418	-	-	0/49/69/69	0/1/1/1
27	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	B	618	-	-	0/29/63/63	0/2/2/2
29	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	BCR	B	620	-	-	0/29/63/63	0/2/2/2
30	SQD	B	621	-	-	0/49/69/69	0/1/1/1
31	LMG	B	622	-	-	0/46/66/70	0/1/1/1
27	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	513	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	C	514	-	-	0/29/63/63	0/2/2/2
29	BCR	C	515	-	-	0/29/63/63	0/2/2/2
29	BCR	C	516	-	-	0/29/63/63	0/2/2/2
29	BCR	C	517	-	-	0/29/63/63	0/2/2/2
32	DGD	C	518	-	-	0/44/84/95	0/2/2/2
32	DGD	C	519	-	-	0/51/91/95	0/2/2/2
32	DGD	C	520	-	-	0/51/91/95	0/2/2/2
31	LMG	C	521	-	-	0/46/66/70	0/1/1/1
33	BCT	D	401	-	-	0/0/0/0	0/0/0/0
27	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	D	404	-	-	0/29/63/63	0/2/2/2
34	PL9	D	405	-	-	0/53/73/73	0/1/1/1
35	LHG	D	408	-	-	0/47/47/53	0/0/0/0
35	LHG	D	409	-	-	0/53/53/53	0/0/0/0
35	LHG	D	410	-	-	0/41/41/53	0/0/0/0
31	LMG	D	411	-	-	0/41/61/70	0/1/1/1
36	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
38	LUT	G	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	G	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	G	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	G	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	G	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	G	601	7	-	0/41/177/177	0/0/9/9
27	CLA	G	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	G	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	G	605	7	-	0/20/156/177	0/0/9/9
37	CHL	G	606	-	-	0/22/158/177	0/0/9/9
37	CHL	G	607	-	-	0/22/158/177	0/0/9/9
37	CHL	G	608	-	-	0/22/158/177	0/0/9/9
37	CHL	G	609	7	-	0/22/158/177	0/0/9/9
27	CLA	G	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	G	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	614	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	H	101	-	-	0/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	L	101	-	-	0/53/53/53	0/0/0/0
38	LUT	N	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	N	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	N	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	N	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	N	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	N	601	7	-	0/22/158/177	0/0/9/9
27	CLA	N	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	N	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	N	605	7	-	0/20/156/177	0/0/9/9
37	CHL	N	606	-	-	0/22/158/177	0/0/9/9
37	CHL	N	607	-	-	0/41/177/177	0/0/9/9
37	CHL	N	608	-	-	0/22/158/177	0/0/9/9
37	CHL	N	609	7	-	0/22/158/177	0/0/9/9
27	CLA	N	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	N	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	614	-	3/3/16/25	0/18/116/135	0/0/9/9
35	LHG	R	2630	27	-	0/53/53/53	0/0/0/0
27	CLA	R	601	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	602	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	R	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	R	606	-	-	0/22/158/177	0/0/9/9
37	CHL	R	607	-	-	0/22/158/177	0/0/9/9
37	CHL	R	608	-	-	0/22/158/177	0/0/9/9
27	CLA	R	609	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	610	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	R	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	612	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	613	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	616	17	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	R	620	-	-	0/29/67/67	0/2/2/2
39	XAT	R	622	-	-	0/31/93/93	0/2/4/4
40	NEX	R	623	-	-	0/27/83/83	0/2/3/3
38	LUT	S	1620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
40	NEX	S	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	S	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	S	601	18	-	0/25/161/177	0/0/9/9
27	CLA	S	602	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	603	-	2/2/16/25	0/18/116/135	0/0/9/9
27	CLA	S	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	S	606	-	-	0/22/158/177	0/0/9/9
37	CHL	S	607	-	-	0/22/158/177	0/0/9/9
37	CHL	S	608	-	-	0/21/157/177	0/0/9/9
27	CLA	S	609	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	610	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	612	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	613	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	614	-	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	Y	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	Y	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	Y	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	Y	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	Y	601	7	-	0/41/177/177	0/0/9/9
27	CLA	Y	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	Y	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	Y	605	7	-	0/20/156/177	0/0/9/9
37	CHL	Y	606	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	607	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	608	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	609	7	-	0/41/177/177	0/0/9/9
27	CLA	Y	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	611	35	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	612	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	613	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	614	-	3/3/16/25	0/18/116/135	0/0/9/9
31	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
24	OEX	a	401	1,3	-	0/0/68/68	0/0/6/6
27	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	a	407	-	3/3/16/25	0/18/116/135	0/0/9/9
28	PHO	a	408	-	-	0/53/103/103	0/1/6/6
28	PHO	a	409	-	-	0/53/103/103	0/1/6/6
27	CLA	a	410	-	3/3/19/25	0/31/129/135	0/0/9/9
29	BCR	a	411	-	-	0/29/63/63	0/2/2/2
30	SQD	a	412	-	-	0/49/69/69	0/1/1/1
31	LMG	a	413	-	-	0/43/63/70	0/1/1/1
30	SQD	a	418	-	-	0/49/69/69	0/1/1/1
27	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	BCR	b	619	-	-	0/29/63/63	0/2/2/2
29	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	SQD	b	621	-	-	0/49/69/69	0/1/1/1
31	LMG	b	622	-	-	0/46/66/70	0/1/1/1
27	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	513	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	c	514	-	-	0/29/63/63	0/2/2/2
29	BCR	c	515	-	-	0/29/63/63	0/2/2/2
29	BCR	c	516	-	-	0/29/63/63	0/2/2/2
29	BCR	c	517	-	-	0/29/63/63	0/2/2/2
32	DGD	c	518	-	-	0/44/84/95	0/2/2/2
32	DGD	c	519	-	-	0/51/91/95	0/2/2/2
32	DGD	c	520	-	-	0/51/91/95	0/2/2/2
31	LMG	c	521	-	-	0/46/66/70	0/1/1/1
33	BCT	d	401	-	-	0/0/0/0	0/0/0/0
27	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	d	404	-	-	0/29/63/63	0/2/2/2
34	PL9	d	405	-	-	0/53/73/73	0/1/1/1
35	LHG	d	408	-	-	0/47/47/53	0/0/0/0
35	LHG	d	409	-	-	0/53/53/53	0/0/0/0
35	LHG	d	410	-	-	0/41/41/53	0/0/0/0
31	LMG	d	411	-	-	0/41/61/70	0/1/1/1
36	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
38	LUT	g	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	g	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	g	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	g	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	g	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	g	601	7	-	0/41/177/177	0/0/9/9
27	CLA	g	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	g	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	g	605	7	-	0/20/156/177	0/0/9/9
37	CHL	g	606	-	-	0/22/158/177	0/0/9/9
37	CHL	g	607	-	-	0/22/158/177	0/0/9/9
37	CHL	g	608	-	-	0/22/158/177	0/0/9/9
37	CHL	g	609	7	-	0/22/158/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	g	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	g	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	614	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	h	101	-	-	0/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
35	LHG	l	101	-	-	0/53/53/53	0/0/0/0
38	LUT	n	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	n	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	n	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	n	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	n	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	n	601	7	-	0/22/158/177	0/0/9/9
27	CLA	n	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	n	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	n	605	7	-	0/20/156/177	0/0/9/9
37	CHL	n	606	-	-	0/22/158/177	0/0/9/9
37	CHL	n	607	-	-	0/41/177/177	0/0/9/9
37	CHL	n	608	-	-	0/22/158/177	0/0/9/9
37	CHL	n	609	7	-	0/22/158/177	0/0/9/9
27	CLA	n	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	n	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	614	-	3/3/16/25	0/18/116/135	0/0/9/9
35	LHG	r	2630	27	-	0/53/53/53	0/0/0/0
27	CLA	r	601	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	602	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	r	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	r	606	-	-	0/22/158/177	0/0/9/9
37	CHL	r	607	-	-	0/22/158/177	0/0/9/9
37	CHL	r	608	-	-	0/22/158/177	0/0/9/9
27	CLA	r	609	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	610	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	r	611	35	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	r	612	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	613	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	616	17	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	r	620	-	-	0/29/67/67	0/2/2/2
39	XAT	r	622	-	-	0/31/93/93	0/2/4/4
40	NEX	r	623	-	-	0/27/83/83	0/2/3/3
38	LUT	s	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
40	NEX	s	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	s	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	s	601	18	-	0/25/161/177	0/0/9/9
27	CLA	s	602	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	603	-	2/2/16/25	0/18/116/135	0/0/9/9
27	CLA	s	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	s	606	-	-	0/22/158/177	0/0/9/9
37	CHL	s	607	-	-	0/22/158/177	0/0/9/9
37	CHL	s	608	-	-	0/21/157/177	0/0/9/9
27	CLA	s	609	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	610	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	612	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	613	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	614	-	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	y	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	y	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	y	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	y	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	y	601	7	-	0/41/177/177	0/0/9/9
27	CLA	y	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	y	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	y	605	7	-	0/20/156/177	0/0/9/9
37	CHL	y	606	-	-	0/22/158/177	0/0/9/9
37	CHL	y	607	-	-	0/22/158/177	0/0/9/9
37	CHL	y	608	-	-	0/22/158/177	0/0/9/9
37	CHL	y	609	7	-	0/41/177/177	0/0/9/9
27	CLA	y	610	7	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	y	611	35	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	612	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	613	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	614	-	3/3/16/25	0/18/116/135	0/0/9/9
31	LMG	z	101	-	-	0/46/66/70	0/1/1/1

The worst 5 of 2657 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	601	CHL	C3D-C4D	-20.31	1.32	1.54
37	g	601	CHL	C3D-C4D	-20.27	1.32	1.54
37	R	608	CHL	C3D-C4D	-20.19	1.32	1.54
37	r	608	CHL	C3D-C4D	-20.19	1.32	1.54
37	Y	608	CHL	C3D-C4D	-20.18	1.32	1.54

The worst 5 of 2930 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	1622	XAT	C31-C30-C29	-6.86	117.25	127.22
39	n	1622	XAT	C31-C30-C29	-6.85	117.26	127.22
29	C	516	BCR	C24-C23-C22	-6.56	116.30	126.21
29	c	516	BCR	C24-C23-C22	-6.54	116.33	126.21
29	D	404	BCR	C11-C10-C9	-6.39	117.94	127.22

5 of 466 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	y	603	CLA	NC
27	y	603	CLA	ND
27	y	603	CLA	NA
27	N	611	CLA	NC
27	N	611	CLA	ND

There are no torsion outliers.

There are no ring outliers.

155 monomers are involved in 855 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	401	OEX	2	0
27	A	405	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	406	CLA	8	0
27	A	407	CLA	7	0
28	A	408	PHO	5	0
28	A	409	PHO	5	0
27	A	410	CLA	8	0
29	A	411	BCR	6	0
30	A	412	SQD	3	0
31	A	413	LMG	8	0
30	A	418	SQD	3	0
27	B	602	CLA	7	0
27	B	603	CLA	11	0
27	B	604	CLA	10	0
27	B	605	CLA	9	0
27	B	606	CLA	7	0
27	B	607	CLA	7	0
27	B	608	CLA	6	0
27	B	609	CLA	9	0
27	B	610	CLA	12	0
27	B	611	CLA	3	0
27	B	612	CLA	5	0
27	B	613	CLA	13	0
27	B	614	CLA	7	0
27	B	615	CLA	6	0
27	B	616	CLA	7	0
27	B	617	CLA	4	0
29	B	618	BCR	10	0
29	B	619	BCR	8	0
29	B	620	BCR	2	0
30	B	621	SQD	3	0
31	B	622	LMG	10	0
27	C	501	CLA	3	0
27	C	502	CLA	9	0
27	C	503	CLA	8	0
27	C	504	CLA	6	0
27	C	505	CLA	8	0
27	C	506	CLA	8	0
27	C	507	CLA	5	0
27	C	508	CLA	5	0
27	C	509	CLA	5	0
27	C	510	CLA	9	0
27	C	511	CLA	10	0
27	C	512	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	513	CLA	5	0
29	C	514	BCR	7	0
29	C	515	BCR	6	0
29	C	516	BCR	10	0
29	C	517	BCR	8	0
32	C	518	DGD	5	0
32	C	519	DGD	6	0
32	C	520	DGD	20	0
31	C	521	LMG	5	0
33	D	401	BCT	5	0
27	D	402	CLA	9	0
27	D	403	CLA	7	0
29	D	404	BCR	5	0
34	D	405	PL9	9	0
35	D	408	LHG	5	0
35	D	409	LHG	4	0
35	D	410	LHG	5	0
31	D	411	LMG	3	0
36	F	101	HEM	5	0
38	G	1620	LUT	9	0
38	G	1621	LUT	7	0
39	G	1622	XAT	8	0
40	G	1623	NEX	3	0
35	G	2630	LHG	14	0
37	G	601	CHL	14	0
27	G	602	CLA	8	0
27	G	603	CLA	2	0
27	G	604	CLA	3	0
37	G	605	CHL	6	0
37	G	606	CHL	3	0
37	G	607	CHL	5	0
37	G	608	CHL	6	0
37	G	609	CHL	5	0
27	G	610	CLA	14	0
27	G	611	CLA	9	0
27	G	612	CLA	1	0
27	G	613	CLA	4	0
27	G	614	CLA	3	0
29	H	101	BCR	7	0
32	H	102	DGD	10	0
35	L	101	LHG	7	0
38	N	1620	LUT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	N	1621	LUT	8	0
39	N	1622	XAT	8	0
40	N	1623	NEX	3	0
35	N	2630	LHG	7	0
37	N	601	CHL	9	0
27	N	602	CLA	10	0
27	N	603	CLA	1	0
37	N	605	CHL	6	0
37	N	606	CHL	4	0
37	N	607	CHL	10	0
37	N	608	CHL	5	0
37	N	609	CHL	7	0
27	N	610	CLA	12	0
27	N	611	CLA	3	0
27	N	612	CLA	3	0
27	N	613	CLA	3	0
27	N	614	CLA	3	0
35	R	2630	LHG	3	0
27	R	601	CLA	5	0
27	R	602	CLA	14	0
27	R	604	CLA	5	0
37	R	606	CHL	6	0
37	R	607	CHL	4	0
37	R	608	CHL	11	0
27	R	609	CLA	5	0
27	R	610	CLA	11	0
27	R	611	CLA	4	0
27	R	612	CLA	1	0
27	R	613	CLA	9	0
27	R	616	CLA	6	0
38	R	620	LUT	13	0
39	R	622	XAT	8	0
40	R	623	NEX	6	0
38	S	1620	LUT	8	0
38	S	1621	LUT	11	0
40	S	1623	NEX	5	0
35	S	2630	LHG	3	0
37	S	601	CHL	2	0
27	S	602	CLA	5	0
27	S	603	CLA	3	0
27	S	604	CLA	7	0
37	S	606	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	S	607	CHL	3	0
37	S	608	CHL	4	0
27	S	609	CLA	4	0
27	S	610	CLA	13	0
27	S	611	CLA	2	0
27	S	612	CLA	3	0
27	S	613	CLA	4	0
27	S	614	CLA	4	0
38	Y	1620	LUT	8	0
38	Y	1621	LUT	9	0
39	Y	1622	XAT	10	0
40	Y	1623	NEX	5	0
35	Y	2630	LHG	8	0
37	Y	601	CHL	9	0
27	Y	602	CLA	10	0
27	Y	603	CLA	5	0
27	Y	604	CLA	4	0
37	Y	605	CHL	5	0
37	Y	607	CHL	6	0
37	Y	608	CHL	3	0
37	Y	609	CHL	8	0
27	Y	610	CLA	9	0
27	Y	611	CLA	7	0
27	Y	612	CLA	5	0
27	Y	613	CLA	7	0
27	Y	614	CLA	2	0
31	Z	101	LMG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.