



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 11, 2017 – 05:04 PM EST

PDB ID : 2AXT  
Title : Crystal Structure of Photosystem II from *Thermosynechococcus elongatus*  
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.  
Deposited on : unknown  
Resolution : 3.00 Å(reported)

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

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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

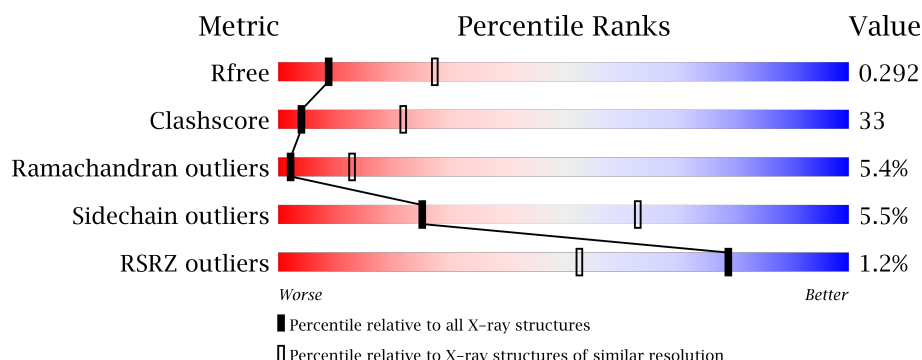
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




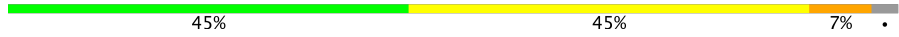

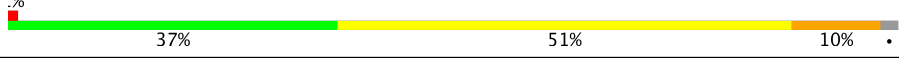
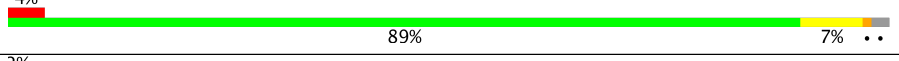
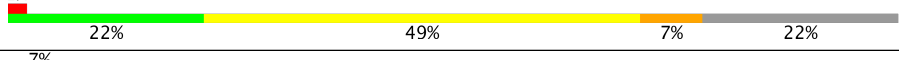
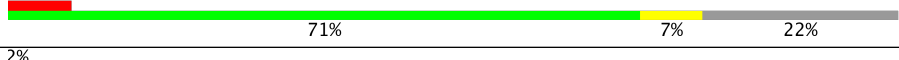
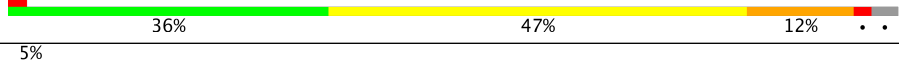
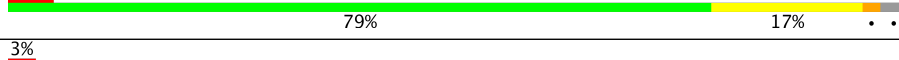
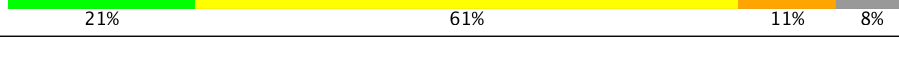


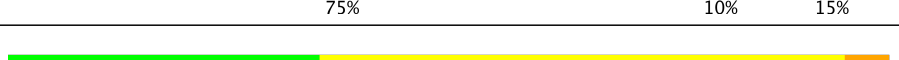

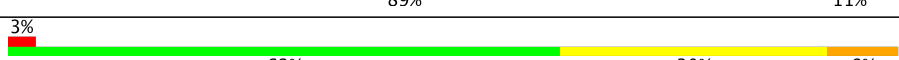
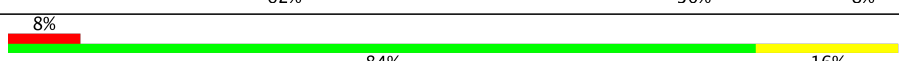
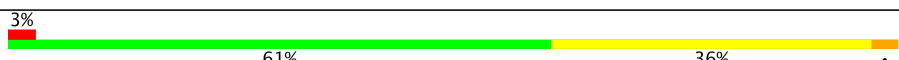
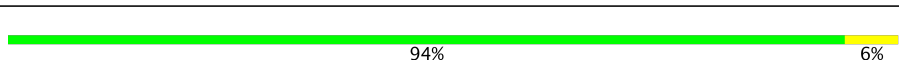
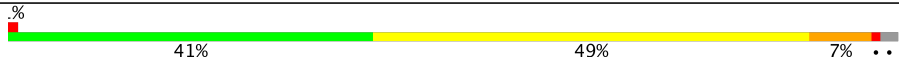


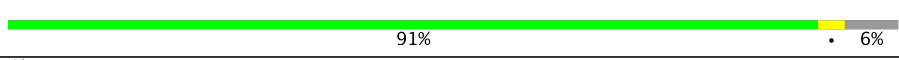

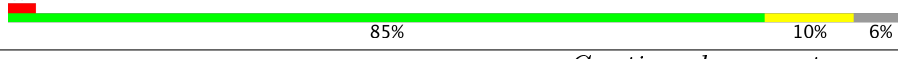

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>42%</div> <div>48%</div> <div>6%</div> <div>...</div> </div>
1	a	344	<div> <div>88%</div> <div>9%</div> <div>...</div> </div>
2	B	510	<div> <div>55%</div> <div>36%</div> <div>5%</div> <div>...</div> </div>
2	b	510	<div> <div>89%</div> <div>6%</div> <div>...</div> </div>
3	C	473	<div> <div>40%</div> <div>48%</div> <div>6%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	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
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	X
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	498	X	-	-	-
20	CLA	C	499	X	-	-	-
20	CLA	C	500	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	D	354	X	-	-	-
20	CLA	D	355	X	-	-	-
20	CLA	a	5558	X	-	-	-
20	CLA	a	5559	X	-	-	-
20	CLA	a	5560	X	-	-	X
20	CLA	a	5563	X	-	-	X
20	CLA	b	5511	X	-	-	X
20	CLA	b	5512	X	-	-	-
20	CLA	b	5513	X	-	-	-
20	CLA	b	5514	X	-	-	-
20	CLA	b	5515	X	-	-	-
20	CLA	b	5516	X	-	-	-
20	CLA	b	5517	X	-	-	-
20	CLA	b	5518	X	-	-	-
20	CLA	b	5519	X	-	-	-
20	CLA	b	5520	X	-	-	-
20	CLA	b	5521	X	-	-	-
20	CLA	b	5522	X	-	-	-
20	CLA	b	5523	X	-	-	-
20	CLA	b	5524	X	-	-	-
20	CLA	b	5525	X	-	-	-
20	CLA	b	5526	X	-	-	-
20	CLA	c	5491	X	-	-	-
20	CLA	c	5492	X	-	-	-
20	CLA	c	5493	X	-	-	-
20	CLA	c	5494	X	-	-	-
20	CLA	c	5495	X	-	-	-
20	CLA	c	5496	X	-	-	-
20	CLA	c	5497	X	-	-	-
20	CLA	c	5498	X	-	-	-
20	CLA	c	5499	X	-	-	-
20	CLA	c	5500	X	-	-	-
20	CLA	c	5501	X	-	-	-
20	CLA	c	5502	X	-	-	-
20	CLA	c	5503	X	-	-	X
20	CLA	d	5354	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	X	-	-	-
22	PQ9	A	564	-	-	-	X
22	PQ9	a	5564	-	-	-	X
24	BCR	B	528	-	-	-	X
24	BCR	C	504	-	-	-	X
24	BCR	C	505	-	-	-	X
24	BCR	D	357	-	-	-	X
24	BCR	H	107	-	-	-	X
24	BCR	X	130	-	-	-	X
24	BCR	b	5529	-	-	-	X
24	BCR	c	5504	-	-	-	X
24	BCR	d	5357	-	-	-	X
24	BCR	h	5107	-	-	-	X
24	BCR	x	5130	-	-	-	X
27	LMT	A	569	-	-	-	X
27	LMT	M	5216	-	-	-	X
27	LMT	T	217	-	-	-	X
27	LMT	a	5568	-	-	-	X
27	LMT	t	5217	-	-	-	X
28	MGE	d	5359	-	-	-	X
29	UNK	C	481	-	-	-	X
29	UNK	C	482	-	-	-	X
29	UNK	C	489	-	-	-	X
29	UNK	c	5474	-	-	-	X
29	UNK	c	5477	-	-	-	X
29	UNK	c	5484	-	-	-	X
29	UNK	c	5485	-	-	-	X
29	UNK	c	5489	-	-	-	X
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

- Molecule 14 is a protein called Photosystem II reaction center T protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

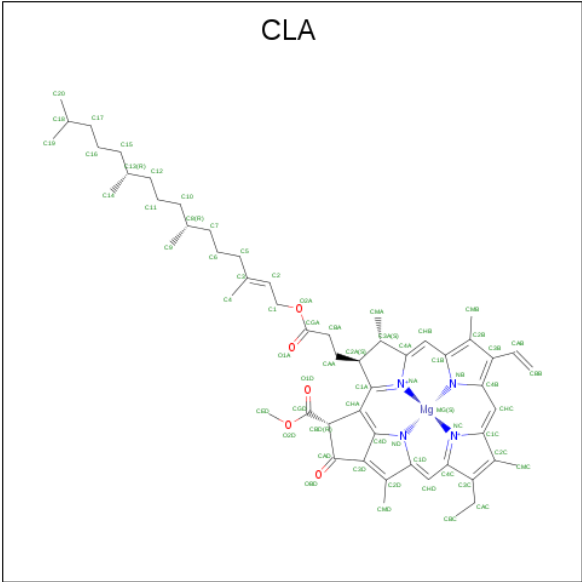
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

- Molecule 19 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	Fe	0	0
			1	1		
19	a	1	Total	Fe	0	0
			1	1		

- Molecule 20 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					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
20	C	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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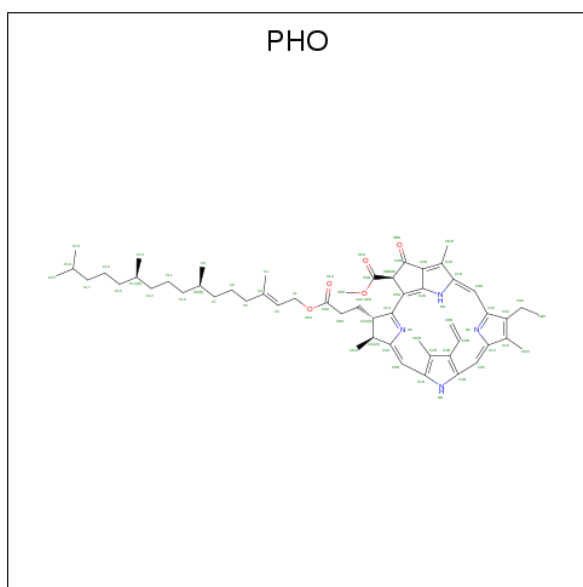
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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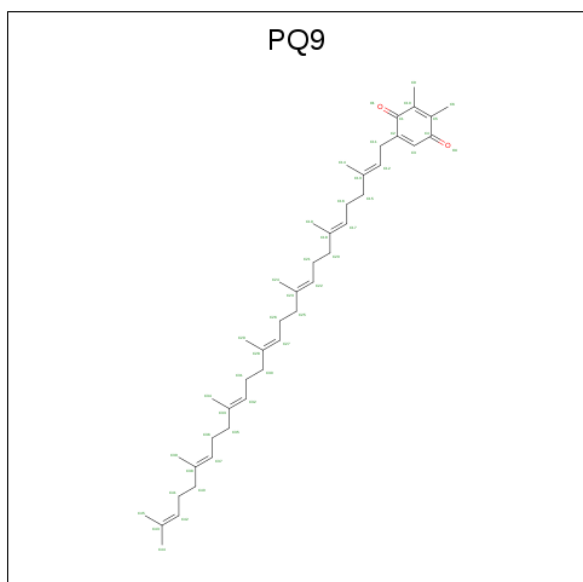
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



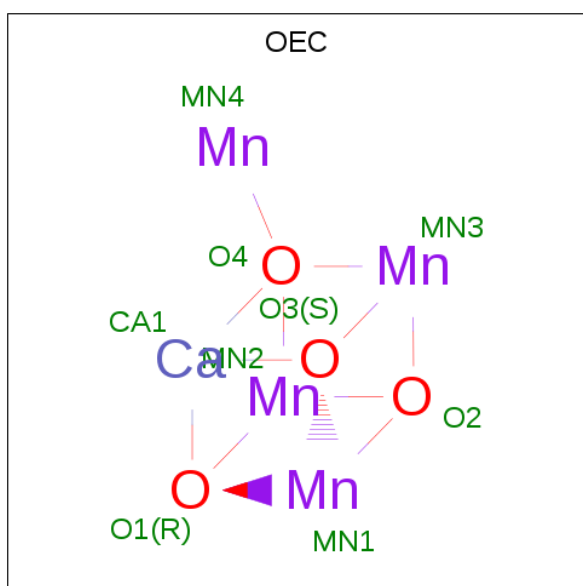
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: C<sub>43</sub>H<sub>64</sub>O<sub>2</sub>).



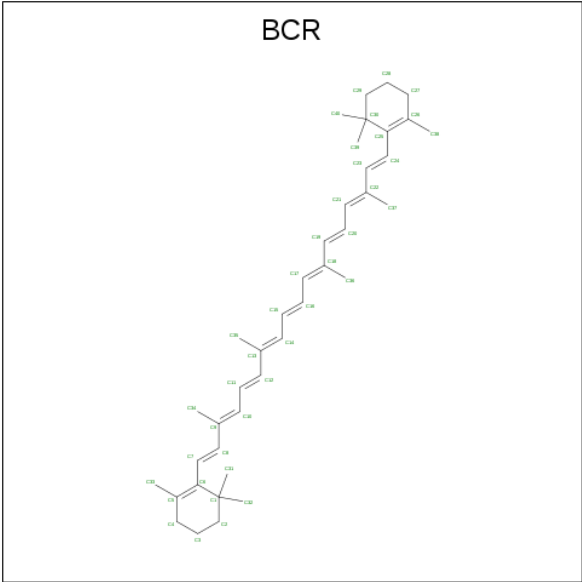
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Ca	Mn	0	0
			5	1	4		
23	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).



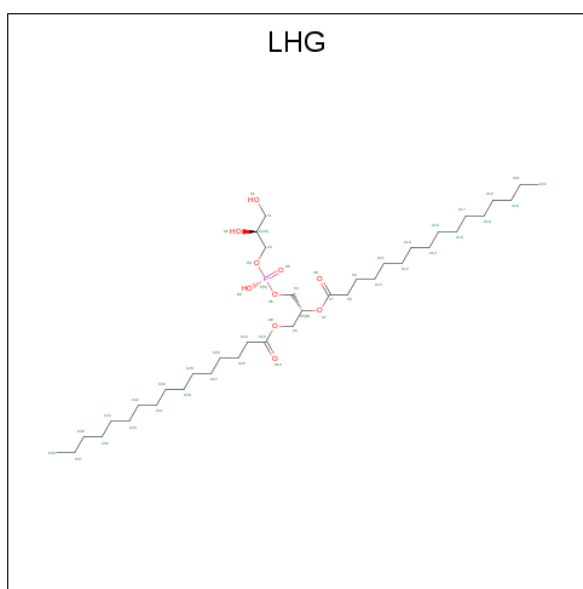
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

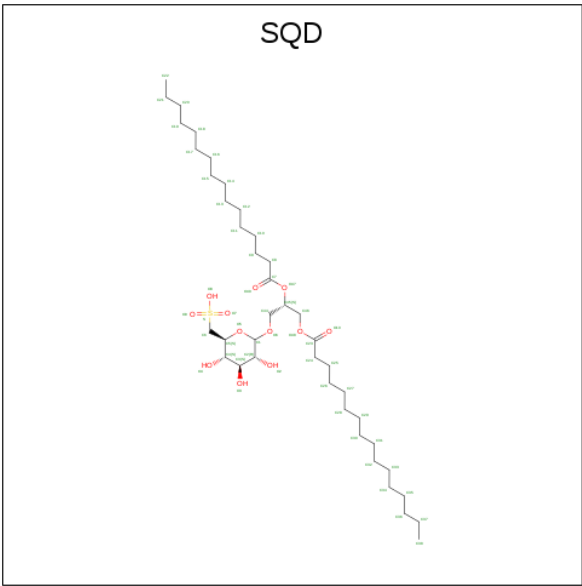
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 39 28 10 1	0	0
25	a	1	Total C O P 39 28 10 1	0	0

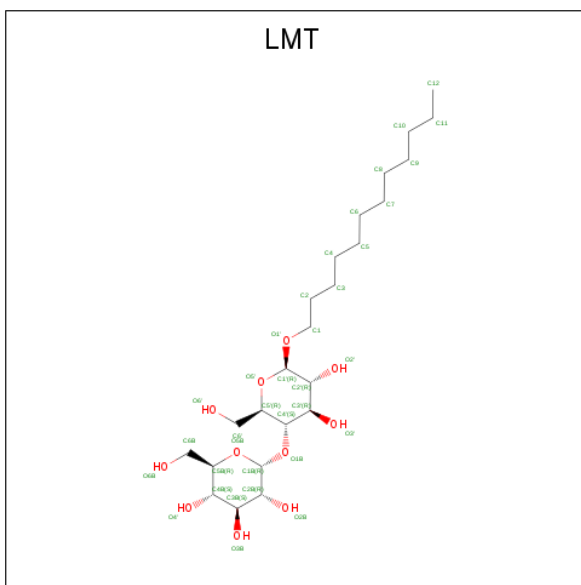
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



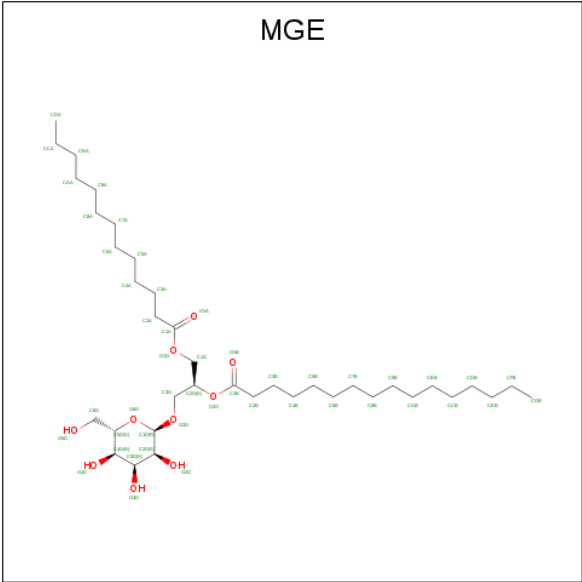
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total 35	C 24	O 11	0	0
27	M	1	Total 35	C 24	O 11	0	0
27	T	1	Total 35	C 24	O 11	0	0
27	a	1	Total 35	C 24	O 11	0	0
27	m	1	Total 35	C 24	O 11	0	0
27	t	1	Total 35	C 24	O 11	0	0

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula:  $C_{38}H_{72}O_{10}$ ).

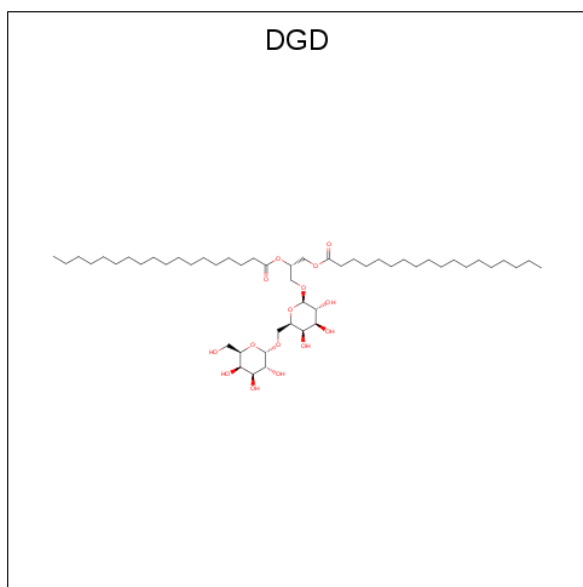


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	C	O	0	0
			47	37	10		
28	d	1	Total	C	O	0	0
			41	31	10		
28	d	1	Total	C	O	0	0
			48	38	10		
28	i	1	Total	C	O	0	0
			48	38	10		
28	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).

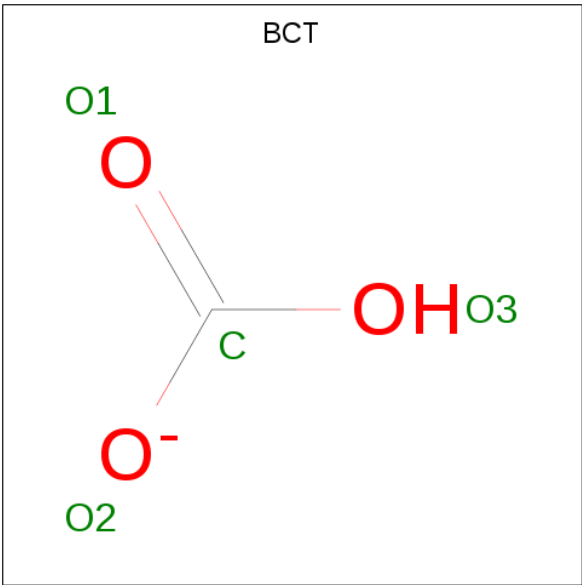
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



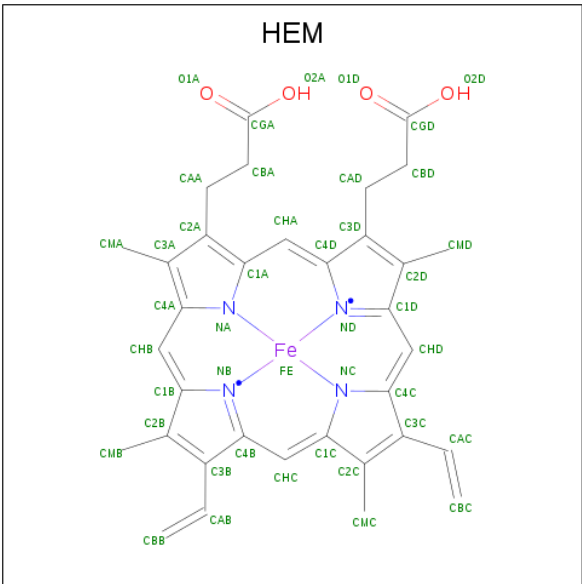
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total	C	O	0	0
			54	39	15		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



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

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
32	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
32	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

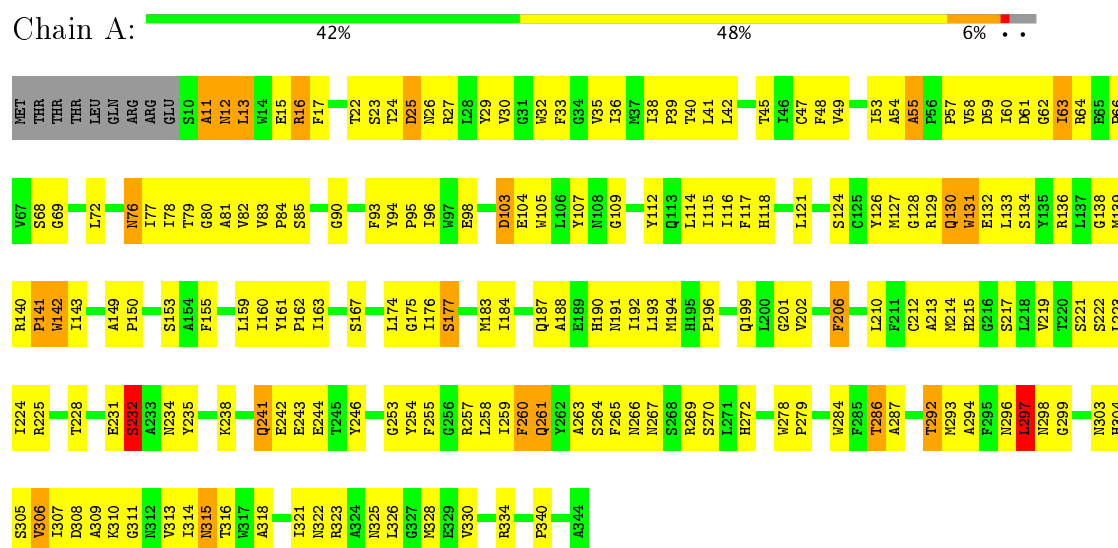
- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total	Ca	0	0
			1	1		
33	k	1	Total	Ca	0	0
			1	1		

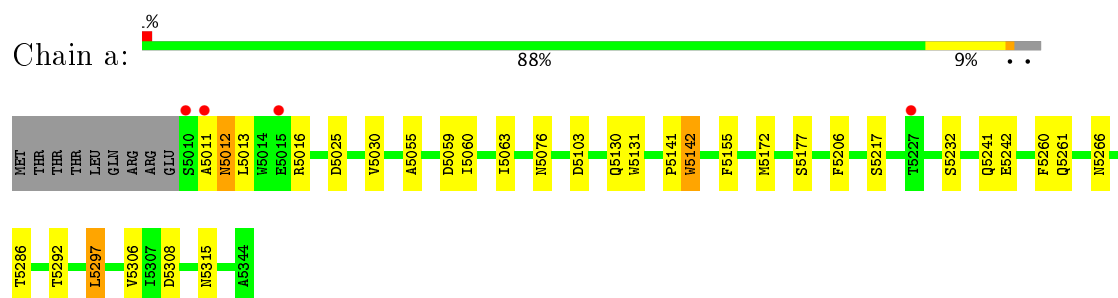
### 3 Residue-property plots

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

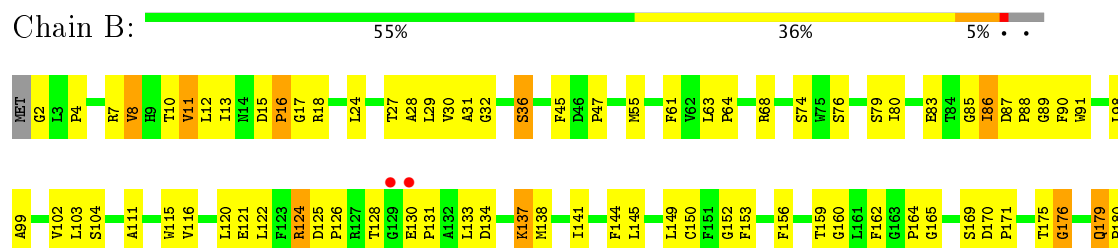
#### • Molecule 1: Photosystem Q(B) protein

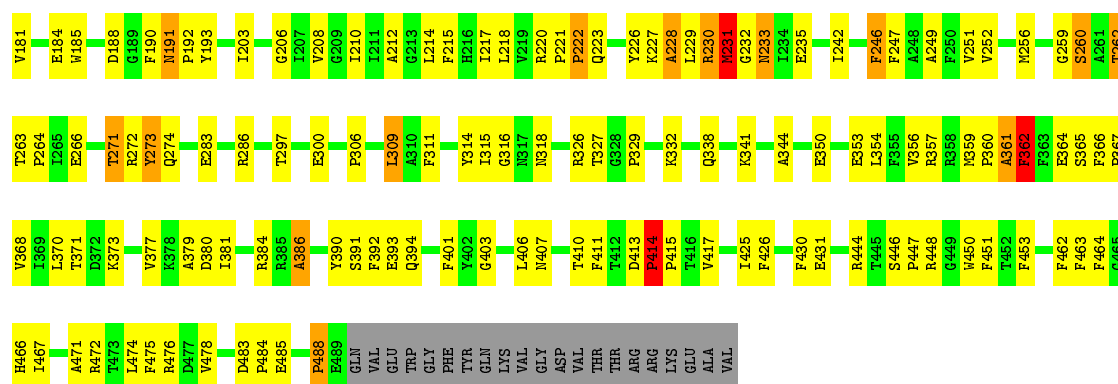


#### • Molecule 1: Photosystem Q(B) protein



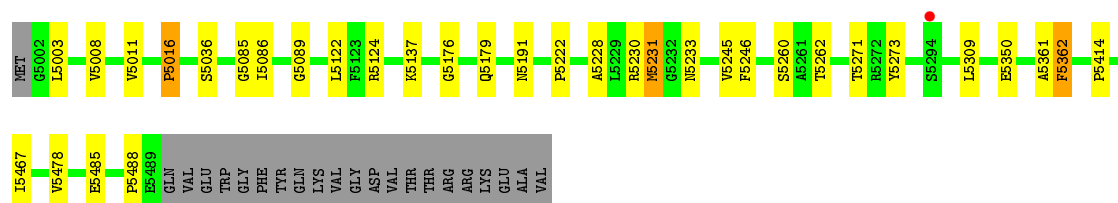
#### • Molecule 2: CP47 protein





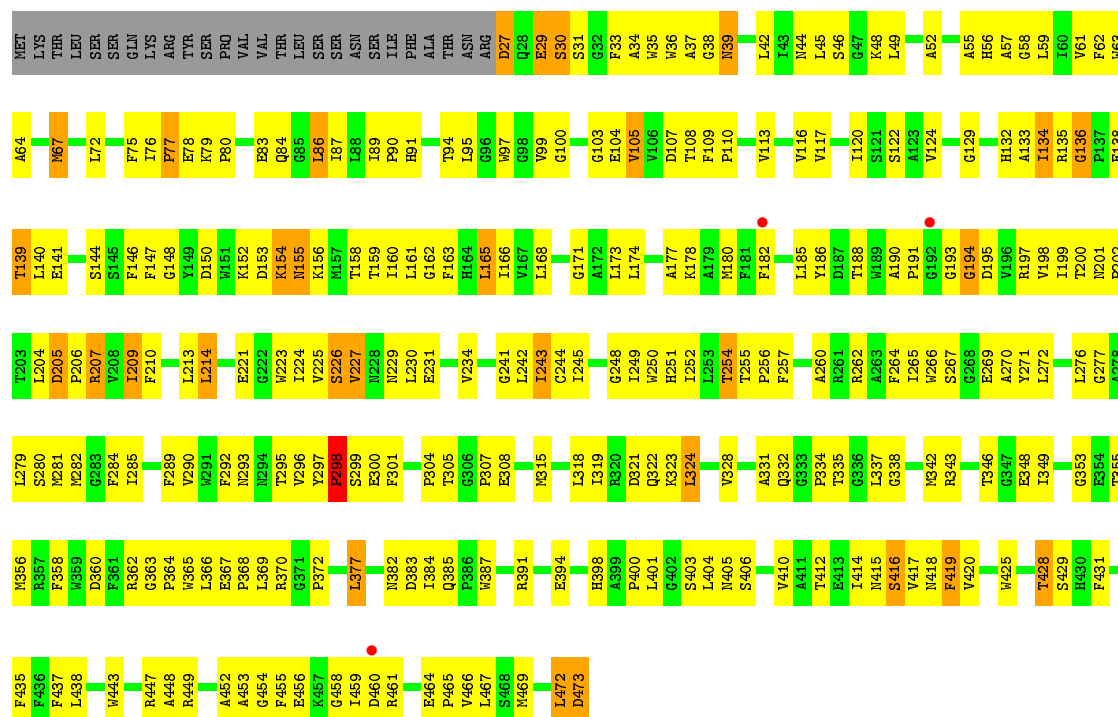
• Molecule 2: CP47 protein

Chain b: 89% 6% . .



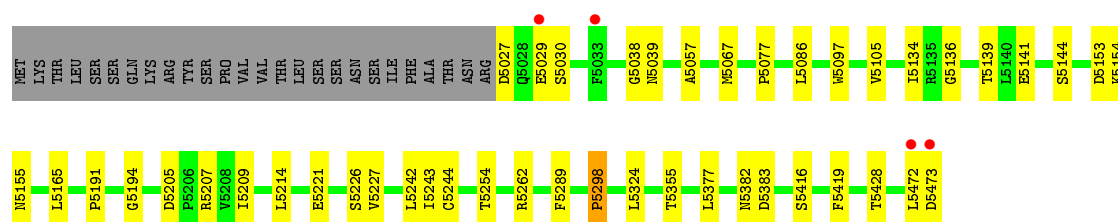
• Molecule 3: photosystem II CP43 protein

Chain C: 40% 48% 6% 5%



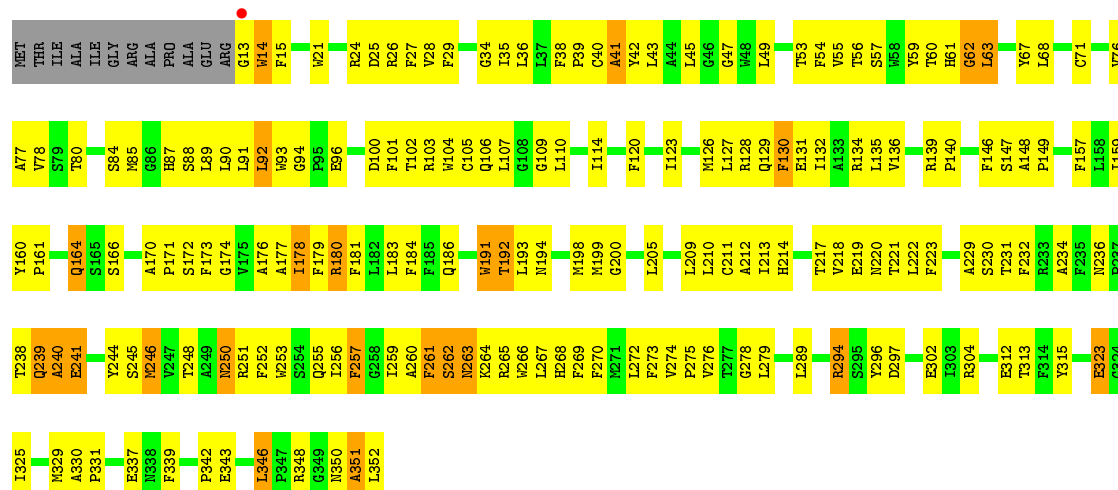
• Molecule 3: photosystem II CP43 protein

Chain c: 85% 10% 5%



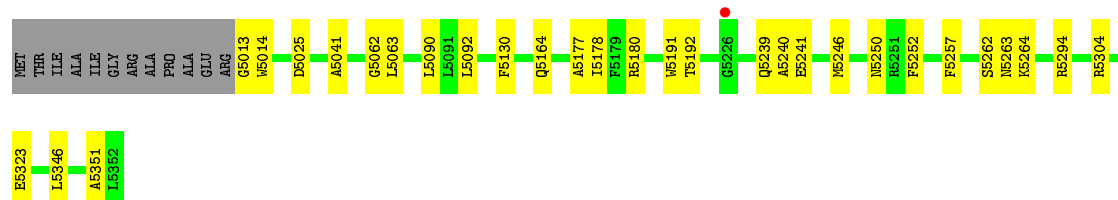
• Molecule 4: photosystem II reaction center D2 protein

Chain D: 45% 45% 7% .



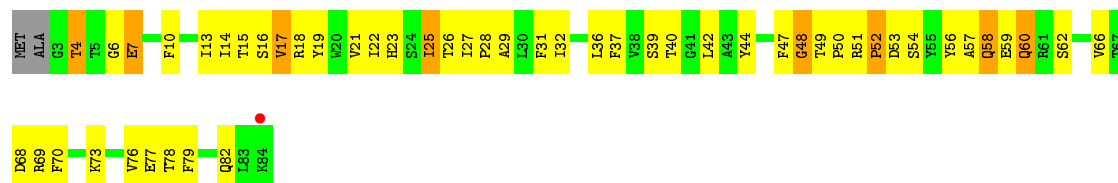
• Molecule 4: photosystem II reaction center D2 protein

Chain d: 88% 9% .



• Molecule 5: Cytochrome b559 alpha subunit

Chain E: 37% 51% 10% .



• Molecule 5: Cytochrome b559 alpha subunit

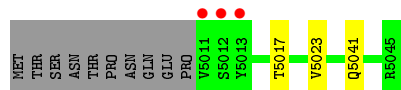
Chain e: 4% 89% 7% .



- Molecule 6: Cytochrome b559 beta subunit



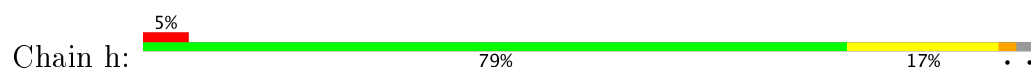
- Molecule 6: Cytochrome b559 beta subunit



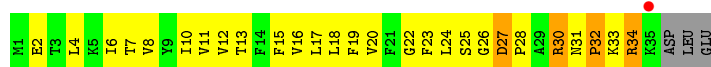
- Molecule 7: Photosystem II reaction center H protein



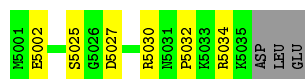
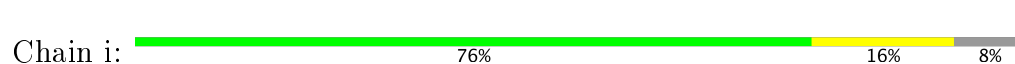
- Molecule 7: Photosystem II reaction center H protein



- Molecule 8: Photosystem II reaction center I protein



- Molecule 8: Photosystem II reaction center I protein



- Molecule 9: Photosystem II reaction center J protein





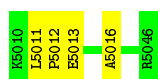
- Molecule 9: Photosystem II reaction center J protein



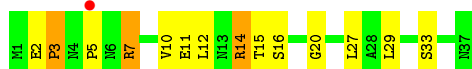
- Molecule 10: Photosystem II reaction center protein K



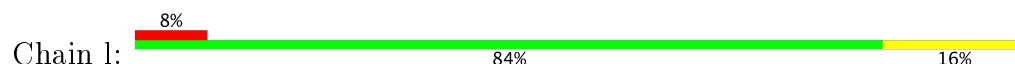
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center L protein



- Molecule 11: Photosystem II reaction center L protein

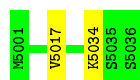


- Molecule 12: Photosystem II reaction center M protein

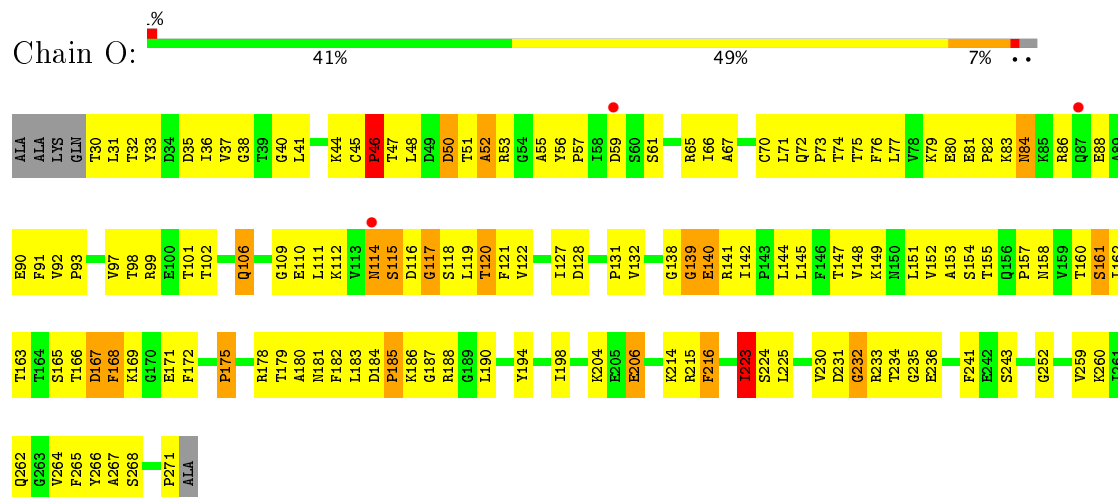


- Molecule 12: Photosystem II reaction center M protein

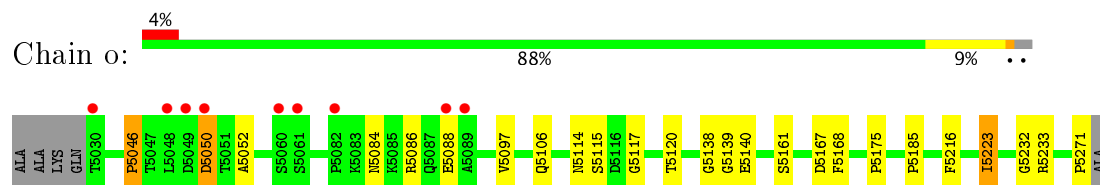




- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



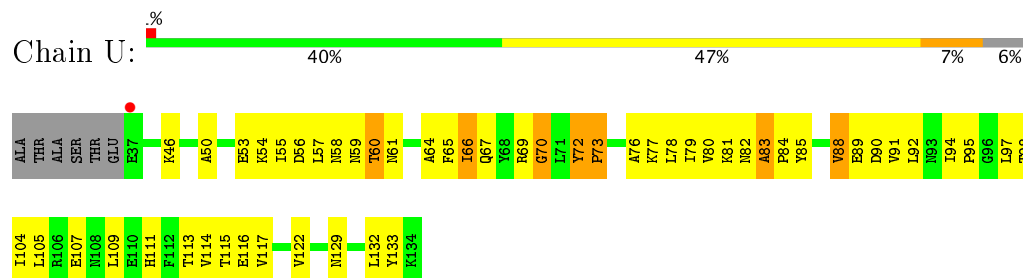
- Molecule 14: Photosystem II reaction center T protein



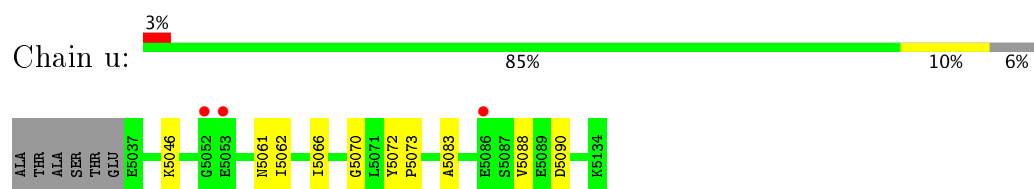
- Molecule 14: Photosystem II reaction center T protein



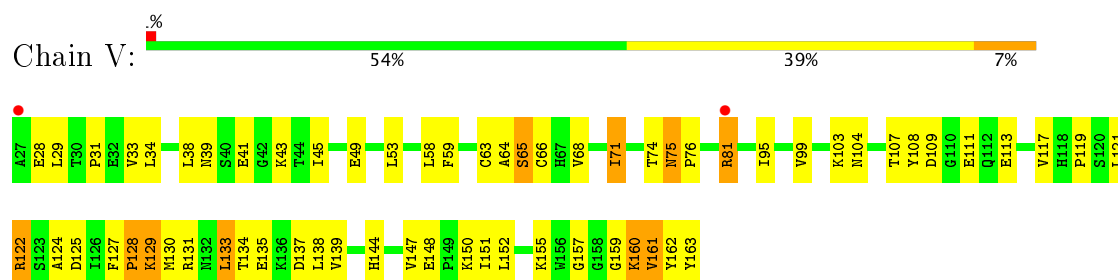
- Molecule 15: Photosystem II 12 kDa extrinsic protein



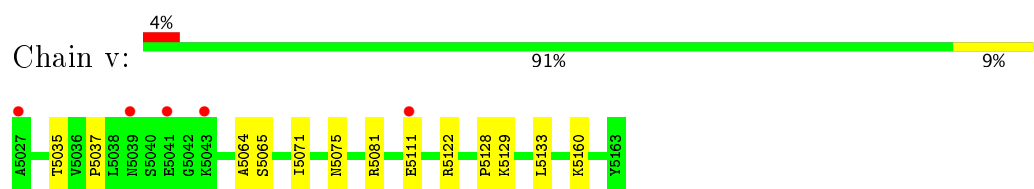
- Molecule 15: Photosystem II 12 kDa extrinsic protein



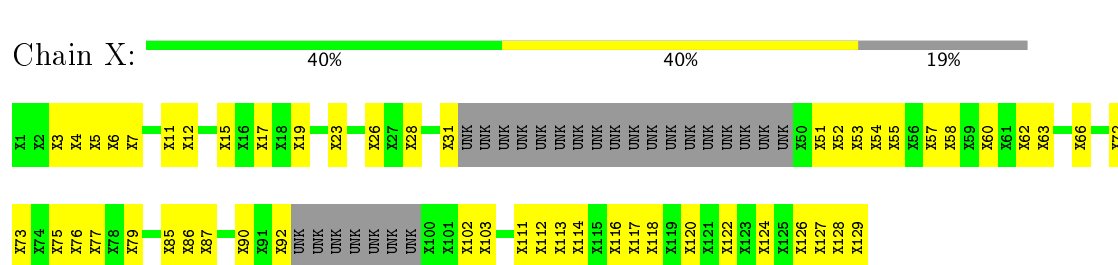
- Molecule 16: Cytochrome c-550



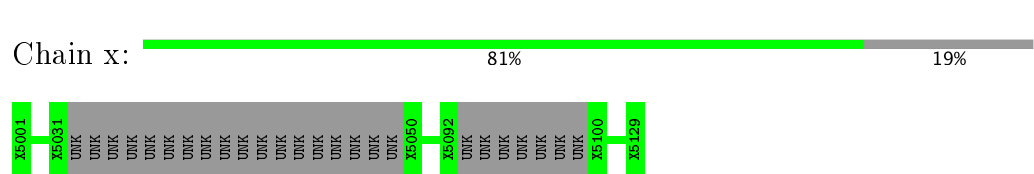
- Molecule 16: Cytochrome c-550



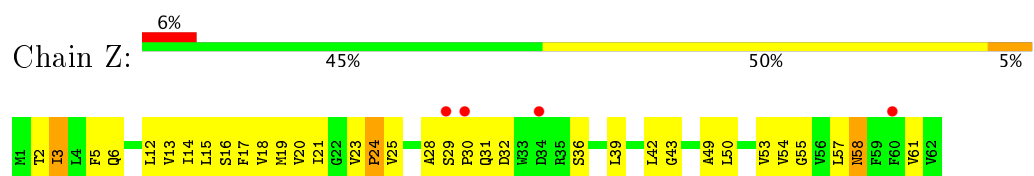
- Molecule 17: Unassigned subunits



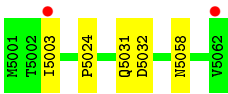
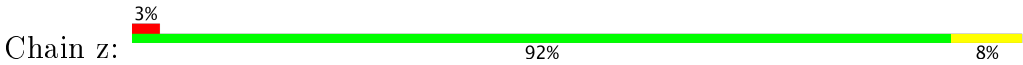
- Molecule 17: Unassigned subunits



- Molecule 18: Photosystem II reaction center Z protein



- Molecule 18: Photosystem II reaction center Z protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.234 , 0.286 0.242 , 0.292	Depositor DCC
$R_{free}$ test set	1733 reflections (1.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, MGE, DGD, CA, LMT, CLA, BCT, FE2, PQ9, OEC, HEM, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (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
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	Sidechain

## 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	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	57	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	A	1	0	0	0	0
19	a	1	0	0	0	0
20	A	250	0	265	15	0
20	B	1007	0	1088	74	0
20	C	774	0	783	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	115	0	111	8	0
20	a	250	0	265	0	0
20	b	1007	0	1088	0	0
20	c	774	0	783	0	0
20	d	115	0	111	0	0
21	A	128	0	148	12	0
21	a	128	0	148	0	0
22	A	30	0	37	2	0
22	D	30	0	37	7	0
22	a	30	0	37	0	0
22	d	30	0	37	0	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	6	0
24	C	120	0	168	20	0
24	D	40	0	56	4	0
24	H	40	0	56	3	0
24	T	40	0	56	5	0
24	X	40	0	56	9	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	t	40	0	56	0	0
24	x	40	0	56	0	0
25	A	39	0	51	4	0
25	a	39	0	51	0	0
26	A	80	0	92	0	0
26	L	47	0	60	0	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	0	0
27	A	35	0	46	0	0
27	M	35	0	46	0	0
27	T	35	0	46	3	0
27	a	35	0	46	0	0
27	m	35	0	46	0	0
27	t	35	0	46	0	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	0	0
28	d	136	0	194	0	0
28	i	48	0	72	0	0
28	l	48	0	72	0	0
29	C	152	0	17	2	0
29	c	152	0	17	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	0	0
32	v	43	0	30	0	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47107	1538	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 33.

The worst 5 of 1538 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)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:CD	17:X:26:UNK:NE2	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	3	17
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	14
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	3	20
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	4	23
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	12
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	2	11
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	3	16
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	19
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	6
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	6
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	10
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	10
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	1	3
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	1	3
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	5	27
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	5	27
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	1	3
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	1	3
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	12
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	4
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	12
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	4
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	2	11
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	2	11
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	6
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	1	6
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1	6
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	14
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	14
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	7
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	7
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	2	13

5 of 269 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	251 (93%)	18 (7%)	19	54
1	a	269/280 (96%)	252 (94%)	17 (6%)	21	57
2	B	378/407 (93%)	361 (96%)	17 (4%)	32	71
2	b	378/407 (93%)	360 (95%)	18 (5%)	30	69
3	C	341/374 (91%)	320 (94%)	21 (6%)	21	58
3	c	341/374 (91%)	320 (94%)	21 (6%)	21	58
4	D	273/283 (96%)	259 (95%)	14 (5%)	28	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	273/283 (96%)	258 (94%)	15 (6%)	25	63
5	E	68/73 (93%)	65 (96%)	3 (4%)	33	72
5	e	68/73 (93%)	66 (97%)	2 (3%)	48	82
6	F	27/39 (69%)	26 (96%)	1 (4%)	39	76
6	f	27/39 (69%)	26 (96%)	1 (4%)	39	76
7	H	50/55 (91%)	42 (84%)	8 (16%)	3	14
7	h	50/55 (91%)	43 (86%)	7 (14%)	4	18
8	I	32/35 (91%)	27 (84%)	5 (16%)	3	15
8	i	32/35 (91%)	27 (84%)	5 (16%)	3	15
9	J	22/28 (79%)	21 (96%)	1 (4%)	32	71
9	j	22/28 (79%)	21 (96%)	1 (4%)	32	71
10	K	29/30 (97%)	28 (97%)	1 (3%)	42	78
10	k	29/30 (97%)	28 (97%)	1 (3%)	42	78
11	L	34/35 (97%)	31 (91%)	3 (9%)	12	41
11	l	34/35 (97%)	31 (91%)	3 (9%)	12	41
12	M	32/33 (97%)	32 (100%)	0	100	100
12	m	32/33 (97%)	32 (100%)	0	100	100
13	O	181/208 (87%)	171 (94%)	10 (6%)	25	63
13	o	181/208 (87%)	172 (95%)	9 (5%)	28	67
14	T	26/29 (90%)	25 (96%)	1 (4%)	38	75
14	t	26/29 (90%)	25 (96%)	1 (4%)	38	75
15	U	83/89 (93%)	80 (96%)	3 (4%)	40	77
15	u	83/89 (93%)	80 (96%)	3 (4%)	40	77
16	V	117/117 (100%)	113 (97%)	4 (3%)	42	78
16	v	117/117 (100%)	111 (95%)	6 (5%)	28	66
18	Z	43/52 (83%)	42 (98%)	1 (2%)	56	85
18	z	43/52 (83%)	42 (98%)	1 (2%)	56	85
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	25	63

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	216	PHE

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Mol	Chain	Res	Type
1	a	5286	THR
13	o	5106	GLN
15	U	46	LYS
1	a	5013	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	130	GLN
1	a	5165	GLN
13	o	5106	GLN
15	U	108	ASN
1	a	5012	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 34 are unknown and 4 are monoatomic - leaving 142 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
26	SQD	A	5212	-	25,26,54	2.82	12 (48%)	35,37,65	3.15	13 (37%)
20	CLA	A	558	1	56,73,73	1.32	5 (8%)	65,113,113	1.54	14 (21%)
20	CLA	A	559	-	56,73,73	1.36	4 (7%)	65,113,113	1.44	9 (13%)
20	CLA	A	560	-	56,73,73	1.35	5 (8%)	65,113,113	1.56	15 (23%)
21	PHO	A	561	-	67,69,69	1.01	4 (5%)	87,99,99	1.42	16 (18%)
21	PHO	A	562	-	67,69,69	1.03	6 (8%)	87,99,99	1.48	15 (17%)
20	CLA	A	563	-	46,63,73	1.42	6 (13%)	53,101,113	1.65	14 (26%)
22	PQ9	A	564	-	30,30,45	0.85	1 (3%)	39,39,57	1.45	8 (20%)
23	OEC	A	565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
24	BCR	A	566	-	41,41,41	1.57	7 (17%)	56,56,56	2.09	21 (37%)
25	LHG	A	567	-	38,38,48	1.87	5 (13%)	39,44,54	1.49	4 (10%)
26	SQD	A	568	-	53,54,54	2.45	28 (52%)	63,65,65	3.02	20 (31%)
27	LMT	A	569	-	36,36,36	1.53	6 (16%)	47,47,47	1.09	2 (4%)
20	CLA	B	511	-	32,49,73	1.88	9 (28%)	37,84,113	1.75	9 (24%)
20	CLA	B	512	2	56,73,73	1.31	3 (5%)	65,113,113	1.52	14 (21%)
20	CLA	B	513	2	56,73,73	1.42	6 (10%)	65,113,113	1.57	13 (20%)
20	CLA	B	514	2	56,73,73	1.44	5 (8%)	65,113,113	1.47	13 (20%)
20	CLA	B	515	-	56,73,73	1.37	6 (10%)	65,113,113	1.64	14 (21%)
20	CLA	B	516	-	56,73,73	1.31	4 (7%)	65,113,113	1.53	11 (16%)
20	CLA	B	517	-	56,73,73	1.41	5 (8%)	65,113,113	1.67	15 (23%)
20	CLA	B	518	2	56,73,73	1.38	5 (8%)	65,113,113	1.59	14 (21%)
20	CLA	B	519	-	56,73,73	1.48	4 (7%)	65,113,113	1.49	14 (21%)
20	CLA	B	520	-	56,73,73	1.37	7 (12%)	65,113,113	1.48	13 (20%)
20	CLA	B	521	2	56,73,73	1.44	7 (12%)	65,113,113	1.56	13 (20%)
20	CLA	B	522	-	56,73,73	1.36	4 (7%)	65,113,113	1.50	9 (13%)
20	CLA	B	523	-	56,73,73	1.49	4 (7%)	65,113,113	1.53	13 (20%)
20	CLA	B	524	2	47,64,73	1.45	4 (8%)	54,102,113	1.63	12 (22%)
20	CLA	B	525	-	56,73,73	1.39	4 (7%)	65,113,113	1.53	12 (18%)
20	CLA	B	526	-	56,73,73	1.53	8 (14%)	65,113,113	1.55	13 (20%)
24	BCR	B	527	-	41,41,41	1.70	8 (19%)	56,56,56	2.03	16 (28%)
24	BCR	B	528	-	41,41,41	1.86	6 (14%)	56,56,56	1.97	15 (26%)
24	BCR	B	529	-	41,41,41	1.79	8 (19%)	56,56,56	2.17	20 (35%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.21	6 (10%)
20	CLA	C	491	3	56,73,73	1.39	5 (8%)	65,113,113	1.40	10 (15%)
20	CLA	C	492	3	51,68,73	1.36	7 (13%)	59,107,113	1.58	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	C	493	3	56,73,73	1.36	4 (7%)	65,113,113	1.56	15 (23%)
20	CLA	C	494	-	37,54,73	1.62	4 (10%)	43,90,113	1.81	11 (25%)
20	CLA	C	495	-	56,73,73	1.52	6 (10%)	65,113,113	1.65	14 (21%)
20	CLA	C	496	3	56,73,73	1.46	7 (12%)	65,113,113	1.55	15 (23%)
20	CLA	C	497	-	56,73,73	1.34	5 (8%)	65,113,113	1.61	13 (20%)
20	CLA	C	498	3	56,73,73	1.29	4 (7%)	65,113,113	1.50	13 (20%)
20	CLA	C	499	-	38,55,73	1.64	4 (10%)	44,91,113	1.73	14 (31%)
20	CLA	C	500	-	56,73,73	1.29	6 (10%)	65,113,113	1.47	12 (18%)
20	CLA	C	501	3	56,73,73	1.50	4 (7%)	65,113,113	1.48	11 (16%)
20	CLA	C	502	-	42,59,73	1.66	8 (19%)	48,96,113	1.79	13 (27%)
20	CLA	C	503	3	41,58,73	1.63	4 (9%)	47,95,113	1.68	12 (25%)
24	BCR	C	504	-	41,41,41	1.83	7 (17%)	56,56,56	2.16	22 (39%)
24	BCR	C	505	-	41,41,41	1.91	8 (19%)	56,56,56	2.08	16 (28%)
24	BCR	C	506	-	41,41,41	1.71	9 (21%)	56,56,56	2.17	21 (37%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.51	7 (10%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.72	11 (17%)
30	DGD	C	509	-	58,58,67	1.11	6 (10%)	72,72,81	1.43	7 (9%)
31	BCT	D	353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	D	354	4	56,73,73	1.36	6 (10%)	65,113,113	1.53	12 (18%)
20	CLA	D	355	-	41,58,73	1.71	5 (12%)	47,95,113	1.73	12 (25%)
22	PQ9	D	356	-	30,30,45	0.86	1 (3%)	39,39,57	1.61	8 (20%)
24	BCR	D	357	-	41,41,41	1.90	9 (21%)	56,56,56	2.22	20 (35%)
28	MGE	D	358	-	47,47,48	1.21	5 (10%)	55,55,56	1.00	3 (5%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.07	5 (10%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.16	4 (7%)
32	HEM	F	51	5,6	28,50,50	1.95	10 (35%)	17,82,82	2.55	6 (35%)
24	BCR	H	107	-	41,41,41	2.07	7 (17%)	56,56,56	2.24	24 (42%)
30	DGD	H	208	-	55,55,67	1.47	10 (18%)	69,69,81	1.55	8 (11%)
28	MGE	I	201	-	48,48,48	1.10	6 (12%)	56,56,56	1.12	5 (8%)
28	MGE	L	210	-	48,48,48	0.98	3 (6%)	56,56,56	1.19	5 (8%)
26	SQD	L	5213	-	46,47,54	2.70	24 (52%)	56,58,65	2.84	15 (26%)
27	LMT	M	5216	-	36,36,36	1.46	8 (22%)	47,47,47	0.94	2 (4%)
27	LMT	T	217	-	36,36,36	1.41	7 (19%)	47,47,47	1.06	4 (8%)
24	BCR	T	5104	-	41,41,41	1.51	9 (21%)	56,56,56	2.26	22 (39%)
32	HEM	V	552	16	28,50,50	1.86	10 (35%)	17,82,82	2.19	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	X	130	-	41,41,41	1.89	10 (24%)	56,56,56	2.49	24 (42%)
26	SQD	a	212	-	25,26,54	3.07	13 (52%)	35,37,65	3.30	15 (42%)
20	CLA	a	5558	1	56,73,73	1.32	7 (12%)	65,113,113	1.48	12 (18%)
20	CLA	a	5559	-	56,73,73	1.27	3 (5%)	65,113,113	1.44	10 (15%)
20	CLA	a	5560	-	56,73,73	1.31	5 (8%)	65,113,113	1.55	14 (21%)
21	PHO	a	5561	-	67,69,69	1.02	5 (7%)	87,99,99	1.36	13 (14%)
21	PHO	a	5562	-	67,69,69	1.03	5 (7%)	87,99,99	1.47	15 (17%)
20	CLA	a	5563	-	46,63,73	1.46	6 (13%)	53,101,113	1.59	12 (22%)
22	PQ9	a	5564	-	30,30,45	0.89	1 (3%)	39,39,57	1.42	8 (20%)
23	OEC	a	5565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
24	BCR	a	5566	-	41,41,41	1.64	7 (17%)	56,56,56	2.09	22 (39%)
25	LHG	a	5567	-	38,38,48	1.91	5 (13%)	39,44,54	1.45	3 (7%)
27	LMT	a	5568	-	36,36,36	1.45	6 (16%)	47,47,47	1.12	1 (2%)
20	CLA	b	5511	-	32,49,73	2.03	8 (25%)	37,84,113	1.76	10 (27%)
20	CLA	b	5512	2	56,73,73	1.32	5 (8%)	65,113,113	1.52	13 (20%)
20	CLA	b	5513	2	56,73,73	1.34	5 (8%)	65,113,113	1.56	14 (21%)
20	CLA	b	5514	2	56,73,73	1.40	4 (7%)	65,113,113	1.51	12 (18%)
20	CLA	b	5515	-	56,73,73	1.37	7 (12%)	65,113,113	1.62	14 (21%)
20	CLA	b	5516	-	56,73,73	1.40	5 (8%)	65,113,113	1.59	12 (18%)
20	CLA	b	5517	-	56,73,73	1.34	5 (8%)	65,113,113	1.58	13 (20%)
20	CLA	b	5518	2	56,73,73	1.34	4 (7%)	65,113,113	1.60	17 (26%)
20	CLA	b	5519	-	56,73,73	1.44	5 (8%)	65,113,113	1.52	13 (20%)
20	CLA	b	5520	-	56,73,73	1.42	6 (10%)	65,113,113	1.48	13 (20%)
20	CLA	b	5521	2	56,73,73	1.25	4 (7%)	65,113,113	1.55	15 (23%)
20	CLA	b	5522	-	56,73,73	1.38	5 (8%)	65,113,113	1.48	9 (13%)
20	CLA	b	5523	-	56,73,73	1.45	5 (8%)	65,113,113	1.59	13 (20%)
20	CLA	b	5524	2	47,64,73	1.42	3 (6%)	54,102,113	1.57	11 (20%)
20	CLA	b	5525	-	56,73,73	1.44	4 (7%)	65,113,113	1.51	12 (18%)
20	CLA	b	5526	-	56,73,73	1.64	8 (14%)	65,113,113	1.61	14 (21%)
24	BCR	b	5527	-	41,41,41	1.52	8 (19%)	56,56,56	1.95	14 (25%)
24	BCR	b	5528	-	41,41,41	1.68	6 (14%)	56,56,56	2.00	17 (30%)
24	BCR	b	5529	-	41,41,41	1.67	8 (19%)	56,56,56	2.09	18 (32%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.15	6 (10%)
20	CLA	c	5491	3	56,73,73	1.35	5 (8%)	65,113,113	1.50	11 (16%)
20	CLA	c	5492	3	51,68,73	1.37	6 (11%)	59,107,113	1.53	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	c	5493	3	56,73,73	1.37	5 (8%)	65,113,113	1.56	15 (23%)
20	CLA	c	5494	-	37,54,73	1.63	4 (10%)	43,90,113	1.72	11 (25%)
20	CLA	c	5495	-	56,73,73	1.45	6 (10%)	65,113,113	1.66	16 (24%)
20	CLA	c	5496	-	56,73,73	1.47	8 (14%)	65,113,113	1.50	12 (18%)
20	CLA	c	5497	-	56,73,73	1.43	6 (10%)	65,113,113	1.57	14 (21%)
20	CLA	c	5498	3	56,73,73	1.36	6 (10%)	65,113,113	1.51	14 (21%)
20	CLA	c	5499	-	38,55,73	1.61	6 (15%)	44,91,113	1.65	10 (22%)
20	CLA	c	5500	-	56,73,73	1.37	5 (8%)	65,113,113	1.50	14 (21%)
20	CLA	c	5501	3	56,73,73	1.39	4 (7%)	65,113,113	1.44	10 (15%)
20	CLA	c	5502	-	42,59,73	1.73	7 (16%)	48,96,113	1.76	12 (25%)
20	CLA	c	5503	3	41,58,73	1.78	6 (14%)	47,95,113	1.64	9 (19%)
24	BCR	c	5504	-	41,41,41	2.11	6 (14%)	56,56,56	2.13	22 (39%)
24	BCR	c	5505	-	41,41,41	1.93	8 (19%)	56,56,56	2.09	18 (32%)
24	BCR	c	5506	-	41,41,41	1.92	9 (21%)	56,56,56	2.10	20 (35%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.50	6 (8%)
30	DGD	c	5508	-	48,48,67	1.48	9 (18%)	62,62,81	1.76	12 (19%)
30	DGD	c	5509	-	58,58,67	1.34	7 (12%)	72,72,81	1.42	6 (8%)
31	BCT	d	5353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	d	5354	4	56,73,73	1.32	7 (12%)	65,113,113	1.53	12 (18%)
20	CLA	d	5355	-	41,58,73	1.81	7 (17%)	47,95,113	1.68	11 (23%)
22	PQ9	d	5356	-	30,30,45	0.78	0	39,39,57	1.60	6 (15%)
24	BCR	d	5357	-	41,41,41	1.95	8 (19%)	56,56,56	2.28	21 (37%)
26	SQD	d	5358	-	53,54,54	2.44	27 (50%)	63,65,65	2.90	20 (31%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	1.00	3 (5%)
28	MGE	d	5360	-	41,41,48	1.20	6 (14%)	49,49,56	1.09	5 (10%)
28	MGE	d	5361	-	48,48,48	1.05	4 (8%)	56,56,56	1.10	3 (5%)
32	HEM	f	5051	5,6	28,50,50	1.99	10 (35%)	17,82,82	2.54	8 (47%)
24	BCR	h	5107	-	41,41,41	1.97	7 (17%)	56,56,56	2.24	25 (44%)
30	DGD	h	5208	-	55,55,67	1.38	9 (16%)	69,69,81	1.56	8 (11%)
28	MGE	i	5201	-	48,48,48	1.25	8 (16%)	56,56,56	1.13	4 (7%)
28	MGE	l	5210	-	48,48,48	0.90	3 (6%)	56,56,56	1.16	5 (8%)
27	LMT	m	216	-	36,36,36	1.47	7 (19%)	47,47,47	1.00	3 (6%)
24	BCR	t	104	-	41,41,41	1.63	9 (21%)	56,56,56	2.22	22 (39%)
26	SQD	t	213	-	46,47,54	2.69	22 (47%)	56,58,65	2.95	17 (30%)
27	LMT	t	5217	-	36,36,36	1.46	5 (13%)	47,47,47	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	HEM	v	5552	16	28,50,50	2.01	9 (32%)	17,82,82	2.26	6 (35%)
24	BCR	x	5130	-	41,41,41	1.93	8 (19%)	56,56,56	2.48	24 (42%)

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
26	SQD	A	5212	-	-	0/19/39/69	0/1/1/1
20	CLA	A	558	1	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	559	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	560	-	3/3/20/25	0/37/135/135	0/0/9/9
21	PHO	A	561	-	-	0/53/103/103	0/1/6/6
21	PHO	A	562	-	-	0/53/103/103	0/1/6/6
20	CLA	A	563	-	3/3/18/25	0/25/123/135	0/0/9/9
22	PQ9	A	564	-	-	0/23/43/61	0/1/1/1
23	OEC	A	565	1,3	-	0/0/0/54	0/0/0/5
24	BCR	A	566	-	-	0/29/63/63	0/2/2/2
25	LHG	A	567	-	-	0/43/43/53	0/0/0/0
26	SQD	A	568	-	-	0/49/69/69	0/1/1/1
27	LMT	A	569	-	-	0/21/61/61	0/2/2/2
20	CLA	B	511	-	3/3/15/25	0/8/106/135	0/0/9/9
20	CLA	B	512	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	513	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	514	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	515	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	516	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	517	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	518	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	519	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	520	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	521	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	522	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	523	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	524	2	3/3/18/25	0/27/125/135	0/0/9/9
20	CLA	B	525	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	526	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	527	-	-	0/29/63/63	0/2/2/2
24	BCR	B	528	-	-	0/29/63/63	0/2/2/2
24	BCR	B	529	-	-	0/29/63/63	0/2/2/2
28	MGE	B	530	-	-	0/43/63/63	0/1/1/1
20	CLA	C	491	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	492	3	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	C	493	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	494	-	3/3/16/25	0/15/113/135	0/0/9/9
20	CLA	C	495	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	496	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	497	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	498	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	499	-	3/3/16/25	0/16/114/135	0/0/9/9
20	CLA	C	500	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	501	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	502	-	3/3/17/25	0/21/119/135	0/0/9/9
20	CLA	C	503	3	3/3/17/25	0/19/117/135	0/0/9/9
24	BCR	C	504	-	-	0/29/63/63	0/2/2/2
24	BCR	C	505	-	-	0/29/63/63	0/2/2/2
24	BCR	C	506	-	-	0/29/63/63	0/2/2/2
30	DGD	C	507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	C	509	-	3/3/13/13	0/46/86/95	0/2/2/2
31	BCT	D	353	19	-	0/0/0/0	0/0/0/0
20	CLA	D	354	4	3/3/20/25	1/37/135/135	0/0/9/9
20	CLA	D	355	-	3/3/17/25	0/19/117/135	0/0/9/9
22	PQ9	D	356	-	-	0/23/43/61	0/1/1/1
24	BCR	D	357	-	-	0/29/63/63	0/2/2/2
28	MGE	D	358	-	-	0/42/62/63	0/1/1/1
28	MGE	D	359	-	-	0/36/56/63	0/1/1/1
28	MGE	D	360	-	-	0/43/63/63	0/1/1/1
32	HEM	F	51	5,6	-	0/6/54/54	0/0/8/8
24	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/43/83/95	0/2/2/2
28	MGE	I	201	-	-	0/43/63/63	0/1/1/1
28	MGE	L	210	-	-	0/43/63/63	0/1/1/1
26	SQD	L	5213	-	-	0/42/62/69	0/1/1/1
27	LMT	M	5216	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	T	217	-	-	0/21/61/61	0/2/2/2
24	BCR	T	5104	-	-	0/29/63/63	0/2/2/2
32	HEM	V	552	16	-	0/6/54/54	0/0/8/8
24	BCR	X	130	-	-	0/29/63/63	0/2/2/2
26	SQD	a	212	-	-	0/19/39/69	0/1/1/1
20	CLA	a	5558	1	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	5559	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	5560	-	3/3/20/25	0/37/135/135	0/0/9/9
21	PHO	a	5561	-	-	0/53/103/103	0/1/6/6
21	PHO	a	5562	-	-	0/53/103/103	0/1/6/6
20	CLA	a	5563	-	3/3/18/25	0/25/123/135	0/0/9/9
22	PQ9	a	5564	-	-	0/23/43/61	0/1/1/1
23	OEC	a	5565	1,3	-	0/0/0/54	0/0/0/5
24	BCR	a	5566	-	-	0/29/63/63	0/2/2/2
25	LHG	a	5567	-	-	0/43/43/53	0/0/0/0
27	LMT	a	5568	-	-	0/21/61/61	0/2/2/2
20	CLA	b	5511	-	3/3/15/25	0/8/106/135	0/0/9/9
20	CLA	b	5512	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5513	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5514	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5515	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5516	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5517	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5518	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5519	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5520	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5521	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5522	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5523	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5524	2	3/3/18/25	0/27/125/135	0/0/9/9
20	CLA	b	5525	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5526	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	5527	-	-	0/29/63/63	0/2/2/2
24	BCR	b	5528	-	-	0/29/63/63	0/2/2/2
24	BCR	b	5529	-	-	0/29/63/63	0/2/2/2
28	MGE	b	5530	-	-	0/43/63/63	0/1/1/1
20	CLA	c	5491	3	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	5492	3	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	c	5493	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5494	-	3/3/16/25	0/15/113/135	0/0/9/9
20	CLA	c	5495	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5496	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5497	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5498	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5499	-	3/3/16/25	0/16/114/135	0/0/9/9
20	CLA	c	5500	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5501	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5502	-	3/3/17/25	0/21/119/135	0/0/9/9
20	CLA	c	5503	3	3/3/17/25	0/19/117/135	0/0/9/9
24	BCR	c	5504	-	-	0/29/63/63	0/2/2/2
24	BCR	c	5505	-	-	0/29/63/63	0/2/2/2
24	BCR	c	5506	-	-	0/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	c	5509	-	3/3/13/13	0/46/86/95	0/2/2/2
31	BCT	d	5353	19	-	0/0/0/0	0/0/0/0
20	CLA	d	5354	4	3/3/20/25	1/37/135/135	0/0/9/9
20	CLA	d	5355	-	3/3/17/25	0/19/117/135	0/0/9/9
22	PQ9	d	5356	-	-	0/23/43/61	0/1/1/1
24	BCR	d	5357	-	-	0/29/63/63	0/2/2/2
26	SQD	d	5358	-	-	0/49/69/69	0/1/1/1
28	MGE	d	5359	-	-	0/42/62/63	0/1/1/1
28	MGE	d	5360	-	-	0/36/56/63	0/1/1/1
28	MGE	d	5361	-	-	0/43/63/63	0/1/1/1
32	HEM	f	5051	5,6	-	0/6/54/54	0/0/8/8
24	BCR	h	5107	-	-	0/29/63/63	0/2/2/2
30	DGD	h	5208	-	3/3/13/13	0/43/83/95	0/2/2/2
28	MGE	i	5201	-	-	0/43/63/63	0/1/1/1
28	MGE	l	5210	-	-	0/43/63/63	0/1/1/1
27	LMT	m	216	-	-	0/21/61/61	0/2/2/2
24	BCR	t	104	-	-	0/29/63/63	0/2/2/2
26	SQD	t	213	-	-	0/42/62/69	0/1/1/1
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
32	HEM	v	5552	16	-	0/6/54/54	0/0/8/8
24	BCR	x	5130	-	-	0/29/63/63	0/2/2/2

The worst 5 of 915 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	v	5552	HEM	CAD-C3D	-4.12	1.44	1.52
32	V	552	HEM	CAD-C3D	-3.60	1.45	1.52
20	A	563	CLA	C1B-CHB	-3.46	1.31	1.40
20	D	354	CLA	C1B-CHB	-3.42	1.31	1.40
32	f	5051	HEM	C4D-ND	-3.37	1.32	1.36

The worst 5 of 1678 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	568	SQD	O8-S-C6	-6.98	97.49	106.01
26	a	212	SQD	O8-S-C6	-6.58	97.98	106.01
26	d	5358	SQD	O8-S-C6	-6.50	98.07	106.01
32	F	51	HEM	CBD-CAD-C3D	-5.98	101.06	112.47
26	t	213	SQD	O8-S-C6	-5.88	98.83	106.01

5 of 234 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	b	5526	CLA	NC
20	b	5526	CLA	ND
20	b	5526	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	ND

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	d	5354	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C4

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	558	CLA	10	0
20	A	559	CLA	5	0
20	A	560	CLA	1	0
21	A	561	PHO	7	0
21	A	562	PHO	5	0
22	A	564	PQ9	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	566	BCR	1	0
25	A	567	LHG	4	0
20	B	511	CLA	1	0
20	B	512	CLA	2	0
20	B	513	CLA	8	0
20	B	514	CLA	5	0
20	B	515	CLA	12	0
20	B	516	CLA	6	0
20	B	517	CLA	9	0
20	B	518	CLA	11	0
20	B	519	CLA	5	0
20	B	520	CLA	6	0
20	B	521	CLA	2	0
20	B	522	CLA	4	0
20	B	523	CLA	2	0
20	B	524	CLA	4	0
20	B	525	CLA	4	0
20	B	526	CLA	2	0
24	B	527	BCR	2	0
24	B	528	BCR	2	0
24	B	529	BCR	2	0
28	B	530	MGE	1	0
20	C	491	CLA	4	0
20	C	492	CLA	2	0
20	C	493	CLA	7	0
20	C	494	CLA	2	0
20	C	495	CLA	9	0
20	C	496	CLA	2	0
20	C	497	CLA	5	0
20	C	498	CLA	6	0
20	C	499	CLA	2	0
20	C	500	CLA	3	0
20	C	501	CLA	13	0
20	C	502	CLA	2	0
20	C	503	CLA	1	0
24	C	504	BCR	7	0
24	C	505	BCR	6	0
24	C	506	BCR	7	0
30	C	507	DGD	6	0
30	C	508	DGD	2	0
30	C	509	DGD	10	0
20	D	354	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	355	CLA	3	0
22	D	356	PQ9	7	0
24	D	357	BCR	4	0
28	D	358	MGE	2	0
28	D	359	MGE	1	0
28	D	360	MGE	7	0
32	F	51	HEM	3	0
24	H	107	BCR	3	0
30	H	208	DGD	3	0
28	I	201	MGE	1	0
28	L	210	MGE	2	0
27	T	217	LMT	3	0
24	T	5104	BCR	5	0
32	V	552	HEM	2	0
24	X	130	BCR	9	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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	-0.59	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.54	4 (1%) 79 53	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.53	2 (0%) 92 77	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.50	1 (0%) 94 85	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.52	3 (0%) 87 67	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.35	4 (0%) 84 61	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 93 82	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.57	1 (0%) 93 82	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.19	1 (1%) 79 53	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.01	3 (3%) 42 18	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.22	1 (2%) 52 24	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	3 (8%) 11 4	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.38	1 (1%) 72 44	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.21	3 (4%) 32 13	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	1 (2%) 52 24	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.34	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.60	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.50	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.54	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.41	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.14	1 (2%) 55 26	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.35	3 (8%) 13 5	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.42	1 (2%) 53 25	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.36	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/247 (97%)	-0.39	3 (1%) 79 53	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.30	9 (3%) 42 18	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.48	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.73	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.39	1 (1%) 82 58	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.41	3 (3%) 49 22	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.47	2 (1%) 74 47	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.23	5 (3%) 43 18	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.26	4 (6%) 20 7	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.19	2 (3%) 48 21	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.45	63 (1%) 79 53	35, 66, 85, 101	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	5010	SER	4.6
3	c	5473	ASP	4.4
13	o	5049	ASP	4.3
4	D	13	GLY	4.1
11	l	5001	MET	4.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMT	A	569	35/35	0.72	0.47	7.86	80,89,92,93	0
29	UNK	c	5484	5/-	0.84	0.53	6.31	69,69,70,72	0
20	CLA	B	511	41/65	0.73	0.41	6.16	88,90,92,98	0
27	LMT	a	5568	35/35	0.81	0.43	6.11	79,92,94,96	0
27	LMT	t	5217	35/35	0.68	0.46	6.11	76,95,104,105	0
24	BCR	H	107	40/40	0.82	0.29	5.91	77,83,88,89	0
29	UNK	C	489	7/-	0.78	0.44	5.91	75,76,77,78	0
29	UNK	c	5489	7/-	0.78	0.41	5.88	73,73,74,74	0
29	UNK	c	5485	5/-	0.85	0.39	5.12	68,69,69,70	0
20	CLA	c	5503	50/65	0.85	0.28	4.62	88,91,92,93	0
22	PQ9	a	5564	30/45	0.87	0.32	4.56	51,55,62,62	30
29	UNK	c	5477	7/-	0.90	0.33	4.56	67,68,70,70	0
20	CLA	b	5511	41/65	0.64	0.40	4.31	88,92,95,96	0
22	PQ9	A	564	30/45	0.77	0.37	4.06	54,57,63,64	30
29	UNK	C	481	13/-	0.73	0.36	4.05	61,64,68,69	0
24	BCR	C	505	40/40	0.81	0.43	4.04	75,81,91,92	0
27	LMT	T	217	35/35	0.75	0.31	3.66	83,93,96,97	0
24	BCR	x	5130	40/40	0.79	0.42	3.65	77,81,85,86	0
29	UNK	c	5474	15/-	0.89	0.24	3.37	39,50,56,56	0
20	CLA	a	5560	65/65	0.90	0.22	3.30	62,68,100,101	0
24	BCR	X	130	40/40	0.84	0.32	3.05	68,71,80,81	0
24	BCR	h	5107	40/40	0.86	0.28	3.04	74,79,82,83	0
24	BCR	d	5357	40/40	0.83	0.37	2.98	61,72,86,88	0
28	MGE	d	5359	47/48	0.76	0.30	2.84	72,81,96,98	0
24	BCR	B	528	40/40	0.84	0.25	2.73	54,68,74,75	0
20	CLA	a	5563	55/65	0.84	0.31	2.72	59,65,102,103	0
24	BCR	c	5504	40/40	0.86	0.29	2.72	73,80,88,89	0
24	BCR	b	5529	40/40	0.86	0.34	2.67	69,72,74,74	0
24	BCR	C	504	40/40	0.91	0.27	2.50	57,64,70,70	0
24	BCR	D	357	40/40	0.89	0.26	2.27	61,66,78,80	0
29	UNK	C	482	13/-	0.84	0.25	2.08	64,66,67,67	0
27	LMT	M	5216	35/35	0.77	0.31	2.02	58,83,90,90	0
20	CLA	A	563	55/65	0.88	0.26	1.96	43,49,75,78	0
20	CLA	B	519	65/65	0.88	0.26	1.93	73,82,85,87	0
24	BCR	T	5104	40/40	0.88	0.25	1.90	67,71,78,79	0
20	CLA	c	5498	65/65	0.85	0.25	1.86	81,90,93,93	0
28	MGE	D	358	47/48	0.82	0.24	1.85	65,72,79,81	0
20	CLA	B	526	65/65	0.79	0.28	1.82	71,82,97,98	0
30	DGD	C	507	53/66	0.89	0.25	1.81	55,66,86,88	0
24	BCR	c	5505	40/40	0.88	0.31	1.80	84,87,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MGE	d	5361	48/48	0.89	0.22	1.78	61,68,78,83	0
20	CLA	c	5501	65/65	0.88	0.26	1.77	82,91,94,95	0
20	CLA	b	5516	65/65	0.82	0.28	1.76	62,66,84,86	0
29	UNK	c	5476	9/-	0.79	0.33	1.68	58,60,62,62	0
27	LMT	m	216	35/35	0.80	0.28	1.68	62,87,89,91	0
20	CLA	D	355	50/65	0.91	0.22	1.60	63,65,68,70	0
20	CLA	b	5519	65/65	0.89	0.24	1.59	70,75,80,81	0
20	CLA	B	515	65/65	0.93	0.21	1.59	55,66,71,72	0
26	SQD	A	568	54/54	0.84	0.32	1.58	76,82,90,90	0
21	PHO	a	5562	64/64	0.91	0.22	1.57	70,75,81,82	0
20	CLA	C	495	65/65	0.92	0.21	1.55	58,68,74,76	0
20	CLA	B	520	65/65	0.90	0.23	1.53	62,67,76,79	0
20	CLA	b	5520	65/65	0.90	0.24	1.49	63,72,74,76	0
24	BCR	c	5506	40/40	0.76	0.32	1.44	75,81,86,86	0
24	BCR	t	104	40/40	0.91	0.20	1.44	65,72,84,85	0
24	BCR	A	566	40/40	0.92	0.24	1.43	50,57,64,66	0
25	LHG	A	567	39/49	0.92	0.23	1.41	57,73,79,81	0
20	CLA	C	501	65/65	0.89	0.25	1.39	70,78,83,85	0
20	CLA	C	498	65/65	0.88	0.22	1.39	64,74,98,101	0
20	CLA	c	5497	65/65	0.89	0.23	1.38	66,82,84,87	0
22	PQ9	D	356	30/45	0.91	0.21	1.31	49,67,80,83	0
20	CLA	B	512	65/65	0.91	0.24	1.29	68,75,78,79	0
28	MGE	b	5530	48/48	0.89	0.18	1.27	59,64,71,73	0
24	BCR	a	5566	40/40	0.90	0.25	1.27	59,75,78,79	0
20	CLA	B	522	65/65	0.94	0.21	1.25	54,65,75,77	0
32	HEM	f	5051	43/43	0.94	0.28	1.25	80,84,97,101	0
29	UNK	C	485	5/-	0.90	0.23	1.24	57,59,61,61	0
20	CLA	c	5495	65/65	0.91	0.21	1.22	74,81,86,88	0
20	CLA	b	5515	65/65	0.94	0.21	1.21	46,51,74,76	0
20	CLA	A	560	65/65	0.91	0.20	1.20	49,57,86,88	0
20	CLA	C	503	50/65	0.86	0.26	1.16	83,86,88,94	0
20	CLA	b	5512	65/65	0.92	0.23	1.14	68,72,75,76	0
30	DGD	c	5509	57/66	0.86	0.28	1.10	67,72,77,78	0
20	CLA	C	497	65/65	0.88	0.24	1.07	74,78,80,82	0
28	MGE	D	359	41/48	0.88	0.23	1.04	60,67,76,79	0
22	PQ9	d	5356	30/45	0.93	0.20	1.02	51,57,66,66	0
24	BCR	B	529	40/40	0.89	0.24	1.00	62,69,80,80	0
20	CLA	B	516	65/65	0.82	0.27	0.98	61,76,92,97	0
20	CLA	d	5354	65/65	0.95	0.17	0.98	39,47,64,65	0
30	DGD	c	5507	53/66	0.89	0.23	0.98	66,74,90,91	0
29	UNK	c	5481	13/-	0.87	0.23	0.96	60,62,66,66	0
28	MGE	l	5210	48/48	0.90	0.21	0.95	59,69,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	b	5513	65/65	0.94	0.20	0.95	54,61,84,90	0
20	CLA	c	5496	65/65	0.82	0.27	0.95	79,83,95,97	0
32	HEM	F	51	43/43	0.95	0.26	0.93	78,84,92,95	0
28	MGE	d	5360	41/48	0.90	0.21	0.93	68,72,78,80	0
28	MGE	L	210	48/48	0.88	0.24	0.88	59,68,73,75	0
29	UNK	C	474	15/-	0.89	0.18	0.88	26,37,40,40	0
26	SQD	a	212	26/54	0.79	0.26	0.87	82,94,101,103	0
25	LHG	a	5567	39/49	0.90	0.26	0.87	65,68,74,80	0
24	BCR	b	5527	40/40	0.92	0.20	0.85	58,63,72,72	0
28	MGE	D	360	48/48	0.91	0.20	0.85	52,60,63,68	0
32	HEM	v	5552	43/43	0.96	0.22	0.85	65,67,70,70	0
20	CLA	B	514	65/65	0.93	0.21	0.83	59,64,82,83	0
30	DGD	C	508	47/66	0.91	0.19	0.79	61,71,80,83	0
30	DGD	H	208	54/66	0.90	0.20	0.75	61,69,75,76	0
28	MGE	i	5201	48/48	0.84	0.27	0.74	67,83,88,90	0
26	SQD	d	5358	54/54	0.80	0.29	0.72	74,85,106,107	0
26	SQD	A	5212	26/54	0.81	0.24	0.72	75,100,107,107	0
29	UNK	C	476	9/-	0.81	0.29	0.72	61,62,63,64	0
28	MGE	I	201	48/48	0.87	0.23	0.71	73,81,89,90	0
20	CLA	C	496	65/65	0.84	0.26	0.70	71,78,88,89	0
20	CLA	B	513	65/65	0.94	0.18	0.68	56,61,67,67	0
20	CLA	C	502	51/65	0.88	0.21	0.67	74,80,83,84	0
21	PHO	a	5561	64/64	0.94	0.18	0.67	51,55,66,68	0
32	HEM	V	552	43/43	0.97	0.18	0.63	37,54,58,59	0
20	CLA	B	525	65/65	0.93	0.20	0.62	67,84,91,92	0
26	SQD	t	213	47/54	0.85	0.26	0.61	61,95,116,117	0
29	UNK	C	477	7/-	0.96	0.16	0.60	47,49,51,51	0
26	SQD	L	5213	47/54	0.80	0.27	0.60	52,85,106,108	0
20	CLA	b	5522	65/65	0.94	0.20	0.59	60,66,75,76	0
28	MGE	B	530	48/48	0.88	0.19	0.58	55,64,70,72	0
30	DGD	C	509	57/66	0.91	0.20	0.55	52,60,69,70	0
20	CLA	c	5502	51/65	0.87	0.24	0.51	93,96,97,98	0
29	UNK	c	5482	13/-	0.90	0.19	0.51	60,61,71,72	0
31	BCT	D	353	4/4	0.96	0.19	0.51	72,73,73,74	0
21	PHO	A	562	64/64	0.94	0.17	0.49	47,53,63,66	0
20	CLA	d	5355	50/65	0.87	0.23	0.48	74,77,80,81	0
24	BCR	b	5528	40/40	0.93	0.18	0.48	61,64,72,73	0
20	CLA	c	5500	65/65	0.92	0.20	0.42	64,69,82,83	0
20	CLA	C	500	65/65	0.94	0.16	0.41	59,63,73,74	0
20	CLA	b	5526	65/65	0.79	0.28	0.37	66,71,92,95	0
20	CLA	D	354	65/65	0.95	0.17	0.36	35,43,63,66	0
20	CLA	b	5514	65/65	0.94	0.18	0.32	41,51,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	C	499	47/65	0.95	0.17	0.31	57,60,66,69	0
24	BCR	C	506	40/40	0.88	0.22	0.30	68,72,79,80	0
24	BCR	B	527	40/40	0.91	0.18	0.30	58,65,68,69	0
20	CLA	C	491	65/65	0.95	0.18	0.27	63,70,77,79	0
20	CLA	B	518	65/65	0.93	0.19	0.27	53,64,79,79	0
29	UNK	C	484	5/-	0.86	0.21	0.26	47,51,52,53	0
20	CLA	C	492	60/65	0.95	0.17	0.23	53,58,76,77	0
20	CLA	B	521	65/65	0.95	0.17	0.21	58,63,66,68	0
21	PHO	A	561	64/64	0.95	0.16	0.18	32,52,55,59	0
20	CLA	C	493	65/65	0.94	0.18	0.17	67,71,77,79	0
20	CLA	c	5491	65/65	0.92	0.20	0.16	70,78,81,86	0
20	CLA	b	5525	65/65	0.93	0.19	0.13	71,77,80,82	0
20	CLA	c	5493	65/65	0.90	0.21	0.05	67,81,86,86	0
20	CLA	a	5559	65/65	0.95	0.16	-0.02	42,49,60,60	0
20	CLA	c	5499	47/65	0.92	0.20	-0.04	60,69,76,78	0
30	DGD	c	5508	47/66	0.91	0.18	-0.04	66,76,82,84	0
20	CLA	b	5517	65/65	0.95	0.15	-0.05	54,58,66,71	0
20	CLA	B	523	65/65	0.95	0.16	-0.06	47,56,73,74	0
20	CLA	B	524	56/65	0.93	0.19	-0.09	67,72,77,80	0
30	DGD	h	5208	54/66	0.93	0.17	-0.10	57,68,73,75	0
20	CLA	b	5523	65/65	0.95	0.15	-0.13	45,52,74,75	0
20	CLA	C	494	46/65	0.95	0.15	-0.18	59,66,68,72	0
20	CLA	a	5558	65/65	0.95	0.16	-0.22	41,50,55,61	0
20	CLA	b	5524	56/65	0.93	0.18	-0.23	63,68,89,91	0
20	CLA	A	559	65/65	0.96	0.14	-0.31	39,43,49,52	0
20	CLA	B	517	65/65	0.96	0.14	-0.35	37,44,56,57	0
20	CLA	c	5492	60/65	0.93	0.17	-0.38	57,61,83,84	0
20	CLA	b	5518	65/65	0.95	0.16	-0.38	60,64,69,75	0
20	CLA	c	5494	46/65	0.93	0.16	-0.47	72,77,86,88	0
23	OEC	a	5565	5/9	0.96	0.13	-0.50	63,64,71,87	0
20	CLA	b	5521	65/65	0.94	0.15	-0.63	48,57,63,64	0
20	CLA	A	558	65/65	0.97	0.14	-0.73	41,46,50,51	0
23	OEC	A	565	5/9	0.96	0.13	-0.75	62,63,65,66	0
31	BCT	d	5353	4/4	0.98	0.15	-1.06	75,75,76,77	0
19	FE2	a	5557	1/1	1.00	0.11	-2.30	75,75,75,75	0
19	FE2	A	557	1/1	0.95	0.05	-3.60	60,60,60,60	0
29	UNK	C	480	7/-	0.92	0.21	-	35,36,38,38	0
29	UNK	C	490	4/-	0.96	0.15	-	67,67,68,68	0
29	UNK	C	488	5/-	0.87	0.16	-	41,45,47,47	0
29	UNK	c	5475	12/-	0.75	0.34	-	74,78,84,84	0
29	UNK	C	479	11/-	0.85	0.26	-	58,64,67,67	0
29	UNK	c	5487	7/-	0.88	0.20	-	57,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	CA	k	5056	1/1	0.94	0.19	-	119,119,119,119	0
29	UNK	C	475	12/-	0.73	0.32	-	68,69,72,73	0
29	UNK	c	5488	5/-	0.92	0.21	-	59,59,59,60	0
29	UNK	C	483	13/-	0.89	0.22	-	61,68,78,78	0
29	UNK	c	5486	8/-	0.89	0.30	-	63,64,65,66	0
29	UNK	c	5480	7/-	0.89	0.27	-	65,66,66,67	0
29	UNK	C	486	8/-	0.80	0.36	-	55,56,59,60	0
29	UNK	c	5483	13/-	0.88	0.25	-	71,75,80,82	0
33	CA	K	56	1/1	0.96	0.09	-	119,119,119,119	0
29	UNK	C	478	11/-	0.85	0.23	-	58,65,66,66	0
29	UNK	C	487	7/-	0.86	0.23	-	49,52,52,53	0
29	UNK	c	5479	11/-	0.85	0.23	-	76,77,77,77	0
29	UNK	c	5478	11/-	0.70	0.39	-	76,79,81,81	0
29	UNK	c	5490	4/-	0.71	0.34	-	91,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.