



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2017 – 04:49 PM EST

PDB ID : 5GTI  
Title : Native XFEL structure of photosystem II (two flash dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-08-20  
Resolution : 2.50 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-20029077
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-20029077

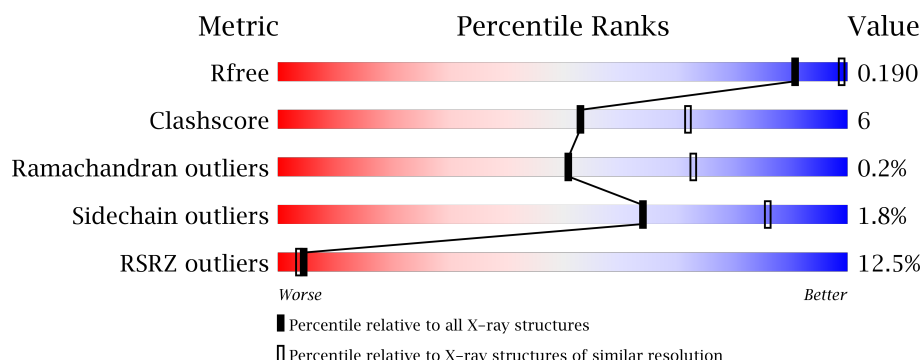
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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>3%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	a	344	<div> <div>4%</div> <div>97%</div> <div>.</div> <div>..</div> </div>
2	B	505	<div> <div>12%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
2	b	505	<div> <div>14%</div> <div>97%</div> <div>.</div> </div>
3	C	455	<div> <div>16%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
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	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	B	627	-	-	-	X
27	GOL	B	628	-	-	-	X
27	GOL	a	412	-	-	-	X
27	GOL	d	401	-	-	-	X
29	PL9	A	413	-	-	-	X
29	PL9	a	415	-	-	-	X
30	UNL	D	410	-	-	-	X
30	UNL	D	411	-	-	-	X
30	UNL	I	101	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	X	101	-	-	-	X
30	UNL	b	629	-	-	-	X
30	UNL	d	409	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	102	-	-	-	X
30	UNL	x	101	-	-	-	X
31	LHG	e	101	-	-	-	X
34	LMG	C	521	-	-	-	X
34	LMG	c	520	-	-	-	X
35	LMT	B	632	-	-	-	X
35	LMT	B	633	-	-	-	X
35	LMT	B	634	-	-	-	X
35	LMT	C	522	-	-	-	X
35	LMT	D	403	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	M	103	-	-	-	X
35	LMT	a	418	-	-	-	X
35	LMT	b	628	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	103	-	-	-	X
36	HTG	B	624	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	C	524	-	-	-	X
36	HTG	D	412	-	-	-	X
36	HTG	V	203	-	-	-	X
36	HTG	b	621	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	HTG	b	622	-	-	-	X
36	HTG	c	522	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 52752 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 II D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

- Molecule 10 is a protein called Photosystem II PsbK protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- Molecule 12 is a protein called Photosystem II PsbM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- 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 Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

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

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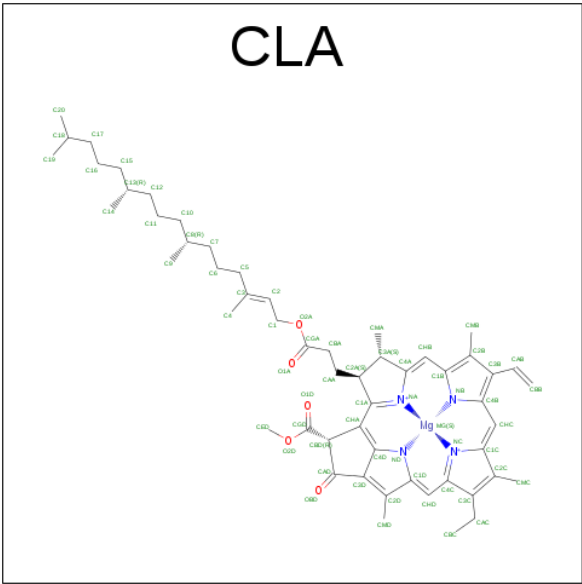
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 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
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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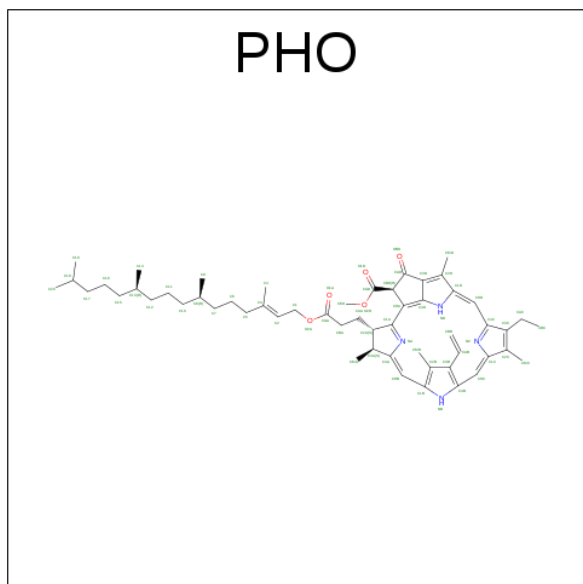
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

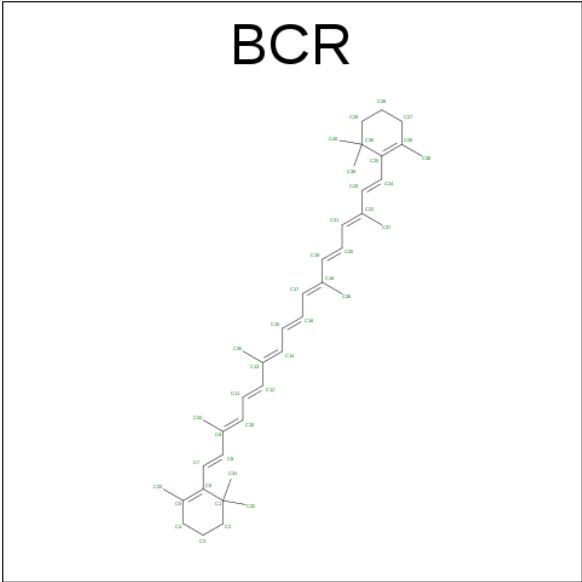
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





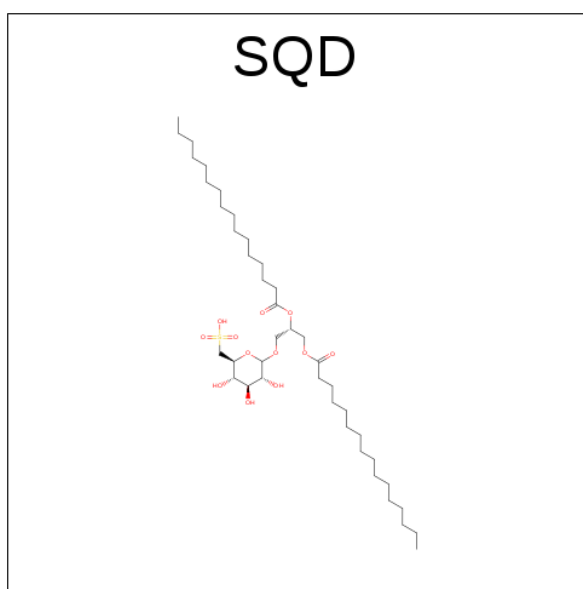
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



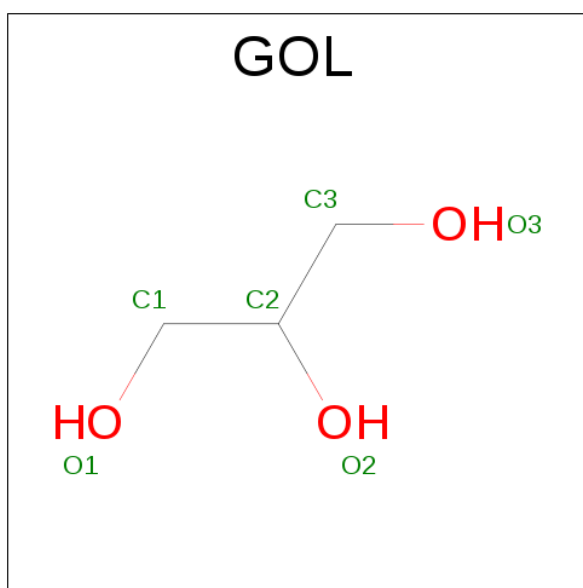
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



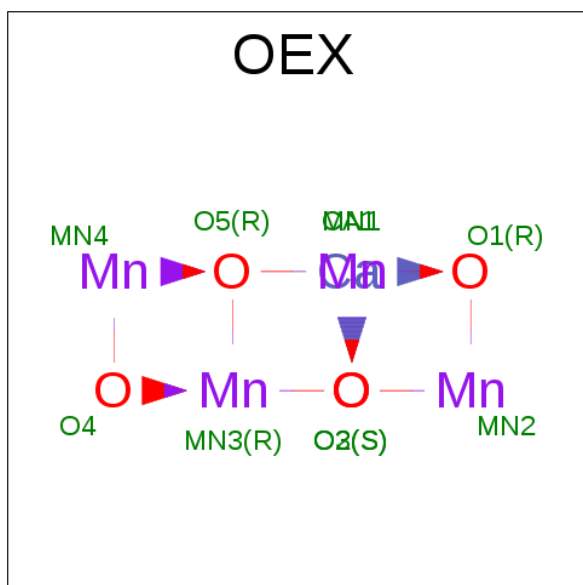
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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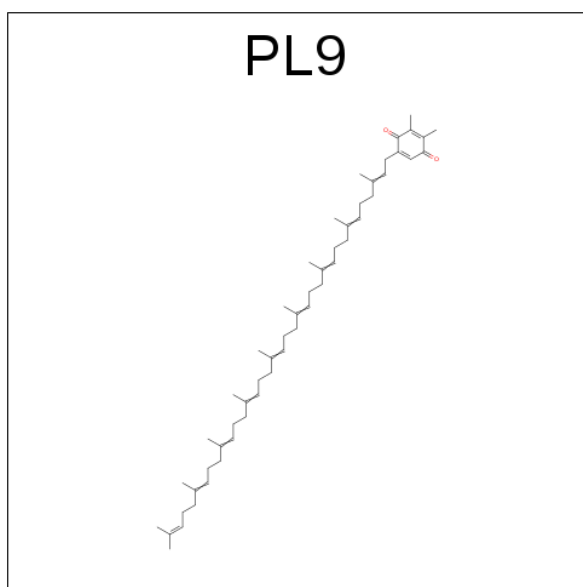
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	b	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 29 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

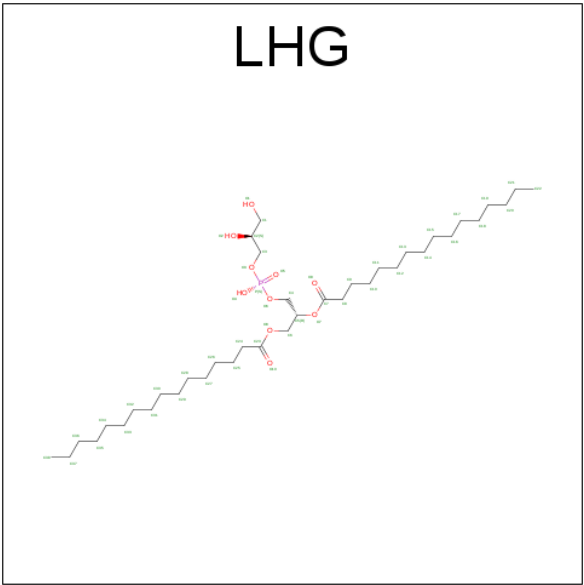
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
			30	25	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	x	1	Total	C	O	0	0
			18	16	2		
30	A	1	Total	C	O	0	0
			28	23	5		
30	j	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	d	1	Total	C	O	0	0
			17	16	1		
30	m	1	Total	C		0	0
			10	10			
30	b	2	Total	C	O	0	0
			69	59	10		
30	M	1	Total	C		0	0
			10	10			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



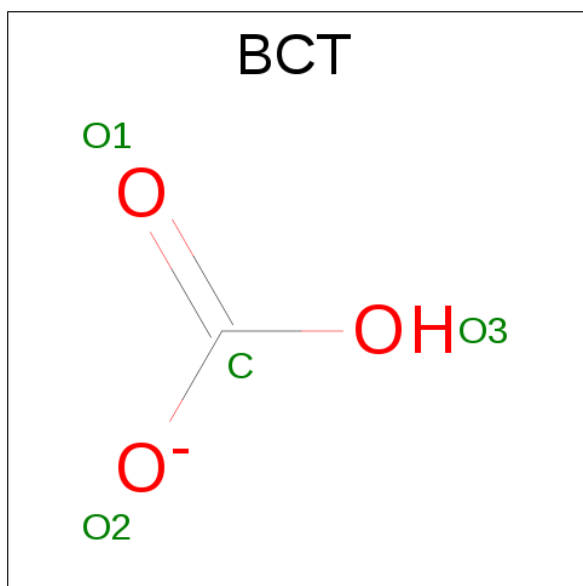
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).

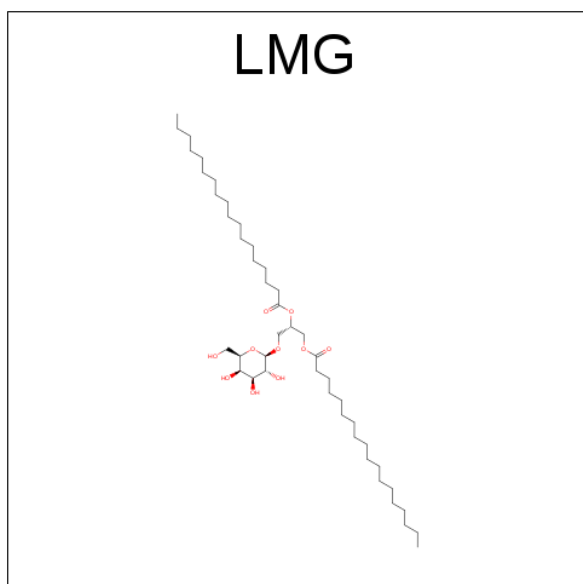


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	C	1	Total Ca 1 1	0	0
33	V	1	Total Ca 1 1	0	0
33	c	2	Total Ca 2 2	0	0
33	O	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0

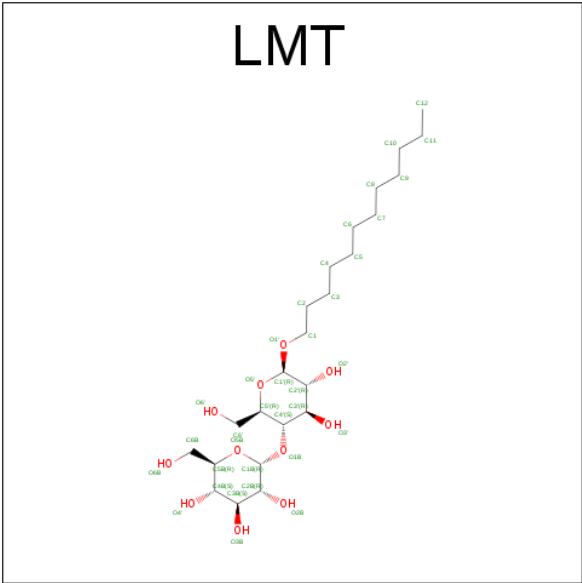
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



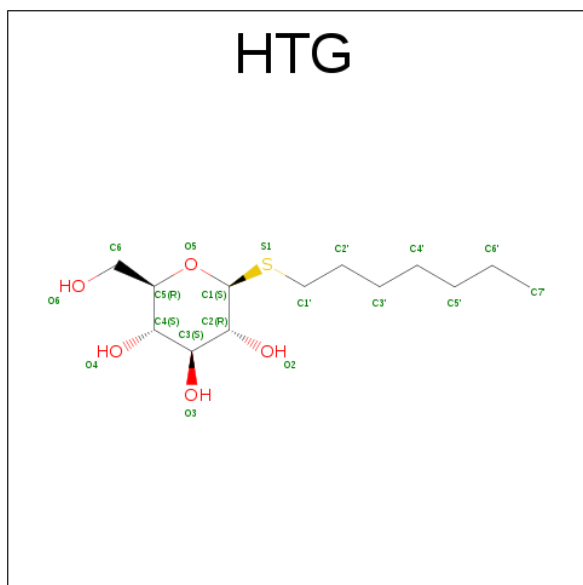
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			25	19	6		
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			26	19	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			35	24	11		
35	D	1	Total	C	O	0	0
			35	24	11		
35	E	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	a	1	Total	C	O	0	0
			35	24	11		
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



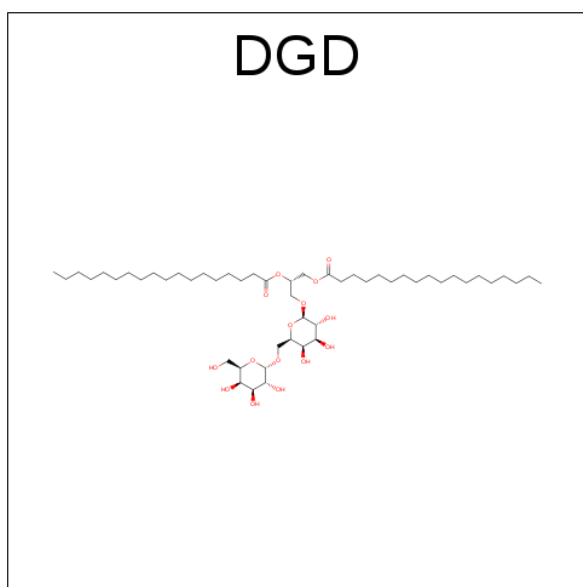
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	S		0	0
			9	8	1			
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O		0	0
			11	6	5			
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	135	Total O 135 135	0	0
40	B	195	Total O 195 195	0	0
40	C	151	Total O 151 151	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	D	118	Total 118	O 118	0	0
40	E	25	Total 25	O 25	0	0
40	F	5	Total 5	O 5	0	0
40	H	22	Total 22	O 22	0	0
40	I	6	Total 6	O 6	0	0
40	J	4	Total 4	O 4	0	0
40	K	6	Total 6	O 6	0	0
40	L	6	Total 6	O 6	0	0
40	M	15	Total 15	O 15	0	0
40	O	105	Total 105	O 105	0	0
40	T	13	Total 13	O 13	0	0
40	U	51	Total 51	O 51	0	0
40	V	81	Total 81	O 81	0	0
40	X	4	Total 4	O 4	0	0
40	Y	1	Total 1	O 1	0	0
40	Z	1	Total 1	O 1	0	0
40	R	1	Total 1	O 1	0	0
40	a	132	Total 132	O 132	0	0
40	b	206	Total 206	O 206	0	0
40	c	153	Total 153	O 153	0	0
40	d	115	Total 115	O 115	0	0

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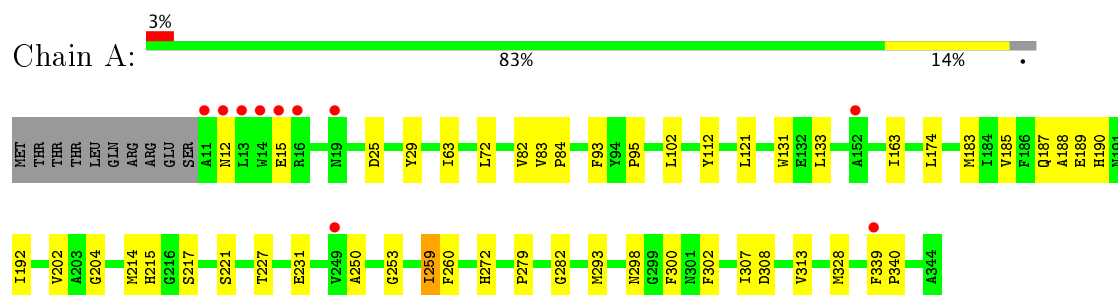
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	e	16	Total 16	O 16	0	0
40	f	5	Total 5	O 5	0	0
40	h	27	Total 27	O 27	0	0
40	i	3	Total 3	O 3	0	0
40	j	3	Total 3	O 3	0	0
40	k	6	Total 6	O 6	0	0
40	l	9	Total 9	O 9	0	0
40	m	18	Total 18	O 18	0	0
40	o	115	Total 115	O 115	0	0
40	t	9	Total 9	O 9	0	0
40	u	62	Total 62	O 62	0	0
40	v	78	Total 78	O 78	0	0
40	x	8	Total 8	O 8	0	0
40	z	1	Total 1	O 1	0	0

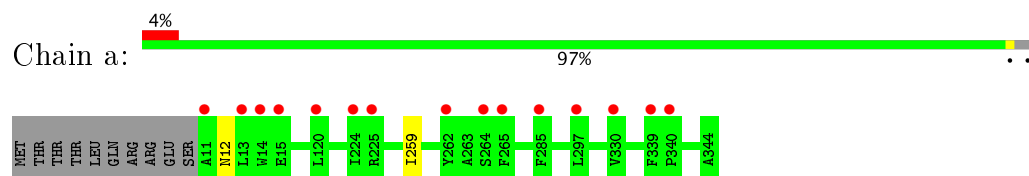
### 3 Residue-property plots [i](#)

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.

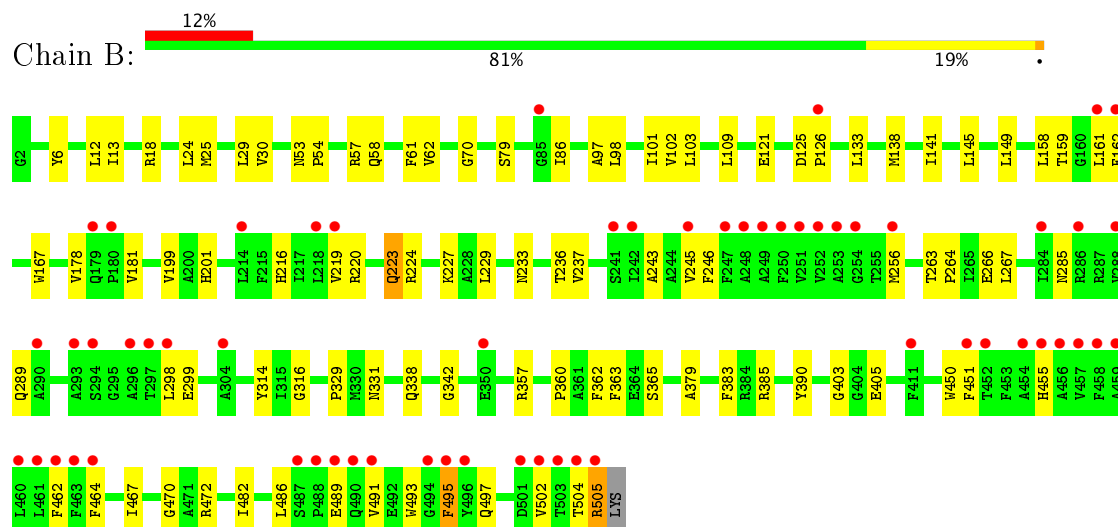
- Molecule 1: Photosystem II D1 protein



- Molecule 1: Photosystem II D1 protein



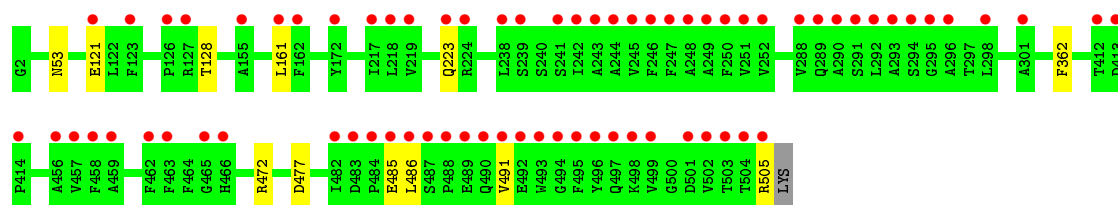
- Molecule 2: Photosystem II CP47 reaction center protein



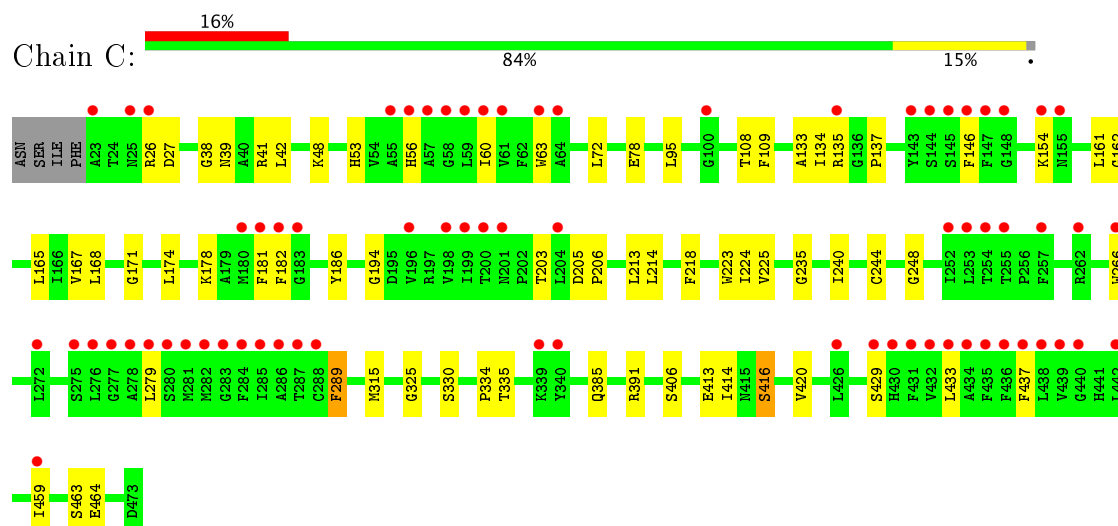
- Molecule 2: Photosystem II CP47 reaction center protein



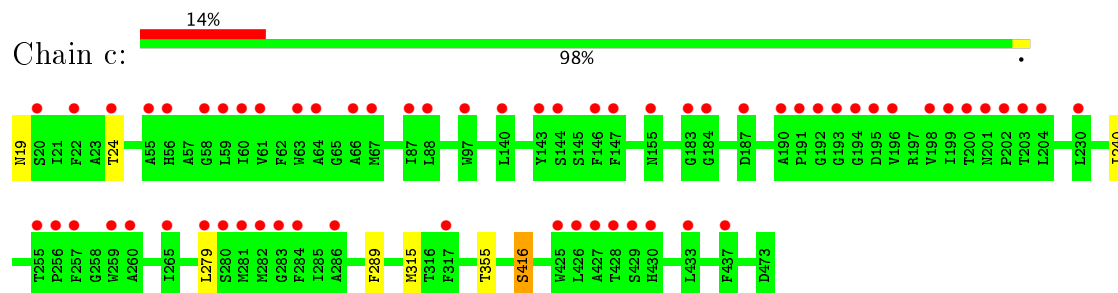




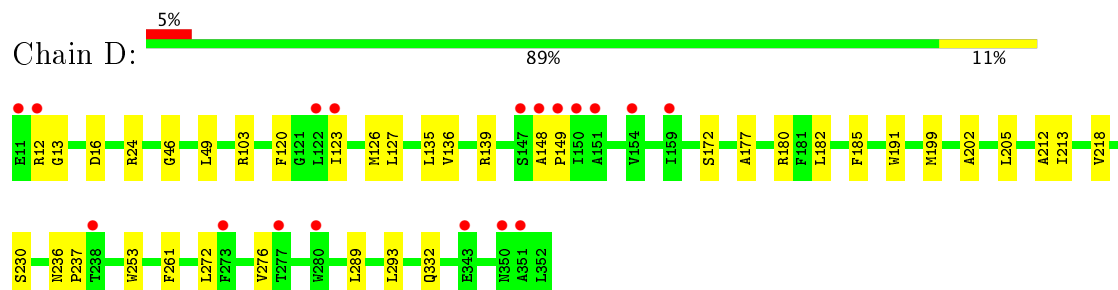
• Molecule 3: Photosystem II CP43 protein



• Molecule 3: Photosystem II CP43 protein

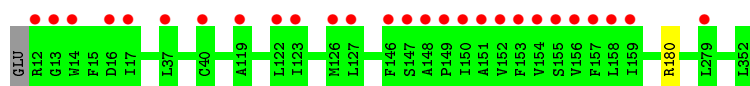


• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

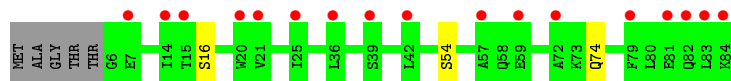
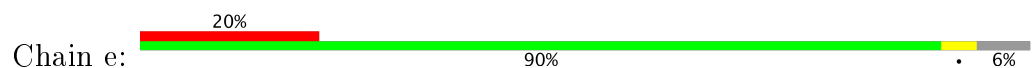




- Molecule 5: Cytochrome b559 subunit alpha



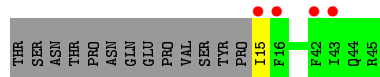
- Molecule 5: Cytochrome b559 subunit alpha



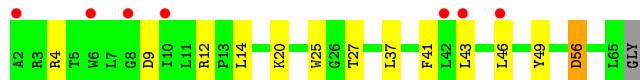
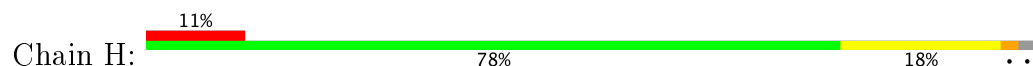
- Molecule 6: Cytochrome b559 subunit beta



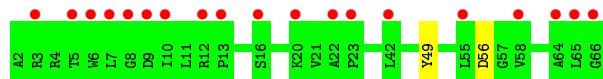
- Molecule 6: Cytochrome b559 subunit beta



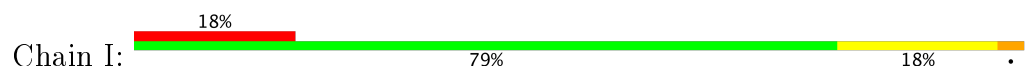
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

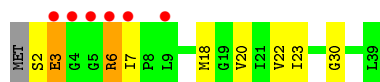




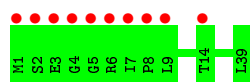
- Molecule 8: Photosystem II reaction center protein I



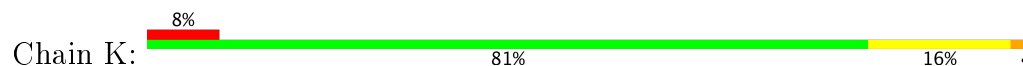
- Molecule 9: Photosystem II reaction center protein J



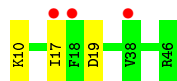
- Molecule 9: Photosystem II reaction center protein J



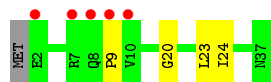
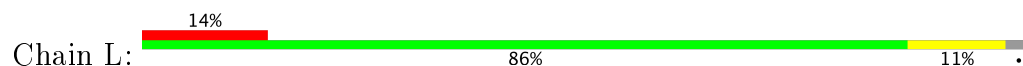
- Molecule 10: Photosystem II PsbK protein



- Molecule 10: Photosystem II PsbK protein

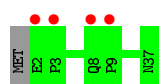


- Molecule 11: Photosystem II reaction center protein L

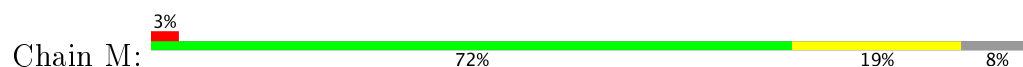


- Molecule 11: Photosystem II reaction center protein L

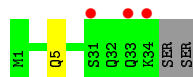




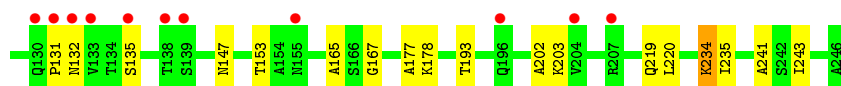
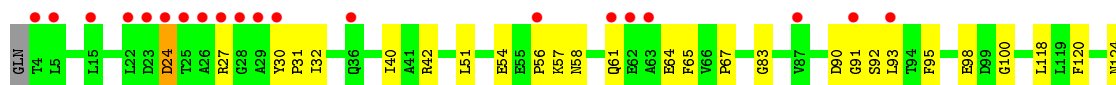
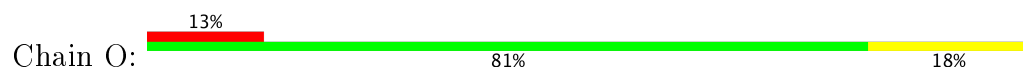
- Molecule 12: Photosystem II PsbM protein



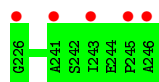
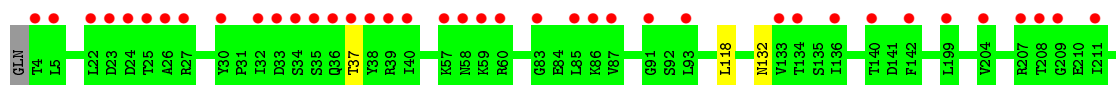
- Molecule 12: Photosystem II PsbM protein



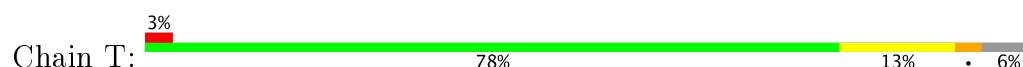
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

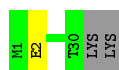


- Molecule 14: Photosystem II reaction center protein T

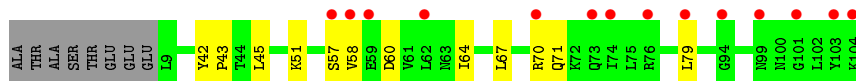
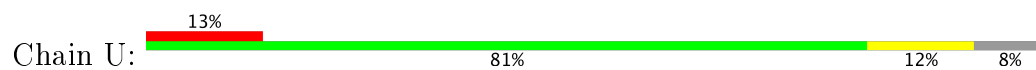


- Molecule 14: Photosystem II reaction center protein T

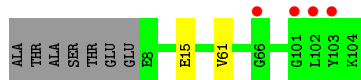




- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



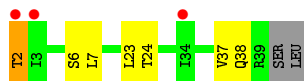
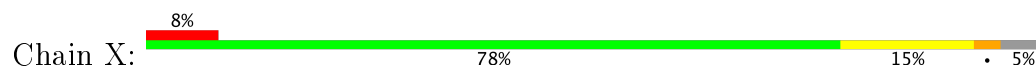
- Molecule 16: Cytochrome c-550



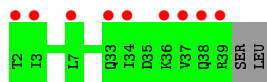
- Molecule 16: Cytochrome c-550



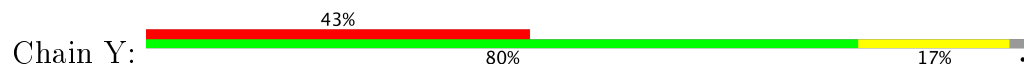
- Molecule 17: Photosystem II reaction center protein X



- Molecule 17: Photosystem II reaction center protein X

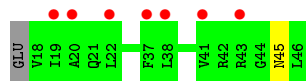


- Molecule 18: Photosystem II reaction center protein Ycf12

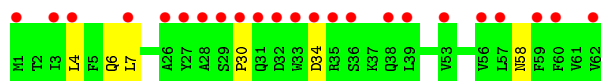
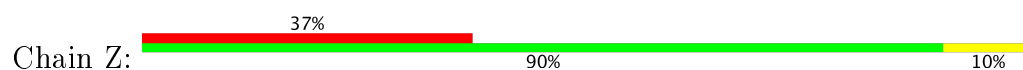




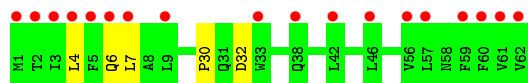
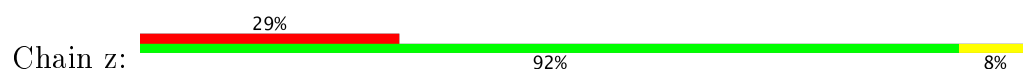
- Molecule 18: Photosystem II reaction center protein Ycf12



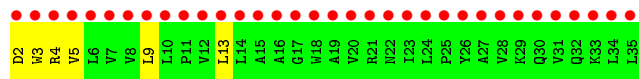
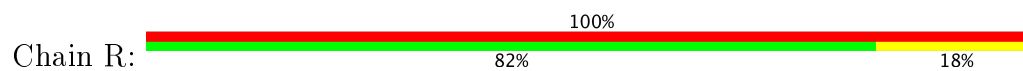
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 46.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 100.0 (46.51-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.139 , 0.187 0.146 , 0.190	Depositor DCC
$R_{free}$ test set	14584 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, HTG, 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  > 5$	RMSZ	# $ Z  > 5$
1	A	0.44	0/2705	0.56	0/3689
1	a	0.43	0/2705	0.54	0/3689
2	B	0.42	0/4109	0.54	0/5600
2	b	0.41	0/4109	0.54	0/5600
3	C	0.39	0/3599	0.51	0/4900
3	c	0.39	0/3633	0.53	0/4946
4	D	0.43	0/2821	0.54	0/3844
4	d	0.43	0/2812	0.54	0/3832
5	E	0.35	0/681	0.53	0/928
5	e	0.37	0/667	0.49	0/908
6	F	0.34	0/284	0.48	0/387
6	f	0.40	0/257	0.49	0/349
7	H	0.36	0/519	0.53	0/708
7	h	0.35	0/524	0.49	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.36	0/311	0.54	0/419
9	J	0.36	0/278	0.46	0/376
9	j	0.35	0/283	0.47	0/383
10	K	0.35	0/303	0.53	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.42	0/303	0.51	0/412
11	l	0.38	0/303	0.53	0/412
12	M	0.44	0/253	0.58	0/346
12	m	0.42	0/262	0.58	0/357
13	O	0.38	0/1896	0.58	0/2571
13	o	0.39	0/1896	0.58	0/2571
14	T	0.54	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.57	0/1052
15	u	0.41	0/785	0.57	0/1064
16	V	0.37	0/1085	0.52	0/1473



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1085	0.53	0/1473
17	X	0.33	0/284	0.49	0/384
17	x	0.31	0/284	0.46	0/384
18	Y	0.30	0/216	0.44	0/289
18	y	0.31	0/216	0.50	0/289
19	Z	0.32	0/490	0.46	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.27	0/279	0.43	0/383
All	All	0.40	0/42631	0.53	0/58018

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2620	0	2517	42	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	96	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	75	0
3	c	3519	0	3437	0	0
4	D	2726	0	2627	36	0
4	d	2717	0	2621	0	0
5	E	662	0	648	20	0
5	e	648	0	634	0	0
6	F	275	0	282	8	0
6	f	250	0	261	0	0
7	H	506	0	529	12	0
7	h	511	0	532	0	0
8	I	314	0	328	6	0
8	i	314	0	328	0	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	296	0	304	4	0
11	l	296	0	304	0	0
12	M	260	0	275	6	0
12	m	269	0	288	0	0
13	O	1865	0	1838	33	0
13	o	1865	0	1838	0	0
14	T	258	0	261	6	0
14	t	258	0	261	0	0
15	U	765	0	767	7	0
15	u	774	0	773	0	0
16	V	1064	0	1073	6	0
16	v	1064	0	1073	0	0
17	X	281	0	312	9	0
17	x	281	0	312	0	0
18	Y	215	0	246	4	0
18	y	215	0	246	0	0
19	Z	479	0	516	2	0
19	z	479	0	516	0	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	21	0
23	B	1040	0	1152	104	0
23	C	845	0	936	96	0
23	D	195	0	216	10	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	2	0
24	D	64	0	74	5	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	12	0
25	C	120	0	168	7	0
25	D	40	0	56	2	0
25	H	40	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	3	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	h	40	0	56	0	0
25	k	40	0	56	0	0
25	t	40	0	56	0	0
25	y	40	0	56	0	0
26	A	108	0	156	5	0
26	B	54	0	78	2	0
26	D	43	0	53	2	0
26	L	54	0	78	4	0
26	a	108	0	156	0	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	12	0	16	4	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	0	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	5	0
29	D	55	0	80	2	0
29	a	55	0	80	0	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	49	0	74	4	0
31	D	98	0	148	11	0
31	E	42	0	57	2	0
31	L	49	0	74	0	0
31	b	49	0	74	0	0
31	d	147	0	222	0	0
31	e	42	0	57	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0
33	c	2	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	7	0
34	J	51	0	72	4	0
34	Z	37	0	44	3	0
34	a	51	0	72	0	0
34	c	102	0	144	0	0
34	j	51	0	71	0	0
34	m	51	0	72	0	0
34	z	39	0	48	0	0
35	B	121	0	162	9	0
35	C	35	0	46	1	0
35	D	35	0	46	0	0
35	E	35	0	46	1	0
35	M	70	0	92	4	0
35	a	35	0	46	0	0
35	b	50	0	70	0	0
35	e	35	0	46	0	0
35	m	35	0	46	0	0
36	B	95	0	130	6	0
36	C	28	0	41	2	0
36	D	16	0	17	1	0
36	V	11	0	10	0	0
36	b	95	0	130	0	0
36	c	38	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	h	16	0	17	0	0
37	C	186	0	246	10	0
37	H	62	0	82	0	0
37	c	186	0	246	0	0
37	h	62	0	82	0	0
38	E	43	0	30	6	0
38	V	43	0	30	0	0
38	e	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	135	0	0	2	0
40	B	195	0	0	18	0
40	C	151	0	0	11	0
40	D	118	0	0	8	0
40	E	25	0	0	3	0
40	F	5	0	0	0	0
40	H	22	0	0	3	0
40	I	6	0	0	1	0
40	J	4	0	0	0	0
40	K	6	0	0	0	0
40	L	6	0	0	0	0
40	M	15	0	0	2	0
40	O	105	0	0	0	0
40	R	1	0	0	0	0
40	T	13	0	0	0	0
40	U	51	0	0	0	0
40	V	81	0	0	3	0
40	X	4	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	1	0
40	a	132	0	0	0	0
40	b	206	0	0	0	0
40	c	153	0	0	0	0
40	d	115	0	0	0	0
40	e	16	0	0	0	0
40	f	5	0	0	0	0
40	h	27	0	0	0	0
40	i	3	0	0	0	0
40	j	3	0	0	0	0
40	k	6	0	0	0	0
40	l	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	m	18	0	0	0	0
40	o	115	0	0	0	0
40	t	9	0	0	0	0
40	u	62	0	0	0	0
40	v	78	0	0	0	0
40	x	8	0	0	0	0
40	z	1	0	0	0	0
All	All	52752	0	51821	559	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 559 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)
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.54	0.94
23:B:605:CLA:H42	23:B:606:CLA:H2	1.48	0.93
4:D:199:MET:O	40:D:501:HOH:O	1.96	0.83
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.38	0.81
25:B:618:BCR:H363	25:T:101:BCR:H19C	31.54	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	44 66
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	44 66
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100 100
2	b	502/505 (99%)	494 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	51	73
3	c	453/455 (100%)	442 (98%)	10 (2%)	1 (0%)	51	73
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	8
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
13	o	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	4	5
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5212/5384 (97%)	5097 (98%)	107 (2%)	8 (0%)	51	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	30	PRO
1	a	259	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	269/279 (96%)	269 (100%)	0	100	100
1	a	269/279 (96%)	268 (100%)	1 (0%)	93	98
2	B	402/403 (100%)	395 (98%)	7 (2%)	66	87
2	b	402/403 (100%)	390 (97%)	12 (3%)	46	74
3	C	352/356 (99%)	349 (99%)	3 (1%)	82	94
3	c	356/356 (100%)	348 (98%)	8 (2%)	57	82
4	D	277/277 (100%)	276 (100%)	1 (0%)	93	98
4	d	276/277 (100%)	275 (100%)	1 (0%)	93	98
5	E	72/73 (99%)	71 (99%)	1 (1%)	71	90
5	e	70/73 (96%)	67 (96%)	3 (4%)	33	58
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/54 (100%)	51 (94%)	3 (6%)	25	45
7	h	54/54 (100%)	52 (96%)	2 (4%)	39	66
8	I	34/34 (100%)	33 (97%)	1 (3%)	48	75
8	i	34/34 (100%)	32 (94%)	2 (6%)	23	42
9	J	26/27 (96%)	24 (92%)	2 (8%)	15	28
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	17
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	17
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	70
13	O	206/207 (100%)	201 (98%)	5 (2%)	54	80
13	o	206/207 (100%)	203 (98%)	3 (2%)	70	89
14	T	26/28 (93%)	25 (96%)	1 (4%)	38	64
14	t	26/28 (93%)	25 (96%)	1 (4%)	38	64
15	U	83/89 (93%)	82 (99%)	1 (1%)	75	91
15	u	84/89 (94%)	82 (98%)	2 (2%)	54	80
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	30 (97%)	1 (3%)	44	71
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	22 (100%)	0	100	100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	23	43
19	z	52/52 (100%)	48 (92%)	4 (8%)	15	28
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4317/4403 (98%)	4241 (98%)	76 (2%)	64	86

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	121	GLU

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Mol	Chain	Res	Type
2	b	486	LEU
15	u	15	GLU
2	b	128	THR
2	b	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
19	Z	58	ASN
2	b	223	GLN
13	o	130	GLN
2	b	53	ASN
2	b	331	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
8	FME	I	1	8	9,9,10	0.58	0	7,9,11	1.25	1 (14%)
12	FME	M	1	12	9,9,10	0.53	0	7,9,11	1.50	1 (14%)
14	FME	T	1	14	9,9,10	0.73	0	7,9,11	1.14	1 (14%)
8	FME	i	1	8	9,9,10	0.56	0	7,9,11	1.53	2 (28%)
12	FME	m	1	12	9,9,10	0.70	0	7,9,11	1.45	2 (28%)
14	FME	t	1	14	9,9,10	0.65	0	7,9,11	1.74	2 (28%)

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
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.17	117.76	125.15
12	M	1	FME	O-C-CA	-2.99	118.17	125.15
8	i	1	FME	O-C-CA	-2.75	118.75	125.15
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
8	I	1	FME	O-C-CA	-2.42	119.51	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 218 ligands modelled in this entry, 18 are unknown and 15 are monoatomic - leaving 185 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
23	CLA	A	404	1	56,73,73	1.97	12 (21%)	65,113,113	2.31	23 (35%)
23	CLA	A	405	40	56,73,73	1.94	12 (21%)	65,113,113	2.10	20 (30%)
24	PHO	A	406	-	67,69,69	2.17	17 (25%)	87,99,99	1.99	23 (26%)
23	CLA	A	407	1	56,73,73	1.94	11 (19%)	65,113,113	2.09	18 (27%)
25	BCR	A	408	-	41,41,41	0.97	1 (2%)	56,56,56	1.65	16 (28%)
26	SQD	A	409	-	53,54,54	0.96	3 (5%)	63,65,65	1.98	13 (20%)
27	GOL	A	410	-	5,5,5	0.36	0	5,5,5	0.22	0
26	SQD	A	411	-	53,54,54	1.01	3 (5%)	63,65,65	1.22	6 (9%)
28	OEX	A	412	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	A	413	-	55,55,55	0.61	1 (1%)	69,69,69	1.90	21 (30%)
31	LHG	A	415	-	48,48,48	0.84	2 (4%)	49,54,54	1.24	6 (12%)
32	BCT	A	416	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	602	40	56,73,73	1.98	12 (21%)	65,113,113	2.16	21 (32%)
23	CLA	B	603	2	56,73,73	1.99	12 (21%)	65,113,113	2.25	20 (30%)
23	CLA	B	604	2	56,73,73	1.95	12 (21%)	65,113,113	2.27	21 (32%)
23	CLA	B	605	2	56,73,73	1.92	10 (17%)	65,113,113	2.33	19 (29%)
23	CLA	B	606	2	56,73,73	1.90	13 (23%)	65,113,113	2.19	22 (33%)
23	CLA	B	607	2	56,73,73	1.86	11 (19%)	65,113,113	2.19	21 (32%)
23	CLA	B	608	40	56,73,73	1.96	12 (21%)	65,113,113	2.17	23 (35%)
23	CLA	B	609	2	56,73,73	1.87	11 (19%)	65,113,113	2.25	20 (30%)
23	CLA	B	610	2	56,73,73	1.91	11 (19%)	65,113,113	2.18	16 (24%)
23	CLA	B	611	40	56,73,73	1.99	12 (21%)	65,113,113	2.27	23 (35%)
23	CLA	B	612	2	56,73,73	1.97	11 (19%)	65,113,113	2.32	22 (33%)
23	CLA	B	613	2	56,73,73	1.94	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	B	614	2	56,73,73	1.99	12 (21%)	65,113,113	2.22	19 (29%)
23	CLA	B	615	2	56,73,73	1.89	12 (21%)	65,113,113	2.29	18 (27%)
23	CLA	B	616	2	56,73,73	1.90	11 (19%)	65,113,113	2.21	22 (33%)
23	CLA	B	617	2	56,73,73	1.95	11 (19%)	65,113,113	2.24	20 (30%)
25	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.63	10 (17%)
25	BCR	B	619	-	41,41,41	0.95	1 (2%)	56,56,56	1.55	12 (21%)
25	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	12 (21%)
26	SQD	B	621	-	53,54,54	1.02	3 (5%)	63,65,65	1.62	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.19	5 (8%)
35	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.19	4 (8%)
36	HTG	B	624	-	19,19,19	0.96	1 (5%)	23,24,24	1.43	4 (17%)
36	HTG	B	625	-	19,19,19	0.81	1 (5%)	23,24,24	1.86	1 (4%)
36	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.83	2 (8%)
27	GOL	B	627	-	5,5,5	0.33	0	5,5,5	0.36	0
27	GOL	B	628	-	5,5,5	0.52	0	5,5,5	0.47	0
36	HTG	B	629	-	19,19,19	0.95	2 (10%)	23,24,24	1.47	3 (13%)
36	HTG	B	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.57	1 (4%)
35	LMT	B	632	-	25,25,36	0.44	0	30,30,47	0.72	0
35	LMT	B	633	-	36,36,36	0.55	1 (2%)	47,47,47	1.03	1 (2%)
35	LMT	B	634	-	26,26,36	0.49	0	31,31,47	0.92	1 (3%)
34	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.28	6 (10%)
23	CLA	C	502	3	56,73,73	1.92	12 (21%)	65,113,113	2.36	23 (35%)
23	CLA	C	503	3	56,73,73	1.90	11 (19%)	65,113,113	2.12	18 (27%)
23	CLA	C	504	3	56,73,73	1.89	12 (21%)	65,113,113	2.12	18 (27%)
23	CLA	C	505	40	56,73,73	2.00	12 (21%)	65,113,113	2.33	22 (33%)
23	CLA	C	506	3	56,73,73	1.89	12 (21%)	65,113,113	2.28	19 (29%)
23	CLA	C	507	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	23 (35%)
23	CLA	C	508	40	56,73,73	1.90	12 (21%)	65,113,113	2.23	21 (32%)
23	CLA	C	509	3	56,73,73	2.04	11 (19%)	65,113,113	2.40	20 (30%)
23	CLA	C	510	3	56,73,73	1.97	12 (21%)	65,113,113	2.21	20 (30%)
23	CLA	C	511	3	56,73,73	1.92	11 (19%)	65,113,113	2.27	19 (29%)
23	CLA	C	512	3	56,73,73	1.99	12 (21%)	65,113,113	2.09	18 (27%)
23	CLA	C	513	3	56,73,73	1.94	11 (19%)	65,113,113	2.18	22 (33%)
23	CLA	C	514	3	56,73,73	1.92	11 (19%)	65,113,113	2.15	20 (30%)
25	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.54	7 (12%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	9 (16%)
37	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.23	8 (10%)
37	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
37	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	5 (6%)
34	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	3 (5%)
34	LMG	C	521	-	51,51,55	0.97	3 (5%)	59,59,63	1.23	4 (6%)
35	LMT	C	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.07	5 (10%)
36	HTG	C	523	-	19,19,19	0.94	1 (5%)	23,24,24	1.69	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	C	524	-	8,8,19	0.38	0	7,7,24	1.11	1 (14%)
27	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.19	0
25	BCR	C	527	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	D	401	40	56,73,73	1.94	11 (19%)	65,113,113	2.12	22 (33%)
24	PHO	D	402	-	67,69,69	2.13	17 (25%)	87,99,99	2.01	24 (27%)
35	LMT	D	403	-	36,36,36	0.57	1 (2%)	47,47,47	1.25	4 (8%)
23	CLA	D	404	4	56,73,73	1.99	12 (21%)	65,113,113	2.34	20 (30%)
23	CLA	D	405	4	56,73,73	1.95	11 (19%)	65,113,113	2.14	21 (32%)
25	BCR	D	406	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	13 (23%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	69,69,69	1.61	18 (26%)
31	LHG	D	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.04	3 (6%)
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	49,54,54	1.10	3 (6%)
36	HTG	D	412	-	16,16,19	1.01	2 (12%)	20,21,24	1.69	1 (5%)
26	SQD	D	413	-	42,43,54	1.12	3 (7%)	52,54,65	1.77	14 (26%)
31	LHG	E	101	-	41,41,48	1.01	2 (4%)	42,47,54	1.15	3 (7%)
35	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.91	2 (4%)
38	HEM	E	103	5,6	28,50,50	0.88	2 (7%)	17,82,82	2.25	4 (23%)
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.59	11 (19%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.01	3 (3%)
34	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.10	5 (8%)
31	LHG	L	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.20	4 (8%)
26	SQD	L	102	-	53,54,54	1.01	3 (5%)	63,65,65	1.69	12 (19%)
35	LMT	M	101	-	36,36,36	0.56	0	47,47,47	1.13	4 (8%)
35	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.84	2 (4%)
27	GOL	O	302	-	5,5,5	0.31	0	5,5,5	0.32	0
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	12 (21%)
38	HEM	V	202	16	28,50,50	0.98	3 (10%)	17,82,82	1.41	2 (11%)
36	HTG	V	203	-	11,11,19	0.28	0	13,15,24	1.40	1 (7%)
25	BCR	Y	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.81	18 (32%)
34	LMG	Z	101	-	37,37,55	0.97	3 (8%)	45,45,63	1.59	8 (17%)
23	CLA	a	404	1	56,73,73	1.93	11 (19%)	65,113,113	2.27	25 (38%)
23	CLA	a	405	40	56,73,73	1.98	11 (19%)	65,113,113	2.29	22 (33%)
23	CLA	a	406	40	56,73,73	1.92	11 (19%)	65,113,113	2.15	21 (32%)
24	PHO	a	407	-	67,69,69	2.12	16 (23%)	87,99,99	2.02	26 (29%)
24	PHO	a	408	-	67,69,69	2.22	15 (22%)	87,99,99	1.87	24 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	a	409	1	56,73,73	1.93	12 (21%)	65,113,113	2.19	26 (40%)
25	BCR	a	410	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	11 (19%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	63,65,65	1.75	15 (23%)
27	GOL	a	412	-	5,5,5	0.42	0	5,5,5	0.26	0
26	SQD	a	413	-	53,54,54	1.06	4 (7%)	63,65,65	1.37	8 (12%)
28	OEX	a	414	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	a	415	-	55,55,55	0.63	1 (1%)	69,69,69	1.94	19 (27%)
34	LMG	a	417	-	51,51,55	0.94	3 (5%)	59,59,63	1.13	3 (5%)
35	LMT	a	418	-	36,36,36	0.49	0	47,47,47	0.78	1 (2%)
32	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	601	40	56,73,73	1.98	11 (19%)	65,113,113	2.13	19 (29%)
23	CLA	b	602	2	56,73,73	1.98	12 (21%)	65,113,113	2.28	27 (41%)
23	CLA	b	603	2	56,73,73	1.91	12 (21%)	65,113,113	2.29	20 (30%)
23	CLA	b	604	2	56,73,73	1.86	11 (19%)	65,113,113	2.30	20 (30%)
23	CLA	b	605	2	56,73,73	1.92	12 (21%)	65,113,113	2.30	21 (32%)
23	CLA	b	606	2	56,73,73	1.85	11 (19%)	65,113,113	2.19	20 (30%)
23	CLA	b	607	40	56,73,73	1.87	12 (21%)	65,113,113	2.35	20 (30%)
23	CLA	b	608	2	56,73,73	1.97	11 (19%)	65,113,113	2.15	20 (30%)
23	CLA	b	609	2	56,73,73	1.95	11 (19%)	65,113,113	2.15	19 (29%)
23	CLA	b	610	40	56,73,73	2.00	12 (21%)	65,113,113	2.25	22 (33%)
23	CLA	b	611	2	56,73,73	1.95	12 (21%)	65,113,113	2.48	19 (29%)
23	CLA	b	612	2	56,73,73	1.98	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	b	613	2	56,73,73	2.02	11 (19%)	65,113,113	2.18	19 (29%)
23	CLA	b	614	2	56,73,73	1.98	12 (21%)	65,113,113	2.21	20 (30%)
23	CLA	b	615	2	56,73,73	1.88	11 (19%)	65,113,113	2.20	20 (30%)
23	CLA	b	616	2	56,73,73	1.95	12 (21%)	65,113,113	2.32	21 (32%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	6 (10%)
25	BCR	b	618	-	41,41,41	0.96	1 (2%)	56,56,56	1.53	13 (23%)
25	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.81	12 (21%)
35	LMT	b	620	-	25,25,36	0.46	0	30,30,47	0.69	0
36	HTG	b	621	-	19,19,19	1.22	2 (10%)	23,24,24	1.96	5 (21%)
36	HTG	b	622	-	19,19,19	0.99	2 (10%)	23,24,24	1.53	2 (8%)
36	HTG	b	623	-	19,19,19	1.06	2 (10%)	23,24,24	1.85	3 (13%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.38	0
36	HTG	b	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.61	3 (13%)
36	HTG	b	626	-	19,19,19	1.06	2 (10%)	23,24,24	1.41	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMT	b	628	-	25,25,36	0.53	1 (4%)	30,30,47	1.29	4 (13%)
31	LHG	b	630	-	48,48,48	0.92	2 (4%)	49,54,54	1.10	2 (4%)
23	CLA	c	501	3	56,73,73	1.91	12 (21%)	65,113,113	2.20	20 (30%)
23	CLA	c	502	3	56,73,73	2.00	11 (19%)	65,113,113	2.22	18 (27%)
23	CLA	c	503	3	56,73,73	1.91	12 (21%)	65,113,113	2.23	21 (32%)
23	CLA	c	504	40	56,73,73	1.98	12 (21%)	65,113,113	2.26	21 (32%)
23	CLA	c	505	3	56,73,73	1.92	12 (21%)	65,113,113	2.21	18 (27%)
23	CLA	c	506	3	56,73,73	1.88	11 (19%)	65,113,113	2.22	21 (32%)
23	CLA	c	507	40	56,73,73	1.92	12 (21%)	65,113,113	2.16	21 (32%)
23	CLA	c	508	3	56,73,73	2.00	12 (21%)	65,113,113	2.32	18 (27%)
23	CLA	c	509	3	56,73,73	1.96	12 (21%)	65,113,113	2.25	21 (32%)
23	CLA	c	510	3	56,73,73	1.91	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	c	511	3	56,73,73	1.96	12 (21%)	65,113,113	2.15	19 (29%)
23	CLA	c	512	3	56,73,73	1.92	12 (21%)	65,113,113	2.31	21 (32%)
23	CLA	c	513	3	56,73,73	1.95	12 (21%)	65,113,113	2.18	22 (33%)
25	BCR	c	514	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	13 (23%)
25	BCR	c	515	-	41,41,41	0.96	1 (2%)	56,56,56	1.67	15 (26%)
37	DGD	c	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	6 (7%)
37	DGD	c	517	-	63,63,67	0.90	3 (4%)	77,77,81	1.01	4 (5%)
37	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.12	5 (6%)
34	LMG	c	519	-	51,51,55	0.95	3 (5%)	59,59,63	1.09	5 (8%)
34	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.23	7 (11%)
36	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.71	1 (4%)
36	HTG	c	522	-	19,19,19	0.98	2 (10%)	23,24,24	1.61	3 (13%)
27	GOL	d	401	-	5,5,5	0.29	0	5,5,5	0.52	0
23	CLA	d	402	4	56,73,73	1.91	12 (21%)	65,113,113	2.31	20 (30%)
23	CLA	d	403	4	56,73,73	1.94	11 (19%)	65,113,113	2.14	19 (29%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.67	14 (25%)
29	PL9	d	405	-	55,55,55	0.62	1 (1%)	69,69,69	1.79	22 (31%)
31	LHG	d	406	-	48,48,48	0.85	2 (4%)	49,54,54	1.13	5 (10%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	49,54,54	0.97	4 (8%)
31	LHG	d	408	-	48,48,48	0.94	2 (4%)	49,54,54	1.03	4 (8%)
31	LHG	e	101	-	41,41,48	1.01	2 (4%)	42,47,54	0.98	2 (4%)
35	LMT	e	102	-	36,36,36	0.47	0	47,47,47	0.90	3 (6%)
38	HEM	e	103	5,6	28,50,50	0.93	2 (7%)	17,82,82	1.90	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	52,54,65	1.69	8 (15%)
36	HTG	h	101	-	16,16,19	1.07	2 (12%)	20,21,24	1.50	1 (5%)
25	BCR	h	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	10 (17%)
37	DGD	h	103	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	3 (3%)
34	LMG	j	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.11	5 (8%)
25	BCR	k	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	13 (23%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.20	6 (10%)
35	LMT	m	103	-	36,36,36	0.50	0	47,47,47	0.97	2 (4%)
25	BCR	t	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.83	14 (25%)
38	HEM	v	201	16	28,50,50	0.91	3 (10%)	17,82,82	1.61	3 (17%)
25	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.66	12 (21%)
34	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.15	4 (8%)

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
23	CLA	A	404	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6
23	CLA	A	407	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
26	SQD	A	409	-	-	0/49/69/69	0/1/1/1
27	GOL	A	410	-	-	0/4/4/4	0/0/0/0
26	SQD	A	411	-	-	0/49/69/69	0/1/1/1
28	OEX	A	412	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	A	413	-	-	0/53/73/73	0/1/1/1
31	LHG	A	415	-	-	0/53/53/53	0/0/0/0
32	BCT	A	416	21	-	0/0/0/0	0/0/0/0
23	CLA	B	602	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	609	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	2	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
34	LMG	B	622	-	-	0/46/66/70	0/1/1/1
35	LMT	B	623	-	-	0/21/61/61	0/2/2/2
36	HTG	B	624	-	-	0/10/30/30	0/1/1/1
36	HTG	B	625	-	-	0/10/30/30	0/1/1/1
36	HTG	B	626	-	-	0/10/30/30	0/1/1/1
27	GOL	B	627	-	-	0/4/4/4	0/0/0/0
27	GOL	B	628	-	-	0/4/4/4	0/0/0/0
36	HTG	B	629	-	-	0/10/30/30	0/1/1/1
36	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	LMT	B	632	-	-	0/17/37/61	0/1/1/2
35	LMT	B	633	-	-	0/21/61/61	0/2/2/2
35	LMT	B	634	-	-	0/17/38/61	0/1/1/2
34	LMG	C	501	-	-	1/46/66/70	0/1/1/1
23	CLA	C	502	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	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
23	CLA	C	514	3	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
37	DGD	C	517	-	-	0/51/91/95	0/2/2/2
37	DGD	C	518	-	-	0/51/91/95	0/2/2/2
37	DGD	C	519	-	-	0/51/91/95	0/2/2/2
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	LMG	C	521	-	-	0/46/66/70	0/1/1/1
35	LMT	C	522	-	-	1/21/61/61	0/2/2/2
36	HTG	C	523	-	-	0/10/30/30	0/1/1/1
36	HTG	C	524	-	-	0/6/6/30	0/0/0/1
27	GOL	C	525	-	-	0/4/4/4	0/0/0/0
25	BCR	C	527	-	-	0/29/63/63	0/2/2/2
23	CLA	D	401	40	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
35	LMT	D	403	-	-	0/21/61/61	0/2/2/2
23	CLA	D	404	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	405	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	406	-	-	0/29/63/63	0/2/2/2
29	PL9	D	407	-	-	0/53/73/73	0/1/1/1
31	LHG	D	408	-	-	0/53/53/53	0/0/0/0
31	LHG	D	409	-	-	0/53/53/53	0/0/0/0
36	HTG	D	412	-	-	0/7/27/30	0/1/1/1
26	SQD	D	413	-	-	2/38/58/69	0/1/1/1
31	LHG	E	101	-	-	0/46/46/53	0/0/0/0
35	LMT	E	102	-	-	0/21/61/61	0/2/2/2
38	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
25	BCR	H	101	-	-	0/29/63/63	0/2/2/2
37	DGD	H	102	-	-	0/51/91/95	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	102	-	-	0/49/69/69	0/1/1/1
35	LMT	M	101	-	-	0/21/61/61	0/2/2/2
35	LMT	M	103	-	-	0/21/61/61	0/2/2/2
27	GOL	O	302	-	-	0/4/4/4	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
38	HEM	V	202	16	-	0/6/54/54	0/0/8/8
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	2/31/51/70	0/1/1/1
23	CLA	a	404	1	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	405	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
23	CLA	a	409	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
26	SQD	a	411	-	-	0/49/69/69	0/1/1/1
27	GOL	a	412	-	-	0/4/4/4	0/0/0/0
26	SQD	a	413	-	-	0/49/69/69	0/1/1/1
28	OEX	a	414	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	a	415	-	-	0/53/73/73	0/1/1/1
34	LMG	a	417	-	-	0/46/66/70	0/1/1/1
35	LMT	a	418	-	-	0/21/61/61	0/2/2/2
32	BCT	a	419	21	-	0/0/0/0	0/0/0/0
23	CLA	b	601	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	602	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	603	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	604	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	2	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
35	LMT	b	620	-	-	0/17/37/61	0/1/1/2
36	HTG	b	621	-	-	0/10/30/30	0/1/1/1
36	HTG	b	622	-	-	0/10/30/30	0/1/1/1
36	HTG	b	623	-	-	0/10/30/30	0/1/1/1
27	GOL	b	624	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	b	625	-	-	0/10/30/30	0/1/1/1
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
35	LMT	b	628	-	-	0/17/37/61	0/1/1/2
31	LHG	b	630	-	-	0/53/53/53	0/0/0/0
23	CLA	c	501	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	3	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
37	DGD	c	516	-	-	0/51/91/95	0/2/2/2
37	DGD	c	517	-	-	0/51/91/95	0/2/2/2
37	DGD	c	518	-	-	0/51/91/95	0/2/2/2
34	LMG	c	519	-	-	0/46/66/70	0/1/1/1
34	LMG	c	520	-	-	0/46/66/70	0/1/1/1
36	HTG	c	521	-	-	0/10/30/30	0/1/1/1
36	HTG	c	522	-	-	0/10/30/30	0/1/1/1
27	GOL	d	401	-	-	0/4/4/4	0/0/0/0
23	CLA	d	402	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	d	404	-	-	0/29/63/63	0/2/2/2
29	PL9	d	405	-	-	0/53/73/73	0/1/1/1
31	LHG	d	406	-	-	0/53/53/53	0/0/0/0
31	LHG	d	407	-	-	0/53/53/53	0/0/0/0
31	LHG	d	408	-	-	0/53/53/53	0/0/0/0
31	LHG	e	101	-	-	0/46/46/53	0/0/0/0
35	LMT	e	102	-	-	0/21/61/61	0/2/2/2
38	HEM	e	103	5,6	-	0/6/54/54	0/0/8/8
26	SQD	f	101	-	-	2/38/58/69	0/1/1/1
36	HTG	h	101	-	-	0/7/27/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
37	DGD	h	103	-	-	0/51/91/95	0/2/2/2
34	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
34	LMG	m	101	-	-	0/46/66/70	0/1/1/1
35	LMT	m	103	-	-	0/21/61/61	0/2/2/2
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
38	HEM	v	201	16	-	0/6/54/54	0/0/8/8
25	BCR	y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	z	101	-	-	0/34/54/70	0/1/1/1

The worst 5 of 1036 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	BCR	C23-C22	-5.44	1.34	1.45
25	y	101	BCR	C23-C22	-5.17	1.34	1.45
25	b	619	BCR	C23-C22	-5.09	1.34	1.45
25	k	101	BCR	C23-C22	-5.09	1.34	1.45
25	B	620	BCR	C23-C22	-4.97	1.35	1.45

The worst 5 of 2182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CHD-C4C-C3C	-6.86	114.58	124.92
23	B	609	CLA	CHD-C4C-C3C	-6.81	114.66	124.92
23	b	607	CLA	C1C-NC-C4C	-6.63	103.24	107.06
23	B	617	CLA	CHD-C4C-C3C	-6.56	115.03	124.92
23	B	611	CLA	CHD-C4C-C3C	-6.56	115.04	124.92

5 of 194 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	C	522	LMT	C1-O1'-C1'-O5'

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	C8-O7-C10-C11
34	Z	101	LMG	C8-O7-C10-O9
34	Z	101	LMG	C8-O7-C10-C11
26	D	413	SQD	C45-O47-C7-O49

There are no ring outliers.

86 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	10	0
23	A	405	CLA	7	0
24	A	406	PHO	2	0
23	A	407	CLA	5	0
25	A	408	BCR	2	0
26	A	409	SQD	2	0
26	A	411	SQD	3	0
29	A	413	PL9	5	0
31	A	415	LHG	4	0
23	B	602	CLA	6	0
23	B	603	CLA	6	0
23	B	604	CLA	8	0
23	B	605	CLA	12	0
23	B	606	CLA	14	0
23	B	607	CLA	5	0
23	B	608	CLA	7	0
23	B	609	CLA	5	0
23	B	610	CLA	6	0
23	B	611	CLA	5	0
23	B	612	CLA	8	0
23	B	613	CLA	12	0
23	B	614	CLA	6	0
23	B	615	CLA	15	0
23	B	616	CLA	7	0
23	B	617	CLA	5	0
25	B	618	BCR	6	0
25	B	619	BCR	4	0
25	B	620	BCR	2	0
26	B	621	SQD	2	0
34	B	622	LMG	2	0
35	B	623	LMT	3	0
36	B	624	HTG	3	0
36	B	625	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	626	HTG	1	0
27	B	627	GOL	1	0
27	B	628	GOL	3	0
36	B	629	HTG	1	0
35	B	632	LMT	1	0
35	B	633	LMT	3	0
35	B	634	LMT	2	0
34	C	501	LMG	3	0
23	C	502	CLA	11	0
23	C	503	CLA	6	0
23	C	504	CLA	6	0
23	C	505	CLA	5	0
23	C	506	CLA	9	0
23	C	507	CLA	17	0
23	C	508	CLA	12	0
23	C	509	CLA	9	0
23	C	510	CLA	8	0
23	C	511	CLA	9	0
23	C	512	CLA	13	0
23	C	513	CLA	7	0
23	C	514	CLA	3	0
25	C	515	BCR	2	0
25	C	516	BCR	4	0
37	C	517	DGD	6	0
37	C	518	DGD	3	0
37	C	519	DGD	1	0
34	C	520	LMG	3	0
34	C	521	LMG	1	0
35	C	522	LMT	1	0
36	C	523	HTG	1	0
36	C	524	HTG	1	0
25	C	527	BCR	1	0
23	D	401	CLA	5	0
24	D	402	PHO	5	0
23	D	404	CLA	4	0
23	D	405	CLA	1	0
25	D	406	BCR	2	0
29	D	407	PL9	2	0
31	D	408	LHG	7	0
31	D	409	LHG	4	0
36	D	412	HTG	1	0
26	D	413	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	E	101	LHG	2	0
35	E	102	LMT	1	0
38	E	103	HEM	6	0
25	H	101	BCR	5	0
34	J	101	LMG	4	0
26	L	102	SQD	4	0
35	M	101	LMT	1	0
35	M	103	LMT	3	0
25	T	101	BCR	6	0
25	Y	101	BCR	3	0
34	Z	101	LMG	3	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	0.06	10 (2%) 51 53	22, 33, 58, 97	0
1	a	334/344 (97%)	0.21	15 (4%) 34 36	24, 36, 65, 113	0
2	B	504/505 (99%)	0.32	59 (11%) 5 4	24, 38, 68, 118	0
2	b	504/505 (99%)	0.48	72 (14%) 3 2	25, 40, 77, 122	0
3	C	451/455 (99%)	0.65	71 (15%) 2 2	27, 48, 70, 108	0
3	c	455/455 (100%)	0.46	62 (13%) 3 3	32, 52, 72, 118	0
4	D	342/342 (100%)	0.09	18 (5%) 27 28	22, 35, 58, 113	0
4	d	341/342 (99%)	0.29	27 (7%) 13 13	24, 39, 59, 124	0
5	E	81/84 (96%)	0.35	6 (7%) 15 15	40, 59, 90, 125	0
5	e	79/84 (94%)	0.96	17 (21%) 1 1	45, 62, 100, 125	0
6	F	34/44 (77%)	-0.08	1 (2%) 52 55	41, 51, 81, 96	0
6	f	31/44 (70%)	-0.07	4 (12%) 4 3	48, 53, 84, 128	0
7	H	64/65 (98%)	0.37	7 (10%) 6 6	37, 51, 72, 104	0
7	h	65/65 (100%)	1.15	19 (29%) 1 0	40, 54, 79, 152	0
8	I	37/38 (97%)	0.44	7 (18%) 1 1	36, 48, 98, 129	0
8	i	37/38 (97%)	0.24	3 (8%) 13 12	38, 49, 107, 137	0
9	J	38/39 (97%)	0.29	6 (15%) 2 2	37, 55, 113, 156	0
9	j	39/39 (100%)	0.88	10 (25%) 1 0	46, 56, 109, 137	0
10	K	37/37 (100%)	0.14	3 (8%) 13 12	49, 58, 81, 98	0
10	k	37/37 (100%)	0.41	3 (8%) 13 12	52, 60, 82, 99	0
11	L	36/37 (97%)	0.52	5 (13%) 3 3	23, 30, 98, 143	0
11	l	36/37 (97%)	0.21	4 (11%) 6 5	24, 31, 97, 143	0
12	M	32/36 (88%)	-0.19	1 (3%) 49 52	24, 31, 53, 125	0
12	m	33/36 (91%)	-0.28	3 (9%) 10 10	24, 32, 66, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.36	31 (12%) 4 3	22, 50, 103, 163	0
13	o	243/244 (99%)	0.57	44 (18%) 1 1	26, 50, 108, 151	0
14	T	29/32 (90%)	0.30	1 (3%) 46 48	26, 31, 68, 97	0
14	t	29/32 (90%)	-0.02	0 100 100	26, 31, 69, 98	0
15	U	96/104 (92%)	0.57	14 (14%) 3 2	32, 44, 72, 86	0
15	u	97/104 (93%)	-0.08	4 (4%) 38 40	37, 47, 72, 105	0
16	V	137/137 (100%)	0.18	5 (3%) 43 45	30, 46, 75, 111	0
16	v	137/137 (100%)	0.47	20 (14%) 3 2	37, 54, 79, 112	0
17	X	38/40 (95%)	0.41	3 (7%) 13 13	49, 58, 80, 121	0
17	x	38/40 (95%)	1.09	9 (23%) 1 0	50, 60, 84, 123	0
18	Y	29/30 (96%)	1.73	13 (44%) 0 0	60, 76, 112, 120	0
18	y	29/30 (96%)	1.06	7 (24%) 1 0	63, 76, 107, 118	0
19	Z	62/62 (100%)	1.46	23 (37%) 0 0	57, 77, 127, 161	0
19	z	62/62 (100%)	1.60	18 (29%) 1 0	61, 79, 127, 161	0
20	R	34/34 (100%)	6.41	34 (100%) 0 0	92, 116, 145, 149	0
All	All	5284/5384 (98%)	0.44	659 (12%) 4 4	22, 45, 88, 163	0

The worst 5 of 659 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	11.0
20	R	20	VAL	10.2
2	b	495	PHE	9.4
20	R	35	LEU	9.0
20	R	14	LEU	8.3

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

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
8	FME	i	1	10/11	0.96	0.10	-	38,50,63,74	0
12	FME	M	1	10/11	0.97	0.16	-	33,41,72,72	0
12	FME	m	1	10/11	0.96	0.11	-	26,43,69,74	0
14	FME	T	1	10/11	0.98	0.09	-	19,37,45,52	0
8	FME	I	1	10/11	0.97	0.17	-	29,49,53,54	0
14	FME	t	1	10/11	0.97	0.10	-	22,34,47,66	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	GOL	d	401	6/6	0.76	0.68	29.98	36,51,76,77	0
30	UNL	i	101	40/-	0.74	0.38	26.06	56,91,147,151	0
36	HTG	b	622	19/19	0.76	0.83	16.83	77,105,127,134	0
30	UNL	j	102	10/-	0.73	0.31	12.64	57,81,94,94	0
30	UNL	K	101	34/-	0.73	0.32	10.65	62,102,116,137	0
36	HTG	B	625	19/19	0.72	0.44	10.00	43,101,109,111	0
35	LMT	M	103	35/35	0.68	0.34	9.83	37,128,152,157	0
36	HTG	V	203	11/19	0.86	0.60	9.71	88,101,107,108	0
27	GOL	B	627	6/6	0.95	0.36	9.70	60,77,93,95	0
35	LMT	D	403	35/35	0.61	0.39	8.48	40,112,125,126	0
36	HTG	C	524	9/19	0.56	1.22	8.27	70,90,106,139	0
35	LMT	B	633	35/35	0.58	0.44	8.16	39,117,133,139	0
35	LMT	E	102	35/35	0.72	0.56	7.32	91,129,157,163	0
35	LMT	e	102	35/35	0.65	0.80	6.25	75,139,161,171	0
30	UNL	I	101	40/-	0.70	0.32	5.73	39,89,141,148	0
27	GOL	a	412	6/6	0.88	0.25	5.61	56,70,85,86	0
30	UNL	D	410	17/-	0.87	0.37	5.55	46,64,94,102	0
29	PL9	A	413	55/55	0.78	0.35	5.24	44,83,100,110	0
36	HTG	c	522	19/19	0.70	0.82	5.07	83,139,149,158	0
30	UNL	D	411	40/-	0.84	0.28	4.94	49,76,125,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	HTG	D	412	16/19	0.47	0.41	4.58	43,118,136,138	0
30	UNL	X	101	18/-	0.89	0.20	4.55	39,66,83,87	0
35	LMT	a	418	35/35	0.85	0.54	3.91	97,118,139,139	0
36	HTG	b	621	19/19	0.78	0.26	3.74	33,91,127,144	0
30	UNL	b	629	36/-	0.81	0.33	3.59	46,85,130,141	0
34	LMG	C	521	51/55	0.52	0.51	3.39	50,107,149,153	0
30	UNL	x	101	18/-	0.84	0.31	3.27	47,66,104,105	0
31	LHG	e	101	42/49	0.73	0.43	3.03	63,119,140,150	0
35	LMT	B	634	26/35	0.88	0.18	3.01	48,90,109,115	0
35	LMT	b	628	25/35	0.78	0.28	2.84	37,63,135,142	0
30	UNL	d	409	17/-	0.94	0.38	2.76	48,58,94,99	0
35	LMT	C	522	35/35	0.60	0.64	2.74	83,119,141,151	0
27	GOL	B	628	6/6	0.86	0.26	2.67	47,58,65,72	0
29	PL9	a	415	55/55	0.75	0.34	2.61	56,82,108,115	0
34	LMG	c	520	51/55	0.64	0.43	2.59	62,104,135,147	0
35	LMT	m	103	35/35	0.64	0.49	2.40	40,85,113,117	0
35	LMT	B	632	25/35	0.82	0.27	2.20	41,68,135,136	0
36	HTG	B	624	19/19	0.88	0.21	2.08	33,71,128,130	0
31	LHG	D	408	49/49	0.96	0.26	1.96	25,37,56,78	0
31	LHG	d	407	49/49	0.91	0.25	1.92	24,38,58,65	0
31	LHG	A	415	49/49	0.90	0.34	1.90	29,46,67,82	0
34	LMG	Z	101	37/55	0.72	0.40	1.73	57,103,134,149	0
29	PL9	d	405	55/55	0.95	0.21	1.71	24,33,49,66	0
23	CLA	b	601	65/65	0.92	0.27	1.71	46,70,107,135	0
26	SQD	A	411	54/54	0.85	0.25	1.68	41,71,114,129	0
31	LHG	E	101	42/49	0.80	0.27	1.66	47,95,114,121	0
26	SQD	L	102	54/54	0.79	0.26	1.64	39,73,114,123	0
23	CLA	c	503	65/65	0.93	0.44	1.63	44,55,67,84	0
27	GOL	A	410	6/6	0.96	0.13	1.60	45,57,60,90	0
29	PL9	D	407	55/55	0.95	0.24	1.56	20,30,44,53	0
31	LHG	L	101	49/49	0.93	0.25	1.53	26,39,54,75	0
27	GOL	C	525	6/6	0.93	0.26	1.50	45,56,66,73	0
22	CL	a	403	1/1	0.98	0.27	1.50	41,41,41,41	0
34	LMG	z	101	39/55	0.85	0.24	1.49	69,117,144,151	0
23	CLA	B	602	65/65	0.94	0.21	1.48	39,61,93,123	0
35	LMT	M	101	35/35	0.68	0.34	1.47	40,85,105,107	0
25	BCR	T	101	40/40	0.97	0.24	1.42	21,37,55,60	0
31	LHG	d	406	49/49	0.94	0.23	1.37	27,48,81,84	0
23	CLA	c	502	65/65	0.91	0.43	1.37	40,55,70,74	0
25	BCR	t	101	40/40	0.96	0.24	1.34	23,43,64,68	0
34	LMG	J	101	51/55	0.91	0.20	1.31	33,54,96,105	0
26	SQD	a	413	54/54	0.89	0.22	1.31	37,73,134,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	SQD	f	101	43/54	0.79	0.32	1.26	86,117,154,157	0
34	LMG	c	519	51/55	0.87	0.28	1.22	47,78,122,143	0
23	CLA	b	605	65/65	0.95	0.26	1.13	26,34,51,76	0
31	LHG	D	409	49/49	0.94	0.21	1.13	32,50,107,117	0
31	LHG	d	408	49/49	0.94	0.21	1.12	40,55,105,111	0
36	HTG	B	629	19/19	0.90	0.19	1.10	47,59,78,83	0
23	CLA	C	511	65/65	0.95	0.48	1.09	36,48,61,67	0
37	DGD	c	516	62/66	0.94	0.24	1.06	35,47,74,93	0
31	LHG	b	630	49/49	0.91	0.17	1.04	26,43,59,64	0
23	CLA	B	611	65/65	0.96	0.23	1.02	29,41,55,70	0
26	SQD	B	621	54/54	0.81	0.24	0.98	44,82,109,118	0
24	PHO	a	408	64/64	0.96	0.28	0.97	30,40,53,60	0
24	PHO	a	407	64/64	0.98	0.20	0.96	24,31,45,50	0
34	LMG	C	501	51/55	0.83	0.29	0.96	40,81,110,113	0
25	BCR	B	618	40/40	0.96	0.18	0.90	24,37,48,49	0
37	DGD	H	102	62/66	0.90	0.29	0.90	29,42,64,68	0
37	DGD	h	103	62/66	0.88	0.29	0.89	34,46,67,76	0
24	PHO	A	406	64/64	0.97	0.20	0.87	22,29,39,46	0
23	CLA	a	409	65/65	0.96	0.18	0.87	30,44,124,130	0
37	DGD	C	518	62/66	0.88	0.23	0.86	35,51,111,119	0
23	CLA	B	606	65/65	0.95	0.21	0.84	24,33,46,51	0
23	CLA	c	501	65/65	0.94	0.23	0.82	43,53,67,72	0
25	BCR	C	516	40/40	0.92	0.22	0.81	38,50,63,68	0
23	CLA	A	407	65/65	0.97	0.15	0.80	28,38,98,117	0
37	DGD	c	518	62/66	0.95	0.20	0.80	39,50,74,97	0
23	CLA	B	604	65/65	0.96	0.27	0.78	30,43,56,67	0
37	DGD	C	517	62/66	0.92	0.26	0.77	30,41,77,88	0
35	LMT	B	623	35/35	0.84	0.26	0.77	50,95,120,122	0
36	HTG	h	101	16/19	0.79	0.38	0.77	71,110,125,143	0
24	PHO	D	402	64/64	0.97	0.24	0.75	25,31,44,55	0
37	DGD	C	519	62/66	0.93	0.17	0.72	30,44,80,109	0
39	MG	J	103	1/1	0.97	0.17	0.70	43,43,43,43	0
25	BCR	d	404	40/40	0.94	0.15	0.69	43,55,79,81	0
23	CLA	C	506	65/65	0.95	0.28	0.68	33,44,75,82	0
23	CLA	C	509	65/65	0.94	0.32	0.67	33,46,93,103	0
25	BCR	D	406	40/40	0.92	0.19	0.65	35,46,78,84	0
37	DGD	c	517	62/66	0.93	0.23	0.64	42,55,110,126	0
23	CLA	b	603	65/65	0.95	0.27	0.64	32,44,61,70	0
25	BCR	B	620	40/40	0.92	0.16	0.63	30,43,67,78	0
23	CLA	b	604	65/65	0.95	0.33	0.62	24,33,95,101	0
34	LMG	j	101	51/55	0.93	0.17	0.62	41,56,92,119	0
23	CLA	C	503	65/65	0.93	0.36	0.60	33,43,60,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	610	65/65	0.95	0.22	0.60	35,44,56,61	0
25	BCR	h	102	40/40	0.71	0.29	0.59	42,57,71,74	0
23	CLA	b	608	65/65	0.95	0.29	0.59	34,44,67,72	0
23	CLA	C	510	65/65	0.94	0.32	0.59	39,53,71,79	0
26	SQD	a	411	54/54	0.94	0.19	0.56	44,69,108,113	0
23	CLA	c	508	65/65	0.93	0.20	0.55	39,53,121,131	0
23	CLA	b	612	65/65	0.93	0.28	0.55	28,35,48,69	0
23	CLA	c	509	65/65	0.92	0.25	0.53	46,56,73,79	0
23	CLA	D	405	65/65	0.93	0.18	0.52	33,48,111,119	0
25	BCR	b	618	40/40	0.96	0.22	0.51	22,36,51,56	0
23	CLA	c	510	65/65	0.95	0.34	0.51	39,51,67,71	0
22	CL	A	403	1/1	0.99	0.25	0.50	27,27,27,27	0
34	LMG	a	417	51/55	0.87	0.22	0.50	42,79,99,115	0
23	CLA	B	613	65/65	0.94	0.25	0.49	26,33,45,65	0
23	CLA	B	608	65/65	0.96	0.23	0.49	20,28,59,67	0
27	GOL	b	624	6/6	0.92	0.15	0.48	75,92,97,104	0
25	BCR	B	619	40/40	0.96	0.23	0.47	21,36,52,60	0
25	BCR	A	408	40/40	0.97	0.17	0.47	23,34,48,56	0
23	CLA	B	612	65/65	0.92	0.26	0.46	24,32,49,54	0
34	LMG	B	622	51/55	0.87	0.23	0.45	35,53,83,101	0
23	CLA	B	605	65/65	0.94	0.31	0.44	22,31,101,111	0
23	CLA	C	514	65/65	0.89	0.26	0.43	50,65,100,107	0
25	BCR	H	101	40/40	0.82	0.23	0.43	35,46,66,73	0
23	CLA	B	614	65/65	0.97	0.32	0.37	23,31,72,87	0
23	CLA	c	511	65/65	0.92	0.19	0.35	47,56,78,89	0
34	LMG	m	101	51/55	0.90	0.20	0.35	33,52,85,99	0
23	CLA	c	504	65/65	0.95	0.30	0.34	41,52,94,117	0
23	CLA	b	602	65/65	0.89	0.25	0.34	36,48,68,77	0
34	LMG	C	520	51/55	0.83	0.28	0.32	43,75,125,134	0
26	SQD	D	413	43/54	0.90	0.30	0.31	58,106,117,124	0
23	CLA	D	401	65/65	0.97	0.16	0.29	21,28,43,47	0
25	BCR	Y	101	40/40	0.94	0.15	0.29	40,51,62,71	0
38	HEM	e	103	43/43	0.97	0.21	0.29	52,78,106,116	0
23	CLA	B	603	65/65	0.90	0.23	0.28	31,41,57,69	0
23	CLA	d	403	65/65	0.92	0.17	0.27	41,52,102,116	0
23	CLA	c	512	65/65	0.89	0.22	0.26	53,66,96,104	0
23	CLA	b	607	65/65	0.96	0.18	0.25	21,30,58,67	0
25	BCR	y	101	40/40	0.89	0.18	0.24	48,60,74,77	0
23	CLA	c	505	65/65	0.93	0.20	0.23	36,46,76,82	0
23	CLA	B	609	65/65	0.97	0.24	0.23	30,42,56,66	0
23	CLA	b	611	65/65	0.96	0.21	0.21	27,35,57,62	0
23	CLA	C	513	65/65	0.88	0.23	0.20	46,60,106,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	502	65/65	0.92	0.23	0.18	36,45,67,70	0
23	CLA	C	508	65/65	0.91	0.24	0.16	40,51,66,78	0
35	LMT	b	620	25/35	0.79	0.24	0.16	55,88,143,147	0
25	BCR	b	617	40/40	0.95	0.16	0.15	21,35,45,51	0
23	CLA	C	504	65/65	0.91	0.29	0.15	37,47,66,75	0
26	SQD	A	409	54/54	0.94	0.16	0.12	41,66,99,109	0
23	CLA	c	513	65/65	0.90	0.22	0.10	58,74,112,119	0
23	CLA	b	613	65/65	0.96	0.26	0.08	24,36,79,89	0
23	CLA	d	402	65/65	0.96	0.22	0.08	27,32,58,72	0
23	CLA	a	406	65/65	0.97	0.21	0.07	30,38,98,103	0
23	CLA	B	610	65/65	0.91	0.17	0.05	31,42,53,89	0
25	BCR	a	410	40/40	0.96	0.15	0.05	28,38,55,58	0
23	CLA	D	404	65/65	0.94	0.18	0.02	21,29,50,56	0
23	CLA	b	609	65/65	0.90	0.17	-0.00	39,48,63,74	0
25	BCR	b	619	40/40	0.94	0.15	-0.02	33,46,69,80	0
23	CLA	a	404	65/65	0.96	0.19	-0.03	27,33,52,66	0
23	CLA	C	505	65/65	0.93	0.23	-0.04	32,46,91,111	0
25	BCR	c	515	40/40	0.96	0.14	-0.04	41,54,66,70	0
23	CLA	B	617	65/65	0.94	0.21	-0.04	33,45,121,132	0
23	CLA	a	405	65/65	0.96	0.15	-0.05	23,29,52,60	0
25	BCR	C	527	40/40	0.93	0.17	-0.09	43,55,71,72	0
23	CLA	C	512	65/65	0.90	0.18	-0.11	39,54,77,85	0
23	CLA	b	614	65/65	0.95	0.15	-0.12	25,35,93,107	0
38	HEM	v	201	43/43	0.98	0.14	-0.13	44,53,63,82	0
23	CLA	c	507	65/65	0.90	0.19	-0.14	43,57,70,72	0
23	CLA	c	506	65/65	0.96	0.15	-0.15	47,65,98,117	0
23	CLA	A	405	65/65	0.96	0.15	-0.16	24,33,85,94	0
25	BCR	k	101	40/40	0.93	0.18	-0.16	50,60,84,87	0
23	CLA	B	615	65/65	0.93	0.18	-0.17	23,32,86,95	0
23	CLA	b	606	65/65	0.94	0.15	-0.18	29,42,91,110	0
23	CLA	B	607	65/65	0.94	0.14	-0.18	28,37,76,93	0
33	CA	c	523	1/1	0.96	0.18	-0.21	68,68,68,68	0
23	CLA	A	404	65/65	0.96	0.17	-0.24	22,25,39,58	0
23	CLA	b	615	65/65	0.91	0.18	-0.32	33,43,65,87	0
33	CA	C	526	1/1	0.98	0.26	-0.33	59,59,59,59	0
39	MG	j	103	1/1	0.96	0.14	-0.38	48,48,48,48	0
23	CLA	C	507	65/65	0.93	0.16	-0.46	42,57,106,115	0
25	BCR	C	515	40/40	0.94	0.17	-0.47	49,60,74,82	0
22	CL	a	402	1/1	1.00	0.13	-0.52	28,28,28,28	0
23	CLA	B	616	65/65	0.93	0.15	-0.53	29,38,60,67	0
38	HEM	V	202	43/43	0.98	0.12	-0.57	33,36,48,70	0
36	HTG	b	625	19/19	0.93	0.11	-0.59	40,60,90,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	616	65/65	0.90	0.20	-0.63	34,51,101,111	0
38	HEM	E	103	43/43	0.98	0.09	-0.75	43,56,69,83	0
25	BCR	c	514	40/40	0.94	0.14	-0.76	58,68,80,83	0
22	CL	A	402	1/1	0.99	0.11	-1.19	24,24,24,24	0
32	BCT	a	419	4/4	0.98	0.07	-1.36	41,45,48,58	0
32	BCT	A	416	4/4	0.98	0.08	-1.58	32,45,46,51	0
28	OEX	A	412	10/10	0.99	0.10	-1.66	23,32,46,47	0
28	OEX	a	414	10/10	0.99	0.09	-2.18	29,36,46,48	0
33	CA	O	301	1/1	0.86	0.13	-2.38	101,101,101,101	0
33	CA	c	524	1/1	0.98	0.08	-2.71	66,66,66,66	0
33	CA	o	301	1/1	0.93	0.12	-3.86	89,89,89,89	0
21	FE2	a	401	1/1	0.99	0.04	-3.93	47,47,47,47	0
21	FE2	A	401	1/1	0.99	0.05	-4.16	46,46,46,46	0
33	CA	V	201	1/1	0.93	0.11	-	94,94,94,94	0
36	HTG	C	523	19/19	0.80	0.43	-	95,107,121,133	0
36	HTG	c	521	19/19	0.81	0.37	-	71,125,137,163	0
36	HTG	B	630	19/19	0.82	0.27	-	67,116,145,154	0
30	UNL	B	631	33/-	0.68	0.26	-	36,92,134,151	0
30	UNL	m	102	10/-	0.75	0.32	-	36,47,64,66	0
30	UNL	c	525	32/-	0.72	0.33	-	74,104,124,132	0
30	UNL	M	102	10/-	0.85	0.28	-	38,51,60,60	0
30	UNL	a	416	30/-	0.55	0.50	-	86,102,121,129	0
30	UNL	A	414	28/-	0.27	0.57	-	66,93,121,126	0
30	UNL	J	102	10/-	0.66	0.45	-	59,66,85,90	0
36	HTG	B	626	19/19	0.48	0.70	-	51,135,163,189	0
33	CA	B	601	1/1	0.77	0.12	-	144,144,144,144	0
36	HTG	b	623	19/19	0.58	0.63	-	73,116,140,180	0
30	UNL	b	627	33/-	0.59	0.45	-	53,80,145,147	0
27	GOL	O	302	6/6	0.83	0.27	-	63,68,72,78	0
36	HTG	b	626	19/19	0.82	0.25	-	66,114,151,181	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.