



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2017 – 04:47 PM EST

PDB ID : 5GTH
Title : Native XFEL structure of photosystem II (dark 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

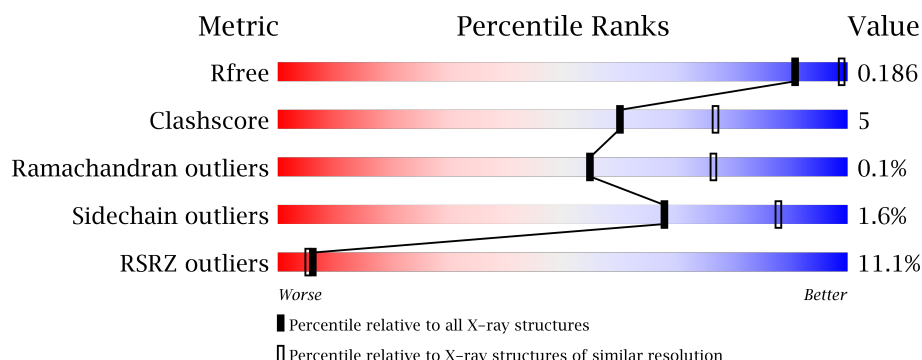
1 Overall quality at a glance

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 ≥ 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>85%</div> <div>12%</div> <div>.</div> </div>
1	a	344	<div> <div>3%</div> <div>97%</div> <div>.</div> <div>..</div> </div>
2	B	505	<div> <div>10%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	b	505	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>14%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	406	X	-	-	-
23	CLA	A	408	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	502	X	-	-	-
23	CLA	C	503	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	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	-	-	-
23	CLA	c	510	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
27	GOL	A	411	-	-	-	X
27	GOL	B	625	-	-	-	X
27	GOL	B	626	-	-	-	X
27	GOL	a	411	-	-	-	X
27	GOL	d	402	-	-	-	X
29	PL9	A	414	-	-	-	X
29	PL9	a	414	-	-	-	X
30	UNL	D	410	-	-	-	X
30	UNL	D	411	-	-	-	X
30	UNL	I	102	-	-	-	X
30	UNL	J	102	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	X	101	-	-	-	X
30	UNL	b	629	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	102	-	-	-	X
30	UNL	x	101	-	-	-	X
31	LHG	E	101	-	-	-	X
31	LHG	e	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	z	101	-	-	-	X
34	HTG	B	622	-	-	-	X
34	HTG	B	623	-	-	-	X
34	HTG	C	522	-	-	-	X
34	HTG	D	412	-	-	-	X
34	HTG	V	203	-	-	-	X
34	HTG	b	622	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	b	628	-	-	-	X
34	HTG	c	522	-	-	-	X
35	LMT	B	630	-	-	-	X
35	LMT	B	631	-	-	-	X
35	LMT	D	402	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	I	101	-	-	-	X
35	LMT	M	103	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	LMT	a	417	-	-	-	X
35	LMT	b	627	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	102	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 52773 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 protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	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	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	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	1	0
			665	434	107	124			
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	1	0
			514	344	84	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 reaction center protein K.

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

Continued on next page...

Continued from previous page...

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	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

- 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		

Continued on next page...

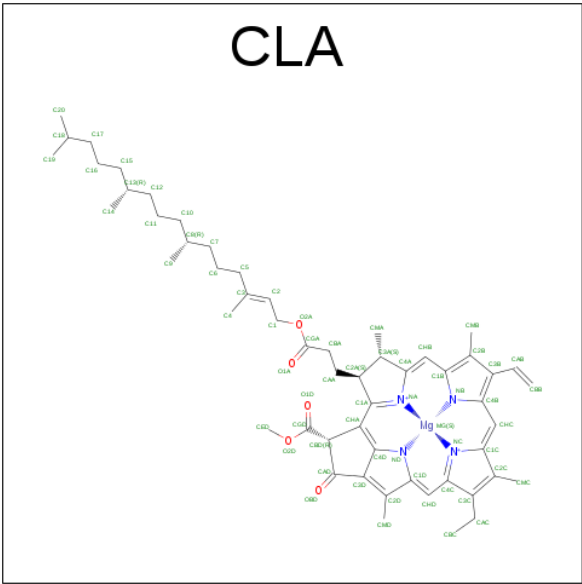
Continued from previous page...

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: C₅₅H₇₂MgN₄O₅).



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	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	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	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
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

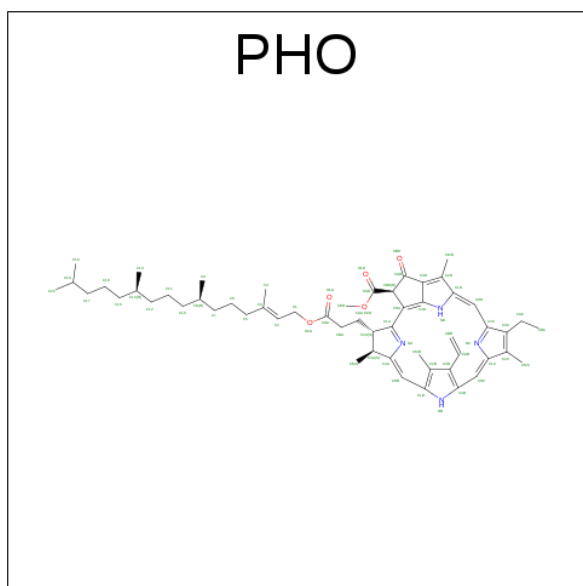
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

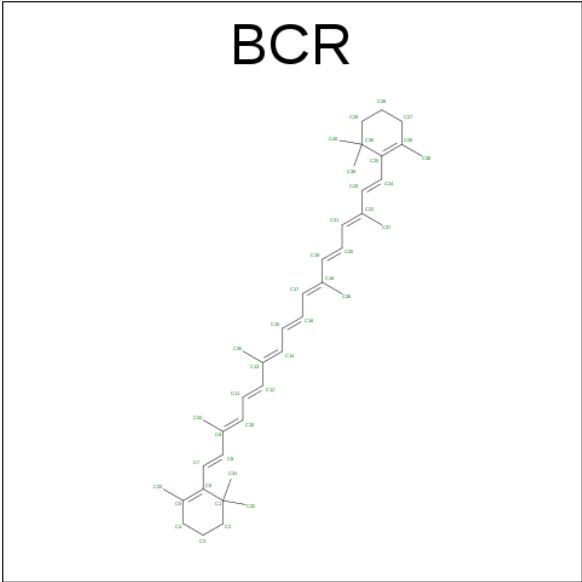
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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: $C_{40}H_{56}$).



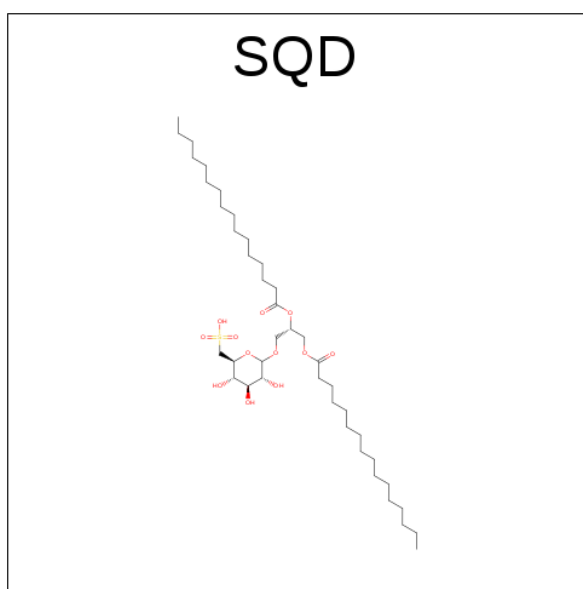
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

Continued on next page...

Continued from previous page...

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: $C_{41}H_{78}O_{12}S$).



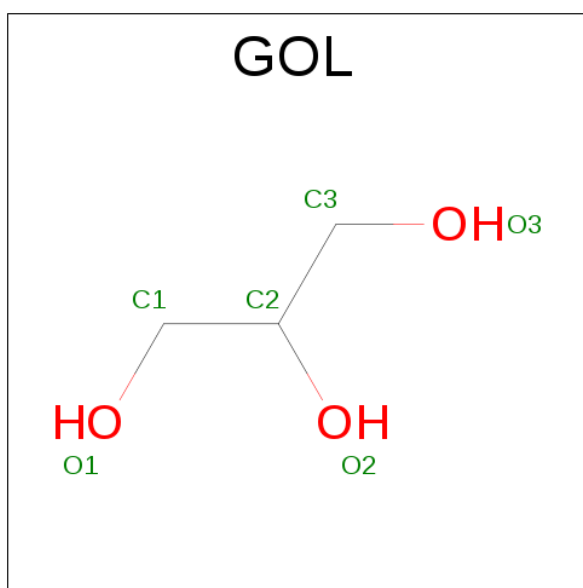
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

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: $C_3H_8O_3$).



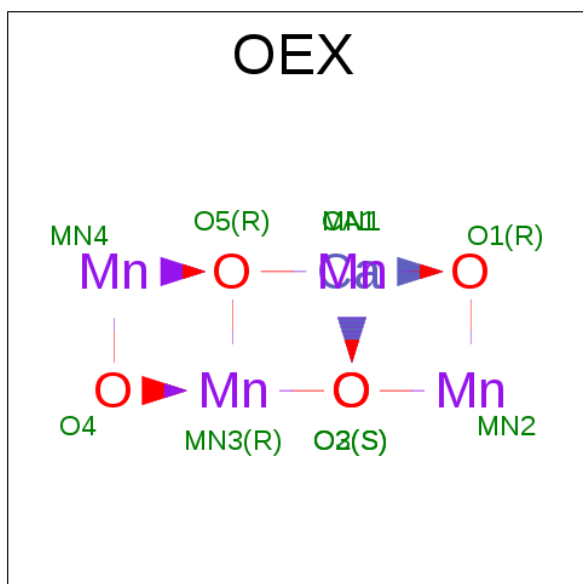
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

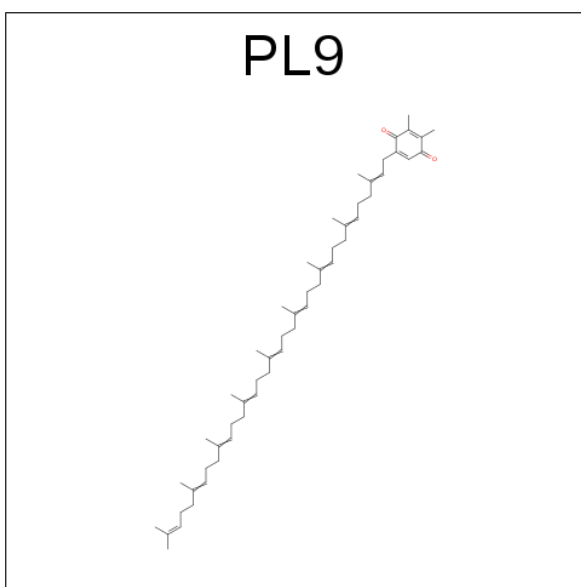
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_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:).

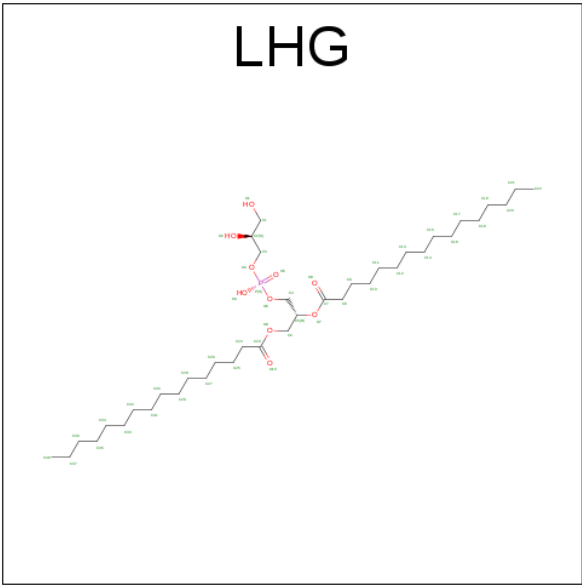
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
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

Continued on next page...

Continued from previous page...

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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



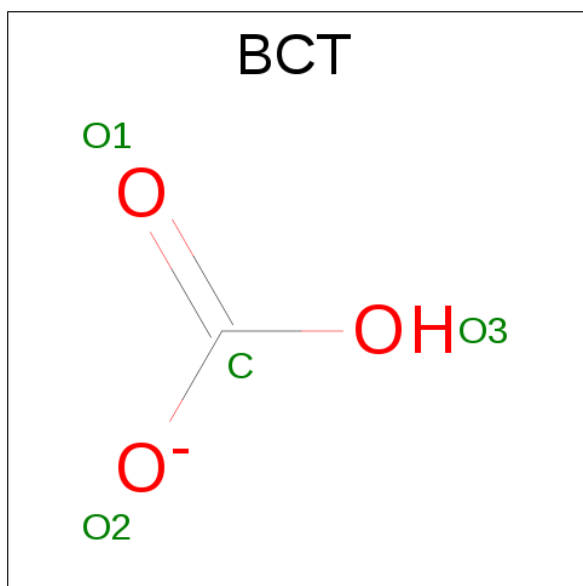
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O P 49 38 10 1	0	0
31	A	1	Total C O P 49 38 10 1	0	0
31	D	1	Total C O P 49 38 10 1	0	0

Continued on next page...

Continued from previous page...

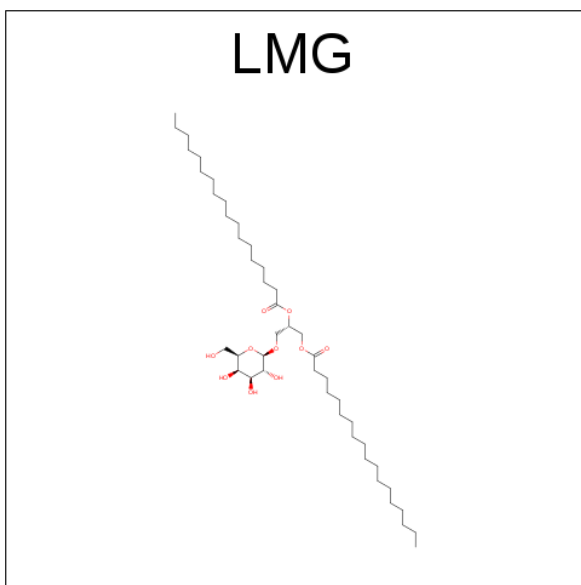
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



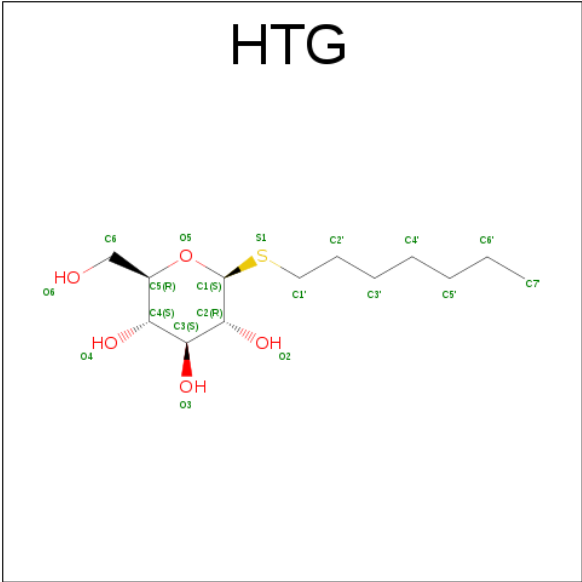
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



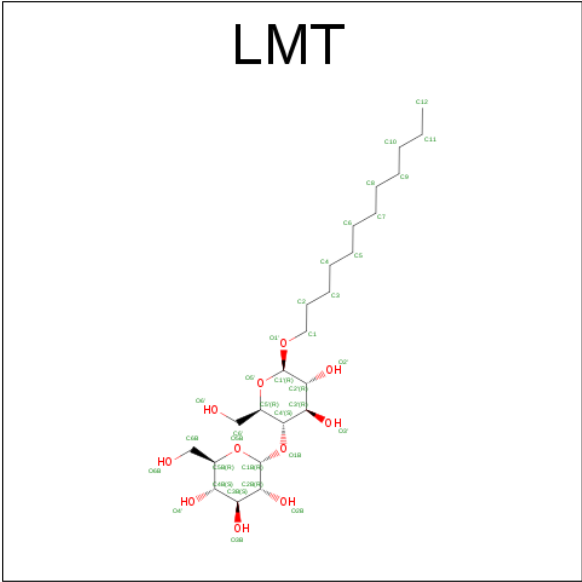
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



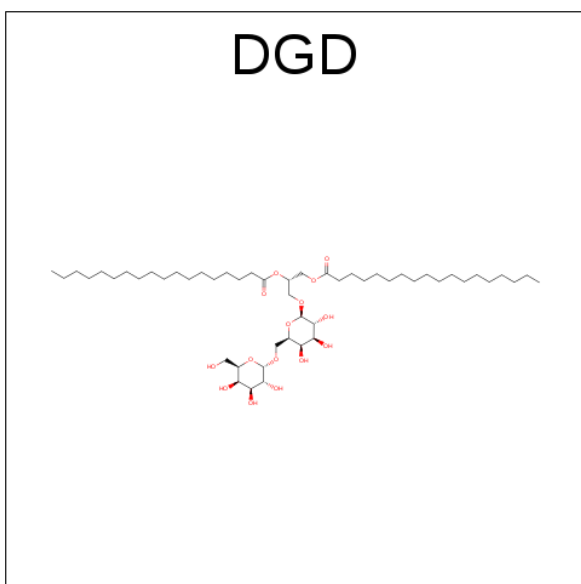
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O		0	0
			25	19	6			
35	B	1	Total	C	O		0	0
			35	24	11			
35	B	1	Total	C	O		0	0
			26	19	7			
35	D	1	Total	C	O		0	0
			35	24	11			
35	D	1	Total	C	O		0	0
			35	24	11			
35	E	1	Total	C	O		0	0
			35	24	11			
35	I	1	Total	C	O		0	0
			35	24	11			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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

Continued on next page...

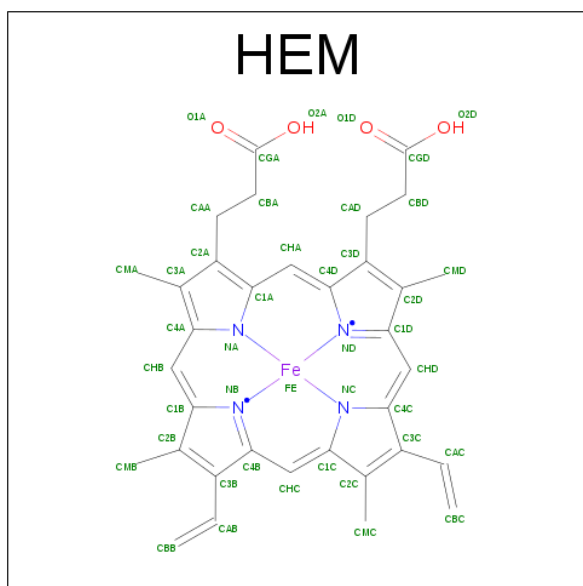
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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	C	Fe	N	O	0
			43	34	1	4	4	0
38	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
38	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	127	Total	O	0	0
			127	127		
40	B	175	Total	O	0	0
			175	175		
40	C	148	Total	O	0	0
			148	148		
40	D	111	Total	O	0	0
			111	111		
40	E	18	Total	O	0	0
			18	18		
40	F	5	Total	O	0	0
			5	5		
40	H	19	Total	O	0	0
			19	19		
40	I	6	Total	O	0	0
			6	6		
40	J	5	Total	O	0	0
			5	5		
40	K	6	Total	O	0	0
			6	6		
40	L	9	Total	O	0	0
			9	9		
40	M	14	Total	O	0	0
			14	14		
40	O	100	Total	O	0	0
			100	100		
40	T	10	Total	O	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	46	Total 46	O 46	0	0
40	V	78	Total 79	O 79	0	1
40	X	3	Total 3	O 3	0	0
40	Y	1	Total 1	O 1	0	0
40	a	130	Total 130	O 130	0	0
40	b	192	Total 192	O 192	0	0
40	c	136	Total 136	O 136	0	0
40	d	108	Total 108	O 108	0	0
40	e	15	Total 15	O 15	0	0
40	f	5	Total 5	O 5	0	0
40	h	28	Total 28	O 28	0	0
40	i	4	Total 4	O 4	0	0
40	j	3	Total 3	O 3	0	0
40	k	4	Total 4	O 4	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	109	Total 109	O 109	0	0
40	t	7	Total 7	O 7	0	0
40	u	64	Total 64	O 64	0	0
40	v	71	Total 71	O 71	0	0
40	x	4	Total 4	O 4	0	0

Continued on next page...

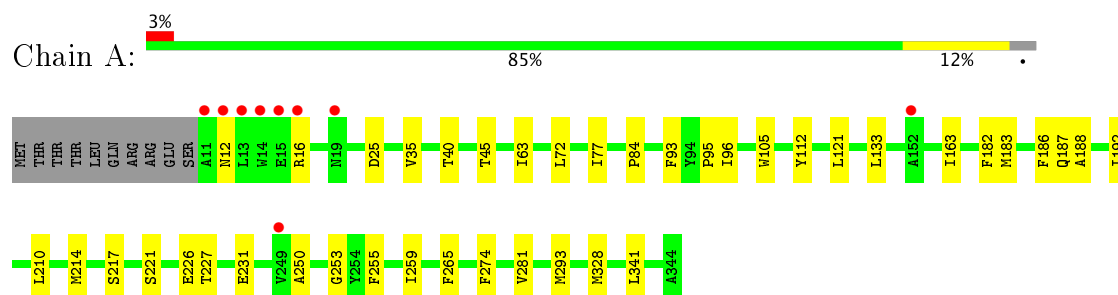
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	y	2	Total	O	0	0
			2	2		

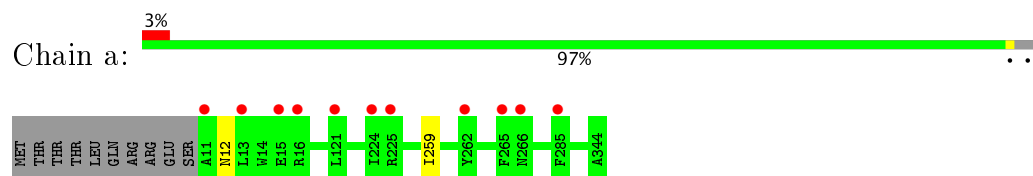
3 Residue-property plots [i](#)

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.

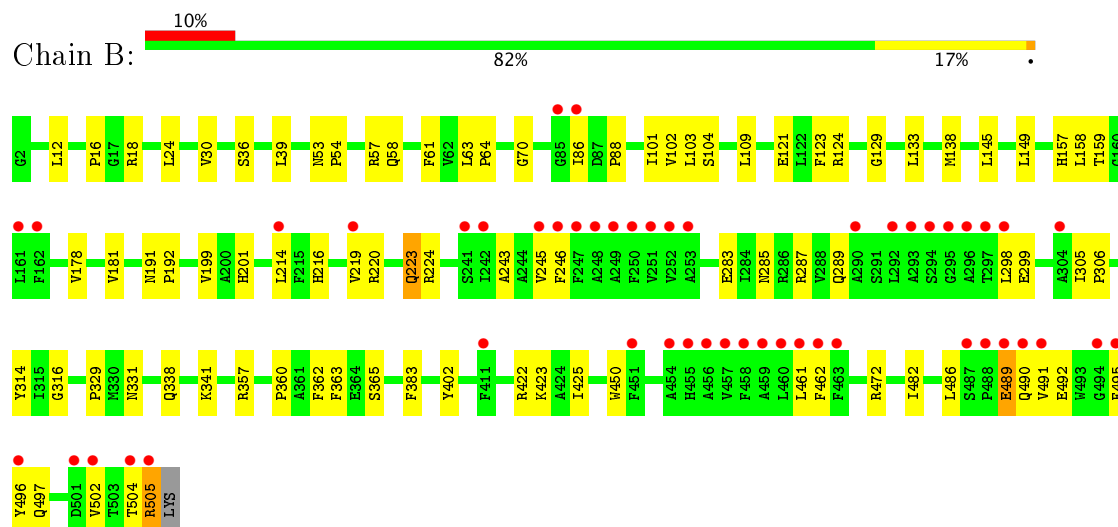
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

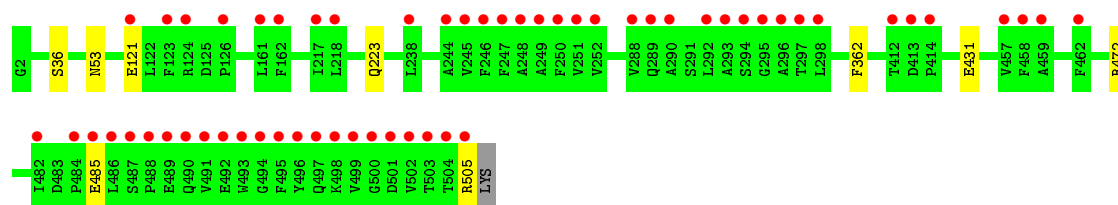


- Molecule 2: Photosystem II CP47 reaction center protein

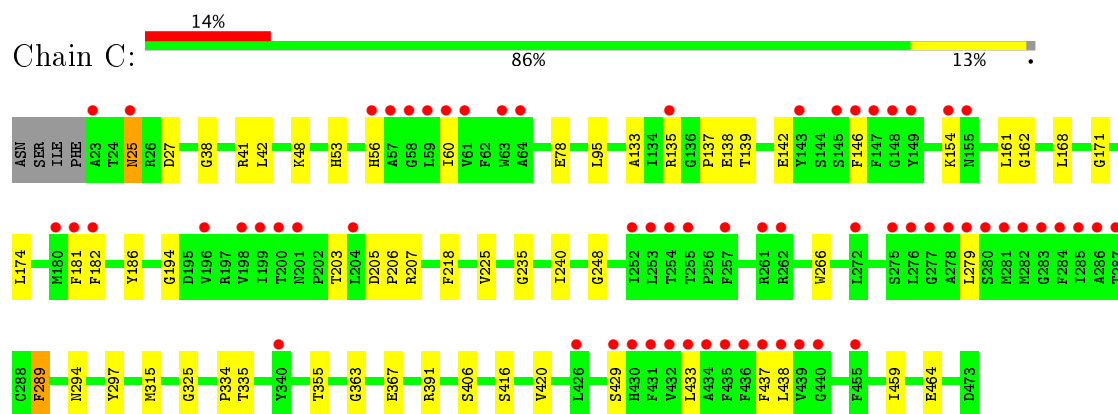


- Molecule 2: Photosystem II CP47 reaction center protein

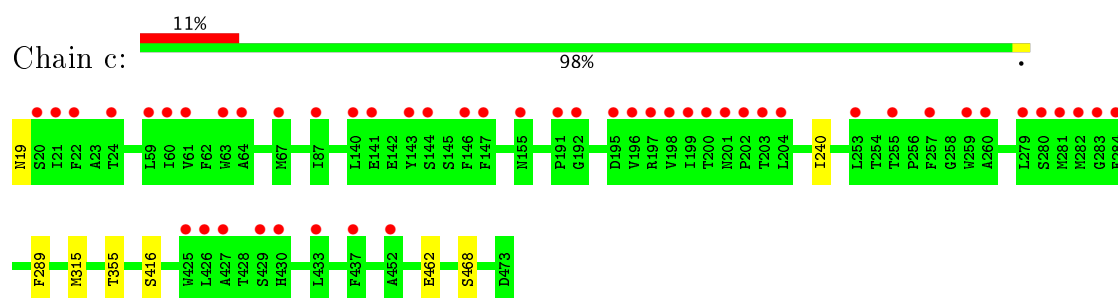




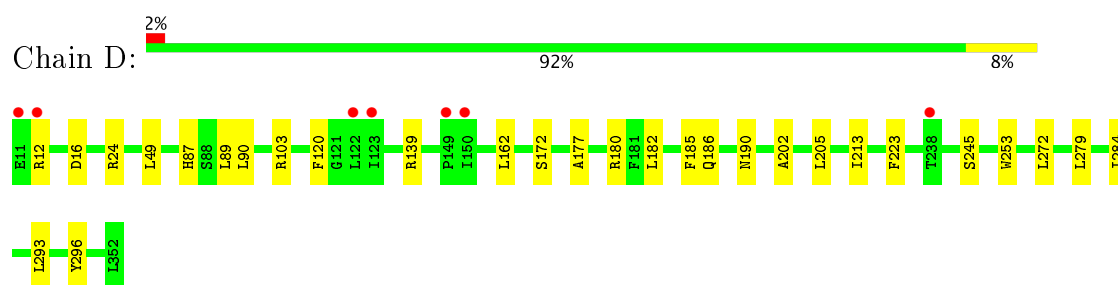
• Molecule 3: Photosystem II CP43 reaction center protein



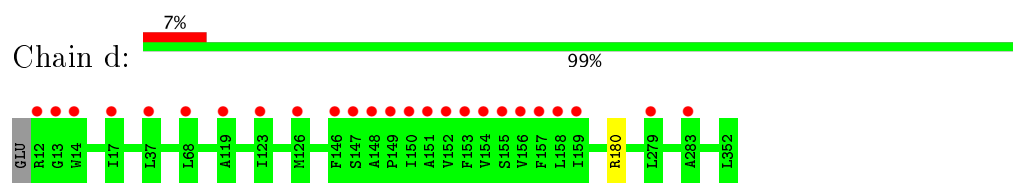
• Molecule 3: Photosystem II CP43 reaction center protein



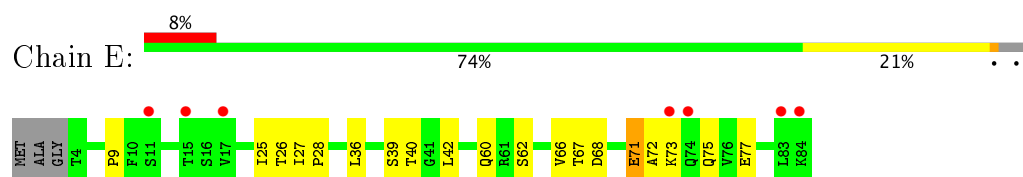
• Molecule 4: Photosystem II D2 protein



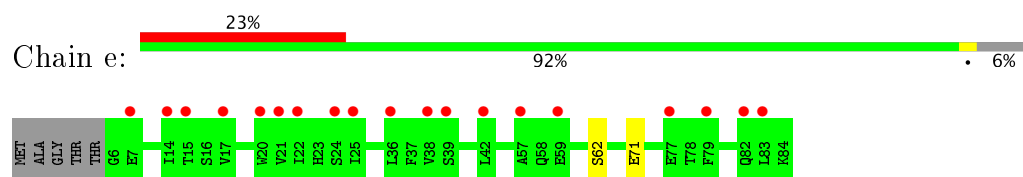
• Molecule 4: Photosystem II D2 protein



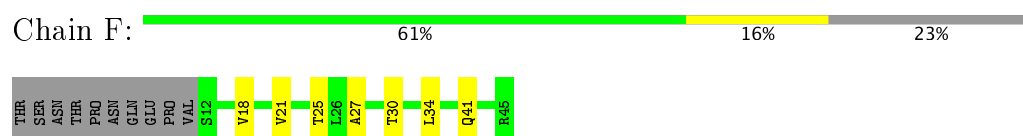
• Molecule 5: Cytochrome b559 subunit alpha



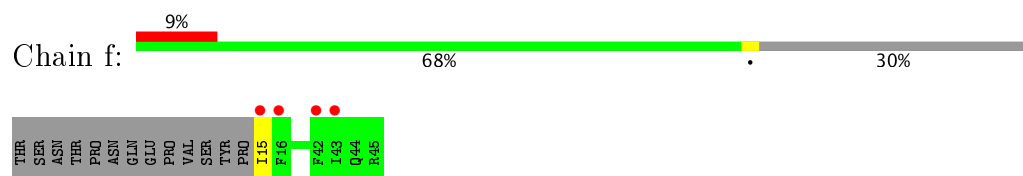
- Molecule 5: Cytochrome b559 subunit alpha



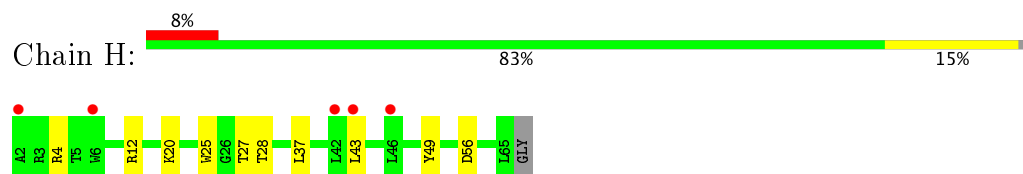
- Molecule 6: Cytochrome b559 subunit beta



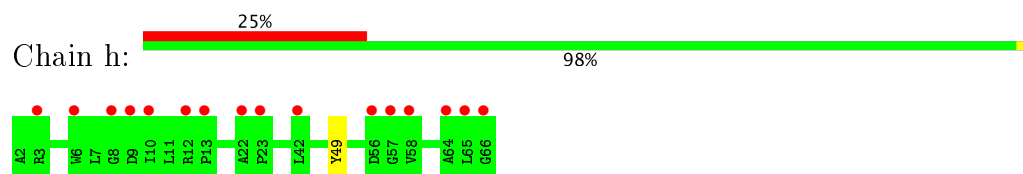
- Molecule 6: Cytochrome b559 subunit beta



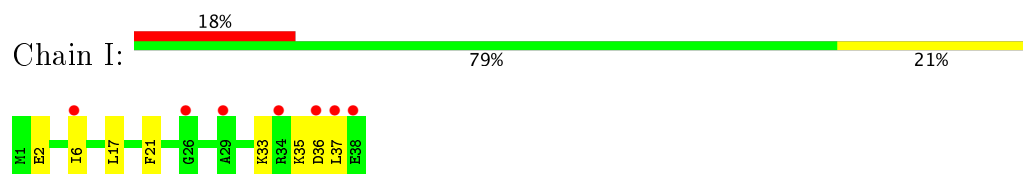
- Molecule 7: Photosystem II reaction center protein H



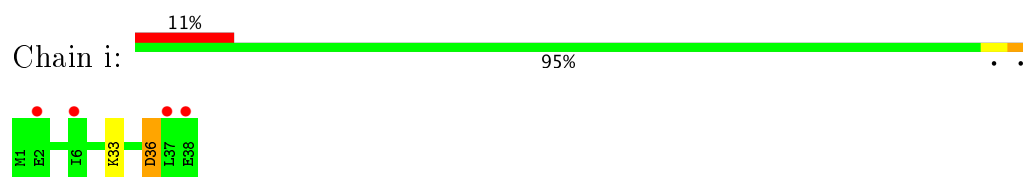
- Molecule 7: Photosystem II reaction center protein H



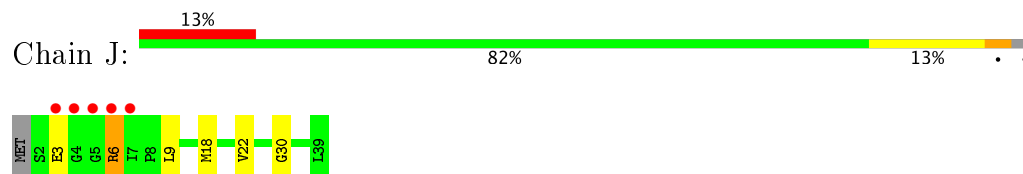
- Molecule 8: Photosystem II reaction center protein I



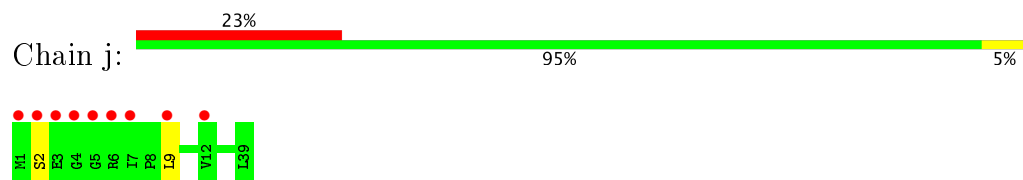
- Molecule 8: Photosystem II reaction center protein I



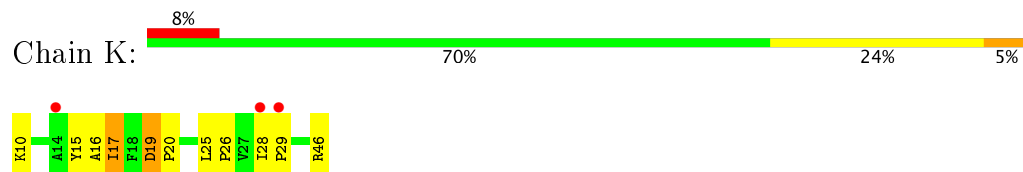
- Molecule 9: Photosystem II reaction center protein J



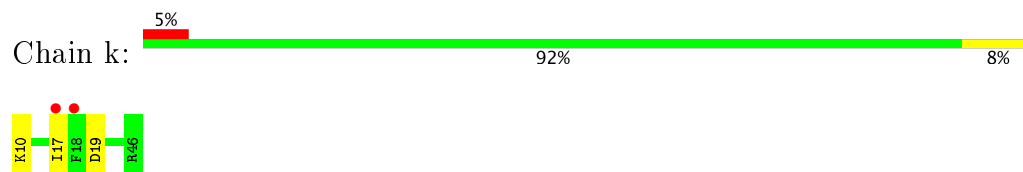
- Molecule 9: Photosystem II reaction center protein J



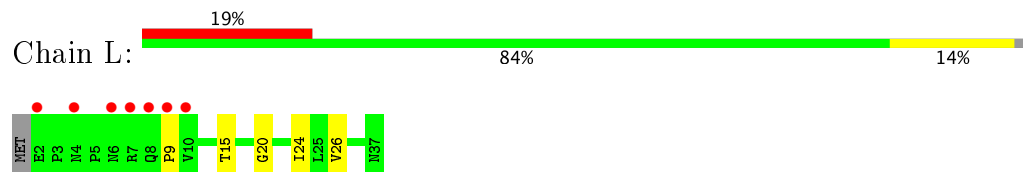
- Molecule 10: Photosystem II reaction center protein K



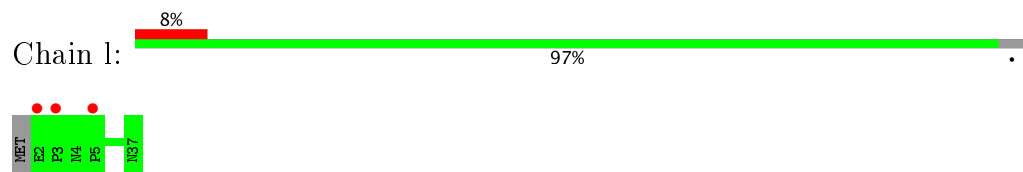
- Molecule 10: Photosystem II reaction center protein K



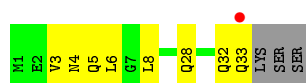
- Molecule 11: Photosystem II reaction center protein L



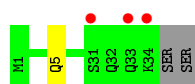
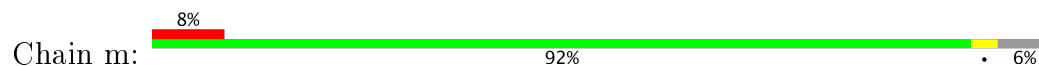
- Molecule 11: Photosystem II reaction center protein L



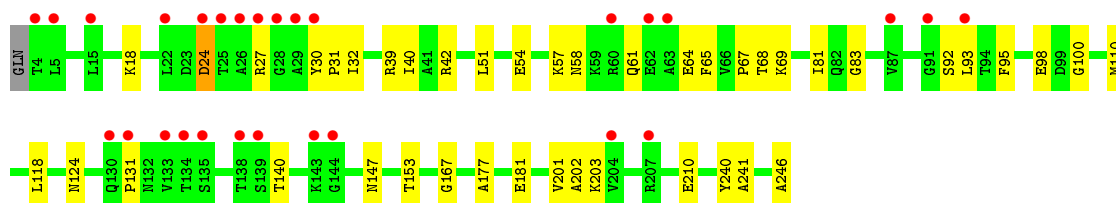
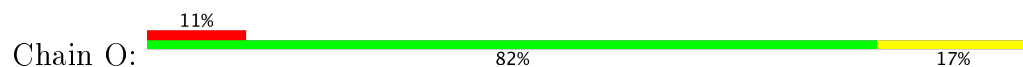
- Molecule 12: Photosystem II reaction center protein M



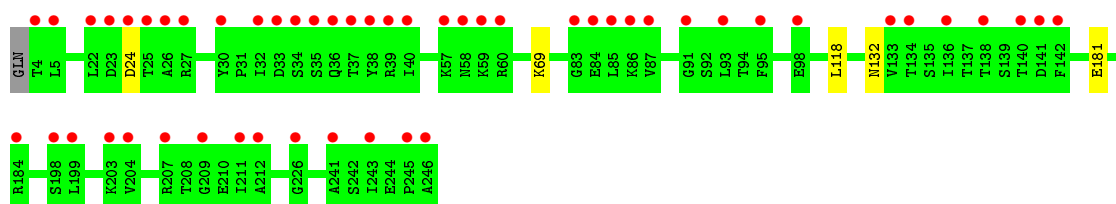
- Molecule 12: Photosystem II reaction center protein M



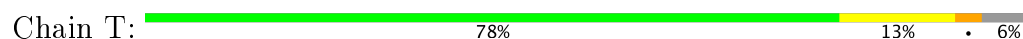
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



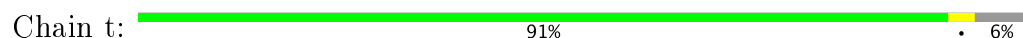
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



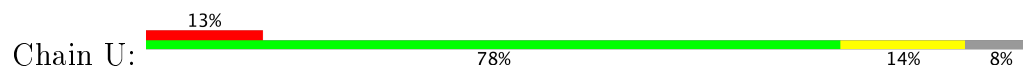
- Molecule 14: Photosystem II reaction center protein T

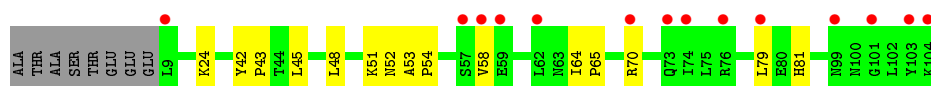


- Molecule 14: Photosystem II reaction center protein T

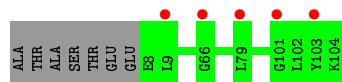


- Molecule 15: Photosystem II 12 kDa extrinsic protein





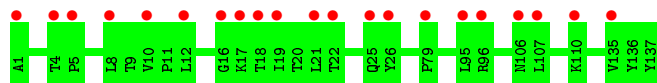
- Molecule 15: Photosystem II 12 kDa extrinsic protein



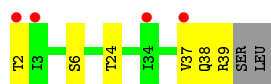
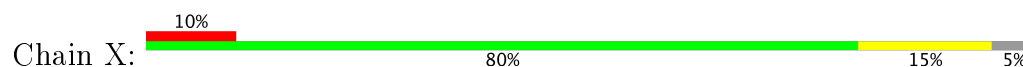
- Molecule 16: Cytochrome c-550



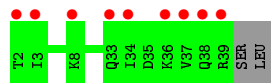
- Molecule 16: Cytochrome c-550



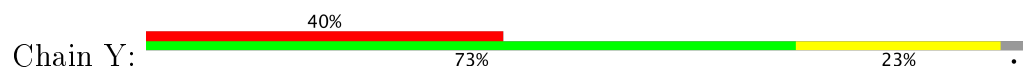
- Molecule 17: Photosystem II reaction center protein X



- Molecule 17: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein Ycf12

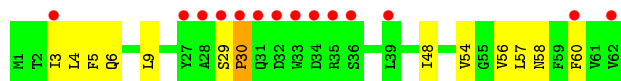
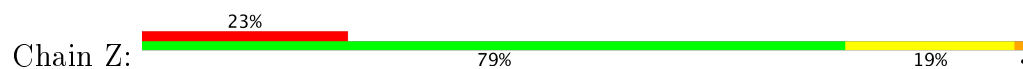


- Molecule 18: Photosystem II reaction center protein Ycf12

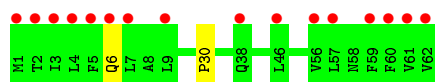




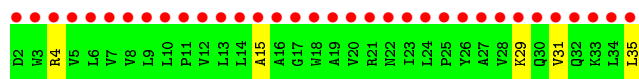
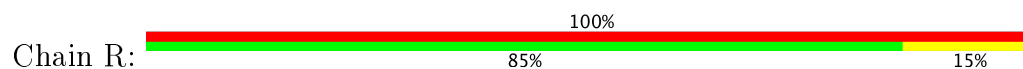
- Molecule 19: Photosystem II reaction center protein Z



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.147 , 0.186	Depositor DCC
R_{free} test set	14584 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 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	0/2728	0.56	0/3719
1	a	0.45	0/2739	0.56	0/3735
2	B	0.42	0/4171	0.55	0/5683
2	b	0.42	0/4138	0.55	0/5640
3	C	0.40	0/3626	0.53	0/4936
3	c	0.41	0/3670	0.53	0/4996
4	D	0.45	0/2827	0.55	0/3852
4	d	0.45	0/2818	0.53	0/3840
5	E	0.34	0/687	0.53	0/936
5	e	0.34	0/667	0.50	0/908
6	F	0.34	0/284	0.47	0/387
6	f	0.38	0/257	0.48	0/349
7	H	0.35	0/530	0.51	0/723
7	h	0.34	0/524	0.50	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.37	0/311	0.52	0/419
9	J	0.36	0/278	0.48	0/376
9	j	0.37	0/283	0.50	0/383
10	K	0.36	0/303	0.54	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.43	0/311	0.48	0/423
11	l	0.39	0/311	0.50	0/423
12	M	0.44	0/261	0.55	0/357
12	m	0.44	0/262	0.60	0/357
13	O	0.37	0/1935	0.57	0/2623
13	o	0.37	0/1910	0.56	0/2589
14	T	0.51	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.58	0/1052
15	u	0.40	0/785	0.57	0/1064
16	V	0.38	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1085	0.52	0/1473
17	X	0.35	0/284	0.48	0/384
17	x	0.31	0/284	0.49	0/384
18	Y	0.30	0/216	0.45	0/289
18	y	0.32	0/216	0.52	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.34	0/490	0.45	0/669
20	R	0.28	0/279	0.43	0/383
All	All	0.41	0/42949	0.54	0/58445

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	2634	0	2546	32	0
1	a	2639	0	2554	0	0
2	B	4007	0	3879	73	0
2	b	3986	0	3855	0	0
3	C	3501	0	3428	52	0
3	c	3537	0	3471	0	0
4	D	2729	0	2632	25	0
4	d	2720	0	2626	0	0
5	E	665	0	653	19	0
5	e	648	0	634	0	0
6	F	275	0	282	7	0
6	f	250	0	261	0	0
7	H	514	0	542	9	0
7	h	511	0	532	0	0
8	I	314	0	328	5	0
8	i	314	0	328	0	0
9	J	272	0	279	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	0	0
10	K	293	0	305	9	0
10	k	293	0	305	0	0
11	L	301	0	315	4	0
11	l	301	0	315	0	0
12	M	265	0	286	8	0
12	m	269	0	288	0	0
13	O	1889	0	1871	27	0
13	o	1873	0	1852	0	0
14	T	258	0	261	6	0
14	t	258	0	261	0	0
15	U	765	0	767	8	0
15	u	774	0	773	0	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	0	0
17	X	281	0	312	7	0
17	x	281	0	312	0	0
18	Y	215	0	246	5	0
18	y	215	0	246	0	0
19	Z	479	0	516	7	0
19	z	479	0	516	0	0
20	R	273	0	305	5	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	260	0	288	22	0
23	B	1040	0	1152	77	0
23	C	845	0	936	86	0
23	D	130	0	144	8	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	1	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	12	0
25	C	80	0	112	8	0
25	D	40	0	56	2	0
25	H	40	0	56	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	K	40	0	56	1	0
25	T	40	0	56	6	0
25	Y	40	0	56	2	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	10	0
26	B	54	0	78	2	0
26	D	43	0	53	1	0
26	L	54	0	78	5	0
26	a	108	0	156	0	0
26	f	43	0	53	0	0
27	A	6	0	8	1	0
27	B	12	0	16	2	0
27	C	6	0	8	1	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	9	0
29	D	55	0	80	3	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

Continued on next page...

Continued from previous page...

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	98	0	148	4	0
31	D	98	0	148	14	0
31	E	42	0	57	3	0
31	d	147	0	222	0	0
31	e	42	0	57	0	0
31	l	49	0	74	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	51	0	72	1	0
33	C	102	0	144	8	0
33	J	51	0	72	4	0
33	Z	88	0	116	4	0
33	a	51	0	72	0	0
33	b	51	0	72	0	0
33	c	102	0	144	0	0
33	j	51	0	72	0	0
33	z	39	0	48	0	0
34	B	76	0	104	6	0
34	C	38	0	52	2	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	76	0	104	0	0
34	c	38	0	52	0	0
34	d	16	0	17	0	0
35	B	86	0	116	4	0
35	D	70	0	92	3	0
35	E	35	0	46	1	0
35	I	35	0	46	1	0
35	M	70	0	92	3	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	C	186	0	246	13	0
36	H	62	0	82	1	0
36	c	186	0	246	0	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	V	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
38	E	43	0	30	5	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	127	0	0	2	0
40	B	175	0	0	4	0
40	C	148	0	0	2	0
40	D	111	0	0	1	0
40	E	18	0	0	1	0
40	F	5	0	0	0	0
40	H	19	0	0	0	0
40	I	6	0	0	1	0
40	J	5	0	0	1	0
40	K	6	0	0	0	0
40	L	9	0	0	0	0
40	M	14	0	0	1	0
40	O	100	0	0	1	0
40	T	10	0	0	1	0
40	U	46	0	0	0	0
40	V	79	0	0	3	0
40	X	3	0	0	0	0
40	Y	1	0	0	0	0
40	a	130	0	0	0	0
40	b	192	0	0	0	0
40	c	136	0	0	0	0
40	d	108	0	0	0	0
40	e	15	0	0	0	0
40	f	5	0	0	0	0
40	h	28	0	0	0	0
40	i	4	0	0	0	0
40	j	3	0	0	0	0
40	k	4	0	0	0	0
40	l	7	0	0	0	0
40	m	11	0	0	0	0
40	o	109	0	0	0	0
40	t	7	0	0	0	0
40	u	64	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	v	71	0	0	0	0
40	x	4	0	0	0	0
40	y	2	0	0	0	0
All	All	52773	0	52080	492	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 5.

The worst 5 of 492 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.46	0.95
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.57	0.91
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.27	0.81
34:B:622:HTG:H1	35:B:630:LMT:H21	1.60	0.81
26:A:410:SQD:H251	31:D:409:LHG:H131	1.66	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	44	66
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	44	66
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	38	59
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	38	59
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	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	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (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%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	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
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	55	73

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

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	272/279 (98%)	271 (100%)	1 (0%)	93	98
1	a	274/279 (98%)	273 (100%)	1 (0%)	93	98
2	B	410/403 (102%)	403 (98%)	7 (2%)	66	87
2	b	406/403 (101%)	397 (98%)	9 (2%)	57	82
3	C	356/356 (100%)	351 (99%)	5 (1%)	71	90
3	c	361/356 (101%)	353 (98%)	8 (2%)	57	82
4	D	278/277 (100%)	277 (100%)	1 (0%)	93	98
4	d	277/277 (100%)	276 (100%)	1 (0%)	93	98
5	E	73/73 (100%)	72 (99%)	1 (1%)	71	90
5	e	70/73 (96%)	68 (97%)	2 (3%)	48	75
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	62
7	H	55/54 (102%)	52 (94%)	3 (6%)	25	46
7	h	54/54 (100%)	53 (98%)	1 (2%)	62	85
8	I	34/34 (100%)	33 (97%)	1 (3%)	48	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	24 (92%)	2 (8%)	15	28
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	17
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	17
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	29 (97%)	1 (3%)	43	70
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	70
13	O	211/207 (102%)	207 (98%)	4 (2%)	62	85
13	o	208/207 (100%)	203 (98%)	5 (2%)	54	80
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%)	84 (100%)	0	100	100
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%)	31 (100%)	0	100	100
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%)	21 (96%)	1 (4%)	32	56
19	Z	52/52 (100%)	50 (96%)	2 (4%)	38	64
19	z	52/52 (100%)	51 (98%)	1 (2%)	62	85
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4360/4403 (99%)	4288 (98%)	72 (2%)	68	87

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	6	GLN
2	b	472	ARG
13	o	118	LEU
1	a	12	ASN
2	b	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	81	HIS
2	b	14	ASN
13	o	124	ASN
17	X	33	GLN
2	b	53	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	0.54	0	7,9,11	1.33	1 (14%)
12	FME	M	1	12	9,9,10	0.55	0	7,9,11	1.60	2 (28%)
14	FME	T	1	14	9,9,10	0.66	0	7,9,11	1.43	1 (14%)
8	FME	i	1	8	9,9,10	0.57	0	7,9,11	1.54	1 (14%)
12	FME	m	1	12	9,9,10	0.61	0	7,9,11	1.33	1 (14%)
14	FME	t	1	14	9,9,10	0.58	0	7,9,11	1.83	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.23	117.62	125.15
8	I	1	FME	O-C-CA	-2.74	118.77	125.15
14	T	1	FME	O-C-CA	-2.69	118.88	125.15
12	M	1	FME	O-C-CA	-2.66	118.95	125.15
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82

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 214 ligands modelled in this entry, 18 are unknown and 14 are monoatomic - leaving 182 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	2.29	25 (38%)
23	CLA	A	405	40	56,73,73	1.99	11 (19%)	65,113,113	2.14	22 (33%)
23	CLA	A	406	40	56,73,73	1.93	12 (21%)	65,113,113	2.05	20 (30%)
24	PHO	A	407	-	67,69,69	2.13	17 (25%)	87,99,99	2.04	26 (29%)
23	CLA	A	408	1	56,73,73	1.89	12 (21%)	65,113,113	2.18	21 (32%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.58	12 (21%)
26	SQD	A	410	-	53,54,54	0.95	3 (5%)	63,65,65	2.01	13 (20%)
27	GOL	A	411	-	5,5,5	0.38	0	5,5,5	0.25	0
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	63,65,65	1.24	7 (11%)
28	OEX	A	413	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	A	414	-	55,55,55	0.63	1 (1%)	69,69,69	1.89	21 (30%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	49,54,54	1.15	4 (8%)
31	LHG	A	417	-	48,48,48	0.92	2 (4%)	49,54,54	1.12	2 (4%)
32	BCT	A	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	601	40	56,73,73	2.00	12 (21%)	65,113,113	2.19	21 (32%)
23	CLA	B	602	2	56,73,73	1.96	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	B	603	2	56,73,73	1.92	11 (19%)	65,113,113	2.28	19 (29%)
23	CLA	B	604	2	56,73,73	1.90	11 (19%)	65,113,113	2.38	19 (29%)
23	CLA	B	605	2	56,73,73	1.90	12 (21%)	65,113,113	2.14	20 (30%)
23	CLA	B	606	2	56,73,73	1.88	11 (19%)	65,113,113	2.21	21 (32%)
23	CLA	B	607	40	56,73,73	1.93	12 (21%)	65,113,113	2.20	22 (33%)
23	CLA	B	608	2	56,73,73	1.90	11 (19%)	65,113,113	2.20	21 (32%)
23	CLA	B	609	2	56,73,73	1.89	11 (19%)	65,113,113	2.17	17 (26%)
23	CLA	B	610	40	56,73,73	2.00	12 (21%)	65,113,113	2.32	21 (32%)
23	CLA	B	611	2	56,73,73	1.95	11 (19%)	65,113,113	2.25	21 (32%)
23	CLA	B	612	2	56,73,73	1.90	11 (19%)	65,113,113	2.40	21 (32%)
23	CLA	B	613	2	56,73,73	1.99	12 (21%)	65,113,113	2.35	21 (32%)
23	CLA	B	614	2	56,73,73	1.90	13 (23%)	65,113,113	2.38	21 (32%)
23	CLA	B	615	2	56,73,73	1.89	11 (19%)	65,113,113	2.18	19 (29%)
23	CLA	B	616	2	56,73,73	1.98	12 (21%)	65,113,113	2.17	18 (27%)
25	BCR	B	617	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	10 (17%)
25	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.66	13 (23%)
25	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	10 (17%)
26	SQD	B	620	-	53,54,54	1.04	4 (7%)	63,65,65	1.64	12 (19%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.15	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	B	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.48	4 (17%)
34	HTG	B	623	-	19,19,19	0.82	1 (5%)	23,24,24	1.94	1 (4%)
34	HTG	B	624	-	19,19,19	0.98	1 (5%)	23,24,24	2.01	2 (8%)
27	GOL	B	625	-	5,5,5	0.35	0	5,5,5	0.35	0
27	GOL	B	626	-	5,5,5	0.49	0	5,5,5	0.41	0
34	HTG	B	627	-	19,19,19	0.95	2 (10%)	23,24,24	1.59	1 (4%)
35	LMT	B	629	-	25,25,36	0.45	0	30,30,47	0.71	0
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.98	2 (4%)
35	LMT	B	631	-	26,26,36	0.49	0	31,31,47	0.82	1 (3%)
33	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	4 (6%)
23	CLA	C	502	3	56,73,73	1.90	12 (21%)	65,113,113	2.37	22 (33%)
23	CLA	C	503	3	56,73,73	1.92	11 (19%)	65,113,113	2.12	18 (27%)
23	CLA	C	504	3	56,73,73	1.88	11 (19%)	65,113,113	2.00	18 (27%)
23	CLA	C	505	40	56,73,73	2.03	12 (21%)	65,113,113	2.37	23 (35%)
23	CLA	C	506	3	56,73,73	1.91	12 (21%)	65,113,113	2.35	20 (30%)
23	CLA	C	507	3	56,73,73	1.93	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	C	508	40	56,73,73	1.92	12 (21%)	65,113,113	2.26	20 (30%)
23	CLA	C	509	3	56,73,73	2.05	12 (21%)	65,113,113	2.44	20 (30%)
23	CLA	C	510	3	56,73,73	2.02	12 (21%)	65,113,113	2.18	21 (32%)
23	CLA	C	511	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	23 (35%)
23	CLA	C	512	3	56,73,73	1.96	12 (21%)	65,113,113	2.20	21 (32%)
23	CLA	C	513	3	56,73,73	1.95	11 (19%)	65,113,113	2.20	24 (36%)
23	CLA	C	514	3	56,73,73	1.93	12 (21%)	65,113,113	2.10	19 (29%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.58	10 (17%)
25	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	10 (17%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.10	7 (9%)
36	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
36	DGD	C	519	-	63,63,67	0.80	2 (3%)	77,77,81	1.02	6 (7%)
33	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	4 (6%)
34	HTG	C	521	-	19,19,19	0.90	1 (5%)	23,24,24	1.59	3 (13%)
34	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	2.01	5 (21%)
27	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.23	0
24	PHO	D	401	-	67,69,69	2.12	16 (23%)	87,99,99	2.08	26 (29%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.31	5 (10%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.39	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	D	404	4	56,73,73	1.95	12 (21%)	65,113,113	2.46	23 (35%)
23	CLA	D	405	4	56,73,73	1.92	11 (19%)	65,113,113	2.23	20 (30%)
25	BCR	D	406	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	14 (25%)
29	PL9	D	407	-	55,55,55	0.63	1 (1%)	69,69,69	1.69	21 (30%)
31	LHG	D	408	-	48,48,48	0.86	2 (4%)	49,54,54	0.99	3 (6%)
31	LHG	D	409	-	48,48,48	0.91	2 (4%)	49,54,54	1.15	5 (10%)
34	HTG	D	412	-	16,16,19	1.02	2 (12%)	20,21,24	1.73	1 (5%)
26	SQD	D	413	-	42,43,54	1.12	3 (7%)	52,54,65	1.92	13 (25%)
31	LHG	E	101	-	41,41,48	1.02	2 (4%)	42,47,54	1.17	4 (9%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.90	1 (2%)
38	HEM	E	103	5,6	28,50,50	0.85	0	17,82,82	2.16	4 (23%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.72	13 (23%)
36	DGD	H	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.03	6 (7%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.14	5 (10%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.01	5 (8%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	9 (16%)
26	SQD	L	101	-	53,54,54	1.00	3 (5%)	63,65,65	1.67	9 (14%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.05	2 (4%)
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.82	1 (2%)
25	BCR	T	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.73	14 (25%)
38	HEM	V	202	16	28,50,50	0.99	3 (10%)	17,82,82	1.59	3 (17%)
34	HTG	V	203	-	11,11,19	0.25	0	13,15,24	1.13	2 (15%)
25	BCR	Y	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.67	10 (17%)
33	LMG	Z	101	-	51,51,55	0.97	2 (3%)	59,59,63	1.29	5 (8%)
33	LMG	Z	102	-	37,37,55	0.99	3 (8%)	45,45,63	1.68	8 (17%)
23	CLA	a	404	1	56,73,73	1.91	11 (19%)	65,113,113	2.42	24 (36%)
23	CLA	a	405	40	56,73,73	1.98	12 (21%)	65,113,113	2.12	23 (35%)
24	PHO	a	406	-	67,69,69	2.09	17 (25%)	87,99,99	1.94	26 (29%)
24	PHO	a	407	-	67,69,69	2.17	15 (22%)	87,99,99	1.98	24 (27%)
23	CLA	a	408	1	56,73,73	1.93	12 (21%)	65,113,113	2.25	24 (36%)
25	BCR	a	409	-	41,41,41	0.93	1 (2%)	56,56,56	1.50	11 (19%)
26	SQD	a	410	-	53,54,54	0.94	3 (5%)	63,65,65	1.88	14 (22%)
27	GOL	a	411	-	5,5,5	0.36	0	5,5,5	0.39	0
26	SQD	a	412	-	53,54,54	1.04	3 (5%)	63,65,65	1.39	8 (12%)
28	OEX	a	413	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	a	414	-	55,55,55	0.63	1 (1%)	69,69,69	1.93	18 (26%)
33	LMG	a	416	-	51,51,55	0.93	2 (3%)	59,59,63	1.09	3 (5%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.81	1 (2%)
32	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	601	40	56,73,73	1.98	12 (21%)	65,113,113	2.15	21 (32%)
23	CLA	b	602	2	56,73,73	1.98	12 (21%)	65,113,113	2.29	25 (38%)
23	CLA	b	603	2	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
23	CLA	b	604	2	56,73,73	1.93	11 (19%)	65,113,113	2.34	18 (27%)
23	CLA	b	605	2	56,73,73	1.94	12 (21%)	65,113,113	2.24	17 (26%)
23	CLA	b	606	2	56,73,73	1.87	11 (19%)	65,113,113	2.20	23 (35%)
23	CLA	b	607	40	56,73,73	1.87	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	b	608	2	56,73,73	2.00	12 (21%)	65,113,113	2.20	19 (29%)
23	CLA	b	609	2	56,73,73	1.91	12 (21%)	65,113,113	2.25	20 (30%)
23	CLA	b	610	40	56,73,73	2.03	12 (21%)	65,113,113	2.31	24 (36%)
23	CLA	b	611	2	56,73,73	1.98	12 (21%)	65,113,113	2.30	20 (30%)
23	CLA	b	612	2	56,73,73	2.01	12 (21%)	65,113,113	2.21	19 (29%)
23	CLA	b	613	2	56,73,73	1.97	12 (21%)	65,113,113	2.29	20 (30%)
23	CLA	b	614	2	56,73,73	1.94	12 (21%)	65,113,113	2.29	22 (33%)
23	CLA	b	615	2	56,73,73	1.85	11 (19%)	65,113,113	2.19	17 (26%)
23	CLA	b	616	2	56,73,73	1.93	11 (19%)	65,113,113	2.18	22 (33%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.51	10 (17%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	8 (14%)
25	BCR	b	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.68	12 (21%)
33	LMG	b	620	-	51,51,55	0.85	2 (3%)	59,59,63	1.29	8 (13%)
35	LMT	b	621	-	25,25,36	0.45	0	30,30,47	0.69	0
34	HTG	b	622	-	19,19,19	0.94	1 (5%)	23,24,24	1.67	2 (8%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	2.06	2 (8%)
27	GOL	b	624	-	5,5,5	0.29	0	5,5,5	0.43	0
34	HTG	b	625	-	19,19,19	0.90	2 (10%)	23,24,24	1.91	3 (13%)
35	LMT	b	627	-	25,25,36	0.55	1 (4%)	30,30,47	1.14	3 (10%)
34	HTG	b	628	-	19,19,19	0.99	1 (5%)	23,24,24	1.96	4 (17%)
23	CLA	c	501	3	56,73,73	1.88	12 (21%)	65,113,113	2.16	20 (30%)
23	CLA	c	502	3	56,73,73	1.96	12 (21%)	65,113,113	2.30	19 (29%)
23	CLA	c	503	3	56,73,73	1.92	12 (21%)	65,113,113	2.24	20 (30%)
23	CLA	c	504	40	56,73,73	1.98	12 (21%)	65,113,113	2.20	24 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	505	3	56,73,73	1.92	11 (19%)	65,113,113	2.24	19 (29%)
23	CLA	c	506	3	56,73,73	1.93	11 (19%)	65,113,113	2.28	22 (33%)
23	CLA	c	507	40	56,73,73	1.91	11 (19%)	65,113,113	2.18	19 (29%)
23	CLA	c	508	3	56,73,73	2.02	12 (21%)	65,113,113	2.31	19 (29%)
23	CLA	c	509	3	56,73,73	1.99	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	c	510	3	56,73,73	1.86	12 (21%)	65,113,113	2.26	23 (35%)
23	CLA	c	511	3	56,73,73	1.98	12 (21%)	65,113,113	2.15	19 (29%)
23	CLA	c	512	3	56,73,73	1.93	12 (21%)	65,113,113	2.28	19 (29%)
23	CLA	c	513	3	56,73,73	1.95	12 (21%)	65,113,113	2.22	22 (33%)
25	BCR	c	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	13 (23%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.70	17 (30%)
36	DGD	c	516	-	63,63,67	0.82	2 (3%)	77,77,81	1.19	7 (9%)
36	DGD	c	517	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
36	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.12	6 (7%)
33	LMG	c	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.06	3 (5%)
33	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.26	6 (10%)
34	HTG	c	521	-	19,19,19	0.89	1 (5%)	23,24,24	1.75	1 (4%)
34	HTG	c	522	-	19,19,19	0.94	2 (10%)	23,24,24	1.63	3 (13%)
23	CLA	d	401	40	56,73,73	1.95	11 (19%)	65,113,113	2.26	22 (33%)
27	GOL	d	402	-	5,5,5	0.26	0	5,5,5	0.55	0
23	CLA	d	403	4	56,73,73	1.92	12 (21%)	65,113,113	2.26	22 (33%)
23	CLA	d	404	4	56,73,73	1.96	11 (19%)	65,113,113	2.09	24 (36%)
25	BCR	d	405	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	14 (25%)
29	PL9	d	406	-	55,55,55	0.61	1 (1%)	69,69,69	1.76	19 (27%)
31	LHG	d	407	-	48,48,48	0.87	2 (4%)	49,54,54	1.08	5 (10%)
31	LHG	d	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.94	3 (6%)
31	LHG	d	409	-	48,48,48	0.95	2 (4%)	49,54,54	1.04	3 (6%)
34	HTG	d	411	-	16,16,19	1.09	2 (12%)	20,21,24	1.76	1 (5%)
31	LHG	e	101	-	41,41,48	1.01	2 (4%)	42,47,54	0.99	2 (4%)
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.87	2 (4%)
38	HEM	e	103	5,6	28,50,50	0.84	1 (3%)	17,82,82	1.87	3 (17%)
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	52,54,65	1.57	9 (17%)
25	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.47	9 (16%)
36	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.05	5 (6%)
33	LMG	j	101	39	51,51,55	0.87	2 (3%)	59,59,63	1.10	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	13 (23%)
31	LHG	l	101	-	48,48,48	0.93	2 (4%)	49,54,54	1.09	4 (8%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.97	2 (4%)
25	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.72	16 (28%)
38	HEM	v	201	16	28,50,50	0.98	3 (10%)	17,82,82	1.61	4 (23%)
25	BCR	y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.63	11 (19%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.13	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	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	40	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	407	-	-	0/53/103/103	0/1/6/6
23	CLA	A	408	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	0/49/69/69	0/1/1/1
27	GOL	A	411	-	-	0/4/4/4	0/0/0/0
26	SQD	A	412	-	-	0/49/69/69	0/1/1/1
28	OEX	A	413	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	A	414	-	-	0/53/73/73	0/1/1/1
31	LHG	A	416	-	-	0/53/53/53	0/0/0/0
31	LHG	A	417	-	-	0/53/53/53	0/0/0/0
32	BCT	A	418	21	-	0/0/0/0	0/0/0/0
23	CLA	B	601	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	2	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	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	2	3/3/20/25	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
26	SQD	B	620	-	-	0/49/69/69	0/1/1/1
33	LMG	B	621	-	-	0/46/66/70	0/1/1/1
34	HTG	B	622	-	-	0/10/30/30	0/1/1/1
34	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	HTG	B	624	-	-	0/10/30/30	0/1/1/1
27	GOL	B	625	-	-	0/4/4/4	0/0/0/0
27	GOL	B	626	-	-	0/4/4/4	0/0/0/0
34	HTG	B	627	-	-	0/10/30/30	0/1/1/1
35	LMT	B	629	-	-	0/17/37/61	0/1/1/2
35	LMT	B	630	-	-	0/21/61/61	0/2/2/2
35	LMT	B	631	-	-	0/17/38/61	0/1/1/2
33	LMG	C	501	-	-	0/46/66/70	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	2/2/20/25	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
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
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
33	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
27	GOL	C	523	-	-	0/4/4/4	0/0/0/0
24	PHO	D	401	-	-	0/53/103/103	0/1/6/6
35	LMT	D	402	-	-	0/21/61/61	0/2/2/2
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
34	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
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
35	LMT	I	101	-	-	0/21/61/61	0/2/2/2
33	LMG	J	101	39	-	0/46/66/70	0/1/1/1
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	SQD	L	101	-	-	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
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
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
33	LMG	Z	102	-	-	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
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
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
23	CLA	a	408	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
26	SQD	a	410	-	-	0/49/69/69	0/1/1/1
27	GOL	a	411	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	412	-	-	0/49/69/69	0/1/1/1
28	OEX	a	413	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	a	414	-	-	0/53/73/73	0/1/1/1
33	LMG	a	416	-	-	0/46/66/70	0/1/1/1
35	LMT	a	417	-	-	0/21/61/61	0/2/2/2
32	BCT	a	418	21	-	0/0/0/0	0/0/0/0
23	CLA	b	601	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	602	2	3/3/20/25	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
33	LMG	b	620	-	-	0/46/66/70	0/1/1/1
35	LMT	b	621	-	-	0/17/37/61	0/1/1/2
34	HTG	b	622	-	-	0/10/30/30	0/1/1/1
34	HTG	b	623	-	-	0/10/30/30	0/1/1/1
27	GOL	b	624	-	-	0/4/4/4	0/0/0/0
34	HTG	b	625	-	-	0/10/30/30	0/1/1/1
35	LMT	b	627	-	-	0/17/37/61	0/1/1/2
34	HTG	b	628	-	-	0/10/30/30	0/1/1/1
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	3	2/2/20/25	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	3/3/20/25	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
36	DGD	c	516	-	-	0/51/91/95	0/2/2/2
36	DGD	c	517	-	-	0/51/91/95	0/2/2/2
36	DGD	c	518	-	-	0/51/91/95	0/2/2/2
33	LMG	c	519	-	-	0/46/66/70	0/1/1/1
33	LMG	c	520	-	-	0/46/66/70	0/1/1/1
34	HTG	c	521	-	-	0/10/30/30	0/1/1/1
34	HTG	c	522	-	-	0/10/30/30	0/1/1/1
23	CLA	d	401	40	3/3/20/25	0/37/135/135	0/0/9/9
27	GOL	d	402	-	-	0/4/4/4	0/0/0/0
23	CLA	d	403	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	d	404	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	d	405	-	-	0/29/63/63	0/2/2/2
29	PL9	d	406	-	-	0/53/73/73	0/1/1/1
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	d	409	-	-	0/53/53/53	0/0/0/0
34	HTG	d	411	-	-	0/7/27/30	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
26	SQD	f	101	-	-	2/38/58/69	0/1/1/1
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2
33	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0
35	LMT	m	102	-	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	z	101	-	-	0/34/54/70	0/1/1/1

The worst 5 of 1031 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	102	BCR	C23-C22	-5.18	1.34	1.45
25	C	515	BCR	C23-C22	-5.16	1.34	1.45
25	k	101	BCR	C23-C22	-5.07	1.34	1.45
25	b	619	BCR	C23-C22	-5.06	1.34	1.45
25	d	405	BCR	C23-C22	-4.98	1.35	1.45

The worst 5 of 2207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	CHD-C4C-C3C	-6.74	114.77	124.92
23	B	609	CLA	CHD-C4C-C3C	-6.47	115.16	124.92
23	C	509	CLA	C1C-NC-C4C	-6.47	103.33	107.06
23	D	404	CLA	C1C-NC-C4C	-6.45	103.34	107.06
23	B	612	CLA	C1C-NC-C4C	-6.40	103.37	107.06

5 of 196 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	d	404	CLA	NC
23	d	404	CLA	ND

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Z	102	LMG	C8-O7-C10-O9
33	Z	102	LMG	C8-O7-C10-C11
26	f	101	SQD	C45-O47-C7-O49
26	D	413	SQD	C45-O47-C7-O49
26	f	101	SQD	C45-O47-C7-C8

There are no ring outliers.

86 monomers are involved in 300 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	5	0
23	A	405	CLA	4	0
23	A	406	CLA	4	0
24	A	407	PHO	6	0
23	A	408	CLA	9	0
25	A	409	BCR	2	0
26	A	410	SQD	7	0
27	A	411	GOL	1	0
26	A	412	SQD	3	0
29	A	414	PL9	9	0
31	A	416	LHG	2	0
31	A	417	LHG	2	0
23	B	601	CLA	4	0
23	B	602	CLA	5	0
23	B	603	CLA	4	0
23	B	604	CLA	6	0
23	B	605	CLA	11	0
23	B	606	CLA	4	0
23	B	607	CLA	3	0
23	B	608	CLA	3	0
23	B	609	CLA	7	0
23	B	610	CLA	2	0
23	B	611	CLA	4	0
23	B	612	CLA	6	0
23	B	613	CLA	7	0
23	B	614	CLA	7	0
23	B	615	CLA	6	0
23	B	616	CLA	8	0
25	B	617	BCR	3	0
25	B	618	BCR	6	0
25	B	619	BCR	3	0
26	B	620	SQD	2	0
33	B	621	LMG	1	0
34	B	622	HTG	5	0
34	B	623	HTG	1	0
27	B	625	GOL	1	0
27	B	626	GOL	1	0
35	B	629	LMT	1	0
35	B	630	LMT	3	0
33	C	501	LMG	7	0
23	C	502	CLA	7	0
23	C	503	CLA	4	0
23	C	504	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	505	CLA	7	0
23	C	506	CLA	14	0
23	C	507	CLA	13	0
23	C	508	CLA	13	0
23	C	509	CLA	8	0
23	C	510	CLA	6	0
23	C	511	CLA	4	0
23	C	512	CLA	8	0
23	C	513	CLA	9	0
23	C	514	CLA	7	0
25	C	515	BCR	5	0
25	C	516	BCR	3	0
36	C	517	DGD	8	0
36	C	518	DGD	5	0
36	C	519	DGD	1	0
33	C	520	LMG	1	0
34	C	521	HTG	1	0
34	C	522	HTG	1	0
27	C	523	GOL	1	0
24	D	401	PHO	1	0
35	D	402	LMT	1	0
35	D	403	LMT	2	0
23	D	404	CLA	8	0
25	D	406	BCR	2	0
29	D	407	PL9	3	0
31	D	408	LHG	3	0
31	D	409	LHG	11	0
26	D	413	SQD	1	0
31	E	101	LHG	3	0
35	E	102	LMT	1	0
38	E	103	HEM	5	0
25	H	101	BCR	7	0
36	H	102	DGD	1	0
35	I	101	LMT	1	0
33	J	101	LMG	4	0
25	K	102	BCR	1	0
26	L	101	SQD	5	0
35	M	101	LMT	2	0
35	M	103	LMT	1	0
25	T	101	BCR	6	0
25	Y	101	BCR	2	0
33	Z	101	LMG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	Z	102	LMG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.06	9 (2%) 55 58	21, 31, 53, 100	0
1	a	334/344 (97%)	0.09	11 (3%) 47 50	23, 33, 62, 108	0
2	B	504/505 (99%)	0.21	50 (9%) 8 7	21, 36, 65, 109	0
2	b	504/505 (99%)	0.35	58 (11%) 5 5	23, 37, 74, 118	0
3	C	451/455 (99%)	0.51	64 (14%) 3 2	26, 45, 67, 117	0
3	c	455/455 (100%)	0.31	49 (10%) 6 6	30, 48, 69, 109	0
4	D	342/342 (100%)	-0.04	7 (2%) 65 67	21, 32, 53, 108	0
4	d	341/342 (99%)	0.22	25 (7%) 16 16	23, 36, 54, 123	0
5	E	81/84 (96%)	0.22	7 (8%) 11 11	37, 54, 82, 120	0
5	e	79/84 (94%)	1.06	19 (24%) 1 0	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.22	0 100 100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.19	4 (12%) 4 3	44, 50, 86, 122	0
7	H	64/65 (98%)	0.25	5 (7%) 14 14	34, 47, 68, 101	0
7	h	65/65 (100%)	1.09	16 (24%) 1 0	37, 51, 74, 141	0
8	I	37/38 (97%)	0.42	7 (18%) 1 1	37, 46, 88, 130	0
8	i	37/38 (97%)	0.21	4 (10%) 6 6	38, 46, 93, 135	0
9	J	38/39 (97%)	0.20	5 (13%) 4 3	32, 52, 106, 147	0
9	j	39/39 (100%)	0.77	9 (23%) 1 0	40, 51, 107, 129	0
10	K	37/37 (100%)	0.00	3 (8%) 13 12	44, 53, 76, 91	0
10	k	37/37 (100%)	0.29	2 (5%) 26 27	47, 54, 78, 93	0
11	L	36/37 (97%)	0.59	7 (19%) 1 1	20, 26, 89, 129	0
11	l	36/37 (97%)	0.23	3 (8%) 12 12	22, 28, 87, 128	0
12	M	32/36 (88%)	-0.03	1 (3%) 49 52	22, 29, 49, 117	0
12	m	33/36 (91%)	-0.23	3 (9%) 10 10	24, 29, 72, 117	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.25	28 (11%) 5 5	22, 45, 100, 157	0
13	o	243/244 (99%)	0.62	52 (21%) 1 1	24, 46, 99, 144	0
14	T	29/32 (90%)	0.21	0 100 100	23, 28, 60, 96	0
14	t	29/32 (90%)	-0.15	0 100 100	23, 29, 61, 97	0
15	U	96/104 (92%)	0.47	14 (14%) 3 2	31, 40, 66, 84	0
15	u	97/104 (93%)	-0.17	5 (5%) 28 29	32, 43, 68, 101	0
16	V	137/137 (100%)	0.08	3 (2%) 62 64	29, 43, 70, 100	0
16	v	137/137 (100%)	0.46	21 (15%) 2 2	34, 50, 74, 101	0
17	X	38/40 (95%)	0.20	4 (10%) 7 6	44, 56, 82, 110	0
17	x	38/40 (95%)	1.15	9 (23%) 1 0	47, 58, 83, 112	0
18	Y	29/30 (96%)	1.76	12 (41%) 0 0	56, 71, 112, 114	0
18	y	29/30 (96%)	0.95	5 (17%) 2 1	58, 70, 110, 114	0
19	Z	62/62 (100%)	1.08	14 (22%) 1 1	57, 72, 117, 152	0
19	z	62/62 (100%)	1.30	16 (25%) 1 0	60, 74, 117, 153	0
20	R	34/34 (100%)	6.09	34 (100%) 0 0	89, 108, 128, 135	0
All	All	5284/5384 (98%)	0.34	585 (11%) 6 5	20, 41, 82, 157	0

The worst 5 of 585 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	10.4
20	R	35	LEU	9.2
20	R	19	ALA	8.8
20	R	20	VAL	8.7
9	J	5	GLY	8.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.97	0.15	-	18,38,70,79	0
14	FME	T	1	10/11	0.98	0.09	-	18,32,46,47	0
8	FME	I	1	10/11	0.98	0.22	-	31,47,56,62	0
8	FME	i	1	10/11	0.97	0.09	-	37,49,57,62	0
14	FME	t	1	10/11	0.98	0.10	-	21,32,41,71	0
12	FME	m	1	10/11	0.96	0.11	-	30,42,63,78	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	GOL	d	402	6/6	0.80	0.60	20.72	33,50,65,68	0
34	HTG	b	622	19/19	0.76	0.89	15.38	74,95,125,130	0
30	UNL	i	101	40/-	0.70	0.42	13.74	48,88,140,147	0
30	UNL	J	102	10/-	0.71	0.39	10.13	55,64,89,90	0
35	LMT	D	402	35/35	0.65	0.37	9.47	31,97,113,115	0
34	HTG	V	203	11/19	0.82	0.56	9.01	71,92,107,108	0
35	LMT	B	630	35/35	0.55	0.46	8.54	33,105,126,134	0
35	LMT	E	102	35/35	0.72	0.55	7.55	78,120,147,150	0
35	LMT	M	103	35/35	0.68	0.34	7.10	40,120,148,154	0
30	UNL	j	102	10/-	0.74	0.29	6.91	60,75,88,89	0
34	HTG	c	522	19/19	0.74	0.85	6.47	79,124,142,146	0
35	LMT	e	102	35/35	0.67	0.79	6.36	76,134,147,156	0
29	PL9	A	414	55/55	0.71	0.40	6.31	41,88,105,119	0
34	HTG	D	412	16/19	0.54	0.43	5.45	48,115,128,130	0
34	HTG	b	623	19/19	0.62	0.66	5.23	71,109,141,169	0
27	GOL	B	625	6/6	0.95	0.29	5.22	48,76,85,89	0
34	HTG	B	623	19/19	0.76	0.41	5.21	60,84,110,115	0
30	UNL	D	411	40/-	0.83	0.24	5.19	40,77,117,122	0
34	HTG	C	522	19/19	0.68	0.91	5.19	58,139,157,179	0
27	GOL	B	626	6/6	0.86	0.31	4.97	38,51,55,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	HTG	b	628	19/19	0.85	0.25	4.41	34,65,115,119	0
35	LMT	a	417	35/35	0.84	0.55	4.29	78,114,130,131	0
30	UNL	D	410	17/-	0.93	0.28	4.13	44,56,91,100	0
30	UNL	K	101	34/-	0.71	0.35	4.09	55,96,114,125	0
27	GOL	a	411	6/6	0.91	0.20	4.08	52,60,62,66	0
27	GOL	A	411	6/6	0.97	0.12	4.01	50,58,65,79	0
30	UNL	I	102	40/-	0.73	0.31	3.93	40,85,135,142	0
29	PL9	a	414	55/55	0.66	0.41	3.40	57,93,112,120	0
35	LMT	I	101	35/35	0.58	0.65	2.93	74,108,131,141	0
33	LMG	Z	101	51/55	0.59	0.43	2.85	46,105,140,150	0
35	LMT	B	631	26/35	0.90	0.18	2.79	52,80,105,109	0
31	LHG	e	101	42/49	0.72	0.42	2.73	81,118,142,148	0
35	LMT	b	627	25/35	0.83	0.25	2.65	29,61,134,139	0
30	UNL	b	629	36/-	0.81	0.29	2.65	49,80,131,138	0
30	UNL	x	101	18/-	0.82	0.29	2.43	44,63,91,92	0
33	LMG	z	101	39/55	0.88	0.25	2.34	63,112,140,147	0
31	LHG	E	101	42/49	0.80	0.27	2.34	41,93,108,124	0
30	UNL	X	101	18/-	0.91	0.19	2.05	40,53,83,90	0
34	HTG	B	622	19/19	0.92	0.21	2.02	34,61,127,132	0
30	UNL	d	410	17/-	0.95	0.29	1.99	42,57,85,90	0
35	LMT	m	102	35/35	0.69	0.47	1.93	34,78,102,109	0
31	LHG	A	416	49/49	0.92	0.32	1.85	26,44,61,77	0
33	LMG	Z	102	37/55	0.74	0.38	1.75	47,97,129,137	0
23	CLA	c	503	65/65	0.94	0.41	1.72	40,51,63,78	0
23	CLA	B	601	65/65	0.94	0.23	1.71	39,57,88,119	0
35	LMT	B	629	25/35	0.84	0.24	1.65	34,68,124,125	0
33	LMG	c	520	51/55	0.70	0.36	1.63	51,102,132,138	0
26	SQD	L	101	54/54	0.77	0.27	1.61	47,71,116,121	0
31	LHG	D	408	49/49	0.96	0.23	1.59	22,34,51,68	0
26	SQD	f	101	43/54	0.77	0.36	1.56	85,111,157,164	0
23	CLA	b	601	65/65	0.93	0.24	1.54	43,69,99,126	0
29	PL9	D	407	55/55	0.95	0.23	1.54	20,31,45,54	0
31	LHG	d	408	49/49	0.93	0.22	1.54	24,35,53,70	0
23	CLA	c	502	65/65	0.91	0.41	1.51	37,48,68,73	0
35	LMT	M	101	35/35	0.70	0.35	1.47	39,80,103,109	0
35	LMT	D	403	35/35	0.81	0.32	1.38	48,91,116,117	0
25	BCR	t	101	40/40	0.96	0.23	1.32	19,42,59,62	0
24	PHO	a	406	64/64	0.98	0.20	1.31	22,31,40,51	0
29	PL9	d	406	55/55	0.94	0.19	1.28	23,30,41,58	0
26	SQD	a	412	54/54	0.88	0.22	1.27	44,73,125,133	0
31	LHG	A	417	49/49	0.94	0.24	1.27	23,37,55,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	610	65/65	0.97	0.22	1.13	27,36,52,69	0
33	LMG	c	519	51/55	0.88	0.27	1.12	43,77,114,124	0
25	BCR	T	101	40/40	0.96	0.22	1.11	20,36,45,53	0
27	GOL	C	523	6/6	0.93	0.24	1.10	44,54,59,60	0
31	LHG	d	409	49/49	0.94	0.20	1.10	33,50,98,110	0
26	SQD	A	412	54/54	0.89	0.21	1.08	39,65,102,118	0
23	CLA	B	605	65/65	0.96	0.20	1.07	22,30,44,48	0
33	LMG	C	501	51/55	0.83	0.28	1.02	35,74,98,102	0
23	CLA	c	501	65/65	0.95	0.23	1.01	38,49,64,71	0
25	BCR	B	618	40/40	0.97	0.23	1.01	21,36,54,69	0
36	DGD	C	519	62/66	0.93	0.17	0.98	28,44,71,95	0
36	DGD	c	516	62/66	0.95	0.23	0.95	33,43,73,95	0
25	BCR	d	405	40/40	0.93	0.16	0.93	40,50,74,81	0
25	BCR	C	516	40/40	0.93	0.21	0.91	36,48,66,73	0
33	LMG	J	101	51/55	0.92	0.18	0.89	30,51,88,99	0
31	LHG	l	101	49/49	0.92	0.17	0.88	25,38,55,60	0
23	CLA	b	604	65/65	0.95	0.31	0.88	23,31,85,96	0
23	CLA	b	605	65/65	0.96	0.23	0.85	24,34,52,97	0
24	PHO	a	407	64/64	0.97	0.26	0.85	28,35,50,52	0
31	LHG	d	407	49/49	0.96	0.20	0.85	25,44,72,87	0
23	CLA	B	603	65/65	0.97	0.26	0.84	26,39,52,57	0
36	DGD	c	518	62/66	0.95	0.19	0.81	36,46,77,96	0
34	HTG	d	411	16/19	0.78	0.37	0.81	81,112,121,122	0
36	DGD	h	102	62/66	0.89	0.27	0.79	31,46,62,73	0
31	LHG	D	409	49/49	0.95	0.19	0.79	29,47,107,124	0
23	CLA	C	511	65/65	0.95	0.42	0.79	33,44,57,61	0
23	CLA	a	408	65/65	0.95	0.19	0.78	28,40,107,115	0
23	CLA	C	506	65/65	0.96	0.26	0.78	31,40,71,78	0
26	SQD	D	413	43/54	0.91	0.27	0.76	64,97,112,116	0
33	LMG	j	101	51/55	0.93	0.18	0.75	37,53,102,123	0
24	PHO	D	401	64/64	0.98	0.18	0.74	21,27,35,45	0
23	CLA	D	405	65/65	0.93	0.19	0.73	31,46,99,111	0
25	BCR	H	101	40/40	0.84	0.23	0.72	33,42,63,67	0
23	CLA	c	511	65/65	0.92	0.21	0.70	43,56,74,82	0
23	CLA	c	508	65/65	0.93	0.19	0.70	35,48,107,118	0
23	CLA	c	509	65/65	0.91	0.24	0.68	43,52,66,73	0
36	DGD	c	517	62/66	0.92	0.22	0.67	38,53,112,129	0
26	SQD	a	410	54/54	0.93	0.18	0.65	41,64,98,105	0
33	LMG	a	416	51/55	0.85	0.25	0.64	41,77,102,118	0
23	CLA	C	513	65/65	0.84	0.27	0.64	43,59,94,101	0
23	CLA	b	608	65/65	0.97	0.28	0.63	32,41,60,68	0
23	CLA	B	612	65/65	0.95	0.23	0.63	24,29,42,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	C	509	65/65	0.94	0.29	0.61	30,43,102,115	0
23	CLA	A	408	65/65	0.97	0.14	0.61	26,36,101,109	0
36	DGD	C	517	62/66	0.93	0.23	0.61	27,36,81,92	0
23	CLA	C	503	65/65	0.93	0.35	0.61	31,42,55,73	0
25	BCR	B	619	40/40	0.94	0.15	0.59	28,42,63,67	0
22	CL	A	403	1/1	1.00	0.24	0.58	27,27,27,27	0
23	CLA	B	613	65/65	0.97	0.32	0.58	21,29,68,78	0
23	CLA	b	603	65/65	0.96	0.24	0.57	30,40,53,74	0
36	DGD	C	518	62/66	0.90	0.21	0.57	29,46,103,110	0
23	CLA	B	604	65/65	0.94	0.30	0.56	21,29,92,104	0
23	CLA	A	405	65/65	0.97	0.16	0.55	19,23,41,47	0
36	DGD	H	102	62/66	0.92	0.25	0.54	26,40,58,66	0
23	CLA	b	610	65/65	0.96	0.20	0.50	30,42,51,60	0
23	CLA	B	607	65/65	0.96	0.22	0.49	18,27,54,66	0
25	BCR	B	617	40/40	0.97	0.15	0.49	22,31,46,49	0
24	PHO	A	407	64/64	0.97	0.21	0.48	23,31,46,51	0
25	BCR	b	618	40/40	0.96	0.21	0.48	21,34,49,55	0
25	BCR	h	101	40/40	0.70	0.27	0.47	39,50,64,77	0
26	SQD	B	620	54/54	0.86	0.21	0.47	41,73,108,113	0
23	CLA	c	510	65/65	0.96	0.31	0.47	39,47,62,66	0
23	CLA	C	510	65/65	0.93	0.29	0.42	36,47,67,69	0
23	CLA	B	602	65/65	0.92	0.23	0.42	29,37,55,67	0
25	BCR	Y	101	40/40	0.94	0.15	0.41	37,49,59,62	0
33	LMG	C	520	51/55	0.83	0.28	0.41	37,69,104,121	0
23	CLA	B	611	65/65	0.94	0.24	0.39	23,30,41,45	0
25	BCR	D	406	40/40	0.94	0.17	0.39	32,42,87,90	0
23	CLA	c	504	65/65	0.95	0.27	0.39	37,50,89,111	0
33	LMG	b	620	51/55	0.90	0.19	0.39	29,50,88,106	0
23	CLA	b	607	65/65	0.96	0.17	0.37	20,31,53,63	0
23	CLA	c	505	65/65	0.94	0.20	0.36	32,45,68,86	0
23	CLA	a	405	65/65	0.97	0.22	0.35	27,36,105,111	0
34	HTG	B	627	19/19	0.91	0.17	0.35	45,63,74,75	0
23	CLA	b	612	65/65	0.94	0.23	0.34	25,35,48,59	0
23	CLA	B	608	65/65	0.97	0.23	0.32	27,37,51,55	0
23	CLA	b	602	65/65	0.92	0.23	0.31	32,44,60,68	0
25	BCR	A	409	40/40	0.97	0.15	0.29	22,34,46,49	0
25	BCR	b	619	40/40	0.94	0.15	0.28	32,45,61,69	0
33	LMG	B	621	51/55	0.88	0.21	0.28	32,49,79,105	0
39	MG	J	103	1/1	0.98	0.14	0.28	39,39,39,39	0
25	BCR	y	101	40/40	0.92	0.16	0.27	44,54,70,72	0
23	CLA	C	514	65/65	0.89	0.23	0.21	46,64,87,95	0
23	CLA	c	513	65/65	0.90	0.22	0.21	52,73,115,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	SQD	A	410	54/54	0.94	0.15	0.18	38,62,99,105	0
25	BCR	b	617	40/40	0.96	0.14	0.18	20,34,41,44	0
23	CLA	C	508	65/65	0.91	0.25	0.18	36,47,60,70	0
23	CLA	d	404	65/65	0.94	0.17	0.17	38,48,98,109	0
35	LMT	b	621	25/35	0.79	0.24	0.15	60,99,144,148	0
23	CLA	C	502	65/65	0.94	0.22	0.15	34,41,60,77	0
23	CLA	b	609	65/65	0.92	0.17	0.13	36,44,63,82	0
23	CLA	b	611	65/65	0.97	0.19	0.13	25,34,49,61	0
38	HEM	e	103	43/43	0.98	0.19	0.12	48,73,98,105	0
23	CLA	B	616	65/65	0.95	0.21	0.12	30,45,113,124	0
23	CLA	C	504	65/65	0.94	0.27	0.07	36,44,65,75	0
23	CLA	B	606	65/65	0.94	0.15	0.07	26,35,76,99	0
23	CLA	c	512	65/65	0.91	0.20	0.06	48,64,90,96	0
39	MG	j	103	1/1	0.96	0.15	0.05	51,51,51,51	0
23	CLA	A	404	65/65	0.96	0.17	0.04	20,23,41,58	0
23	CLA	d	403	65/65	0.97	0.22	0.04	25,29,49,62	0
27	GOL	b	624	6/6	0.94	0.13	0.03	58,76,78,86	0
25	BCR	c	515	40/40	0.96	0.14	0.03	37,52,65,75	0
25	BCR	K	102	40/40	0.94	0.17	0.02	39,47,62,65	0
23	CLA	D	404	65/65	0.96	0.17	-0.04	20,26,46,52	0
23	CLA	B	609	65/65	0.92	0.17	-0.05	29,39,53,63	0
23	CLA	B	614	65/65	0.92	0.18	-0.08	21,31,82,100	0
23	CLA	A	406	65/65	0.97	0.14	-0.09	22,29,80,89	0
23	CLA	b	613	65/65	0.97	0.23	-0.10	22,33,67,78	0
23	CLA	c	507	65/65	0.92	0.18	-0.12	41,53,65,68	0
23	CLA	c	506	65/65	0.96	0.14	-0.14	44,58,90,111	0
23	CLA	C	512	65/65	0.91	0.18	-0.15	36,52,73,84	0
23	CLA	d	401	65/65	0.97	0.15	-0.17	23,26,48,75	0
25	BCR	a	409	40/40	0.97	0.14	-0.17	24,35,45,49	0
23	CLA	b	606	65/65	0.95	0.14	-0.17	27,42,77,106	0
23	CLA	C	505	65/65	0.94	0.21	-0.20	30,41,79,104	0
23	CLA	b	614	65/65	0.95	0.14	-0.22	23,34,76,89	0
25	BCR	k	101	40/40	0.94	0.16	-0.28	47,55,79,81	0
38	HEM	v	201	43/43	0.98	0.13	-0.32	40,50,59,66	0
23	CLA	a	404	65/65	0.97	0.17	-0.39	25,30,50,60	0
37	CA	c	523	1/1	0.94	0.17	-0.40	68,68,68,68	0
23	CLA	b	615	65/65	0.93	0.17	-0.40	29,40,66,81	0
34	HTG	b	625	19/19	0.93	0.11	-0.42	43,56,83,93	0
23	CLA	C	507	65/65	0.93	0.15	-0.49	39,55,102,106	0
22	CL	a	403	1/1	0.98	0.19	-0.53	34,34,34,34	0
25	BCR	C	515	40/40	0.94	0.15	-0.54	46,61,72,73	0
32	BCT	a	418	4/4	0.99	0.10	-0.54	45,52,54,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	CA	C	524	1/1	0.98	0.24	-0.58	62,62,62,62	0
38	HEM	V	202	43/43	0.98	0.11	-0.59	30,33,44,53	0
23	CLA	B	615	65/65	0.95	0.14	-0.60	27,34,61,68	0
38	HEM	E	103	43/43	0.98	0.09	-0.71	40,54,66,73	0
23	CLA	b	616	65/65	0.92	0.18	-0.76	31,46,98,105	0
25	BCR	c	514	40/40	0.95	0.13	-0.84	52,65,76,79	0
32	BCT	A	418	4/4	0.99	0.08	-1.18	34,39,47,65	0
28	OEX	A	413	10/10	0.99	0.09	-1.60	22,30,43,45	0
37	CA	c	524	1/1	0.97	0.09	-1.85	66,66,66,66	0
22	CL	a	402	1/1	0.99	0.10	-1.95	31,31,31,31	0
28	OEX	a	413	10/10	1.00	0.09	-2.11	27,34,45,53	0
21	FE2	a	401	1/1	0.99	0.06	-2.13	45,45,45,45	0
37	CA	O	301	1/1	0.93	0.11	-2.28	87,87,87,87	0
22	CL	A	402	1/1	0.99	0.07	-2.64	24,24,24,24	0
37	CA	o	301	1/1	0.95	0.10	-3.41	85,85,85,85	0
21	FE2	A	401	1/1	0.99	0.04	-4.79	42,42,42,42	0
30	UNL	c	525	32/-	0.73	0.31	-	71,97,113,119	0
34	HTG	B	624	19/19	0.63	0.68	-	57,104,140,144	0
30	UNL	a	415	30/-	0.61	0.50	-	72,90,111,118	0
30	UNL	A	415	28/-	0.19	0.56	-	67,87,108,112	0
37	CA	V	201	1/1	0.93	0.14	-	93,93,93,93	0
30	UNL	m	101	10/-	0.75	0.30	-	40,50,55,56	0
30	UNL	B	628	33/-	0.68	0.28	-	29,76,136,139	0
30	UNL	b	626	33/-	0.58	0.43	-	44,78,131,135	0
34	HTG	c	521	19/19	0.78	0.36	-	68,112,134,140	0
30	UNL	M	102	10/-	0.85	0.26	-	33,52,59,69	0
34	HTG	C	521	19/19	0.78	0.41	-	66,101,116,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.