



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2018 – 10:04 PM EST

PDB ID : 2WSF
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.48 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

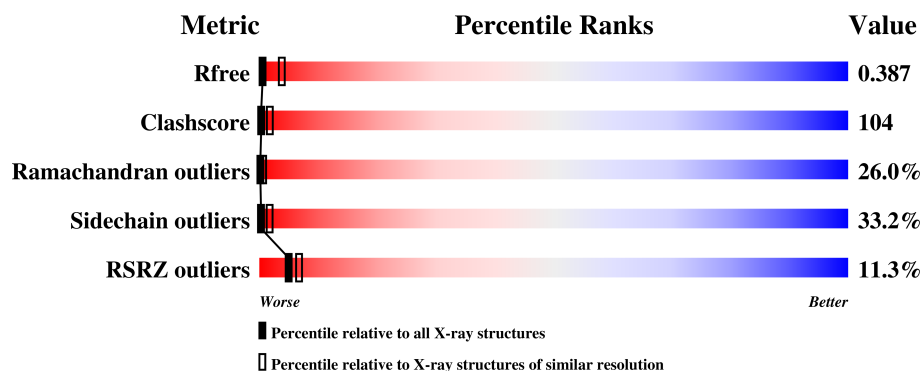
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	111664	1159 (3.56-3.40)
Clashscore	122126	1235 (3.56-3.40)
Ramachandran outliers	120053	1202 (3.56-3.40)
Sidechain outliers	120020	1203 (3.56-3.40)
RSRZ outliers	108989	1080 (3.56-3.40)

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	1	241	<div> <div>16%</div> <div> <div>27%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>32%</div> </div> </div>
2	2	269	<div> <div>13%</div> <div> <div>10%</div> <div>23%</div> <div>23%</div> <div>10%</div> <div>35%</div> </div> </div>
3	3	276	<div> <div>11%</div> <div> <div>15%</div> <div>21%</div> <div>13%</div> <div>5%</div> <div>45%</div> </div> </div>
4	4	251	<div> <div>6%</div> <div> <div>7%</div> <div>22%</div> <div>25%</div> <div>12%</div> <div>34%</div> </div> </div>
5	A	758	<div> <div>7%</div> <div> <div>10%</div> <div>50%</div> <div>30%</div> <div>7%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	

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
19	CLA	1	201	X	-	-	-
19	CLA	1	202	X	-	-	-
19	CLA	1	203	X	-	-	-
19	CLA	1	204	X	-	-	-
19	CLA	1	205	X	-	-	-
19	CLA	1	206	X	-	-	-
19	CLA	1	207	X	-	-	-
19	CLA	1	208	X	-	-	-
19	CLA	1	209	X	-	-	-
19	CLA	1	210	X	-	-	-
19	CLA	1	211	X	-	-	X
19	CLA	1	212	X	-	-	-
19	CLA	1	213	X	-	-	-
19	CLA	1	214	X	-	-	-
19	CLA	1	215	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	301	X	-	-	X
19	CLA	2	302	X	-	-	-
19	CLA	2	303	X	-	X	-
19	CLA	2	304	X	-	-	X
19	CLA	2	305	X	-	-	-
19	CLA	2	306	X	-	-	-
19	CLA	2	307	X	-	X	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	X	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-
19	CLA	2	315	X	-	-	-
19	CLA	2	316	X	-	-	-
19	CLA	2	317	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	302	X	-	-	X
19	CLA	3	303	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	306	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	X
19	CLA	3	313	X	-	-	X
19	CLA	3	314	X	-	-	X
19	CLA	3	315	X	-	-	-
19	CLA	3	316	X	-	-	X
19	CLA	3	317	X	-	-	-
19	CLA	3	318	X	-	-	-
19	CLA	4	301	X	-	X	-
19	CLA	4	302	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	304	X	-	X	-
19	CLA	4	305	X	-	-	X
19	CLA	4	306	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	314	X	-	-	-
19	CLA	4	315	X	-	-	-
19	CLA	4	317	X	-	-	X
19	CLA	4	318	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	X
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	X	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	X	-
19	CLA	A	808	X	-	X	-
19	CLA	A	809	X	-	X	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	X	X
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	X	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	X	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	X	-
19	CLA	A	819	X	-	X	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	X	-
19	CLA	A	825	X	-	X	-
19	CLA	A	826	X	-	X	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	X	-
19	CLA	A	831	X	-	X	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	X	-
19	CLA	A	839	X	-	X	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	849	X	-	X	-
19	CLA	A	850	X	-	X	-
19	CLA	A	851	X	-	X	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	X	-
19	CLA	B	806	X	-	X	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	X	-
19	CLA	B	809	X	-	X	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	X	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	X
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	X	-
19	CLA	B	825	X	-	X	-
19	CLA	B	826	X	-	X	-
19	CLA	B	827	X	-	X	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	X	-
19	CLA	B	830	X	-	X	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	X	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	X	-
19	CLA	B	835	X	-	X	-
19	CLA	B	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	X	-
19	CLA	B	839	X	-	X	-
19	CLA	B	840	X	-	-	-
19	CLA	B	841	X	-	-	-
19	CLA	B	842	X	-	-	-
19	CLA	B	850	X	-	-	-
19	CLA	F	201	X	-	X	-
19	CLA	F	205	X	-	-	-
19	CLA	F	206	X	-	-	-
19	CLA	F	207	X	-	-	-
19	CLA	G	105	X	-	-	X
19	CLA	H	101	X	-	-	X
19	CLA	H	102	X	-	-	-
19	CLA	H	111	X	-	X	-
19	CLA	H	112	X	-	-	-
19	CLA	I	102	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	K	101	X	-	-	-
19	CLA	K	102	X	-	X	-
19	CLA	K	103	X	-	-	-
19	CLA	K	104	X	-	-	-
19	CLA	L	201	X	-	X	-
19	CLA	L	202	X	-	-	X
19	CLA	L	203	X	-	X	-
19	CLA	L	204	X	-	-	X
19	CLA	L	208	X	-	-	-
19	CLA	L	209	X	-	X	-
19	CLA	L	210	X	-	-	-
19	CLA	R	107	X	-	-	-
19	CLA	R	108	X	-	-	-
20	LMU	2	313	-	-	X	-
20	LMU	A	852	-	-	-	X
20	LMU	A	853	-	-	X	-
20	LMU	G	101	-	-	X	-
20	LMU	K	107	-	-	X	-
21	SUC	1	219	X	-	-	-
21	SUC	2	314	X	-	X	-
21	SUC	2	323	X	-	X	-
21	SUC	3	312	X	-	-	-
21	SUC	3	321	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SUC	4	322	X	-	-	-
21	SUC	A	857	X	-	-	-
21	SUC	B	851	X	-	-	-
21	SUC	H	107	X	-	-	-
21	SUC	H	108	X	-	-	X
21	SUC	H	110	X	-	X	-
21	SUC	H	113	X	-	X	-
21	SUC	L	207	X	-	-	-
22	BCR	2	318	-	-	-	X
22	BCR	A	843	-	-	X	X
22	BCR	A	844	-	-	X	-
22	BCR	A	845	-	-	X	-
22	BCR	B	801	-	-	X	-
22	BCR	B	846	-	-	X	-
22	BCR	B	847	-	-	X	-
22	BCR	F	203	-	-	X	-
22	BCR	F	204	-	-	X	-
22	BCR	G	104	-	-	-	X
22	BCR	I	103	-	-	X	X
22	BCR	J	102	-	-	X	-
22	BCR	L	211	-	-	X	X
23	PQN	A	842	X	-	-	-
23	PQN	B	843	X	-	X	-
24	SF4	A	856	-	-	X	-
24	SF4	C	102	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	153	Total	C	N	O	S	0	0	0
			1186	781	193	207	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

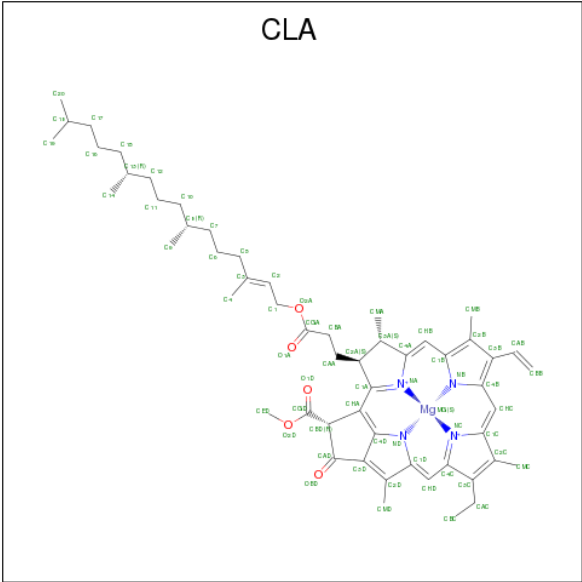
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			42	34	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			36	30	1	4		
19	4	1	Total	C	Mg	N	0	0
			55	45	1	4		
19	4	1	Total	C	Mg	N	0	0
			36	30	1	4		
19	4	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	4	1	Total	C	Mg	N	0	0
			55	45	1	4		
19	4	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	4	1	Total	C	Mg	N	0	0
			52	42	1	4		
19	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	4	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total 25	C 20	Mg 1	N 4	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
19	A	1	Total 52	C 42	Mg 1	N 4 O 5	0	0
19	A	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
19	A	1	Total 58	C 48	Mg 1	N 4 O 5	0	0
19	A	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
19	A	1	Total 42	C 34	Mg 1	N 4 O 3	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 58	C 48	Mg 1	N 4 O 5	0	0
19	A	1	Total 59	C 49	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 45	C 35	Mg 1	N 4 O 5	0	0
19	A	1	Total 46	C 36	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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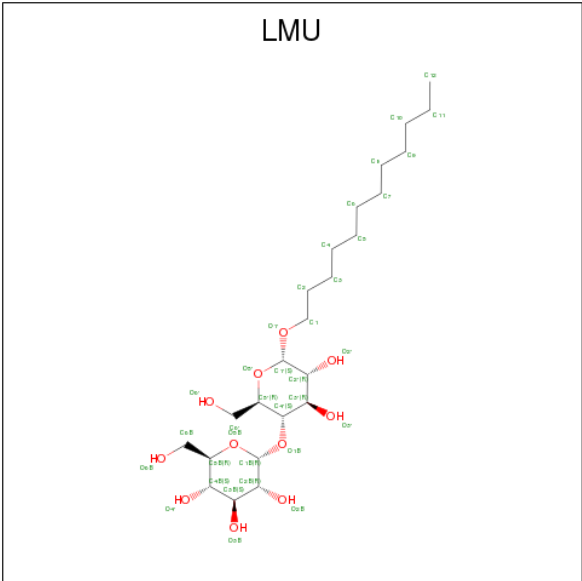
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	3	1	Total	C	O	0	0
			35	24	11		
20	3	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			34	23	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			35	24	11		

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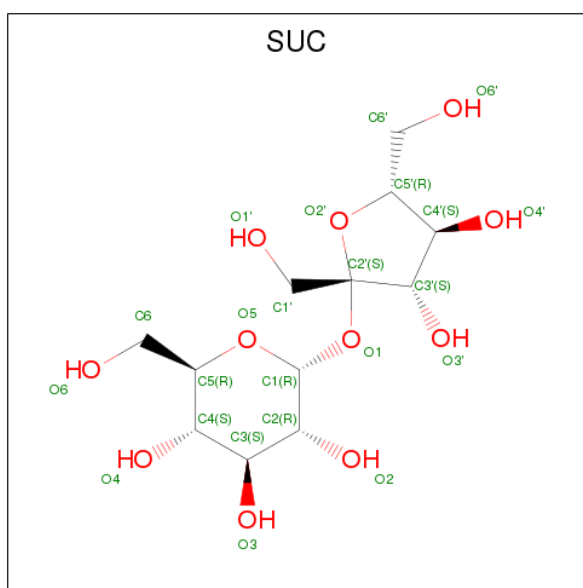
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			25	14	11		
20	C	1	Total	C	O	0	0
			35	24	11		
20	D	1	Total	C	O	0	0
			35	24	11		
20	E	1	Total	C	O	0	0
			35	24	11		
20	F	1	Total	C	O	0	0
			34	23	11		
20	G	1	Total	C	O	0	0
			35	24	11		
20	G	1	Total	C	O	0	0
			35	24	11		
20	G	1	Total	C	O	0	0
			35	24	11		
20	H	1	Total	C	O	0	0
			35	24	11		
20	H	1	Total	C	O	0	0
			35	24	11		
20	H	1	Total	C	O	0	0
			35	24	11		
20	H	1	Total	C	O	0	0
			35	24	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 21 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



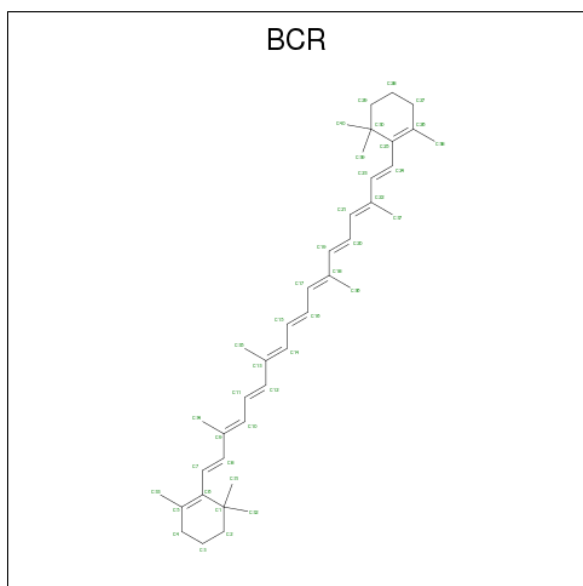
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			23	12	11		
21	2	1	Total	C	O	0	0
			22	12	10		
21	2	1	Total	C	O	0	0
			23	12	11		
21	3	1	Total	C	O	0	0
			23	12	11		
21	3	1	Total	C	O	0	0
			23	12	11		
21	4	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			22	12	10		
21	H	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	L	1	Total	C	O	0	0
			23	12	11		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



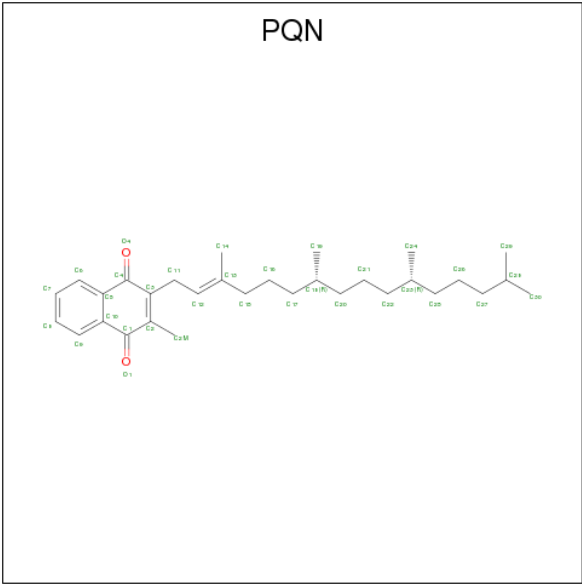
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	2	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		

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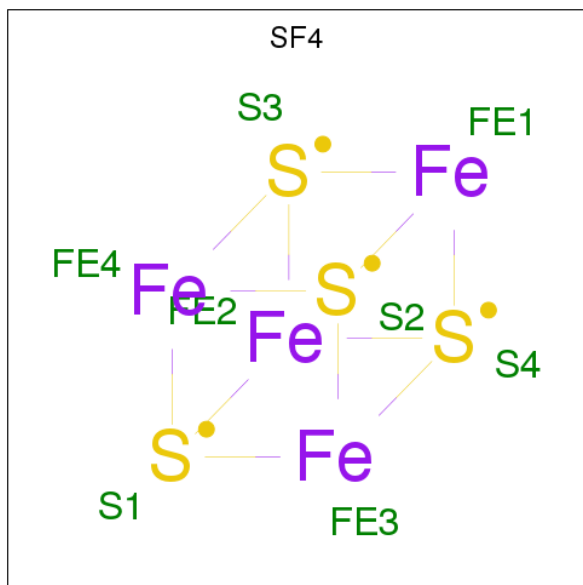
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	I	1	Total C 39 39	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



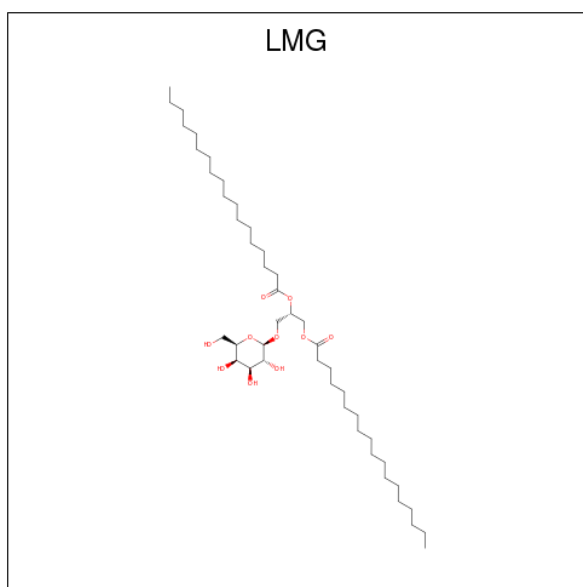
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			33	31	2		
23	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 25 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
25	B	1	Total	C	O	0	0
			49	39	10		

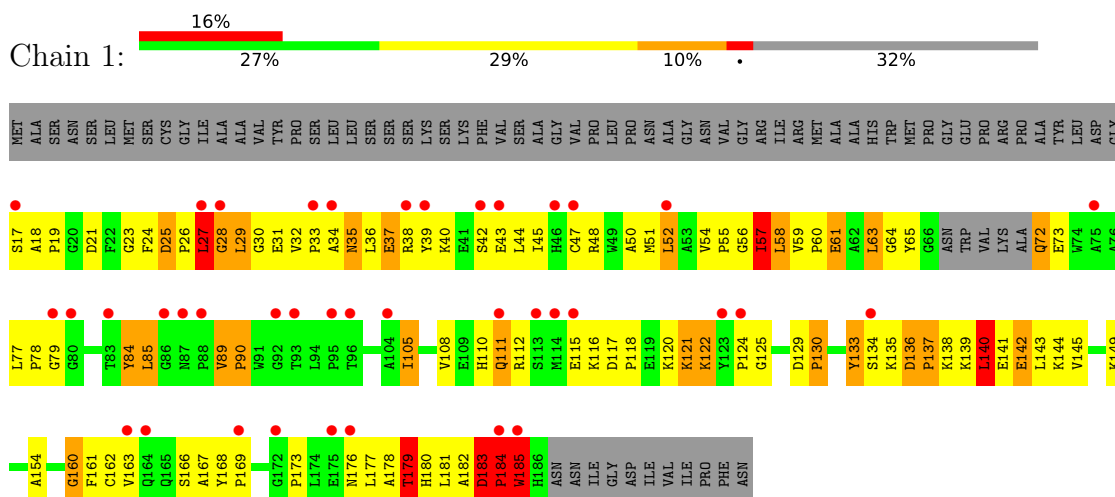
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

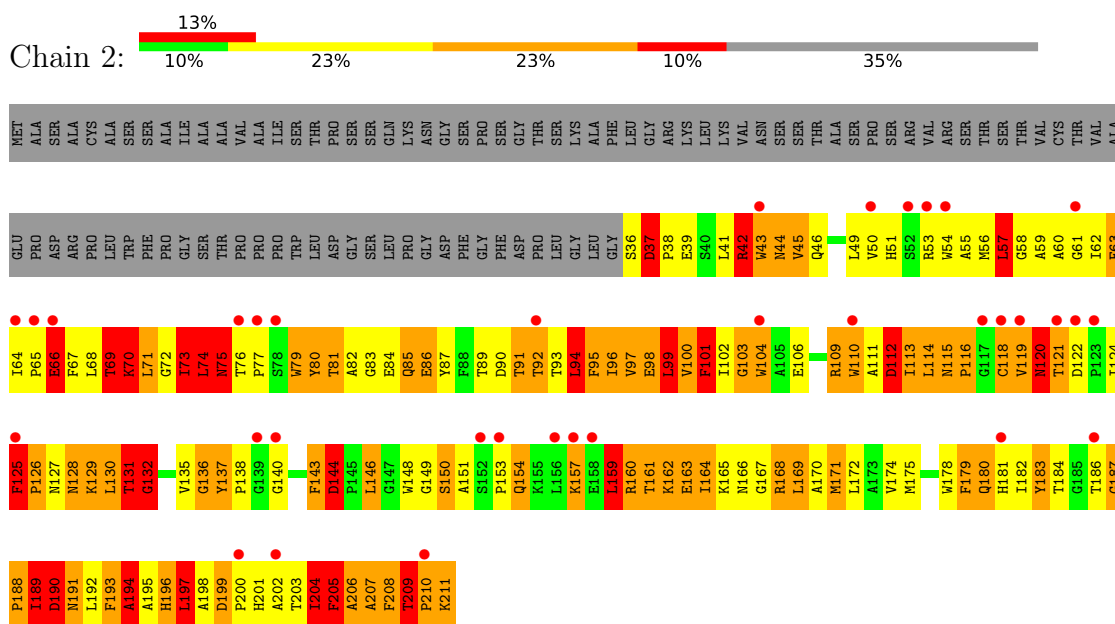
3 Residue-property plots

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

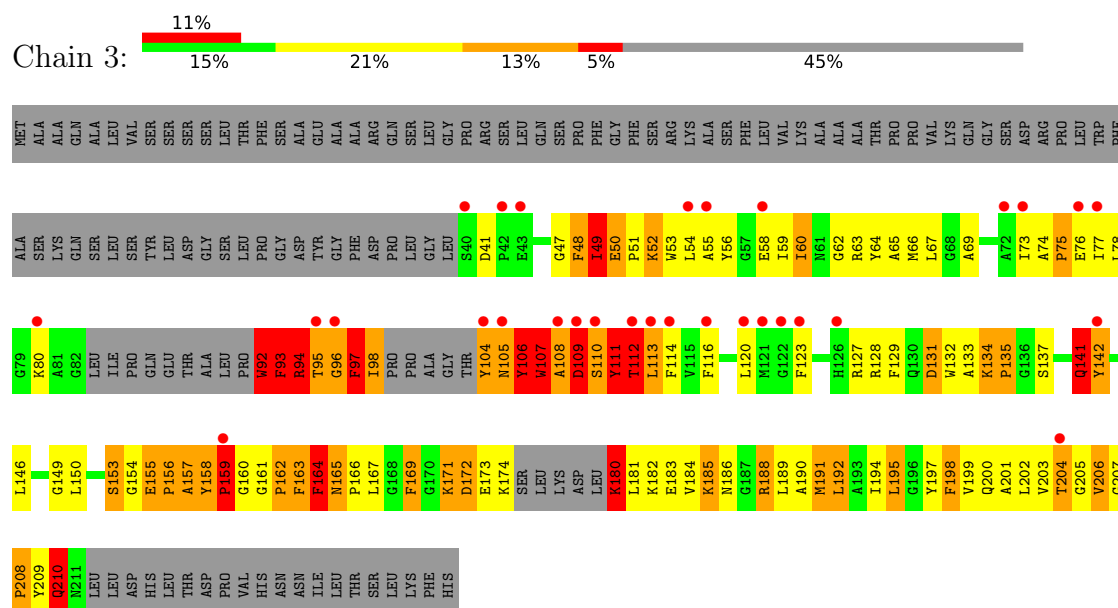
• Molecule 1: AT3G54890



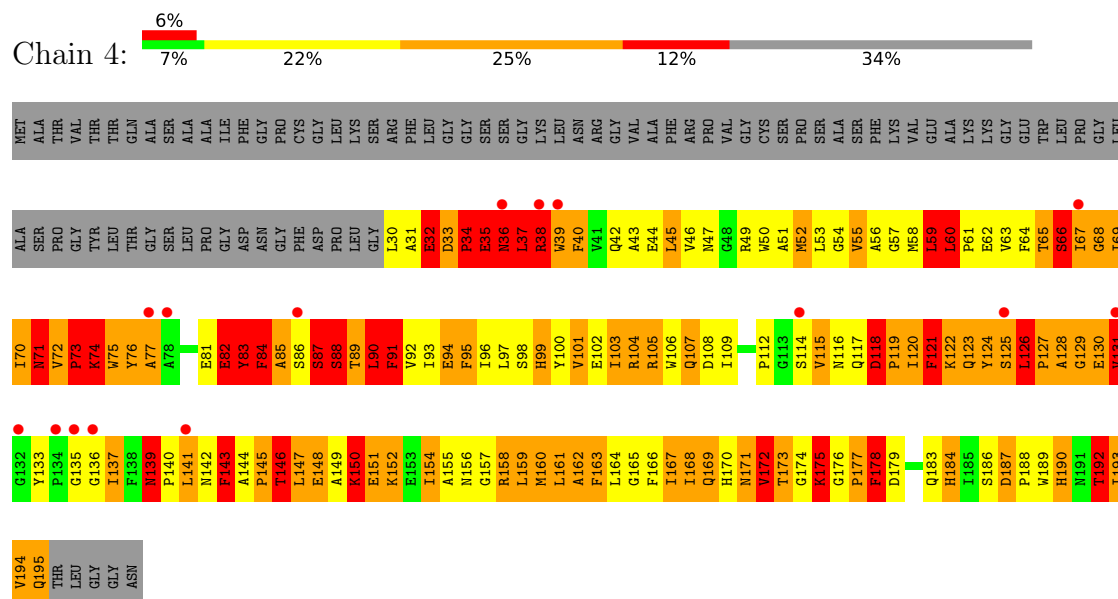
• Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



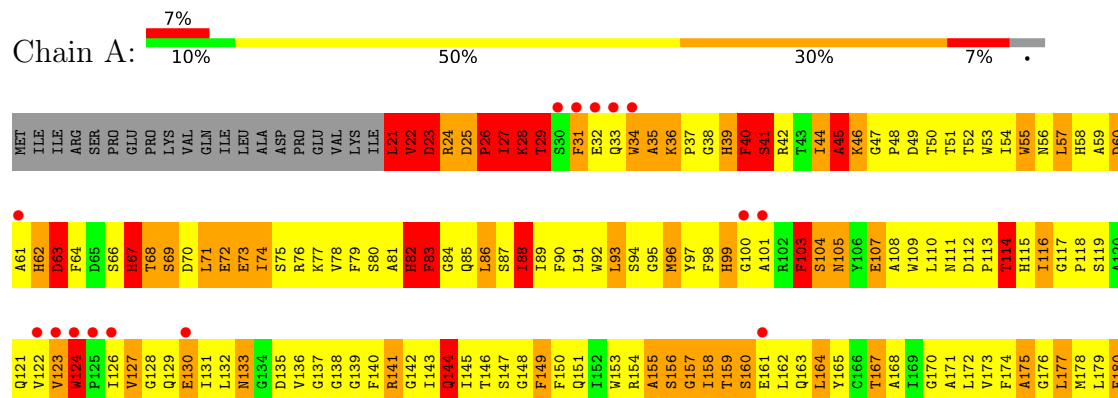
• Molecule 3: LHCA3

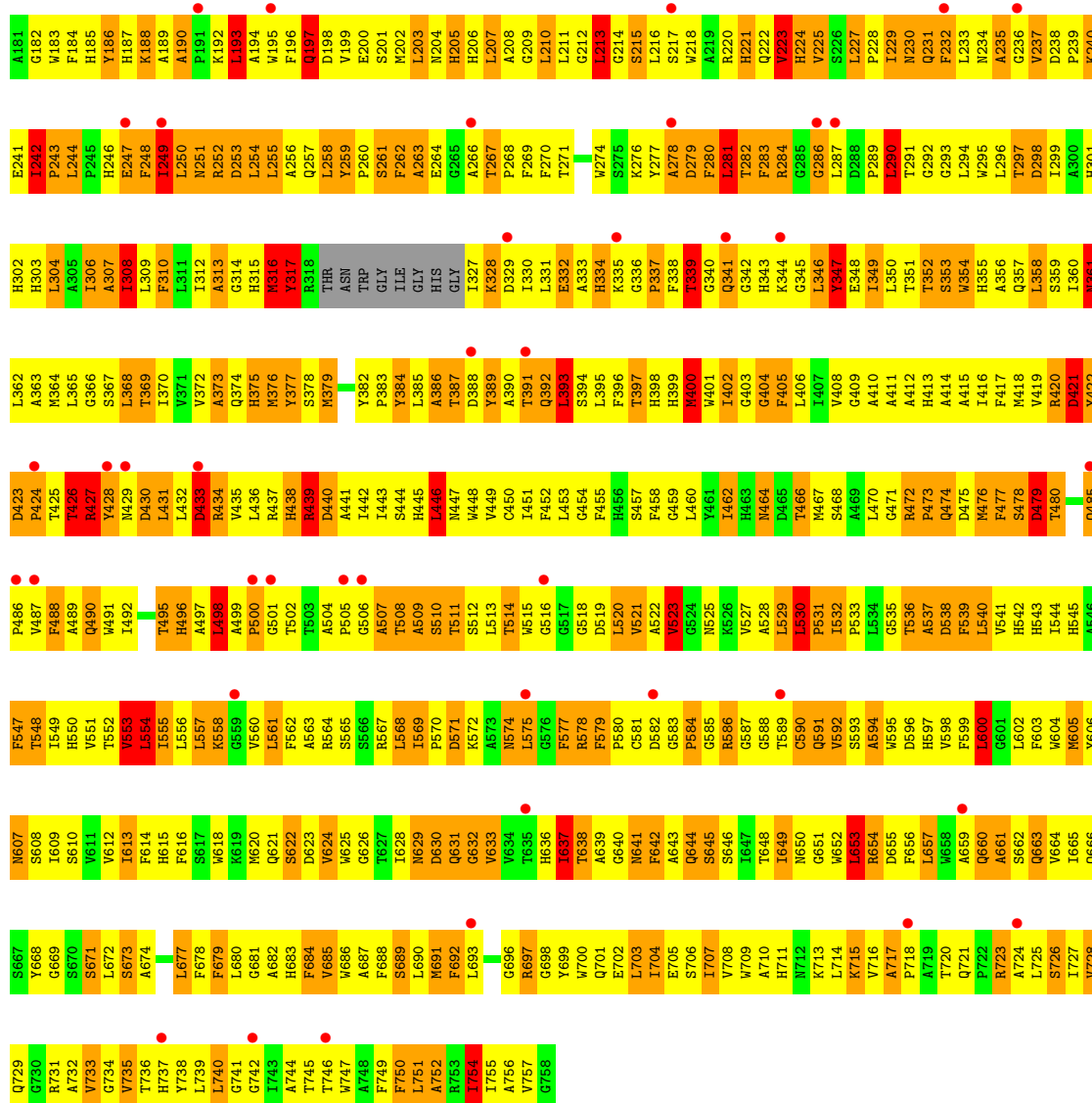


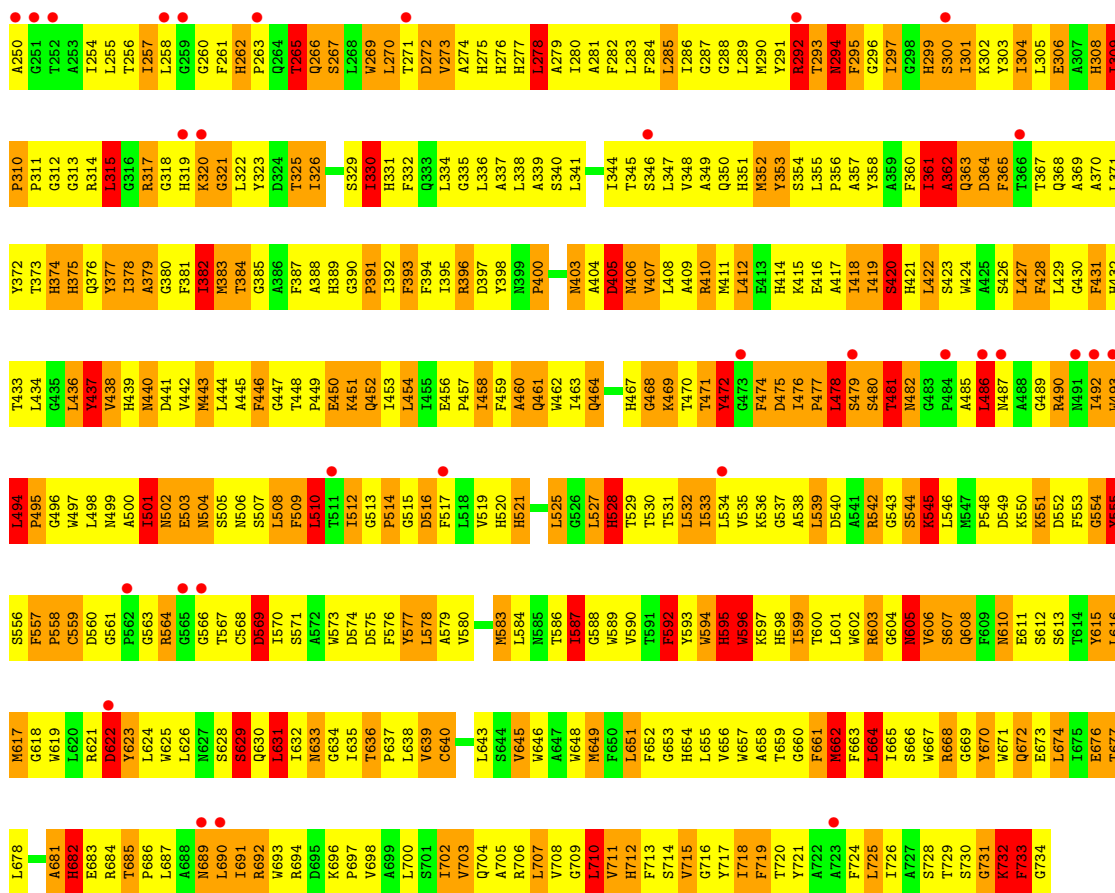
- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



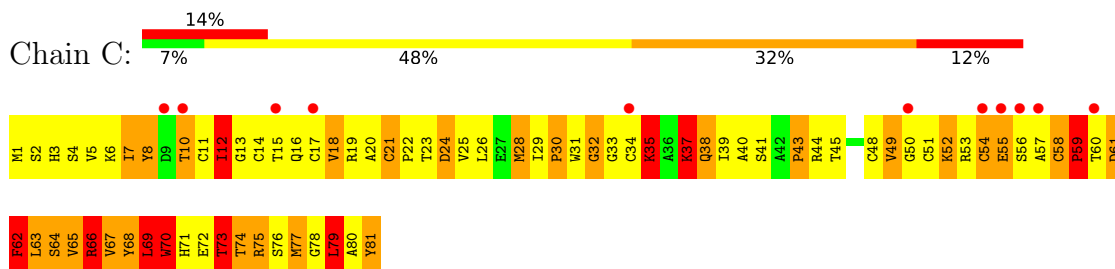
- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



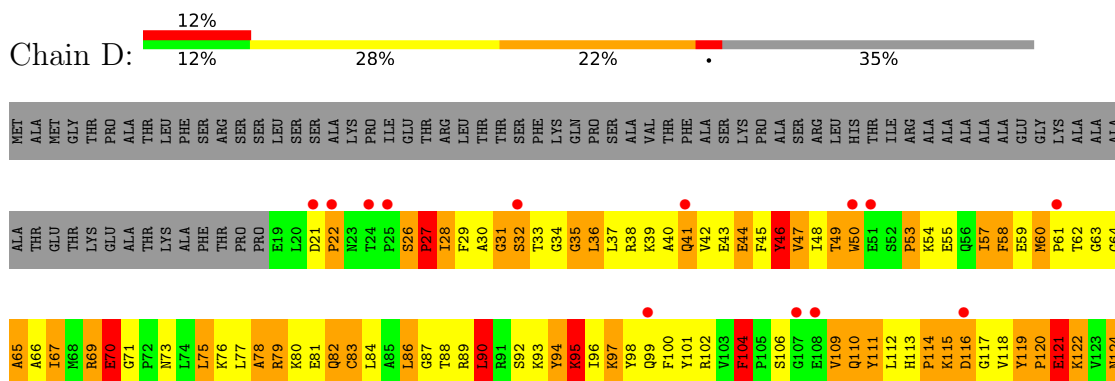


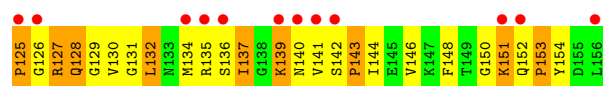


• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

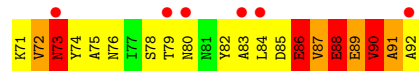
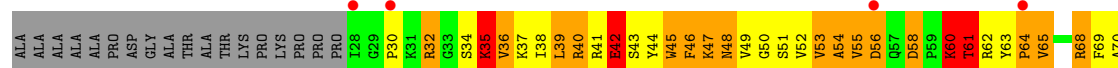
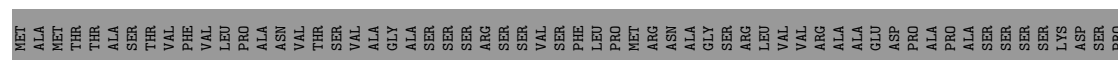
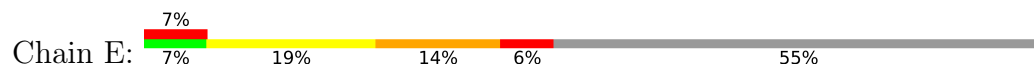


• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

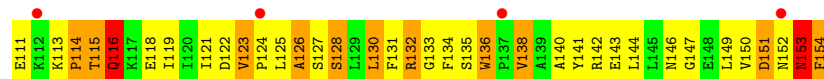
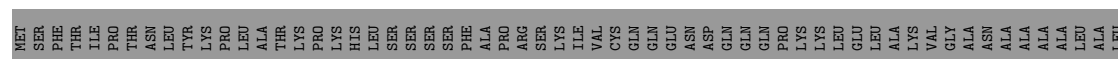




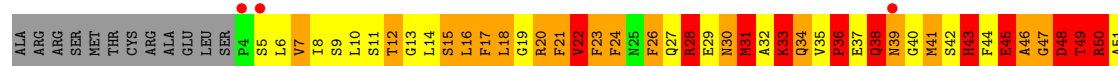
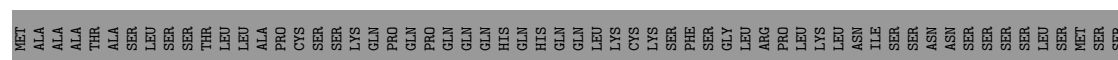
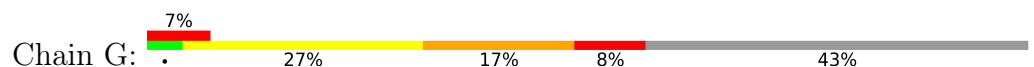
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



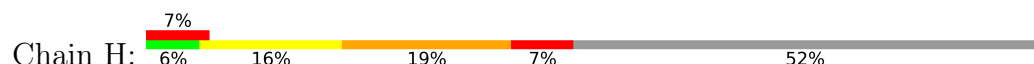
• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

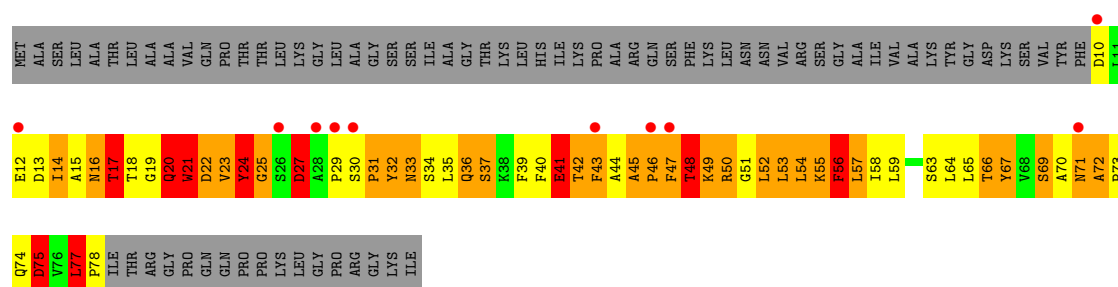


• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

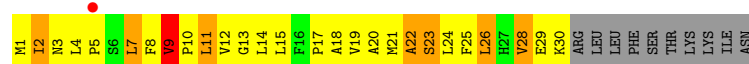


• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC

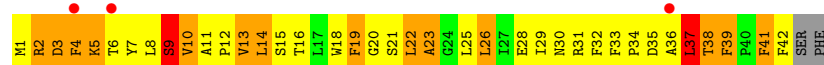




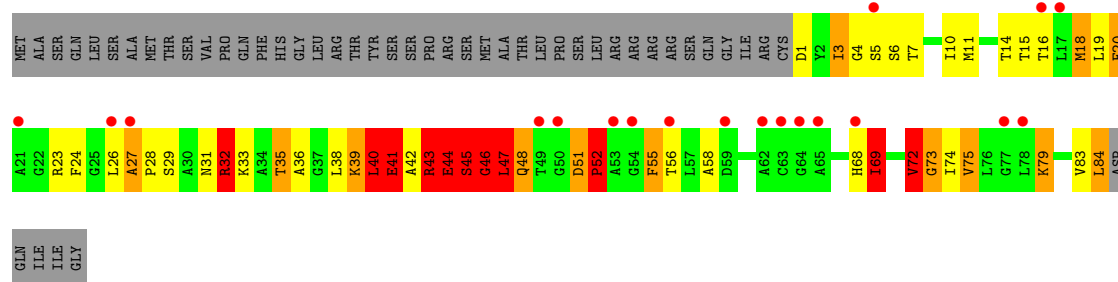
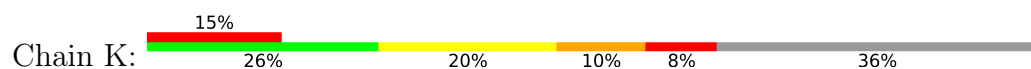
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



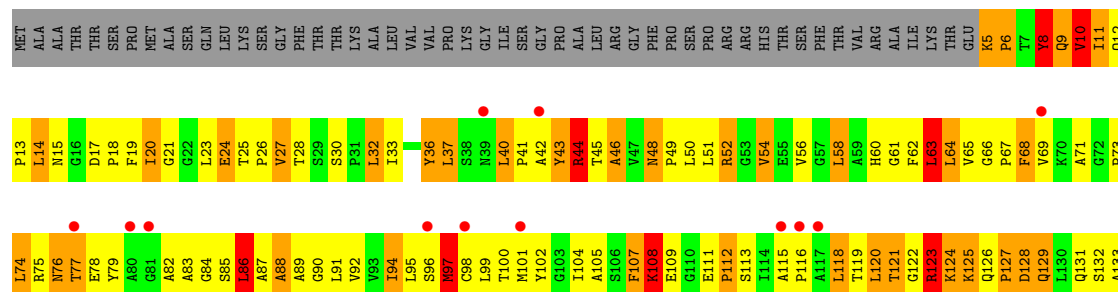
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

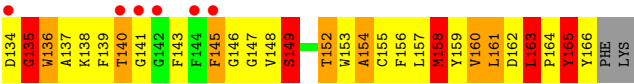


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

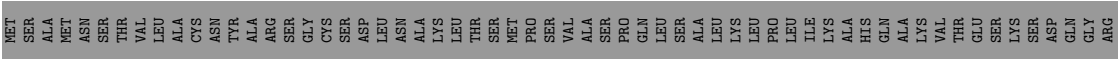
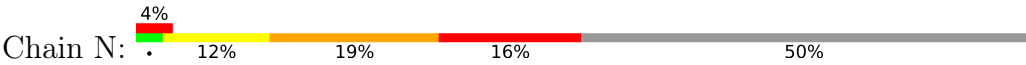


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

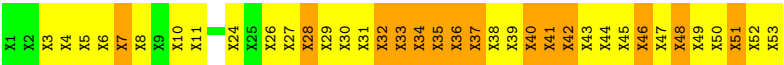
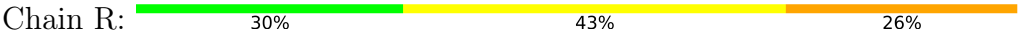




● Molecule 17: PHOTOSYSTEM I-N SUBUNIT



● Molecule 18: PHOTOSYSTEM I-N SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.391 , 0.425 0.383 , 0.387	Depositor DCC
R_{free} test set	1456 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SUC, SF4, CLA, PQN, LMU, UNL, 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	1	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1264	0	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	293	16
4	4	1319	0	1282	610	5
5	A	5745	0	5597	1351	0
6	B	5848	0	5655	1211	15
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	129	0
10	F	1221	0	1249	201	0
11	G	740	0	708	191	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	5
17	N	685	0	668	321	1
18	R	265	0	68	78	0
19	1	617	0	388	89	1
19	2	650	0	465	147	0
19	3	620	0	362	75	0
19	4	694	0	443	167	0
19	A	2346	0	2062	726	0
19	B	2226	0	2061	684	0
19	F	180	0	123	46	0
19	G	51	0	40	4	0
19	H	223	0	197	57	0
19	I	60	0	58	12	0
19	J	109	0	95	26	0
19	K	202	0	158	54	1
19	L	382	0	335	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	R	122	0	123	14	0
20	1	105	0	137	32	0
20	2	175	0	230	45	0
20	3	70	0	92	16	0
20	4	139	0	179	24	3
20	A	245	0	322	53	0
20	B	95	0	115	11	0
20	C	35	0	46	0	0
20	D	35	0	46	3	0
20	E	35	0	46	11	0
20	F	34	0	41	8	0
20	G	105	0	138	27	41
20	H	140	0	184	42	0
20	K	105	0	138	41	0
20	L	105	0	138	2	0
20	R	245	0	322	43	3
21	1	23	0	22	0	0
21	2	45	0	41	21	0
21	3	46	0	44	8	0
21	4	23	0	22	3	0
21	A	23	0	22	1	0
21	B	23	0	22	4	0
21	H	91	0	85	24	41
21	L	23	0	22	4	0
22	2	40	0	54	9	0
22	A	120	0	162	103	0
22	B	200	0	270	114	0
22	F	80	0	108	60	0
22	G	40	0	54	5	0
22	I	79	0	105	46	0
22	J	40	0	54	36	0
22	L	40	0	54	36	0
23	A	33	0	46	7	0
23	B	33	0	46	28	0
24	A	8	0	0	18	0
24	C	16	0	0	5	0
25	B	49	0	71	17	0
26	H	23	0	0	1	0
All	All	36033	0	34517	7362	69

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 104.

The worst 5 of 7362 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)
4:4:160:MET:CE	19:4:306:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	19:1:213:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55

The worst 5 of 69 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:101:LMU:C5B	21:H:110:SUC:O1[1_654]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64
20:G:101:LMU:O4'	21:H:110:SUC:O2[1_654]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1_556]	1.05	1.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0	1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0	0
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	1
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	1
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	0
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	1
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	1
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	0

5 of 803 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

5.3.2 Protein sidechains [i](#)

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	1	127/190 (67%)	100 (79%)	27 (21%)	1	5
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	1
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	2
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	2
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	2
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	2
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	2
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	1
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	2
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	3	16
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	2
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	2
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	2
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	1
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	2

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	121	TYR
6	B	438	VAL
16	L	14	LEU
6	B	142	LEU
6	B	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	67	HIS
6	B	333	GLN
15	K	80	ASN
6	B	71	GLN
6	B	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 1 is unknown - leaving 256 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	$\# Z > 2$
19	CLA	1	201	-	39,54,73	2.33	12 (30%)	44,90,113	3.29	20 (45%)
19	CLA	1	202	-	34,49,73	2.50	11 (32%)	38,84,113	3.32	16 (42%)
19	CLA	1	203	-	40,55,73	2.46	14 (35%)	45,91,113	4.14	18 (40%)
19	CLA	1	204	-	39,54,73	2.46	11 (28%)	44,90,113	3.62	20 (45%)
19	CLA	1	205	-	29,44,73	2.76	10 (34%)	36,78,113	4.24	15 (41%)
19	CLA	1	206	-	54,69,73	2.08	11 (20%)	61,108,113	2.70	21 (34%)
19	CLA	1	207	-	44,59,73	2.35	14 (31%)	49,96,113	3.58	20 (40%)
19	CLA	1	208	-	19,32,73	1.81	4 (21%)	24,54,113	3.00	14 (58%)
19	CLA	1	209	-	19,32,73	2.05	6 (31%)	24,54,113	3.21	14 (58%)
19	CLA	1	210	1	29,44,73	2.59	10 (34%)	36,78,113	4.24	14 (38%)
19	CLA	1	211	-	44,59,73	2.54	15 (34%)	49,96,113	3.62	21 (42%)
19	CLA	1	212	-	19,32,73	1.93	6 (31%)	24,54,113	3.04	13 (54%)
19	CLA	1	213	-	44,59,73	2.52	15 (34%)	49,96,113	4.17	23 (46%)
19	CLA	1	214	-	19,32,73	1.91	5 (26%)	24,54,113	3.26	13 (54%)
19	CLA	1	215	-	44,59,73	2.37	13 (29%)	49,96,113	3.72	18 (36%)
20	LMU	1	216	-	36,36,36	0.45	0	47,47,47	1.37	6 (12%)
20	LMU	1	217	-	36,36,36	0.56	0	47,47,47	0.97	1 (2%)
20	LMU	1	218	-	36,36,36	0.69	0	47,47,47	1.64	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SUC	1	219	-	24,24,24	0.45	0	36,36,36	1.23	2 (5%)
19	CLA	2	301	-	19,32,73	1.88	6 (31%)	24,54,113	3.05	14 (58%)
19	CLA	2	302	-	44,59,73	2.37	12 (27%)	49,96,113	3.32	20 (40%)
19	CLA	2	303	-	51,66,73	2.21	13 (25%)	57,104,113	3.38	20 (35%)
19	CLA	2	304	-	19,32,73	2.03	8 (42%)	24,54,113	3.11	13 (54%)
19	CLA	2	305	-	43,58,73	2.27	10 (23%)	48,95,113	2.92	16 (33%)
19	CLA	2	306	-	19,32,73	1.88	6 (31%)	24,54,113	2.65	13 (54%)
19	CLA	2	307	-	58,73,73	1.97	11 (18%)	66,113,113	2.97	19 (28%)
19	CLA	2	308	-	19,32,73	2.08	9 (47%)	24,54,113	3.31	13 (54%)
19	CLA	2	309	-	19,32,73	2.02	7 (36%)	24,54,113	2.93	13 (54%)
19	CLA	2	310	2	43,58,73	2.38	13 (30%)	48,95,113	3.49	19 (39%)
19	CLA	2	311	-	43,58,73	2.27	11 (25%)	48,95,113	3.58	22 (45%)
19	CLA	2	312	-	54,69,73	2.06	12 (22%)	61,108,113	3.13	25 (40%)
20	LMU	2	313	-	36,36,36	0.51	0	47,47,47	1.57	6 (12%)
21	SUC	2	314	-	23,23,24	0.61	0	35,35,36	1.42	4 (11%)
19	CLA	2	315	-	43,58,73	2.43	13 (30%)	48,95,113	3.13	17 (35%)
19	CLA	2	316	-	19,32,73	1.86	5 (26%)	24,54,113	2.69	12 (50%)
19	CLA	2	317	-	58,73,73	2.02	14 (24%)	66,113,113	3.16	20 (30%)
22	BCR	2	318	-	41,41,41	1.98	3 (7%)	56,56,56	5.72	20 (35%)
20	LMU	2	319	-	36,36,36	0.56	0	47,47,47	0.67	0
20	LMU	2	320	-	36,36,36	0.81	1 (2%)	47,47,47	1.55	11 (23%)
20	LMU	2	321	-	36,36,36	0.45	0	47,47,47	1.26	3 (6%)
20	LMU	2	322	-	36,36,36	0.80	1 (2%)	47,47,47	1.17	4 (8%)
21	SUC	2	323	-	24,24,24	0.53	0	36,36,36	1.22	2 (5%)
19	CLA	3	301	-	29,44,73	2.60	10 (34%)	36,78,113	4.42	16 (44%)
19	CLA	3	302	-	19,32,73	1.91	5 (26%)	24,54,113	2.90	13 (54%)
19	CLA	3	303	-	29,44,73	2.69	9 (31%)	36,78,113	4.24	16 (44%)
19	CLA	3	304	-	19,32,73	1.90	7 (36%)	24,54,113	3.10	14 (58%)
19	CLA	3	305	-	19,32,73	1.83	5 (26%)	24,54,113	2.87	11 (45%)
19	CLA	3	306	-	19,32,73	1.85	5 (26%)	24,54,113	3.07	14 (58%)
19	CLA	3	307	-	35,50,73	2.49	10 (28%)	39,85,113	3.92	18 (46%)
19	CLA	3	308	-	19,32,73	1.85	5 (26%)	24,54,113	3.18	15 (62%)
19	CLA	3	309	-	19,32,73	1.94	7 (36%)	24,54,113	3.37	14 (58%)
19	CLA	3	310	-	58,73,73	1.99	12 (20%)	66,113,113	3.20	25 (37%)
19	CLA	3	311	-	58,73,73	1.97	12 (20%)	66,113,113	2.70	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SUC	3	312	-	24,24,24	0.52	0	36,36,36	1.46	5 (13%)
19	CLA	3	313	-	19,32,73	1.92	4 (21%)	24,54,113	3.07	14 (58%)
19	CLA	3	314	-	43,58,73	2.28	9 (20%)	48,95,113	2.64	18 (37%)
19	CLA	3	315	-	58,73,73	1.95	13 (22%)	66,113,113	3.06	19 (28%)
19	CLA	3	316	-	19,32,73	2.09	8 (42%)	24,54,113	3.28	14 (58%)
19	CLA	3	317	-	19,32,73	1.91	6 (31%)	24,54,113	3.12	13 (54%)
19	CLA	3	318	-	29,44,73	2.63	9 (31%)	36,78,113	4.38	17 (47%)
20	LMU	3	319	-	36,36,36	0.48	0	47,47,47	0.71	1 (2%)
20	LMU	3	320	-	36,36,36	0.43	0	47,47,47	1.10	4 (8%)
21	SUC	3	321	-	24,24,24	0.58	0	36,36,36	0.99	3 (8%)
19	CLA	4	301	-	48,63,73	2.20	12 (25%)	54,101,113	2.96	16 (29%)
19	CLA	4	302	-	29,44,73	2.80	11 (37%)	36,78,113	4.48	17 (47%)
19	CLA	4	303	-	58,73,73	2.07	14 (24%)	66,113,113	3.25	22 (33%)
19	CLA	4	304	-	48,63,73	2.13	11 (22%)	54,101,113	2.79	18 (33%)
19	CLA	4	305	-	43,58,73	2.36	13 (30%)	48,95,113	3.51	19 (39%)
19	CLA	4	306	-	45,60,73	2.39	14 (31%)	50,97,113	3.91	29 (58%)
19	CLA	4	307	-	19,32,73	1.94	6 (31%)	24,54,113	3.01	13 (54%)
19	CLA	4	308	-	19,32,73	1.96	8 (42%)	24,54,113	3.26	14 (58%)
19	CLA	4	309	-	19,32,73	1.85	4 (21%)	24,54,113	3.01	13 (54%)
19	CLA	4	310	-	43,58,73	2.32	13 (30%)	48,95,113	3.40	15 (31%)
19	CLA	4	311	-	19,32,73	1.87	7 (36%)	24,54,113	3.09	13 (54%)
19	CLA	4	312	-	19,32,73	1.87	5 (26%)	24,54,113	3.08	14 (58%)
19	CLA	4	313	-	29,44,73	2.59	10 (34%)	36,78,113	4.38	19 (52%)
19	CLA	4	314	4	19,32,73	1.91	5 (26%)	24,54,113	2.76	14 (58%)
19	CLA	4	315	-	39,54,73	2.37	12 (30%)	44,90,113	2.92	16 (36%)
20	LMU	4	316	-	36,36,36	0.71	1 (2%)	47,47,47	1.07	3 (6%)
19	CLA	4	317	-	45,60,73	2.28	13 (28%)	50,97,113	3.29	21 (42%)
19	CLA	4	318	-	40,55,73	2.34	13 (32%)	45,91,113	3.73	20 (44%)
20	LMU	4	319	-	35,35,36	0.79	2 (5%)	46,46,47	1.79	11 (23%)
20	LMU	4	320	-	36,36,36	0.76	1 (2%)	47,47,47	1.27	7 (14%)
20	LMU	4	321	-	36,36,36	0.45	0	47,47,47	1.44	7 (14%)
21	SUC	4	322	-	24,24,24	0.49	0	36,36,36	0.97	2 (5%)
19	CLA	A	801	-	39,54,73	2.55	12 (30%)	48,90,113	4.55	25 (52%)
19	CLA	A	802	-	19,32,73	1.90	5 (26%)	24,54,113	3.26	14 (58%)
19	CLA	A	803	-	39,54,73	2.54	13 (33%)	44,90,113	3.76	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	804	19	48,63,73	2.28	12 (25%)	54,101,113	2.86	19 (35%)
19	CLA	A	805	-	47,62,73	2.14	12 (25%)	52,99,113	2.93	17 (32%)
19	CLA	A	806	-	49,64,73	2.11	11 (22%)	55,102,113	3.01	18 (32%)
19	CLA	A	807	-	39,54,73	2.33	11 (28%)	44,90,113	3.70	18 (40%)
19	CLA	A	808	5	53,68,73	2.11	13 (24%)	60,107,113	2.83	20 (33%)
19	CLA	A	809	-	45,60,73	2.15	10 (22%)	50,97,113	2.94	20 (40%)
19	CLA	A	810	-	35,53,73	2.46	11 (31%)	38,89,113	3.70	17 (44%)
19	CLA	A	811	19	58,73,73	2.00	12 (20%)	66,113,113	2.46	20 (30%)
19	CLA	A	812	-	47,62,73	2.12	10 (21%)	52,99,113	2.78	15 (28%)
19	CLA	A	813	-	43,58,73	2.23	11 (25%)	48,95,113	3.05	16 (33%)
19	CLA	A	814	-	19,32,73	2.00	8 (42%)	24,54,113	3.11	13 (54%)
19	CLA	A	815	-	43,58,73	2.30	11 (25%)	48,95,113	2.96	20 (41%)
19	CLA	A	816	-	47,62,73	2.20	13 (27%)	52,99,113	3.40	21 (40%)
19	CLA	A	817	-	45,60,73	2.24	12 (26%)	50,97,113	3.17	16 (32%)
19	CLA	A	818	-	53,68,73	2.22	14 (26%)	60,107,113	3.07	23 (38%)
19	CLA	A	819	-	51,66,73	2.10	11 (21%)	57,104,113	3.06	21 (36%)
19	CLA	A	820	-	44,59,73	2.25	11 (25%)	49,96,113	3.15	17 (34%)
19	CLA	A	821	5	35,50,73	2.40	10 (28%)	39,85,113	3.52	14 (35%)
19	CLA	A	822	-	43,58,73	2.27	12 (27%)	48,95,113	3.05	17 (35%)
19	CLA	A	823	-	51,66,73	2.03	11 (21%)	57,104,113	2.55	17 (29%)
19	CLA	A	824	-	52,67,73	2.06	12 (23%)	58,105,113	3.06	19 (32%)
19	CLA	A	825	-	58,73,73	1.91	12 (20%)	66,113,113	2.61	14 (21%)
19	CLA	A	826	-	58,73,73	1.95	12 (20%)	66,113,113	3.08	20 (30%)
19	CLA	A	827	-	48,63,73	2.16	11 (22%)	54,101,113	3.07	19 (35%)
19	CLA	A	828	-	58,73,73	1.97	12 (20%)	66,113,113	2.85	19 (28%)
19	CLA	A	829	-	43,58,73	2.29	13 (30%)	48,95,113	3.32	17 (35%)
19	CLA	A	830	-	58,73,73	1.95	11 (18%)	66,113,113	2.71	16 (24%)
19	CLA	A	831	-	58,73,73	2.03	14 (24%)	66,113,113	3.72	24 (36%)
19	CLA	A	832	-	43,58,73	2.24	12 (27%)	48,95,113	2.96	17 (35%)
19	CLA	A	833	5	35,53,73	2.36	11 (31%)	38,89,113	3.73	17 (44%)
19	CLA	A	834	-	39,54,73	2.40	11 (28%)	44,90,113	3.34	16 (36%)
19	CLA	A	835	-	58,73,73	2.06	12 (20%)	66,113,113	2.90	21 (31%)
19	CLA	A	836	-	40,55,73	2.39	13 (32%)	45,91,113	2.46	13 (28%)
19	CLA	A	837	-	44,59,73	2.30	12 (27%)	49,96,113	3.27	18 (36%)
19	CLA	A	838	-	58,73,73	1.99	11 (18%)	66,113,113	2.83	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	839	-	52,67,73	2.33	15 (28%)	58,105,113	2.90	20 (34%)
19	CLA	A	840	-	48,63,73	2.14	11 (22%)	54,101,113	2.97	17 (31%)
19	CLA	A	841	-	19,32,73	1.99	7 (36%)	24,54,113	3.26	14 (58%)
23	PQN	A	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.16	4 (9%)
22	BCR	A	843	-	41,41,41	1.97	3 (7%)	56,56,56	5.50	21 (37%)
22	BCR	A	844	-	41,41,41	2.03	3 (7%)	56,56,56	5.59	21 (37%)
22	BCR	A	845	-	41,41,41	2.02	4 (9%)	56,56,56	5.73	25 (44%)
20	LMU	A	846	-	36,36,36	0.69	0	47,47,47	1.26	7 (14%)
20	LMU	A	847	-	36,36,36	0.67	1 (2%)	47,47,47	1.40	7 (14%)
20	LMU	A	848	-	36,36,36	0.48	0	47,47,47	0.84	3 (6%)
19	CLA	A	849	-	58,73,73	1.97	13 (22%)	66,113,113	2.94	20 (30%)
19	CLA	A	850	-	58,73,73	2.01	13 (22%)	66,113,113	2.82	20 (30%)
19	CLA	A	851	-	58,73,73	2.05	12 (20%)	66,113,113	2.67	18 (27%)
20	LMU	A	852	-	36,36,36	0.54	1 (2%)	47,47,47	0.84	1 (2%)
20	LMU	A	853	-	36,36,36	0.49	0	47,47,47	1.40	6 (12%)
20	LMU	A	854	-	36,36,36	0.50	0	47,47,47	1.26	7 (14%)
20	LMU	A	855	-	36,36,36	0.64	1 (2%)	47,47,47	1.37	7 (14%)
24	SF4	A	856	5,6	0,12,12	0.00	-	0,24,24	0.00	-
21	SUC	A	857	-	24,24,24	0.53	0	36,36,36	1.66	11 (30%)
22	BCR	B	801	-	41,41,41	2.53	6 (14%)	56,56,56	6.10	21 (37%)
19	CLA	B	802	-	47,62,73	2.18	12 (25%)	52,99,113	3.27	20 (38%)
19	CLA	B	803	-	58,73,73	1.99	11 (18%)	66,113,113	2.70	18 (27%)
20	LMU	B	804	-	36,36,36	0.69	0	47,47,47	1.73	12 (25%)
20	LMU	B	805	-	36,36,36	0.67	1 (2%)	47,47,47	1.64	12 (25%)
19	CLA	B	806	-	58,73,73	2.03	12 (20%)	66,113,113	2.45	17 (25%)
19	CLA	B	807	-	35,53,73	2.45	12 (34%)	38,89,113	3.31	13 (34%)
19	CLA	B	808	-	54,69,73	2.01	13 (24%)	61,108,113	2.85	20 (32%)
19	CLA	B	809	-	58,73,73	2.00	13 (22%)	66,113,113	2.85	21 (31%)
19	CLA	B	810	-	53,68,73	2.11	11 (20%)	60,107,113	2.82	19 (31%)
19	CLA	B	811	6	19,32,73	1.95	8 (42%)	24,54,113	2.83	13 (54%)
19	CLA	B	812	-	47,62,73	2.42	13 (27%)	57,100,113	3.88	23 (40%)
19	CLA	B	813	-	48,63,73	2.07	11 (22%)	54,101,113	2.97	19 (35%)
19	CLA	B	814	-	58,73,73	1.99	11 (18%)	66,113,113	2.83	17 (25%)
19	CLA	B	815	-	53,68,73	2.11	11 (20%)	60,107,113	2.40	15 (25%)
19	CLA	B	816	-	53,68,73	2.03	11 (20%)	60,107,113	2.61	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	817	-	39,54,73	2.34	11 (28%)	44,90,113	3.11	17 (38%)
19	CLA	B	818	-	46,61,73	2.21	11 (23%)	51,98,113	2.72	17 (33%)
19	CLA	B	819	-	34,49,73	2.77	13 (38%)	38,84,113	4.39	16 (42%)
19	CLA	B	820	-	54,69,73	1.97	11 (20%)	61,108,113	3.00	20 (32%)
19	CLA	B	821	-	43,58,73	2.26	12 (27%)	48,95,113	3.24	18 (37%)
19	CLA	B	822	-	39,54,73	2.36	12 (30%)	44,90,113	3.45	15 (34%)
19	CLA	B	823	-	48,63,73	2.18	12 (25%)	54,101,113	2.84	17 (31%)
19	CLA	B	824	-	58,73,73	2.15	14 (24%)	66,113,113	2.86	19 (28%)
19	CLA	B	825	-	47,62,73	2.25	12 (25%)	52,99,113	2.70	19 (36%)
19	CLA	B	826	-	51,66,73	2.11	12 (23%)	57,104,113	2.96	15 (26%)
19	CLA	B	827	-	58,73,73	1.94	12 (20%)	66,113,113	2.93	18 (27%)
19	CLA	B	828	-	58,73,73	1.99	12 (20%)	66,113,113	3.08	20 (30%)
19	CLA	B	829	-	58,73,73	1.99	12 (20%)	66,113,113	2.60	22 (33%)
19	CLA	B	830	-	58,73,73	1.98	13 (22%)	66,113,113	2.46	19 (28%)
19	CLA	B	831	-	43,58,73	2.28	11 (25%)	48,95,113	3.04	18 (37%)
19	CLA	B	832	-	52,67,73	2.15	12 (23%)	58,105,113	2.94	19 (32%)
19	CLA	B	833	-	43,58,73	2.27	11 (25%)	48,95,113	3.44	20 (41%)
19	CLA	B	834	-	35,53,73	2.45	11 (31%)	38,89,113	3.51	13 (34%)
19	CLA	B	835	-	35,53,73	2.45	11 (31%)	38,89,113	3.23	16 (42%)
19	CLA	B	836	-	44,59,73	2.24	12 (27%)	49,96,113	3.33	19 (38%)
19	CLA	B	837	-	53,68,73	2.04	11 (20%)	60,107,113	2.76	15 (25%)
19	CLA	B	838	-	58,73,73	1.91	12 (20%)	66,113,113	2.57	16 (24%)
19	CLA	B	839	-	40,55,73	2.57	14 (35%)	45,91,113	3.93	17 (37%)
19	CLA	B	840	-	58,73,73	1.95	12 (20%)	66,113,113	2.57	18 (27%)
19	CLA	B	841	-	58,73,73	1.91	13 (22%)	66,113,113	2.44	18 (27%)
19	CLA	B	842	-	29,44,73	2.72	12 (41%)	36,78,113	4.46	18 (50%)
23	PQN	B	843	-	34,34,34	1.47	2 (5%)	42,45,45	1.29	5 (11%)
22	BCR	B	844	-	41,41,41	1.87	3 (7%)	56,56,56	5.21	24 (42%)
22	BCR	B	845	-	41,41,41	1.77	3 (7%)	56,56,56	4.80	18 (32%)
22	BCR	B	846	-	41,41,41	1.99	4 (9%)	56,56,56	5.59	21 (37%)
22	BCR	B	847	-	41,41,41	1.96	3 (7%)	56,56,56	5.47	17 (30%)
25	LMG	B	848	-	49,49,55	0.98	2 (4%)	57,57,63	1.09	3 (5%)
20	LMU	B	849	-	26,26,36	0.76	1 (3%)	37,37,47	1.27	6 (16%)
19	CLA	B	850	-	58,73,73	1.95	13 (22%)	66,113,113	2.91	20 (30%)
21	SUC	B	851	-	24,24,24	0.46	0	36,36,36	1.28	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	C	101	-	36,36,36	0.68	1 (2%)	47,47,47	1.24	4 (8%)
24	SF4	C	102	7	0,12,12	0.00	-	0,24,24	0.00	-
24	SF4	C	103	7	0,12,12	0.00	-	0,24,24	0.00	-
20	LMU	D	201	-	36,36,36	0.46	0	47,47,47	1.42	6 (12%)
20	LMU	E	101	-	36,36,36	0.60	0	47,47,47	1.87	12 (25%)
19	CLA	F	201	-	43,58,73	2.37	14 (32%)	48,95,113	3.45	18 (37%)
20	LMU	F	202	-	35,35,36	0.57	0	46,46,47	1.35	5 (10%)
22	BCR	F	203	-	41,41,41	2.02	3 (7%)	56,56,56	5.49	19 (33%)
22	BCR	F	204	-	41,41,41	2.17	5 (12%)	56,56,56	5.77	24 (42%)
19	CLA	F	205	-	29,44,73	2.53	12 (41%)	36,78,113	3.95	18 (50%)
19	CLA	F	206	-	34,49,73	2.55	12 (35%)	38,84,113	3.48	16 (42%)
19	CLA	F	207	-	46,61,73	2.50	18 (39%)	51,98,113	3.51	24 (47%)
20	LMU	G	101	-	36,36,36	1.09	2 (5%)	47,47,47	2.00	11 (23%)
20	LMU	G	102	-	36,36,36	0.60	0	47,47,47	1.57	8 (17%)
20	LMU	G	103	-	36,36,36	0.49	0	47,47,47	0.92	1 (2%)
22	BCR	G	104	-	41,41,41	1.88	3 (7%)	56,56,56	5.75	17 (30%)
19	CLA	G	105	-	44,59,73	2.32	13 (29%)	49,96,113	3.35	17 (34%)
19	CLA	H	101	-	48,63,73	2.24	12 (25%)	54,101,113	3.42	19 (35%)
19	CLA	H	102	-	48,63,73	2.14	11 (22%)	54,101,113	3.04	19 (35%)
20	LMU	H	103	-	36,36,36	0.84	1 (2%)	47,47,47	2.07	12 (25%)
20	LMU	H	104	-	36,36,36	0.59	0	47,47,47	1.61	7 (14%)
20	LMU	H	105	-	36,36,36	0.71	1 (2%)	47,47,47	1.64	8 (17%)
20	LMU	H	106	-	36,36,36	0.59	1 (2%)	47,47,47	1.56	11 (23%)
21	SUC	H	107	-	24,24,24	0.35	0	36,36,36	0.97	1 (2%)
21	SUC	H	108	-	23,23,24	0.63	0	35,35,36	1.45	6 (17%)
21	SUC	H	110	-	24,24,24	1.08	2 (8%)	36,36,36	2.16	11 (30%)
19	CLA	H	111	-	51,66,73	2.27	13 (25%)	57,104,113	2.74	20 (35%)
19	CLA	H	112	-	48,63,73	2.15	10 (20%)	54,101,113	3.18	19 (35%)
21	SUC	H	113	-	24,24,24	0.45	0	36,36,36	0.92	0
22	BCR	I	101	-	40,40,41	1.66	3 (7%)	52,53,56	4.26	19 (36%)
19	CLA	I	102	-	53,68,73	2.04	11 (20%)	60,107,113	2.98	15 (25%)
22	BCR	I	103	-	41,41,41	2.14	5 (12%)	56,56,56	6.17	28 (50%)
19	CLA	J	101	-	41,56,73	2.31	12 (29%)	46,92,113	3.06	14 (30%)
22	BCR	J	102	-	41,41,41	1.94	3 (7%)	56,56,56	5.56	18 (32%)
19	CLA	J	103	-	54,69,73	2.04	12 (22%)	61,108,113	2.64	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	K	101	-	39,54,73	2.37	13 (33%)	44,90,113	3.34	13 (29%)
19	CLA	K	102	-	43,58,73	2.28	12 (27%)	48,95,113	3.20	18 (37%)
19	CLA	K	103	-	43,58,73	2.30	11 (25%)	48,95,113	3.23	20 (41%)
19	CLA	K	104	-	49,64,73	2.16	13 (26%)	55,102,113	3.33	20 (36%)
20	LMU	K	105	-	36,36,36	0.66	1 (2%)	47,47,47	1.53	8 (17%)
20	LMU	K	106	-	36,36,36	0.37	0	47,47,47	1.04	4 (8%)
20	LMU	K	107	-	36,36,36	0.52	0	47,47,47	1.30	6 (12%)
19	CLA	L	201	-	53,68,73	2.09	10 (18%)	60,107,113	2.59	18 (30%)
19	CLA	L	202	-	48,63,73	2.16	12 (25%)	54,101,113	3.00	17 (31%)
19	CLA	L	203	-	58,73,73	1.93	11 (18%)	66,113,113	3.06	20 (30%)
19	CLA	L	204	-	48,63,73	2.25	11 (22%)	54,101,113	2.73	21 (38%)
20	LMU	L	205	-	36,36,36	0.63	0	47,47,47	1.90	13 (27%)
20	LMU	L	206	-	36,36,36	0.51	0	47,47,47	0.98	3 (6%)
21	SUC	L	207	-	24,24,24	0.50	0	36,36,36	1.20	6 (16%)
19	CLA	L	208	16	43,58,73	2.29	12 (27%)	48,95,113	3.18	17 (35%)
19	CLA	L	209	-	40,55,73	2.38	12 (30%)	45,91,113	3.52	17 (37%)
19	CLA	L	210	-	43,58,73	2.36	12 (27%)	48,95,113	3.56	17 (35%)
22	BCR	L	211	-	41,41,41	2.01	4 (9%)	56,56,56	5.66	17 (30%)
20	LMU	L	212	-	36,36,36	0.70	1 (2%)	47,47,47	1.27	4 (8%)
20	LMU	R	101	-	36,36,36	0.84	2 (5%)	47,47,47	2.06	11 (23%)
20	LMU	R	102	-	36,36,36	0.56	0	47,47,47	1.49	9 (19%)
20	LMU	R	103	-	36,36,36	0.69	1 (2%)	47,47,47	1.44	6 (12%)
20	LMU	R	104	-	36,36,36	0.56	0	47,47,47	1.27	5 (10%)
20	LMU	R	105	-	36,36,36	0.73	1 (2%)	47,47,47	1.38	8 (17%)
20	LMU	R	106	-	36,36,36	0.52	0	47,47,47	1.22	4 (8%)
19	CLA	R	107	-	50,65,73	2.13	11 (22%)	56,103,113	3.14	20 (35%)
19	CLA	R	108	-	58,73,73	2.02	11 (18%)	66,113,113	2.60	20 (30%)
20	LMU	R	109	-	36,36,36	0.48	0	47,47,47	0.80	1 (2%)

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
19	CLA	1	201	-	3/3/16/25	0/15/113/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	202	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	1	203	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	204	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	205	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	206	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	207	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	208	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	209	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	210	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	211	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	212	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	213	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	214	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	215	-	4/4/17/25	0/21/119/135	0/0/9/9
20	LMU	1	216	-	-	0/21/61/61	0/2/2/2
20	LMU	1	217	-	-	0/21/61/61	0/2/2/2
20	LMU	1	218	-	-	0/21/61/61	0/2/2/2
21	SUC	1	219	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	2	301	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	302	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	303	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	2	304	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	305	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	306	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	307	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	308	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	309	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	310	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	311	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	312	-	4/4/19/25	0/33/131/135	0/0/9/9
20	LMU	2	313	-	-	0/21/61/61	0/2/2/2
21	SUC	2	314	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	315	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	2	316	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	317	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	2	318	-	-	1/29/63/63	0/2/2/2
20	LMU	2	319	-	-	0/21/61/61	0/2/2/2
20	LMU	2	320	-	-	1/21/61/61	0/2/2/2
20	LMU	2	321	-	-	0/21/61/61	0/2/2/2
20	LMU	2	322	-	-	0/21/61/61	0/2/2/2
21	SUC	2	323	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	301	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	302	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	303	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	304	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	305	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	306	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	307	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	308	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	309	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	310	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	311	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	3	312	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	313	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	314	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	315	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	316	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	317	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	318	-	3/3/14/25	0/0/96/135	0/0/9/9
20	LMU	3	319	-	-	0/21/61/61	0/2/2/2
20	LMU	3	320	-	-	0/21/61/61	0/2/2/2
21	SUC	3	321	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	4	301	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	302	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	303	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	4	304	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	305	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	4	306	-	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	308	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	309	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	310	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	4	311	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	312	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	313	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	314	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	315	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	316	-	-	0/21/61/61	0/2/2/2
19	CLA	4	317	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	318	-	3/3/16/25	0/16/114/135	0/0/9/9
20	LMU	4	319	-	-	0/20/60/61	0/2/2/2
20	LMU	4	320	-	-	0/21/61/61	0/2/2/2
20	LMU	4	321	-	-	0/21/61/61	0/2/2/2
21	SUC	4	322	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	A	801	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	A	802	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	803	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	804	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	805	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	806	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	A	807	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	808	5	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	809	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	810	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	811	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	812	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	813	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	814	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	815	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	816	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	817	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	818	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	819	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	820	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	821	5	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	822	-	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	823	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	824	-	4/4/18/25	1/30/128/135	0/0/9/9
19	CLA	A	825	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	826	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	827	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	828	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	829	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	830	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	831	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	832	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	833	5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	834	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	835	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	836	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	837	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	838	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	839	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	840	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	A	841	-	3/3/7/25	0/0/66/135	0/0/8/9
23	PQN	A	842	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	A	843	-	-	0/29/63/63	0/2/2/2
22	BCR	A	844	-	-	0/29/63/63	0/2/2/2
22	BCR	A	845	-	-	0/29/63/63	0/2/2/2
20	LMU	A	846	-	-	0/21/61/61	0/2/2/2
20	LMU	A	847	-	-	0/21/61/61	0/2/2/2
20	LMU	A	848	-	-	0/21/61/61	0/2/2/2
19	CLA	A	849	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	850	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	851	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	A	852	-	-	0/21/61/61	0/2/2/2
20	LMU	A	853	-	-	0/21/61/61	0/2/2/2
20	LMU	A	854	-	-	0/21/61/61	0/2/2/2
20	LMU	A	855	-	-	0/21/61/61	0/2/2/2
24	SF4	A	856	5,6	-	0/0/48/48	0/6/5/5
21	SUC	A	857	-	1/1/9/9	0/12/51/51	0/2/2/2
22	BCR	B	801	-	-	0/29/63/63	0/2/2/2
19	CLA	B	802	-	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	803	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	B	804	-	-	0/21/61/61	0/2/2/2
20	LMU	B	805	-	-	0/21/61/61	0/2/2/2
19	CLA	B	806	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	807	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	808	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	809	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	810	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	811	6	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	B	812	-	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	813	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	814	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	815	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	816	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	817	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	818	-	3/3/17/25	0/23/121/135	0/0/9/9
19	CLA	B	819	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	B	820	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	821	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	822	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	823	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	824	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	825	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	826	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	827	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	828	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	829	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	830	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	831	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	832	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	833	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	834	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	835	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	836	-	3/3/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	837	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	838	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	839	-	3/3/16/25	1/16/114/135	0/0/9/9
19	CLA	B	840	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	841	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	842	-	3/3/14/25	0/0/96/135	0/0/9/9
23	PQN	B	843	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	BCR	B	845	-	-	0/29/63/63	0/2/2/2
22	BCR	B	846	-	-	0/29/63/63	0/2/2/2
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
25	LMG	B	848	-	-	0/44/64/70	0/1/1/1
20	LMU	B	849	-	-	0/11/51/61	0/2/2/2
19	CLA	B	850	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	B	851	-	1/1/9/9	0/12/51/51	0/2/2/2
20	LMU	C	101	-	-	0/21/61/61	0/2/2/2
24	SF4	C	102	7	-	0/0/48/48	0/6/5/5
24	SF4	C	103	7	-	0/0/48/48	0/6/5/5
20	LMU	D	201	-	-	0/21/61/61	0/2/2/2
20	LMU	E	101	-	-	0/21/61/61	0/2/2/2
19	CLA	F	201	-	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	F	202	-	-	0/20/60/61	0/2/2/2
22	BCR	F	203	-	-	0/29/63/63	0/2/2/2
22	BCR	F	204	-	-	0/29/63/63	0/2/2/2
19	CLA	F	205	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	F	206	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	F	207	-	6/6/17/25	1/23/121/135	0/0/9/9
20	LMU	G	101	-	-	0/21/61/61	0/2/2/2
20	LMU	G	102	-	-	0/21/61/61	0/2/2/2
20	LMU	G	103	-	-	0/21/61/61	0/2/2/2
22	BCR	G	104	-	-	2/29/63/63	0/2/2/2
19	CLA	G	105	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	H	101	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	H	102	-	4/4/18/25	0/25/123/135	0/0/9/9
20	LMU	H	103	-	-	0/21/61/61	0/2/2/2
20	LMU	H	104	-	-	1/21/61/61	0/2/2/2
20	LMU	H	105	-	-	0/21/61/61	0/2/2/2
20	LMU	H	106	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SUC	H	107	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	H	108	-	1/1/9/9	0/10/49/51	0/2/2/2
21	SUC	H	110	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	H	111	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	H	112	-	4/4/18/25	0/25/123/135	0/0/9/9
21	SUC	H	113	-	1/1/9/9	0/12/51/51	0/2/2/2
22	BCR	I	101	-	-	0/29/60/63	0/2/2/2
19	CLA	I	102	-	4/4/19/25	0/31/129/135	0/0/9/9
22	BCR	I	103	-	-	0/29/63/63	0/2/2/2
19	CLA	J	101	-	3/3/16/25	0/17/115/135	0/0/9/9
22	BCR	J	102	-	-	0/29/63/63	0/2/2/2
19	CLA	J	103	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	K	101	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	K	102	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	103	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	104	-	4/4/18/25	0/27/125/135	0/0/9/9
20	LMU	K	105	-	-	0/21/61/61	0/2/2/2
20	LMU	K	106	-	-	0/21/61/61	0/2/2/2
20	LMU	K	107	-	-	0/21/61/61	0/2/2/2
19	CLA	L	201	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	L	202	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	L	203	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	L	204	-	4/4/18/25	0/25/123/135	0/0/9/9
20	LMU	L	205	-	-	0/21/61/61	0/2/2/2
20	LMU	L	206	-	-	0/21/61/61	0/2/2/2
21	SUC	L	207	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	L	208	16	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	L	209	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	210	-	4/4/17/25	0/19/117/135	0/0/9/9
22	BCR	L	211	-	-	0/29/63/63	0/2/2/2
20	LMU	L	212	-	-	0/21/61/61	0/2/2/2
20	LMU	R	101	-	-	0/21/61/61	0/2/2/2
20	LMU	R	102	-	-	0/21/61/61	0/2/2/2
20	LMU	R	103	-	-	0/21/61/61	0/2/2/2
20	LMU	R	104	-	-	0/21/61/61	0/2/2/2
20	LMU	R	105	-	-	0/21/61/61	0/2/2/2
20	LMU	R	106	-	-	0/21/61/61	0/2/2/2
19	CLA	R	107	-	4/4/18/25	0/28/126/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	R	108	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	R	109	-	-	0/21/61/61	0/2/2/2

The worst 5 of 1983 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	BCR	C21-C22	-9.91	1.22	1.35
22	B	801	BCR	C20-C21	-9.39	1.14	1.43
19	1	205	CLA	CAB-C3B	-9.10	1.33	1.51
19	B	812	CLA	CAB-C3B	-9.00	1.33	1.51
19	4	302	CLA	CAB-C3B	-8.76	1.34	1.51

The worst 5 of 3740 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	203	CLA	OBD-CAD-CBD	-18.46	98.80	125.91
19	1	213	CLA	OBD-CAD-CBD	-17.94	99.56	125.91
19	A	831	CLA	OBD-CAD-CBD	-17.87	99.66	125.91
19	B	819	CLA	OBD-CAD-CBD	-17.46	100.26	125.91
19	A	807	CLA	OBD-CAD-CBD	-17.04	100.89	125.91

5 of 617 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	210	CLA	NC
19	1	210	CLA	ND
19	1	210	CLA	NA
19	A	829	CLA	NC
19	A	829	CLA	ND

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	G	104	BCR	C20-C21-C22-C37
22	G	104	BCR	C20-C21-C22-C23
22	B	847	BCR	C20-C21-C22-C23
22	B	847	BCR	C20-C21-C22-C37
22	2	318	BCR	C21-C20-C19-C18

There are no ring outliers.

236 monomers are involved in 2793 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	201	CLA	13	0
19	1	202	CLA	1	0
19	1	203	CLA	8	0
19	1	204	CLA	15	0
19	1	205	CLA	6	0
19	1	206	CLA	9	0
19	1	207	CLA	6	1
19	1	208	CLA	3	0
19	1	209	CLA	1	0
19	1	210	CLA	8	0
19	1	211	CLA	7	0
19	1	212	CLA	2	0
19	1	213	CLA	16	0
19	1	215	CLA	1	0
20	1	216	LMU	3	0
20	1	217	LMU	20	0
20	1	218	LMU	9	0
19	2	302	CLA	13	0
19	2	303	CLA	25	0
19	2	304	CLA	2	0
19	2	305	CLA	16	0
19	2	307	CLA	22	0
19	2	308	CLA	1	0
19	2	310	CLA	21	0
19	2	311	CLA	6	0
19	2	312	CLA	19	0
20	2	313	LMU	29	0
21	2	314	SUC	10	0
19	2	315	CLA	17	0
19	2	317	CLA	11	0
22	2	318	BCR	9	0
20	2	319	LMU	6	0
20	2	320	LMU	5	0
20	2	321	LMU	5	0
21	2	323	SUC	11	0
19	3	301	CLA	1	0
19	3	303	CLA	4	0
19	3	304	CLA	2	0
19	3	305	CLA	3	0
19	3	306	CLA	7	0
19	3	307	CLA	14	0
19	3	308	CLA	2	0
19	3	309	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	310	CLA	17	0
19	3	311	CLA	10	0
21	3	312	SUC	6	0
19	3	314	CLA	1	0
19	3	315	CLA	13	0
20	3	319	LMU	2	0
20	3	320	LMU	14	0
21	3	321	SUC	2	0
19	4	301	CLA	34	0
19	4	302	CLA	3	0
19	4	303	CLA	18	0
19	4	304	CLA	21	0
19	4	305	CLA	5	0
19	4	306	CLA	18	0
19	4	310	CLA	25	0
19	4	311	CLA	3	0
19	4	312	CLA	4	0
19	4	313	CLA	5	0
19	4	314	CLA	10	0
19	4	315	CLA	5	0
20	4	316	LMU	1	0
19	4	317	CLA	3	0
19	4	318	CLA	14	0
20	4	319	LMU	8	3
20	4	320	LMU	2	0
20	4	321	LMU	13	0
21	4	322	SUC	3	0
19	A	801	CLA	9	0
19	A	803	CLA	20	0
19	A	804	CLA	36	0
19	A	805	CLA	16	0
19	A	806	CLA	13	0
19	A	807	CLA	33	0
19	A	808	CLA	21	0
19	A	809	CLA	32	0
19	A	810	CLA	4	0
19	A	811	CLA	22	0
19	A	812	CLA	4	0
19	A	813	CLA	21	0
19	A	814	CLA	14	0
19	A	815	CLA	4	0
19	A	816	CLA	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	817	CLA	8	0
19	A	818	CLA	46	0
19	A	819	CLA	33	0
19	A	820	CLA	8	0
19	A	821	CLA	8	0
19	A	822	CLA	20	0
19	A	823	CLA	10	0
19	A	824	CLA	43	0
19	A	825	CLA	51	0
19	A	826	CLA	49	0
19	A	827	CLA	19	0
19	A	828	CLA	18	0
19	A	829	CLA	7	0
19	A	830	CLA	31	0
19	A	831	CLA	37	0
19	A	832	CLA	19	0
19	A	833	CLA	13	0
19	A	834	CLA	7	0
19	A	835	CLA	15	0
19	A	836	CLA	6	0
19	A	837	CLA	17	0
19	A	838	CLA	33	0
19	A	839	CLA	27	0
19	A	840	CLA	6	0
19	A	841	CLA	1	0
23	A	842	PQN	7	0
22	A	843	BCR	32	0
22	A	844	BCR	23	0
22	A	845	BCR	48	0
20	A	846	LMU	5	0
20	A	847	LMU	4	0
20	A	848	LMU	4	0
19	A	849	CLA	21	0
19	A	850	CLA	30	0
19	A	851	CLA	26	0
20	A	852	LMU	5	0
20	A	853	LMU	21	0
20	A	854	LMU	15	0
24	A	856	SF4	18	0
21	A	857	SUC	1	0
22	B	801	BCR	24	0
19	B	802	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	803	CLA	44	0
20	B	804	LMU	7	0
20	B	805	LMU	3	0
19	B	806	CLA	25	0
19	B	807	CLA	9	0
19	B	808	CLA	31	0
19	B	809	CLA	22	0
19	B	810	CLA	18	0
19	B	811	CLA	4	0
19	B	812	CLA	9	0
19	B	813	CLA	8	0
19	B	814	CLA	30	0
19	B	815	CLA	17	0
19	B	816	CLA	8	0
19	B	817	CLA	19	0
19	B	818	CLA	17	0
19	B	819	CLA	7	0
19	B	820	CLA	17	0
19	B	821	CLA	7	0
19	B	822	CLA	16	0
19	B	823	CLA	15	0
19	B	824	CLA	30	0
19	B	825	CLA	24	0
19	B	826	CLA	39	0
19	B	827	CLA	36	0
19	B	828	CLA	13	0
19	B	829	CLA	25	0
19	B	830	CLA	24	0
19	B	831	CLA	11	0
19	B	832	CLA	24	0
19	B	833	CLA	18	0
19	B	834	CLA	23	0
19	B	835	CLA	30	0
19	B	836	CLA	9	0
19	B	837	CLA	12	0
19	B	838	CLA	42	0
19	B	839	CLA	47	0
19	B	840	CLA	18	0
19	B	841	CLA	17	0
19	B	842	CLA	2	0
23	B	843	PQN	28	0
22	B	844	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	845	BCR	18	0
22	B	846	BCR	32	0
22	B	847	BCR	32	0
25	B	848	LMG	17	0
20	B	849	LMU	1	0
19	B	850	CLA	18	0
21	B	851	SUC	4	0
24	C	102	SF4	4	0
24	C	103	SF4	1	0
20	D	201	LMU	3	0
20	E	101	LMU	11	0
19	F	201	CLA	29	0
20	F	202	LMU	8	0
22	F	203	BCR	26	0
22	F	204	BCR	34	0
19	F	205	CLA	1	0
19	F	206	CLA	5	0
19	F	207	CLA	13	0
20	G	101	LMU	4	41
20	G	102	LMU	7	0
20	G	103	LMU	16	0
22	G	104	BCR	5	0
19	G	105	CLA	4	0
19	H	101	CLA	15	0
19	H	102	CLA	2	0
20	H	103	LMU	6	0
20	H	104	LMU	9	0
20	H	105	LMU	18	0
20	H	106	LMU	9	0
21	H	107	SUC	6	0
21	H	108	SUC	3	0
21	H	110	SUC	1	41
19	H	111	CLA	27	0
19	H	112	CLA	13	0
21	H	113	SUC	14	0
22	I	101	BCR	9	0
19	I	102	CLA	12	0
22	I	103	BCR	38	0
19	J	101	CLA	12	0
22	J	102	BCR	36	0
19	J	103	CLA	14	0
19	K	101	CLA	16	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	K	102	CLA	27	0
19	K	103	CLA	9	0
19	K	104	CLA	17	0
20	K	105	LMU	13	0
20	K	106	LMU	8	0
20	K	107	LMU	21	0
19	L	201	CLA	23	0
19	L	202	CLA	10	0
19	L	203	CLA	29	0
19	L	204	CLA	13	0
20	L	205	LMU	1	0
21	L	207	SUC	4	0
19	L	208	CLA	3	0
19	L	209	CLA	27	0
19	L	210	CLA	9	0
22	L	211	BCR	36	0
20	L	212	LMU	1	0
20	R	101	LMU	3	0
20	R	102	LMU	8	0
20	R	103	LMU	9	0
20	R	104	LMU	5	0
20	R	106	LMU	9	0
19	R	107	CLA	10	0
19	R	108	CLA	4	0
20	R	109	LMU	9	3

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	1	165/241 (68%)	1.34	39 (23%) 0 0	21, 24, 25, 25	0
2	2	176/269 (65%)	0.89	34 (19%) 1 1	21, 23, 24, 25	0
3	3	153/276 (55%)	1.12	30 (19%) 1 1	49, 78, 110, 112	0
4	4	166/251 (66%)	0.57	15 (9%) 9 11	21, 23, 24, 25	0
5	A	730/758 (96%)	0.62	56 (7%) 13 15	20, 22, 23, 25	0
6	B	733/734 (99%)	0.67	53 (7%) 15 16	20, 22, 24, 25	0
7	C	81/81 (100%)	0.83	11 (13%) 3 4	21, 22, 23, 23	0
8	D	138/212 (65%)	0.90	25 (18%) 1 2	21, 23, 24, 25	0
9	E	65/143 (45%)	0.71	10 (15%) 2 3	21, 22, 24, 24	0
10	F	154/231 (66%)	0.60	12 (7%) 13 14	21, 22, 23, 24	0
11	G	95/167 (56%)	0.95	12 (12%) 3 5	21, 23, 24, 25	0
12	H	69/144 (47%)	0.83	10 (14%) 2 3	21, 23, 24, 25	0
13	I	30/40 (75%)	0.32	1 (3%) 46 43	21, 22, 23, 23	0
14	J	42/44 (95%)	0.51	3 (7%) 16 17	21, 23, 23, 24	0
15	K	84/131 (64%)	1.48	19 (22%) 0 1	21, 24, 24, 26	0
16	L	162/216 (75%)	0.60	18 (11%) 5 7	20, 23, 24, 25	0
17	N	85/170 (50%)	0.60	7 (8%) 11 13	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.76	355 (11%) 5 7	20, 23, 25, 112	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	10.2
3	3	40	SER	8.6
1	1	92	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	1	87	ASN	7.4
15	K	64	GLY	7.0

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

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

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. 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	B-factors(Å ²)	Q<0.9
20	LMU	A	852	35/35	0.54	0.49	2,39,60,60	0
19	CLA	H	102	55/65	0.56	0.39	2,49,60,60	0
20	LMU	A	853	35/35	0.57	0.37	2,45,60,60	0
20	LMU	G	103	35/35	0.58	0.30	2,51,60,60	0
20	LMU	4	320	35/35	0.58	0.27	2,43,60,60	0
20	LMU	B	804	35/35	0.58	0.32	2,34,60,60	0
19	CLA	1	211	51/65	0.59	0.52	2,42,60,60	0
20	LMU	2	321	35/35	0.60	0.39	2,40,60,60	0
22	BCR	2	318	40/40	0.60	0.40	2,32,60,60	0
19	CLA	4	317	52/65	0.61	0.42	2,34,60,60	0
20	LMU	L	205	35/35	0.62	0.22	2,31,60,60	0
19	CLA	3	314	50/65	0.62	0.41	2,56,60,60	0
19	CLA	B	835	45/65	0.62	0.36	12,37,60,60	0
22	BCR	A	843	40/40	0.63	0.45	2,45,60,60	0
20	LMU	H	103	35/35	0.63	0.33	2,15,60,60	0
19	CLA	A	802	25/65	0.63	0.53	2,42,60,60	0
20	LMU	2	322	35/35	0.63	0.33	2,40,60,60	0
19	CLA	1	215	51/65	0.63	0.40	2,51,60,60	0
19	CLA	4	303	65/65	0.64	0.36	2,32,60,60	0
19	CLA	B	817	46/65	0.64	0.43	2,28,60,60	0
19	CLA	L	204	55/65	0.64	0.45	2,44,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	3	305	25/65	0.64	0.34	17,42,60,60	0
21	SUC	H	107	23/23	0.64	0.36	9,40,60,60	0
20	LMU	A	848	35/35	0.65	0.29	2,45,60,60	0
19	CLA	K	103	50/65	0.65	0.32	2,60,60,60	0
21	SUC	H	108	22/23	0.65	0.46	6,52,60,60	0
19	CLA	3	318	36/65	0.66	0.40	2,51,60,60	0
19	CLA	3	311	65/65	0.66	0.41	2,46,60,60	0
21	SUC	3	321	23/23	0.67	0.30	2,30,60,60	0
19	CLA	H	112	55/65	0.67	0.34	2,33,60,60	0
19	CLA	B	836	51/65	0.67	0.37	2,45,60,60	0
19	CLA	A	840	55/65	0.67	0.36	2,44,60,60	0
19	CLA	4	308	25/65	0.68	0.30	2,29,60,60	0
19	CLA	F	206	41/65	0.68	0.33	2,41,60,60	0
20	LMU	R	104	35/35	0.68	0.23	2,36,60,60	0
20	LMU	H	106	35/35	0.68	0.29	2,41,60,60	0
22	BCR	I	103	40/40	0.68	0.40	2,38,60,60	0
19	CLA	H	101	55/65	0.68	0.47	2,47,60,60	0
21	SUC	A	857	23/23	0.68	0.32	2,52,60,60	0
19	CLA	1	201	46/65	0.69	0.25	2,56,60,60	0
19	CLA	4	307	25/65	0.69	0.35	2,39,60,60	0
20	LMU	K	106	35/35	0.69	0.24	2,38,60,60	0
19	CLA	4	304	55/65	0.69	0.36	4,39,60,60	0
20	LMU	1	217	35/35	0.69	0.23	2,44,60,60	0
20	LMU	A	846	35/35	0.69	0.25	2,26,60,60	0
22	BCR	G	104	40/40	0.69	0.48	2,33,60,60	0
20	LMU	2	313	35/35	0.69	0.27	2,21,60,60	0
20	LMU	E	101	35/35	0.69	0.28	2,30,60,60	0
19	CLA	3	309	25/65	0.69	0.27	2,47,60,60	0
19	CLA	3	303	36/65	0.70	0.26	2,53,60,60	0
20	LMU	B	805	35/35	0.70	0.29	2,37,60,60	0
19	CLA	3	310	65/65	0.70	0.33	2,26,60,60	0
20	LMU	R	105	35/35	0.70	0.27	2,35,60,60	0
19	CLA	G	105	51/65	0.70	0.42	2,44,60,60	0
19	CLA	3	302	25/65	0.70	0.41	15,54,60,60	0
20	LMU	A	854	35/35	0.70	0.27	2,32,60,60	0
19	CLA	R	108	65/65	0.71	0.34	2,35,60,60	0
20	LMU	K	107	35/35	0.71	0.26	2,38,60,60	0
19	CLA	K	101	46/65	0.71	0.25	2,51,60,60	0
19	CLA	2	312	61/65	0.71	0.25	2,34,60,60	0
20	LMU	R	103	35/35	0.71	0.38	2,35,60,60	0
19	CLA	3	313	25/65	0.71	0.43	2,30,60,60	0
19	CLA	A	841	25/65	0.71	0.30	2,43,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	B	816	60/65	0.72	0.34	2,40,60,60	0
22	BCR	B	845	40/40	0.72	0.38	2,21,60,60	0
19	CLA	R	107	57/65	0.72	0.30	2,38,60,60	0
20	LMU	R	106	35/35	0.72	0.23	2,27,60,60	0
20	LMU	R	101	35/35	0.72	0.32	2,45,60,60	0
22	BCR	L	211	40/40	0.72	0.47	2,18,60,60	0
20	LMU	3	319	35/35	0.72	0.31	2,44,60,60	0
19	CLA	L	202	55/65	0.72	0.44	2,46,60,60	0
19	CLA	2	304	25/65	0.73	0.45	2,27,60,60	0
19	CLA	1	206	61/65	0.73	0.29	2,35,60,60	0
20	LMU	G	102	35/35	0.73	0.26	2,33,60,60	0
19	CLA	A	833	45/65	0.73	0.27	2,37,60,60	0
19	CLA	A	801	46/65	0.73	0.35	2,43,60,60	0
22	BCR	A	844	40/40	0.73	0.39	2,34,60,60	0
19	CLA	2	301	25/65	0.73	0.47	2,48,60,60	0
19	CLA	1	208	25/65	0.73	0.27	2,31,60,60	0
19	CLA	1	205	36/65	0.73	0.29	2,52,60,60	0
19	CLA	1	207	51/65	0.73	0.31	2,36,60,60	0
20	LMU	C	101	35/35	0.74	0.38	2,35,60,60	0
21	SUC	H	113	23/23	0.74	0.27	3,33,60,60	0
19	CLA	2	305	50/65	0.74	0.30	2,48,60,60	0
19	CLA	A	820	51/65	0.74	0.30	2,44,60,60	0
19	CLA	4	301	55/65	0.74	0.35	2,33,60,60	0
19	CLA	3	307	42/65	0.75	0.26	2,53,60,60	0
20	LMU	L	212	35/35	0.75	0.30	2,22,60,60	0
19	CLA	2	311	50/65	0.75	0.31	2,25,60,60	0
19	CLA	3	317	25/65	0.75	0.27	2,42,60,60	0
19	CLA	1	203	47/65	0.75	0.27	2,17,60,60	0
20	LMU	K	105	35/35	0.75	0.26	2,37,60,60	0
20	LMU	2	320	35/35	0.75	0.25	2,29,60,60	0
19	CLA	K	102	50/65	0.75	0.32	2,28,60,60	0
21	SUC	2	314	22/23	0.75	0.29	2,35,60,60	0
19	CLA	A	811	65/65	0.75	0.40	2,15,60,60	0
20	LMU	L	206	35/35	0.75	0.24	2,23,60,60	0
19	CLA	4	305	50/65	0.75	0.41	2,21,60,60	0
21	SUC	L	207	23/23	0.75	0.21	2,31,56,60	0
20	LMU	4	316	35/35	0.76	0.38	2,37,60,60	0
19	CLA	2	302	51/65	0.76	0.23	2,33,60,60	0
19	CLA	2	307	65/65	0.76	0.25	2,24,60,60	0
19	CLA	3	316	25/65	0.76	0.48	2,47,60,60	0
19	CLA	4	315	46/65	0.76	0.31	2,45,60,60	0
19	CLA	4	314	25/65	0.76	0.30	2,35,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	SUC	4	322	23/23	0.76	0.24	6,40,60,60	0
20	LMU	A	847	35/35	0.76	0.26	2,27,60,60	0
19	CLA	3	306	25/65	0.76	0.28	2,56,60,60	0
21	SUC	1	219	23/23	0.76	0.35	2,44,60,60	0
19	CLA	4	318	47/65	0.76	0.28	2,37,60,60	0
19	CLA	1	213	51/65	0.76	0.40	2,39,60,60	0
20	LMU	R	102	35/35	0.77	0.22	2,38,60,60	0
19	CLA	J	101	48/65	0.77	0.28	2,34,60,60	0
19	CLA	2	315	50/65	0.77	0.40	2,33,60,60	0
19	CLA	K	104	56/65	0.77	0.31	2,36,60,60	0
19	CLA	3	301	36/65	0.77	0.28	2,34,60,60	0
25	LMG	B	848	49/55	0.77	0.35	2,20,60,60	0
20	LMU	4	321	35/35	0.77	0.27	2,21,55,60	0
19	CLA	2	310	50/65	0.77	0.32	2,18,60,60	0
19	CLA	1	210	36/65	0.77	0.31	2,35,60,60	0
20	LMU	H	104	35/35	0.77	0.23	2,16,60,60	0
21	SUC	B	851	23/23	0.77	0.25	2,41,60,60	0
19	CLA	4	309	25/65	0.78	0.39	2,40,60,60	0
19	CLA	2	306	25/65	0.78	0.22	2,57,60,60	0
19	CLA	A	821	42/65	0.78	0.29	2,46,60,60	0
19	CLA	J	103	61/65	0.78	0.24	2,19,60,60	0
19	CLA	4	302	36/65	0.78	0.35	2,26,60,60	0
22	BCR	J	102	40/40	0.78	0.35	2,31,60,60	0
19	CLA	B	822	46/65	0.78	0.34	2,34,60,60	0
19	CLA	A	823	58/65	0.78	0.36	2,18,60,60	0
19	CLA	L	208	50/65	0.78	0.31	2,27,60,60	0
19	CLA	B	815	60/65	0.78	0.35	2,19,60,60	0
19	CLA	A	817	52/65	0.79	0.36	2,33,60,60	0
19	CLA	2	316	25/65	0.79	0.28	2,36,60,60	0
19	CLA	A	810	45/65	0.79	0.33	2,38,60,60	0
20	LMU	F	202	34/35	0.79	0.22	2,23,60,60	0
19	CLA	A	814	25/65	0.79	0.29	2,31,60,60	0
19	CLA	3	315	65/65	0.79	0.29	2,33,60,60	0
19	CLA	3	308	25/65	0.79	0.26	2,37,60,60	0
20	LMU	3	320	35/35	0.79	0.20	2,28,59,60	0
19	CLA	B	813	55/65	0.79	0.29	2,28,60,60	0
20	LMU	4	319	34/35	0.80	0.24	2,22,60,60	0
26	UNL	H	109	23/-	0.80	0.22	2,31,60,60	0
19	CLA	1	212	25/65	0.80	0.26	2,42,60,60	0
20	LMU	2	319	35/35	0.80	0.20	2,25,60,60	0
19	CLA	1	204	46/65	0.80	0.28	2,35,60,60	0
19	CLA	A	834	46/65	0.80	0.39	2,20,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	805	54/65	0.80	0.29	2,10,60,60	0
19	CLA	A	839	59/65	0.80	0.29	2,30,60,60	0
19	CLA	4	310	50/65	0.80	0.24	2,20,60,60	0
20	LMU	D	201	35/35	0.81	0.22	2,12,50,57	0
19	CLA	2	309	25/65	0.81	0.42	2,34,60,60	0
19	CLA	L	201	60/65	0.81	0.29	2,18,60,60	0
20	LMU	B	849	25/35	0.81	0.21	2,36,60,60	0
19	CLA	1	214	25/65	0.81	0.29	5,42,60,60	0
20	LMU	1	218	35/35	0.81	0.20	2,46,60,60	0
19	CLA	B	842	36/65	0.81	0.30	2,52,60,60	0
19	CLA	A	825	65/65	0.81	0.32	2,16,60,60	0
19	CLA	A	819	58/65	0.81	0.35	2,20,60,60	0
21	SUC	3	312	23/23	0.81	0.28	2,27,60,60	0
21	SUC	H	110	23/23	0.82	0.28	2,34,60,60	0
19	CLA	3	304	25/65	0.82	0.19	2,28,60,60	0
19	CLA	B	827	65/65	0.82	0.32	2,15,60,60	0
19	CLA	B	812	54/65	0.82	0.25	2,17,60,60	0
19	CLA	A	807	46/65	0.82	0.29	2,20,60,60	0
22	BCR	B	847	40/40	0.82	0.33	2,10,60,60	0
22	BCR	A	845	40/40	0.82	0.34	2,5,44,60	0
19	CLA	2	303	58/65	0.82	0.23	2,22,60,60	0
19	CLA	A	815	50/65	0.82	0.27	2,21,60,60	0
22	BCR	B	846	40/40	0.82	0.33	2,11,60,60	0
19	CLA	H	111	58/65	0.82	0.32	2,15,60,60	0
19	CLA	B	820	61/65	0.82	0.30	2,16,60,60	0
19	CLA	A	824	59/65	0.82	0.29	2,25,60,60	0
19	CLA	L	210	50/65	0.82	0.26	2,18,60,60	0
19	CLA	A	812	54/65	0.82	0.25	2,28,60,60	0
20	LMU	A	855	35/35	0.82	0.22	2,29,60,60	0
20	LMU	R	109	35/35	0.82	0.24	2,21,60,60	0
20	LMU	1	216	35/35	0.83	0.25	2,11,50,60	0
19	CLA	B	806	65/65	0.83	0.28	2,11,60,60	0
19	CLA	A	829	50/65	0.83	0.30	2,32,60,60	0
21	SUC	2	323	23/23	0.83	0.24	2,29,60,60	0
20	LMU	G	101	35/35	0.83	0.25	2,34,60,60	0
19	CLA	B	837	60/65	0.83	0.32	2,2,60,60	0
19	CLA	L	203	65/65	0.83	0.31	2,22,60,60	0
19	CLA	4	306	52/65	0.83	0.25	2,26,60,60	0
19	CLA	2	317	65/65	0.83	0.26	2,15,60,60	0
22	BCR	I	101	39/40	0.83	0.31	2,8,60,60	0
19	CLA	B	834	45/65	0.83	0.28	2,16,60,60	0
19	CLA	A	804	55/65	0.83	0.32	2,11,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	A	816	54/65	0.83	0.28	2,31,60,60	0
19	CLA	4	311	25/65	0.84	0.26	2,15,60,60	0
19	CLA	A	832	50/65	0.84	0.26	2,18,56,60	0
19	CLA	B	807	45/65	0.84	0.27	2,14,56,60	0
19	CLA	F	207	53/65	0.84	0.28	2,22,60,60	0
23	PQN	A	842	33/33	0.84	0.32	2,4,59,60	0
19	CLA	L	209	47/65	0.84	0.26	2,13,45,60	0
19	CLA	B	821	50/65	0.84	0.30	2,37,60,60	0
22	BCR	B	844	40/40	0.84	0.30	2,5,60,60	0
19	CLA	I	102	60/65	0.84	0.29	2,18,60,60	0
19	CLA	A	806	56/65	0.84	0.30	2,2,54,60	0
19	CLA	B	823	55/65	0.84	0.28	2,30,60,60	0
19	CLA	A	818	60/65	0.84	0.33	2,11,52,60	0
19	CLA	A	813	50/65	0.84	0.27	2,29,60,60	0
19	CLA	1	209	25/65	0.84	0.31	11,37,60,60	0
19	CLA	A	835	65/65	0.84	0.29	2,6,60,60	0
19	CLA	B	832	59/65	0.85	0.28	2,6,60,60	0
19	CLA	A	838	65/65	0.85	0.31	2,8,60,60	0
19	CLA	B	826	58/65	0.85	0.31	2,13,60,60	0
20	LMU	H	105	35/35	0.85	0.20	2,31,60,60	0
19	CLA	B	803	65/65	0.85	0.31	2,14,56,60	0
19	CLA	B	825	54/65	0.85	0.31	2,15,60,60	0
19	CLA	A	828	65/65	0.85	0.29	2,12,60,60	0
19	CLA	B	818	53/65	0.85	0.28	2,14,60,60	0
19	CLA	B	840	65/65	0.85	0.30	2,11,60,60	0
19	CLA	B	824	65/65	0.85	0.26	2,17,60,60	0
19	CLA	B	833	50/65	0.85	0.29	2,11,53,60	0
19	CLA	4	313	36/65	0.86	0.24	2,21,60,60	0
19	CLA	B	841	65/65	0.86	0.32	2,2,55,60	0
19	CLA	1	202	41/65	0.86	0.22	2,41,60,60	0
19	CLA	A	827	55/65	0.86	0.30	2,12,60,60	0
19	CLA	A	837	51/65	0.86	0.28	2,12,60,60	0
19	CLA	B	811	25/65	0.86	0.28	2,2,60,60	0
19	CLA	A	803	46/65	0.86	0.30	2,14,49,60	0
23	PQN	B	843	33/33	0.86	0.28	2,2,46,51	0
19	CLA	F	201	50/65	0.86	0.23	2,7,51,60	0
19	CLA	A	851	65/65	0.86	0.28	2,2,60,60	0
19	CLA	2	308	25/65	0.87	0.19	2,12,60,60	0
19	CLA	B	829	65/65	0.87	0.26	2,11,46,60	0
19	CLA	A	830	65/65	0.88	0.25	2,9,59,60	0
19	CLA	4	312	25/65	0.88	0.19	2,2,26,32	0
22	BCR	F	203	40/40	0.88	0.28	2,2,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CLA	F	205	36/65	0.88	0.24	2,17,60,60	0
19	CLA	B	850	65/65	0.88	0.28	2,2,55,60	0
19	CLA	A	831	65/65	0.88	0.25	2,14,60,60	0
19	CLA	A	826	65/65	0.88	0.29	2,2,50,60	0
19	CLA	B	838	65/65	0.88	0.24	2,7,60,60	0
19	CLA	A	850	65/65	0.88	0.27	2,4,48,60	0
19	CLA	B	810	60/65	0.89	0.27	2,2,60,60	0
19	CLA	A	822	50/65	0.89	0.23	2,7,60,60	0
19	CLA	B	839	47/65	0.89	0.25	2,5,55,60	0
22	BCR	F	204	40/40	0.89	0.22	2,6,60,60	0
19	CLA	A	836	47/65	0.89	0.23	2,8,50,60	0
19	CLA	B	808	61/65	0.89	0.27	2,9,48,60	0
19	CLA	B	831	50/65	0.89	0.26	2,12,60,60	0
19	CLA	A	849	65/65	0.90	0.27	2,2,48,60	0
19	CLA	B	809	65/65	0.90	0.26	2,2,53,60	0
19	CLA	B	819	41/65	0.90	0.27	2,5,40,60	0
19	CLA	B	830	65/65	0.90	0.24	2,6,53,60	0
19	CLA	B	828	65/65	0.90	0.26	2,10,56,60	0
19	CLA	B	814	65/65	0.90	0.26	2,13,60,60	0
19	CLA	A	808	60/65	0.91	0.29	2,10,60,60	0
22	BCR	B	801	40/40	0.91	0.23	2,4,50,60	0
19	CLA	A	809	52/65	0.91	0.24	2,10,60,60	0
19	CLA	B	802	54/65	0.92	0.27	2,6,45,60	0
24	SF4	C	103	8/8	0.96	0.08	12,19,20,24	0
24	SF4	C	102	8/8	0.97	0.08	18,22,26,32	0
24	SF4	A	856	8/8	0.98	0.05	23,24,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.