

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 01:28 PM BST

:	5GTI
:	Native XFEL structure of photosystem II (two flash dataset)
:	Suga, M.; Shen, J.R.
:	2016-08-20
:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	÷	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$		
R_{free}	130704	4661(2.50-2.50)		
Ramachandran outliers	138981	5231(2.50-2.50)		
Sidechain outliers	138945	5233(2.50-2.50)		
RSRZ outliers	127900	4559(2.50-2.50)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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
		244	3%
	A	344	97% •
			4%
1	a	344	97% •••
			11%
2	В	505	98% •
			14%
2	b	505	97% •
			16%
3	C	455	98%
			13%
3	с	455	98% •
	_		5%
4	D	342	100%



Mol	Chain	Length	Quality of chain	
4	d	342	8%	
5	E	84	8%	
5		01	23%	
O	e	84	90% 2%	• 6%
6	F	44	77%	23%
6	f	44	68% •	30%
7	Н	65	94%	5% •
7	h	65	97%	•
8	Ι	38	95%	5%
8	i	38	<u>8%</u> 92%	5% •
0	т	20	15%	
9	J		92% 	5% •
9	j	39	100%	
10	К	37	92%	8%
10	k	37	92%	8%
11	L	37	97%	
11	1	37	97%	
10	M	26	3%	01/
	111		8%	• 8%
12	m	36	<u> </u>	6% 6%
13	Ο	244	98%	·
13	0	244	98%	·
14	Т	32	3% 91%	• 6%
14	t	32	88%	6% 6%
15	U	104	13%	• 8%
15	u	104	<u>4%</u> 91%	• 7%
16	V	137	4%	
10	v	101	100%	
16	V	137	100%	



Mol	Chain	Length	Quality of chain	
17	Х	40	93%	• 5%
17	х	40	95%	5%
18	Y	30	40%	•
18	у	30	93%	• •
19	Z	62	37% 94%	6%
19	Z	62	92%	8%
20	R	34	100%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	А	404	Х	-	-	-
23	CLA	А	405	Х	-	-	-
23	CLA	А	407	Х	-	-	-
23	CLA	В	602	Х	-	-	-
23	CLA	В	603	X	-	-	-
23	CLA	В	604	Х	_	-	_
23	CLA	В	605	X	-	-	-
23	CLA	В	606	Х	-	-	_
23	CLA	В	607	X	-	-	-
23	CLA	В	608	Х	_	-	_
23	CLA	В	609	Х	_	-	_
23	CLA	В	610	X	-	-	-
23	CLA	В	611	Х	_	-	_
23	CLA	В	612	Х	-	-	-
23	CLA	В	613	Х	_	-	_
23	CLA	В	614	Х	_	-	_
23	CLA	В	615	Х	-	-	_
23	CLA	В	616	Х	_	-	_
23	CLA	В	617	Х	-	-	-
23	CLA	С	502	Х	-	-	_
23	CLA	С	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X		_	-



Conti	Continued from previous page										
Mol	Type	Chain	\mathbf{Res}	Chirality	Geometry	Clashes	Electron density				
23	CLA	С	508	Х	-	-	-				
23	CLA	С	509	Х	-	-	-				
23	CLA	С	510	Х	-	-	-				
23	CLA	С	511	Х	-	-	-				
23	CLA	С	512	Х	-	-	-				
23	CLA	С	513	Х	-	-	-				
23	CLA	С	514	Х	-	-	-				
23	CLA	D	401	Х	-	-	-				
23	CLA	D	404	Х	-	-	-				
23	CLA	D	405	Х	-	-	-				
23	CLA	a	404	Х	-	-	-				
23	CLA	a	405	Х	-	-	-				
23	CLA	a	406	Х	_	-	-				
23	CLA	a	409	Х	_	-	_				
23	CLA	b	601	Х	_	-	-				
23	CLA	b	602	Х	_	-	_				
23	CLA	b	603	Х	_	-	-				
23	CLA	b	604	Х	_	-	_				
23	CLA	b	605	Х	-	-	-				
23	CLA	b	606	Х	-	-	-				
23	CLA	b	607	Х	-	-	-				
23	CLA	b	608	Х	-	-	-				
23	CLA	b	609	X	-	-	-				
23	CLA	b	610	X	-	-	-				
23	CLA	b	611	X	-	-	-				
23	CLA	b	612	X	-	_	-				
23	CLA	b	613	X	-	-	-				
23	CLA	b	614	X	-	_	-				
23	CLA	b	615	X	-	_	-				
23	CLA	b	616	X	-	_	-				
23	CLA	с	501	X	-	_	-				
23	CLA	с	502	X	-	_	-				
23	CLA	с	503	X	-	_	-				
23	CLA	с	504	X	-	_	_				
23	CLA	с	505	X	_	_	_				
23	CLA	с	506	X	_	_	-				
23	CLA	с	507	X	_	-	_				
23	CLA	с	508	X	_	-	_				
23	CLA	с	509	X	_	-	_				
23	CLA	с	510	X	_	-	_				
23	CLA	c	511	X	_	-	_				
23	CLA	с	512	X	_	_	_				
-		-									



		Chain	Bes	Chirality	Geometry	Clashes	Electron density
23	CLA	chain	513	X	Geometry	-	
20		d	402	X V		_	
20		u d	402			-	-
20	COLA	u J	403	Λ	-	-	- V
21	GOL		401	-	-	_	Λ Υ
30	UNL	A	414	-	-	-	<u>Х</u>
30	UNL	J	102	-	-	-	Х
30	UNL	a	416	-	-	-	Х
30	UNL	b	627	-	_	-	Х
31	LHG	е	101	-	-	-	Х
34	LMG	С	521	-	-	-	Х
34	LMG	с	520	-	-	-	Х
35	LMT	В	633	-	-	-	Х
35	LMT	С	522	_	_	-	Х
35	LMT	Ε	102	-	_	-	Х
35	LMT	е	102	-	_	-	Х
35	LMT	m	103	-	-	-	Х
36	HTG	В	625	_	_	-	Х
36	HTG	В	626	-	-	-	Х
$\overline{36}$	HTG	C	524	_	_	-	Х
36	HTG	b	622			-	Х
36	HTG	b	623	-	-	-	X
36	HTG	с	522		_	-	X



2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 52752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Photosystem II D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	334	Total 2620	C 1716	N 431	O 458	${ m S}$ 15	0	0	0
1	a	334	Total 2620	C 1716	N 431	O 458	S 15	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	504	Total	С	Ν	Ο	S	0	Ο	0
	D	001	3969	2605	661	690	13	0	0	0
0	h	504	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	504	3969	2605	661	690	13	0	0	0

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

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

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

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

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



Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
5	F	81	Total	С	Ν	Ο	0	0	0
0		01	662	432	107	123	0	0	0
5	0	70	Total	С	Ν	Ο	0	0	0
5	е	19	648	424	105	119	0	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
6	F	3.4	Total	С	Ν	Ο	S	0	0	0
0	Г	04	275	187	45	42	1	0	0	0
G	f	21	Total	С	Ν	Ο	S	0	0	0
0	I	10	250	170	42	37	1		0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
7	н	64	Total	С	Ν	Ο	S	0	0	Ο
1	11	04	506	339	81	84	2	0	0	0
7	h	65	Total	С	Ν	Ο	S	0	0	0
1	11	05	511	341	82	86	2	0	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
Q	т	38	Total	С	Ν	Ο	\mathbf{S}	0	0	0
0	L		314	211	48	54	1	0	0	0
0	;	20	Total	С	Ν	Ο	S	0	0	0
0		50	314	211	48	54	1		U	

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

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
0	т	20	Total	С	Ν	Ο	S	0	0	0
9	1		272	182	42	47	1	0	0	0
0	;	20	Total	С	Ν	Ο	S	0	0	0
9	J		277	185	43	48	1	0	0	0

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

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
10	K	37	Total 293	$\begin{array}{c} \mathrm{C} \\ 204 \end{array}$	N 43	O 46	0	0	0



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

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

Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
11	L	36	Total	C 107	N 47	0 52	0	0	0
	1	20	Total	- 197 - C	47 N	$\frac{32}{0}$	0	0	0
		30	296	197	47	52	0	U	

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

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
10	М	22	Total	С	Ν	Ο	S	0	0	0
	IVI		260	173	38	48	1	0	0	0
10		24	Total	С	Ν	Ο	S	0	0	0
	111	04	269	179	40	49	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	0	242	Total	С	Ν	Ο	S	0	0	0
10	0	240	1865	1165	315	381	4	0	0	0
19		942	Total	С	Ν	Ο	S	0	0	0
10	0		1865	1165	315	381	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	т	30	Total	С	Ν	Ο	S	0	0	0
14		50	258	181	36	39	2	0	0	0
14	+	20	Total	С	Ν	Ο	S	0	0	0
14	L L		258	181	36	39	2	0	0	U

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	II	06	Total	С	Ν	Ο	0	0	0
10	U	90	765	486	128	151	0	0	0
15	11	07	Total	С	Ν	Ο	0	0	0
10	u	u 97	774	491	129	154	0	0	0



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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	v	197	Total	С	Ν	Ο	S	0	0	0
10	10 V	137	1064	675	177	208	4	0	0	0
16		127	Total	С	Ν	Ο	S	0	0	0
10	V	197	1064	675	177	208	4	0	0	0

• Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	v	38	Total	С	Ν	Ο	0	0	0
17	Λ		281	188	45	48	0	0	0
17	v	20	Total	С	Ν	Ο	0	0	0
11	А	30	281	188	45	48		U	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	20	Total	С	Ν	Ο	S	0	0	0
10	1	29	215	142	37	33	3	0	0	0
18	Ţ	20	Total	С	Ν	Ο	S	0	0	0
10	У	29	215	142	37	33	3	0	0	

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	7	62	Total	С	Ν	Ο	\mathbf{S}	0	0	0
19	2	02	479	328	72	77	2	0	0	0
10	7	62	Total	С	Ν	Ο	S	0	0	0
19	z	02	479	328	72	77	2	0	0	0

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

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

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

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



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

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

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

• Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf		
23	Δ	1	Total	С	Mg	Ν	Ο	Ο	0		
20	11	I	65	55	1	4	5	0	0		
23	Δ	1	Total	С	Mg	Ν	Ο	0	0		
20	Л	T	65	55	1	4	5	0	0		
23	Δ	1	Total	С	Mg	Ν	Ο	0	0		
20	Л	Л		65	55	1	4	5	0		
23	В	1	Total	С	Mg	Ν	Ο	0	0		
20	D	I	65	55	1	4	5	0	0		
23	В	1	Total	С	Mg	Ν	Ο	0	0		
20	D	T	65	55	1	4	5	0	0		
02	D	1	Total	С	Mg	Ν	Ο	0	0		
	D		65	55	1	4	5	U			



Mol	Chain	Residues	5-	At	oms			ZeroOcc	AltConf
	р		Total	С	Mg	Ν	Ο	0	0
23	В	1	65	55	1	4	5	0	0
	р		Total	С	Mg	Ν	Ο	0	0
23	В	1	65	55	1	4	5	0	0
	Б	1	Total	С	Mg	Ν	Ο	0	0
23	В	1	65	55	1	4	5	0	0
0.2	р	1	Total	С	Mg	Ν	Ο	0	0
23	В	1	65	55	1	4	5	0	0
0.2	р	1	Total	С	Mg	Ν	Ο	0	0
23	В	1	65	55	1	4	5	0	0
	р	1	Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
- 12	D	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 12	D	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 72	В	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 0.2	D	1	Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
2	D	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- <u>72</u>	В	1	Total	С	Mg	Ν	Ο	0	0
20	D	L	65	55	1	4	5	0	0
23	В	1	Total	С	Mg	Ν	Ο	0	0
2.5	D	I	65	55	1	4	5	0	0
23	С	1	Total	С	Mg	Ν	Ο	0	0
20	U	T	65	55	1	4	5	0	0
23	С	1	Total	С	Mg	Ν	Ο	0	0
	0	L	65	55	1	4	5	0	0
23	С	1	Total	С	Mg	Ν	Ο	0	0
	0	L	65	55	1	4	5	0	0
23	С	1	Total	С	Mg	Ν	Ο	0	0
	0	1	65	55	1	4	5	0	0
23	C	1	Total	С	Mg	Ν	Ο	0	0
		L	65	55	1	4	5	0	
23	C	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
		1	65	55	1	4	5		
23	C	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
		L	65	55	1	4	5	0	
23	C	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
			65	55	1	4	5	U U	



Mol	Chain	Residues	5-	At	oms			ZeroOcc	AltConf
	a		Total	С	Mg	Ν	0	0	0
23	C	1	65	55	1	4	5	0	0
	a		Total	С	Mg	Ν	Ο	0	0
23	C	1	65	55	1	4	5	0	0
	a	1	Total	С	Mg	Ν	Ο	0	0
23	C	1	65	55	1	4	5	0	0
0.2	a	1	Total	С	Mg	Ν	Ο	0	0
23	U	1	65	55	1	4	5	0	0
0.2	C	1	Total	С	Mg	Ν	Ο	0	0
23	U	1	65	55	1	4	5	0	0
- 02	р	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 12	р	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 12	п	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
2		1	Total	С	Mg	Ν	Ο	0	0
20	a	1	65	55	1	4	5	0	0
- 0.2	-	1	Total	С	Mg	Ν	Ο	0	0
20	a	1	65	55	1	4	5	0	0
2	0	1	Total	С	Mg	Ν	Ο	0	0
20	a	1	65	55	1	4	5	0	0
- 12		1	Total	С	Mg	Ν	Ο	0	0
20	a	1	65	55	1	4	5	0	0
02	Ь	1	Total	С	Mg	Ν	Ο	0	0
2.5	U	I	65	55	1	4	5	0	0
23	h	1	Total	С	Mg	Ν	Ο	0	0
20	U	T	65	55	1	4	5	0	0
23	h	1	Total	С	Mg	Ν	Ο	0	0
20	U	L	65	55	1	4	5	0	0
23	h	1	Total	С	Mg	Ν	Ο	0	0
	U U	L	65	55	1	4	5	0	0
23	h	1	Total	С	Mg	Ν	Ο	0	0
	0	L	65	55	1	4	5	0	0
23	h	1	Total	С	Mg	Ν	Ο	0	0
		L	65	55	1	4	5	0	
23	h	1	Total	\mathbf{C}	Mg	Ν	Ο	0	
		±	65	55	1	4	5	V	
23	h	1	Total	\mathbf{C}	Mg	Ν	0	0	0
	U	L	65	55	1	4	5	0	
23	h	1	Total	$\overline{\mathrm{C}}$	Mg	N	0	0	0
			65	55	1	4	5		



Mol	Chain	Residues	5-	At	oms			ZeroOcc	AltConf
	1		Total	С	Mg	Ν	Ο	0	0
23	b	1	65	55	1	4	5	0	0
	1		Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
0.2	1.	1	Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
0.2	1.	1	Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
	1.	1	Total	С	Mg	Ν	Ο	0	0
23	D	1	65	55	1	4	5	0	0
	1.	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 12	h	1	Total	С	Mg	Ν	Ο	0	0
20	D	1	65	55	1	4	5	0	0
- 12		1	Total	С	Mg	Ν	Ο	0	0
20	C	1	65	55	1	4	5	0	0
- 02		1	Total	С	Mg	Ν	Ο	0	0
20	C	1	65	55	1	4	5	0	0
- 0.2	_	1	Total	С	Mg	Ν	Ο	0	0
20	С	1	65	55	1	4	5	0	0
2	0	1	Total	С	Mg	Ν	Ο	0	0
20	C	1	65	55	1	4	5	0	0
- <u>72</u>		1	Total	С	Mg	Ν	Ο	0	0
20	C	L	65	55	1	4	5	0	0
23	0	1	Total	С	Mg	Ν	Ο	0	0
2.5	C	I	65	55	1	4	5	0	0
93	C	1	Total	С	Mg	Ν	Ο	0	0
_ 20	C	T	65	55	1	4	5	0	0
- 23	C	1	Total	С	Mg	Ν	Ο	0	0
	Č.	L	65	55	1	4	5	0	0
23	C	1	Total	С	Mg	Ν	Ο	0	0
	C C	L	65	55	1	4	5	0	0
23	C	1	Total	С	Mg	Ν	Ο	0	0
	Č	1	65	55	1	4	5	0	0
23	c	1	Total	С	Mg	Ν	Ο	0	0
		L	65	55	1	4	5	U	
23	C	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
	Ŭ	1	65	55	1	4	5		
23	c	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
		L	65	55	1	4	5	U	
23	d	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
	u		65	55	1	4	5		



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

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

РНО	

Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
24	24 A	1	Total	С	Ν	Ο	0	0
24			64	55	4	5	0	
94	Л	1	Total	С	Ν	Ο	0	0
24	D	L	64	55	4	5	0	0
94	2	1	Total	С	Ν	Ο	0	0
24	a	L	64	55	4	5	0	
94	0	1	Total	С	Ν	Ο	0	0
	a		64	55	4	5	0	U

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	А	1	Total C 40 40	0	0
25	В	1	Total C 40 40	0	0
25	В	1	Total C 40 40	0	0
25	В	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 40 & 40 \end{array}$	0	0
25	D	1	Total C 40 40	0	0
25	Н	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 40 & 40 \end{array}$	0	0
25	Т	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 40 & 40 \end{array}$	0	0
25	Y	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 40 & 40 \end{array}$	0	0
25	a	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	b	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 40 & 40 \end{array}$	0	0
25	b	1	$\begin{array}{c c} \hline Total & C \\ 40 & 40 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	С	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	d	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	h	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	k	1	$\begin{array}{cc} {\rm Total} & {\rm C} \\ {\rm 40} & {\rm 40} \end{array}$	0	0
25	t	1	Total C 40 40	0	0
25	У	1	Total C 40 40	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	Δ	1	Total	С	Ο	S	0	Ο
20	Л	I	54	41	12	1	0	0
26	Λ	1	Total	С	Ο	S	0	0
20	Л	I	54	41	12	1	0	0
26	В	1	Total	С	Ο	S	0	0
20	D		54	41	12	1	0	U



Mol	Chain	Residues	A	ton	ıs		ZeroOcc	AltConf
26 D	п	1	Total	С	Ο	\mathbf{S}	0	0
	D		43	30	12	1	0	
26	T	1	Total	С	Ο	\mathbf{S}	0	0
20	L	T	54	41	12	1	0	0
26	9	a 1	Total	С	Ο	\mathbf{S}	0	0
20	a		54	41	12	1	0	
26		1	Total	С	Ο	\mathbf{S}	0	0
20	a	I	54	41	12	1	0	0
26	f	1	Total	С	Ō	S	0	0
			43	30	12	1		

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• Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
27	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
27	В	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
27	С	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
27	О	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
27	a	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
27	d	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
28	А	1	Total	Ca	Mn	Ο	0	0
	11	1	10	1	4	5	0	0
20		. 1	Total	Ca	Mn	Ο	0	0
20	a	L	10	1	4	5	0	0

• Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).





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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	J	1	Total C 10 10	0	0
30	i	1	$\begin{array}{ccc} \mathrm{Total} & \mathrm{C} & \mathrm{O} \\ 40 & 35 & 5 \end{array}$	0	0
30	D	2	Total C O 57 51 6	0	0
30	K	1	Total C O 34 29 5	0	0
30	В	1	Total C O 33 28 5	0	0
30	Ι	1	Total C O 40 35 5	0	0
30	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 32 & 27 & 5 \end{array}$	0	0
30	a	1	Total C O 30 25 5	0	0



30

30

b

М

2

1

0

0

0

0

0

0

0

0

69

59 10

10

Total C

10

• Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

0

0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	Λ	1	Total	С	Ο	Р	0	0
101	Л	T	49	38	10	1	0	0
21	п	1	Total	С	Ο	Р	0	0
101	D	T	49	38	10	1	0	0
21	п	1	Total	С	Ο	Р	0	0
	D	L	49	38	10	1		



Chain Residues Atoms ZeroOcc AltConf Mol Total С Ο 0 301 Х 18 16 2Total С Ο 30А 1 0 28235Total C j 301 0 1010Total С Ο Х 1 0 3016 218Total С Ο 30d 1 0 17161 Total С 301 0 m 1010Total C O

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• Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	А	1	Total C O 4 1 3	0	0
32	a	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 1 3 \end{array}$	0	0

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



Chain Residues ZeroOcc AltConf Mol Atoms С Total Р Ο Е 0 310 1 4231101 Total С Ο Р 31 \mathbf{L} 1 0 0 4938101 Total С Р Ο 31b 1 0 0 4938101 Total С Ο Р d 1 0 0 314938101 Total С Ο Р 31d 1 0 0 4938101 Total С Ο Ρ 0 0 31d 1 4938101 С Р Total Ο 0 311 0е 4231101

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	В	1	Total Ca 1 1	0	0
33	С	1	Total Ca 1 1	0	0
33	V	1	Total Ca 1 1	0	0
33	с	2	Total Ca 2 2	0	0
33	Ο	1	Total Ca 1 1	0	0
33	О	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	В	1	Total C O	0	0
			51 41 10		
34	C	1	Total C O	0	0
- 54	U	L	51 41 10	0	0
34	С	1	Total C O	0	0
- 54	U	T	51 41 10	0	
3/	С	1	Total C O	0	0
04	U	T	51 41 10	0	
34	T	1	Total C O	0	0
J4	J	J L	51 41 10		U



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

• Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	В	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 35 & 24 & 11 \end{array}$	0	0
35	В	1	Total C O 25 19 6	0	0
35	В	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 35 & 24 & 11 \end{array}$	0	0
35	В	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 26 & 19 & 7 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	С	1	Total C O	0	0
		-	35 24 11		
35	П	1	Total C O	0	0
00	D	1	35 24 11	0	0
35	F	1	Total C O	0	0
00	Ľ	T	35 24 11	0	0
35	М	1	Total C O	0	0
00	111	T	35 24 11	0	0
25	М	1	Total C O	0	0
00	IVI	L	35 24 11	0	
25		o 1	Total C O	0	0
00	a	L	35 24 11		
25	h	1	Total C O	0	0
00	U	T	25 19 6	0	0
35	Ь	1	Total C O	0	0
00	U	T	25 19 6	0	0
35	0	1	Total C O	0	0
00	e		35 24 11		0
25	m	1	Total C O	0	0
30			35 24 11		U

• Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	В	1	Total 19	C 13	O 5	${ m S}$ 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	В	1	Total C O S 19 13 5 1	0	0
36	В	1	Total C O S 19 13 5 1	0	0
36	В	1	Total C O S 19 13 5 1	0	0
36	В	1	Total C O S 19 13 5 1	0	0
36	С	1	Total C O S 19 13 5 1	0	0
36	С	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm S} \\ 9 & 8 & 1 \end{array}$	0	0
36	D	1	Total C O S 16 10 5 1	0	0
36	V	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 11 & 6 & 5 \end{array}$	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	с	1	Total C O S 19 13 5 1	0	0
36	с	1	Total C O S 19 13 5 1	0	0
36	h	1	Total C O S 16 10 5 1	0	0

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• Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	С	1	Total C O	0	0
57	U	T	62 47 15	0	0
37	С	1	Total C O	0	0
- 57	U	I	62 47 15	0	0
37	С	1	Total C O	0	0
- 57	U	I	62 47 15	0	0
37	н	1	Total C O	0	0
- 57	11	I	62 47 15	0	0
37	c	1	Total C O	0	Ο
	Č.	, I	62 47 15	0	0
37	c	1	Total C O	0	0
	Č.	, I	62 47 15	0	0
37	С	1	Total C O	0	0
	U		62 47 15		0
37	h	1	Total C O	0	0
01	11	1	62 47 15		U

 Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
28	F	1	Total	С	Fe	Ν	Ο	0	0
00	30 E	T	43	34	1	4	4	0	0
20	0	1	Total	С	Fe	Ν	Ο	0	0
38 e	L	43	34	1	4	4	0	0	

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

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

• Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
40	V	1	Total	С	Fe	Ν	Ο	0	0
40	40 1	1	43	34	1	4	4	0	0
40		1	Total	С	Fe	Ν	Ο	0	0
40 V	v	L	43	34	1	4	4		0

• Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	А	135	Total O 135 135	0	0
41	В	195	Total O 195 195	0	0
41	С	151	Total O 151 151	0	0
41	D	118	Total O 118 118	0	0
41	Е	25	TotalO2525	0	0
41	F	5	Total O 5 5	0	0
41	Н	22	TotalO2222	0	0
41	Ι	6	Total O 6 6	0	0
41	J	4	Total O 4 4	0	0
41	K	6	Total O 6 6	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	6	Total O 6 6	0	0
41	М	15	Total O 15 15	0	0
41	О	105	Total O 105 105	0	0
41	Т	13	Total O 13 13	0	0
41	U	51	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 51 & 51 \end{array}$	0	0
41	V	81	Total O 81 81	0	0
41	Х	4	Total O 4 4	0	0
41	Y	1	Total O 1 1	0	0
41	Z	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	132	Total O 132 132	0	0
41	b	206	Total O 206 206	0	0
41	с	153	Total O 153 153	0	0
41	d	115	Total O 115 115	0	0
41	е	16	Total O 16 16	0	0
41	f	5	Total O 5 5	0	0
41	h	27	Total O 27 27	0	0
41	i	3	Total O 3 3	0	0
41	j	3	Total O 3 3	0	0
41	k	6	TotalO66	0	0
41	l	9	Total O 9 9	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	m	18	Total O 18 18	0	0
41	О	115	Total O 115 115	0	0
41	t	9	Total O 9 9	0	0
41	u	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
41	V	78	Total O 78 78	0	0
41	х	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0



3 Residue-property plots (i)

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

• Molecule 1: Photosystem II D1 protein



• Molecule 3: Photosystem II CP43 protein



5GTI
O O I I



• Molecule 6: Cytochrome b559 subunit beta Chain F: 77% 23% THR SER ASN THR PRO GLN GLN GLU • Molecule 6: Cytochrome b559 subunit beta Chain f: 68% 30% THR SER ASN ASN PRO GLU GLU PRO GLU VAL SER TYR PRO • Molecule 7: Photosystem II reaction center protein H 12% Chain H: 94% 5%• W6 L7 G8 G8 D9 L11 L11 • Molecule 7: Photosystem II reaction center protein H 29% Chain h: 97% A2 R3 T5 W6 W6 G8 G8 D9 I10 R12 R12 V21 A22 10 T • Molecule 8: Photosystem II reaction center protein I 18% Chain I: 95% 5% K35 L37 L37 • Molecule 8: Photosystem II reaction center protein I Chain i: 92% 5%• • Molecule 9: Photosystem II reaction center protein J 15% Chain J: 92% 5% •



MET S2 64 64 11 19 19 19 19 19 19 19 139		
• Molecule 9: Photosys	tem II reaction center protein J	
Chain it		
Unain J:	100%	
M1 83 64 65 65 71 18 19 13 14 14 13		
• Molecule 10: Photosy	stem II PsbK protein	
Chain K:	020/	01/
	92%	8%
K10 A14 117 F118 P19 D19 D19 D19 D19 C20 V30 V30 R46		
• Molecule 10: Photosy	stem II PsbK protein	
Chain k:	92%	8%
K10 117 118 118 119 119 119		
• Molecule 11: Photosy	stem II reaction center protein L	
14%		
Chain L:	97%	٠
MET E2 E2 69 99 V10 N37		
• Molecule 11: Photosy	stem II reaction center protein L	
Chain l:	0706	
	5170	
MET 82 89 99 98 1137		
• Molecule 12: Photosy	stem II PsbM protein	
Chain M:	0004	00/
	03.40	• 8%
■ SER SER		

• Molecule 12: Photosystem II PsbM protein



Chain m.	8%	201
Unann m.	89%	6% 6%
M1 831 033 133 133 133 133	ы ы ы ы ы ы ы ы ы ы ы ы ы ы ы ы ы ы ы	
• Molecule	e 13: Photosystem II manganese-stabilizing polypeptide	
Chain O:	98%	
	⁴ ω ω μ α α α α α α α α α α α α α α α α α	4
13 15 12 12 12 12 12 12 12	22 23 25 26 28 28 28 28 28 28 28 28 28 28 28 28 28	
• Molecule	e 13: Photosystem II manganese-stabilizing polypeptide	
Chain o:	98%	
GLN T4 L5 10 10 22 D22	225 226 A26 A26 A26 A26 A26 A26 A26 A26 A26	F142 • L199 • V204 • T208 • C209 • C209 • C209 •
1211 6226 7241 5242 1243 1243	2246 69	
• Molecule	e 14: Photosystem II reaction center protein T	
Chain T:	91%	• 6%
	0170	
M1 E2 T30 LYS LYS		
• Molecule	e 14: Photosystem II reaction center protein T	
Chain t:	88%	6% 6%
HI HI LINS LINS		
• Molecule	e 15: Photosystem II 12 kDa extrinsic protein	
Chain U:	13%	• 8%
ALA THR ALA SER SER CLU GLU GLU	L62 L62 L62 L62 L62 L75 L75 L75 C17 L75 C17 L75 C17 L75 C101 L102 V103 V103 V104	
• Molecule	e 15: Photosystem II 12 kDa extrinsic protein	
Chain u:	01%	. 70⁄2
Juan u.	5170	- 170

L D W I D E


• Molecule 19: Photosystem II reaction center protein Z



	37%	
Chain Z:	94%	6%
M1 13 13 13 14 17 17 17 17 17 17 12 13 12 13 13 13 13 13 13 14 13 14 14 14 14 14 14 14 14 14 14 14 14 14	031 032 032 033 034 033 033 033 033 033 033 033 033	
• Molecule 19: Ph	notosystem II reaction center protein	Z
Chain z:	29%	804
	32.70	070
M1 12 13 13 14 13 14 13 13 13 132	N33 158 158 158 158 158 158 159 159 159 159 159	
• Molecule 20: Ph	notosystem II protein Y	
	100%	
Chain R:	100%	
D2 W3 V5 V5 V5 V7 V7 V12 V12 V12 V12 V12 V12 V12 V12 V12 V12	A16 416 416 416 416 416 416 416 416 416 4	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	126.52Å 231.23 Å 287.46 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}\left(\mathring{A}\right)$	19.98 - 2.50	Depositor
Resolution (A)	46.51 - 2.50	EDS
% Data completeness	100.0 (19.98-2.50)	Depositor
(in resolution range)	$100.0 \ (46.51 - 2.50)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
D D.	0.139 , 0.187	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.142 , 0.189	DCC
R_{free} test set	14614 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33, 68.2	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, LMG, FE2, HEC, BCT, HEM, FME, UNL, HTG, BCR, SQD

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

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.44	0/2705	0.56	0/3689
1	a	0.43	0/2705	0.54	0/3689
2	В	0.42	0/4109	0.54	0/5600
2	b	0.41	0/4109	0.54	0/5600
3	С	0.39	0/3599	0.51	0/4900
3	с	0.39	0/3633	0.53	0/4946
4	D	0.43	0/2821	0.54	0/3844
4	d	0.43	0/2812	0.54	0/3832
5	Е	0.35	0/681	0.53	0/928
5	е	0.37	0/667	0.49	0/908
6	F	0.34	0/284	0.48	0/387
6	f	0.40	0/257	0.49	0/349
7	Н	0.36	0/519	0.53	0/708
7	h	0.35	0/524	0.49	0/713
8	Ι	0.37	0/311	0.51	0/419
8	i	0.36	0/311	0.54	0/419
9	J	0.36	0/278	0.46	0/376
9	j	0.35	0/283	0.47	0/383
10	K	0.35	0/303	0.53	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.42	0/303	0.51	0/412
11	1	0.38	0/303	0.53	0/412
12	М	0.44	0/253	0.58	0/346
12	m	0.42	0/262	0.58	0/357
13	0	0.38	0/1896	0.58	0/2571
13	0	0.39	0/1896	0.58	0/2571
14	Т	0.54	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.57	0/1052
15	u	0.41	0/785	0.57	0/1064
16	V	0.37	0/1085	0.52	0/1473



Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
16	V	0.37	0/1085	0.53	0/1473
17	Х	0.33	0/284	0.49	0/384
17	х	0.31	0/284	0.46	0/384
18	Y	0.30	0/216	0.44	0/289
18	у	0.31	0/216	0.50	0/289
19	Ζ	0.32	0/490	0.46	0/669
19	Z	0.32	0/490	0.43	0/669
20	R	0.27	0/279	0.43	0/383
All	All	0.40	0/42631	0.53	0/58018

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Percen	\mathbf{tiles}
1	А	332/344~(96%)	326~(98%)	5 (2%)	1 (0%)	41	61
1	a	332/344~(96%)	327~(98%)	4 (1%)	1 (0%)	41	61
2	В	502/505~(99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505~(99%)	494 (98%)	8 (2%)	0	100	100
3	С	449/455~(99%)	440 (98%)	8 (2%)	1 (0%)	47	68
3	с	453/455~(100%)	442 (98%)	10 (2%)	1 (0%)	47	68



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	D	340/342~(99%)	330~(97%)	10 (3%)	0	100	100
4	d	339/342~(99%)	333~(98%)	6(2%)	0	100	100
5	Ε	79/84~(94%)	78~(99%)	1 (1%)	0	100	100
5	е	77/84~(92%)	76~(99%)	1 (1%)	0	100	100
6	F	32/44~(73%)	32 (100%)	0	0	100	100
6	f	29/44~(66%)	29 (100%)	0	0	100	100
7	Н	62/65~(95%)	60 (97%)	2(3%)	0	100	100
7	h	63/65~(97%)	59 (94%)	4 (6%)	0	100	100
8	Ι	36/38~(95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38~(95%)	31 (86%)	4 (11%)	1 (3%)	5	7
9	J	36/39~(92%)	36 (100%)	0	0	100	100
9	j	37/39~(95%)	36 (97%)	1 (3%)	0	100	100
10	К	35/37~(95%)	35 (100%)	0	0	100	100
10	k	35/37~(95%)	35 (100%)	0	0	100	100
11	L	34/37~(92%)	34 (100%)	0	0	100	100
11	1	34/37~(92%)	34 (100%)	0	0	100	100
12	М	31/36~(86%)	31 (100%)	0	0	100	100
12	m	32/36~(89%)	31 (97%)	1 (3%)	0	100	100
13	Ο	241/244~(99%)	232~(96%)	9 (4%)	0	100	100
13	О	241/244~(99%)	232~(96%)	9 (4%)	0	100	100
14	Т	28/32~(88%)	28 (100%)	0	0	100	100
14	t	28/32~(88%)	28 (100%)	0	0	100	100
15	U	94/104~(90%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104~(91%)	91 (96%)	4 (4%)	0	100	100
16	V	135/137~(98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137~(98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40~(90%)	36 (100%)	0	0	100	100
17	X	$\overline{36/40}~(90\%)$	36 (100%)	0	0	100	100
18	Y	27/30~(90%)	26 (96%)	1 (4%)	0	100	100
18	у	27/30~(90%)	25 (93%)	1 (4%)	1 (4%)	3	4
19	Z	60/62~(97%)	59 (98%)	0	1 (2%)	9	16



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
19	Z	60/62~(97%)	59~(98%)	0	1 (2%)	9	16
20	R	32/34~(94%)	32~(100%)	0	0	100	100
All	All	5212/5384~(97%)	5097 (98%)	107 (2%)	8 (0%)	47	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}
8	i	36	ASP
3	С	416	SER
3	с	416	SER
19	Ζ	30	PRO
1	a	259	ILE
19	Z	30	PRO
18	у	45	ASN
1	А	259	ILE

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	Percer	ntiles
1	А	269/279~(96%)	269~(100%)	0	100	100
1	a	269/279~(96%)	268~(100%)	1 (0%)	91	97
2	В	402/403~(100%)	395~(98%)	7(2%)	60	82
2	b	402/403~(100%)	390~(97%)	12 (3%)	41	68
3	С	352/356~(99%)	349~(99%)	3~(1%)	78	92
3	с	356/356~(100%)	348~(98%)	8 (2%)	52	77
4	D	277/277~(100%)	276~(100%)	1 (0%)	91	97
4	d	276/277~(100%)	275~(100%)	1 (0%)	91	97
5	Ε	72/73~(99%)	71~(99%)	1 (1%)	67	86
5	е	70/73~(96%)	67~(96%)	3 (4%)	29	53
6	F	28/38~(74%)	28 (100%)	0	100	100



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	f	25/38~(66%)	24~(96%)	1 (4%)	31	56
7	Н	54/54~(100%)	51~(94%)	3~(6%)	21	40
7	h	54/54~(100%)	52~(96%)	2(4%)	34	60
8	Ι	34/34~(100%)	33~(97%)	1 (3%)	42	69
8	i	34/34~(100%)	32~(94%)	2~(6%)	19	37
9	J	26/27~(96%)	24 (92%)	2 (8%)	13	25
9	j	26/27~(96%)	26~(100%)	0	100	100
10	K	30/30~(100%)	27~(90%)	3~(10%)	7	15
10	k	30/30~(100%)	27~(90%)	3~(10%)	7	15
11	L	34/35~(97%)	34 (100%)	0	100	100
11	l	34/35~(97%)	34 (100%)	0	100	100
12	М	29/32~(91%)	29~(100%)	0	100	100
12	m	30/32~(94%)	29~(97%)	1 (3%)	38	64
13	О	206/207~(100%)	201 (98%)	5 (2%)	49	74
13	О	206/207~(100%)	203~(98%)	3 (2%)	65	85
14	Т	26/28~(93%)	25~(96%)	1 (4%)	33	58
14	t	26/28~(93%)	25~(96%)	1 (4%)	33	58
15	U	83/89~(93%)	82~(99%)	1 (1%)	71	88
15	u	84/89~(94%)	82~(98%)	2(2%)	49	74
16	V	117/117~(100%)	117~(100%)	0	100	100
16	v	117/117~(100%)	117 (100%)	0	100	100
17	Х	31/33~(94%)	30 (97%)	1 (3%)	39	65
17	х	31/33~(94%)	31~(100%)	0	100	100
18	Y	22/23~(96%)	22~(100%)	0	100	100
18	у	22/23~(96%)	22 (100%)	0	100	100
19	Ζ	$\overline{52/52}\ (100\%)$	49 (94%)	3 (6%)	20	38
19	Z	52/52~(100%)	48 (92%)	4 (8%)	13	25
20	R	29/29~(100%)	29 (100%)	0	100	100
All	All	4317/4403~(98%)	4241 (98%)	76 (2%)	59	81

All (76) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type		
2	В	53	ASN		
2	В	161	LEU		
2	В	223	GLN		
2	В	362	PHE		
2	В	472	ARG		
2	В	495	PHE		
2	В	505	ARG		
3	С	289	PHE		
3	С	315	MET		
3	С	416	SER		
4	D	180	ARG		
5	Е	54	SER		
7	Н	12	ARG		
7	Н	49	TYR		
7	Н	56	ASP		
8	Ι	33	LYS		
9	J	3	GLU		
9	J	6	ARG		
10	K	10	LYS		
10	K	17	ILE		
10	K	19	ASP		
13	0	24	ASP		
13	0	118	LEU		
13	0	135	SER		
13	0	219	GLN		
13	0	234	LYS		
14	Т	2	GLU		
15	U	70	ARG		
17	Х	2	THR		
19	Z	4	LEU		
19	Z	6	GLN		
19	Z	7	LEU		
1	a	12	ASN		
2	b	53	ASN		
2	b	121	GLU		
2	b	128	THR		
2	b	161	LEU		
2	b	223	GLN		
2	b	362	PHE		
2	b	472	ARG		
2	b	477	ASP		
2	b	485	GLU		
2	b	486	LEU		
	1	L			



Mol	Chain	Res	Type
2	b	491	VAL
2	b	505	ARG
3	с	19	ASN
3	с	24	THR
3	с	240	ILE
3	с	279	LEU
3	с	289	PHE
3	с	315	MET
3	с	355	THR
3	с	416	SER
4	d	180	ARG
5	е	16	SER
5	е	54	SER
5	е	74	GLN
6	f	15	ILE
7	h	49	TYR
7	h	56	ASP
8	i	33	LYS
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	0	37	THR
13	0	118	LEU
13	0	132	ASN
14	t	2	GLU
15	u	15	GLU
15	u	61	VAL
19	Z	4	LEU
19	Z	6	GLN
19	Z	7	LEU
19	Z	32	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	53	ASN
2	В	331	ASN
3	С	201	ASN
4	D	61	HIS
4	D	83	ASN



Mol	Chain	Res	Type
4	D	142	ASN
5	Е	60	GLN
6	F	44	GLN
13	0	124	ASN
13	0	130	GLN
15	U	73	GLN
19	Z	58	ASN
2	b	53	ASN
2	b	223	GLN
2	b	331	ASN
3	с	201	ASN
4	d	83	ASN
4	d	142	ASN
5	е	60	GLN
5	е	75	GLN
6	f	44	GLN
12	m	5	GLN
13	0	124	ASN
13	0	130	GLN
19	Z	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Tyn	Tune	Chain	Dec	Dec	Dec	Dec	Dog	Dog	Rog	Tink	B	ond leng	gths	E	Bond ang	gles
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2						
8	FME	i	1	8	8,9,10	0.61	0	$7,\!9,\!11$	1.26	1 (14%)						
12	FME	М	1	12	8,9,10	0.55	0	7,9,11	1.35	1 (14%)						
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.64	3 (42%)						



Mol Type Chain	Tune	Chain	Dog	Tink	B	Bond lengths			Bond angles		
	Ullain	1105		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
14	FME	Т	1	14	8,9,10	0.64	0	$7,\!9,\!11$	1.22	0	
8	FME	Ι	1	8	8,9,10	0.64	0	$7,\!9,\!11$	1.00	1 (14%)	
14	FME	t	1	14	8,9,10	0.68	0	$7,\!9,\!11$	1.72	2 (28%)	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	2/7/9/11	-
12	FME	М	1	12	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	Т	1	14	-	3/7/9/11	-
8	FME	Ι	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
14	t	1	FME	O-C-CA	-2.68	117.76	124.78
12	М	1	FME	O-C-CA	-2.52	118.17	124.78
12	m	1	FME	CA-N-CN	-2.39	119.15	122.82
8	i	1	FME	O-C-CA	-2.30	118.75	124.78
12	m	1	FME	O1-CN-N	-2.26	119.33	125.27
12	m	1	FME	C-CA-N	2.20	113.70	109.73
8	Ι	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN
14	Т	1	FME	O1-CN-N-CA
14	Т	1	FME	C-CA-CB-CG
14	Т	1	FME	N-CA-CB-CG
8	i	1	FME	CA-CB-CG-SD



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Mol	Chain	Res	Type	Atoms
8	i	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 218 ligands modelled in this entry, 18 are unknown and 15 are monoatomic - leaving 185 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Bog	Link	B	ond leng	gths	Bo	ond angl	es
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
34	LMG	с	520	-	$51,\!51,\!55$	0.97	2 (3%)	$59,\!59,\!63$	1.21	7 (11%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56, 56, 56	1.68	13 (23%)
36	HTG	b	623	-	19,19,19	1.08	2 (10%)	23,24,24	1.63	3 (13%)
27	GOL	А	410	-	5, 5, 5	0.37	0	5, 5, 5	0.25	0
29	PL9	d	405	-	55, 55, 55	0.64	2 (3%)	$68,\!69,\!69$	1.86	22 (32%)
23	CLA	с	502	3	59,73,73	2.04	12 (20%)	67,113,113	2.19	20 (29%)
37	DGD	С	517	-	$63,\!63,\!67$	0.85	2 (3%)	77,77,81	1.19	7 (9%)
24	PHO	a	408	-	67,69,69	2.23	15 (22%)	85,99,99	1.87	22 (25%)
23	CLA	В	608	41	59,73,73	2.05	14 (23%)	67,113,113	2.19	23 (34%)
23	CLA	b	605	2	59,73,73	2.00	13 (22%)	67,113,113	2.24	23 (34%)
23	CLA	b	611	2	59,73,73	2.01	12 (20%)	67,113,113	2.33	22 (32%)
25	BCR	Н	101	-	41,41,41	1.08	1 (2%)	56, 56, 56	1.59	11 (19%)
23	CLA	В	606	2	59,73,73	1.99	14 (23%)	67,113,113	2.17	24 (35%)
25	BCR	Т	101	-	41,41,41	1.04	1 (2%)	56, 56, 56	1.85	10 (17%)



Mal	Tune	Type Chain Res Link		Link	B	ond leng	gths	Bond angles		
	туре	Chan	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
25	BCR	у	101	-	41,41,41	1.09	1 (2%)	$56,\!56,\!56$	1.66	12 (21%)
29	PL9	a	415	-	55, 55, 55	0.65	1 (1%)	$68,\!69,\!69$	2.00	20 (29%)
24	PHO	a	407	-	67,69,69	2.13	17 (25%)	$85,\!99,\!99$	2.02	25 (29%)
23	CLA	А	405	41	59,73,73	2.03	14 (23%)	67,113,113	2.11	23 (34%)
35	LMT	D	403	-	36,36,36	0.57	1 (2%)	47,47,47	1.20	4 (8%)
23	CLA	с	508	3	59,73,73	2.07	13 (22%)	67,113,113	2.23	21 (31%)
26	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.53	10 (16%)
27	GOL	b	624	-	5, 5, 5	0.36	0	5, 5, 5	0.41	0
27	GOL	0	302	-	5, 5, 5	0.34	0	5, 5, 5	0.34	0
25	BCR	А	408	_	41,41,41	0.99	1 (2%)	$56,\!56,\!56$	1.65	16 (28%)
23	CLA	D	404	4	59,73,73	2.04	13 (22%)	$67,\!113,\!113$	2.23	22 (32%)
35	LMT	М	101	-	36,36,36	0.56	0	47,47,47	1.10	3 (6%)
38	HEM	Е	103	5,6	27,50,50	0.83	1 (3%)	17,82,82	2.28	4 (23%)
34	LMG	Z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.12	4 (8%)
31	LHG	d	406	_	48,48,48	0.87	3 (6%)	51,54,54	1.09	<mark>5 (9%)</mark>
23	CLA	с	511	3	59,73,73	2.03	13 (22%)	67,113,113	2.06	20 (29%)
36	HTG	С	524	_	8,8,19	0.39	0	7,7,24	1.15	1 (14%)
36	HTG	В	629	-	19,19,19	0.97	2(10%)	23,24,24	1.35	3 (13%)
27	GOL	a	412	-	5, 5, 5	0.43	0	5, 5, 5	0.27	0
23	CLA	С	504	3	59,73,73	1.97	13 (22%)	67,113,113	2.08	19 (28%)
25	BCR	С	516	_	41,41,41	1.05	1 (2%)	$56,\!56,\!56$	1.50	11 (19%)
27	GOL	В	627	-	5, 5, 5	0.35	0	5, 5, 5	0.37	0
35	LMT	b	628	-	25,25,36	0.54	1 (4%)	$30,\!30,\!47$	1.21	4 (13%)
23	CLA	a	406	41	59,73,73	2.00	10 (16%)	67,113,113	2.19	23 (34%)
23	CLA	В	602	41	59,73,73	2.05	13 (22%)	67,113,113	2.12	23 (34%)
23	CLA	С	507	3	59,73,73	2.01	13 (22%)	67,113,113	2.21	23 (34%)
23	CLA	С	502	3	59,73,73	1.98	13 (22%)	67,113,113	2.31	24 (35%)
23	CLA	a	404	1	59,73,73	2.00	12 (20%)	67,113,113	2.24	27 (40%)
34	LMG	a	417	_	51,51,55	0.96	3(5%)	$59,\!59,\!63$	1.11	4 (6%)
36	HTG	В	630	-	19,19,19	1.01	2 (10%)	23,24,24	1.33	1 (4%)
34	LMG	j	101	39	51,51,55	0.91	2 (3%)	59,59,63	1.08	6 (10%)
40	HEC	V	202	16	26,50,50	1.53	4 (15%)	18,82,82	1.52	6 (33%)
23	CLA	D	401	41	59,73,73	2.02	12 (20%)	67,113,113	2.17	24 (35%)
23	CLA	с	509	3	59,73,73	2.05	14 (23%)	67,113,113	2.19	22 (32%)
36	HTG	b	625	-	19,19,19	0.99	2(10%)	23,24,24	1.48	3 (13%)



Mal	Tune	Chain	Dog	Link	B	ond leng	gths	Bo	nd angl	es
	туре	Chan	ites		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
23	CLA	с	512	3	59,73,73	2.00	13 (22%)	$67,\!113,\!113$	2.27	23 (34%)
26	SQD	А	411	-	53, 54, 54	1.03	3(5%)	$62,\!65,\!65$	1.11	4 (6%)
23	CLA	d	402	4	59,73,73	1.99	14 (23%)	$67,\!113,\!113$	2.16	22 (32%)
24	PHO	D	402	-	67,69,69	2.14	17 (25%)	85,99,99	2.01	23 (27%)
23	CLA	с	506	3	59,73,73	1.98	14 (23%)	67,113,113	2.14	23 (34%)
23	CLA	с	503	3	59,73,73	1.99	13 (22%)	67,113,113	2.17	21 (31%)
23	CLA	В	610	2	59,73,73	2.00	13 (22%)	67,113,113	2.11	17 (25%)
35	LMT	Е	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.86	0
23	CLA	В	609	2	59,73,73	1.93	13 (22%)	67,113,113	2.19	22 (32%)
23	CLA	А	407	1	59,73,73	2.03	13 (22%)	67,113,113	2.09	21 (31%)
37	DGD	С	519	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
29	PL9	А	413	_	55,55,55	0.63	2 (3%)	68,69,69	1.96	22 (32%)
31	LHG	D	408	_	48,48,48	0.90	2 (4%)	51,54,54	1.00	3 (5%)
24	PHO	А	406	-	67,69,69	2.18	17 (25%)	85,99,99	2.00	23 (27%)
23	CLA	С	510	3	59,73,73	2.04	14 (23%)	67,113,113	2.19	21 (31%)
32	BCT	А	416	21	0,3,3	0.00	-	0,3,3	0.00	
23	CLA	С	514	3	59,73,73	2.01	13 (22%)	67,113,113	2.16	24 (35%)
25	BCR	С	515	-	41,41,41	1.03	1 (2%)	$56,\!56,\!56$	1.54	7 (12%)
34	LMG	с	519	-	51,51,55	0.96	3 (5%)	$59,\!59,\!63$	1.05	5 (8%)
31	LHG	b	630	_	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
27	GOL	С	525	-	5, 5, 5	0.39	0	5, 5, 5	0.20	0
23	CLA	В	604	2	59,73,73	2.01	13 (22%)	$67,\!113,\!113$	2.27	23 (34%)
26	SQD	а	413	-	53, 54, 54	1.09	4 (7%)	$62,\!65,\!65$	1.23	8 (12%)
23	CLA	В	605	2	59,73,73	1.98	12 (20%)	$67,\!113,\!113$	2.20	22 (32%)
35	LMT	В	633	-	36,36,36	0.56	1 (2%)	47,47,47	0.97	1(2%)
23	CLA	с	505	3	59,73,73	1.97	13 (22%)	67,113,113	2.09	19 (28%)
23	CLA	b	615	2	59,73,73	1.96	13 (22%)	67,113,113	2.15	23 (34%)
36	HTG	b	621	-	19,19,19	1.24	2(10%)	23,24,24	1.76	5 (21%)
25	BCR	В	618	_	41,41,41	1.04	1 (2%)	$56,\!56,\!56$	1.63	10 (17%)
36	HTG	В	624	-	19,19,19	0.98	1 (5%)	23,24,24	1.38	4 (17%)
34	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.54	8 (17%)
23	CLA	b	602	2	59,73,73	2.04	13 (22%)	67,113,113	2.30	27 (40%)
26	SQD	a	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.60	11 (17%)
23	CLA	b	607	41	59,73,73	1.95	14 (23%)	67,113,113	2.19	22 (32%)
31	LHG	е	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)



Mal	Tune	Chain	Dog	Link	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
23	CLA	b	612	2	59,73,73	2.04	13 (22%)	$67,\!113,\!113$	2.22	21 (31%)
32	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
29	PL9	D	407	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	19 (27%)
23	CLA	с	501	3	59,73,73	2.00	13 (22%)	$67,\!113,\!113$	2.21	23 (34%)
25	BCR	h	102	-	41,41,41	1.05	1 (2%)	$56,\!56,\!56$	1.47	10 (17%)
27	GOL	В	628	-	5, 5, 5	0.54	0	5, 5, 5	0.49	0
37	DGD	с	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.98	4 (5%)
36	HTG	h	101	_	16, 16, 19	1.09	2 (12%)	$20,\!21,\!24$	1.30	1(5%)
31	LHG	Е	101	-	41,41,48	1.02	2(4%)	44,47,54	1.09	3(6%)
23	CLA	b	608	2	59,73,73	2.03	13 (22%)	67,113,113	2.17	24 (35%)
36	HTG	с	522	-	19,19,19	1.00	2(10%)	23,24,24	1.47	3 (13%)
36	HTG	b	626	_	19,19,19	1.08	2(10%)	23,24,24	1.28	2 (8%)
36	HTG	С	523	-	19,19,19	0.96	1(5%)	23,24,24	1.50	3 (13%)
23	CLA	b	606	2	59,73,73	1.92	13 (22%)	67,113,113	2.20	20 (29%)
25	BCR	t	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.84	13 (23%)
23	CLA	С	508	41	59,73,73	1.99	12 (20%)	67,113,113	2.19	23 (34%)
36	HTG	В	626	-	19,19,19	0.96	1 (5%)	23,24,24	1.59	2 (8%)
23	CLA	b	604	2	59,73,73	1.92	12 (20%)	67,113,113	2.23	22 (32%)
28	OEX	a	414	1,3,41	0,15,15	0.00	-	-		
38	HEM	е	103	5,6	27,50,50	0.88	1(3%)	17,82,82	1.93	3 (17%)
34	LMG	С	520	-	51, 51, 55	0.94	2 (3%)	59,59,63	1.08	3 (5%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	$56,\!56,\!56$	1.53	12 (21%)
23	CLA	С	511	3	59,73,73	2.01	11 (18%)	67,113,113	2.21	20 (29%)
23	CLA	С	505	41	59,73,73	2.06	13 (22%)	67,113,113	2.16	24 (35%)
35	LMT	В	632	-	25,25,36	0.45	0	$30,\!30,\!47$	0.71	0
35	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.74	1 (2%)
26	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.53	8 (15%)
26	SQD	А	409	-	53,54,54	0.98	3 (5%)	62,65,65	1.84	13 (20%)
37	DGD	С	518	_	63,63,67	0.86	2 (3%)	77,77,81	0.98	5(6%)
36	HTG	D	412	-	16,16,19	1.03	2 (12%)	20,21,24	1.40	1 (5%)
23	CLA	b	610	41	59,73,73	2.06	13 (22%)	67,113,113	2.24	22 (32%)
36	HTG	с	521	-	19,19,19	0.93	1(5%)	23,24,24	1.46	1 (4%)
23	CLA	с	510	3	59,73,73	1.96	13 (22%)	67,113,113	2.23	25 (37%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.82	17 (30%)
25	BCR	a	410	-	41,41,41	0.99	1 (2%)	56, 56, 56	1.57	13 (23%)



Mol	Type	Chain	Bog	Link	B	ond leng	gths	Bo	ond angl	es
	туре	Cham	Ites		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
23	CLA	В	613	2	59,73,73	2.02	14 (23%)	67,113,113	2.28	23 (34%)
25	BCR	В	619	-	41,41,41	0.97	1 (2%)	$56,\!56,\!56$	1.56	13 (23%)
23	CLA	А	404	1	59,73,73	2.04	12 (20%)	$67,\!113,\!113$	2.29	24 (35%)
35	LMT	М	103	-	36,36,36	0.46	0	$47,\!47,\!47$	0.78	1 (2%)
26	SQD	D	413	-	42,43,54	1.14	3 (7%)	$51,\!54,\!65$	1.63	12 (23%)
23	CLA	В	616	2	59,73,73	1.98	11 (18%)	$67,\!113,\!113$	2.19	24 (35%)
23	CLA	С	509	3	59,73,73	2.09	13 (22%)	$67,\!113,\!113$	2.27	24 (35%)
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	$56,\!56,\!56$	1.61	13 (23%)
27	GOL	d	401	-	5, 5, 5	0.35	0	5, 5, 5	0.52	0
23	CLA	С	512	3	59,73,73	2.06	14 (23%)	$67,\!113,\!113$	2.06	21 (31%)
28	OEX	А	412	1,3,41	0,15,15	0.00	-	-		
40	HEC	V	201	16	26,50,50	1.55	4 (15%)	$18,\!82,\!82$	1.61	5 (27%)
23	CLA	С	503	3	59,73,73	1.98	13 (22%)	$67,\!113,\!113$	2.08	19(28%)
23	CLA	В	607	2	59,73,73	1.94	12 (20%)	$67,\!113,\!113$	2.18	22 (32%)
35	LMT	m	103	-	36,36,36	0.50	0	47,47,47	0.93	1 (2%)
23	CLA	b	603	2	59,73,73	1.99	12 (20%)	$67,\!113,\!113$	2.26	21 (31%)
23	CLA	b	609	2	59,73,73	2.03	13 (22%)	$67,\!113,\!113$	2.21	20 (29%)
36	HTG	b	622	-	19,19,19	1.01	2(10%)	23,24,24	1.39	2 (8%)
25	BCR	С	514	-	41,41,41	1.01	1 (2%)	$56,\!56,\!56$	1.87	15 (26%)
34	LMG	С	521	-	51,51,55	0.98	3 (5%)	$59,\!59,\!63$	1.21	4 (6%)
23	CLA	С	507	41	59,73,73	2.02	13 (22%)	$67,\!113,\!113$	2.18	22 (32%)
31	LHG	А	415	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	6 (11%)
23	CLA	b	614	2	59,73,73	2.03	13 (22%)	67,113,113	2.15	21 (31%)
35	LMT	b	620	_	25,25,36	0.46	0	$30,\!30,\!47$	0.66	0
25	BCR	В	620	-	41,41,41	1.06	1 (2%)	$56,\!56,\!56$	1.50	12 (21%)
23	CLA	В	603	2	59,73,73	2.07	13 (22%)	$67,\!113,\!113$	2.25	21 (31%)
23	CLA	С	513	3	59,73,73	2.01	12 (20%)	67,113,113	2.20	23 (34%)
35	LMT	С	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.02	4 (8%)
31	LHG	d	408	-	48,48,48	0.96	2 (4%)	51,54,54	0.99	3 (5%)
37	DGD	с	518	_	63,63,67	0.86	3 (4%)	77,77,81	1.09	4 (5%)
23	CLA	В	614	2	59,73,73	2.05	13 (22%)	67,113,113	2.11	21 (31%)
25	BCR	С	527	-	41,41,41	1.01	1 (2%)	$56,\!56,\!56$	1.57	12 (21%)
23	CLA	b	613	2	59,73,73	2.08	13 (22%)	67,113,113	2.14	23 (34%)
25	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.81	12 (21%)
35	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.84	3 (6%)



Mol	Type	Chain	Bos	Link	Bond lengths			Bond angles		
	туре	Chan	1105		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	$51,\!54,\!54$	1.06	3 (5%)
23	CLA	с	513	3	59,73,73	2.03	13 (22%)	$67,\!113,\!113$	2.19	22 (32%)
23	CLA	b	616	2	59,73,73	2.03	13 (22%)	$67,\!113,\!113$	2.30	24 (35%)
23	CLA	а	409	1	59,73,73	2.02	14 (23%)	$67,\!113,\!113$	2.22	27 (40%)
23	CLA	В	611	41	59,73,73	2.05	13 (22%)	$67,\!113,\!113$	2.26	24 (35%)
23	CLA	D	405	4	59,73,73	2.01	12 (20%)	$67,\!113,\!113$	2.14	22 (32%)
31	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	0.93	3 (5%)
37	DGD	с	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.08	6 (7%)
35	LMT	В	634	-	26,26,36	0.49	0	31,31,47	0.90	1 (3%)
37	DGD	Н	102	_	63,63,67	0.89	2 (3%)	77,77,81	0.98	<mark>3 (3%)</mark>
23	CLA	a	405	41	59,73,73	2.07	12 (20%)	67,113,113	2.20	26 (38%)
25	BCR	с	515	_	41,41,41	0.98	1 (2%)	$56,\!56,\!56$	1.67	14 (25%)
23	CLA	В	617	2	59,73,73	2.03	13 (22%)	67,113,113	2.27	22 (32%)
34	LMG	В	622	_	51, 51, 55	0.90	2 (3%)	$59,\!59,\!63$	1.15	5 (8%)
37	DGD	h	103	_	63,63,67	0.89	3(4%)	77,77,81	0.96	3 (3%)
34	LMG	J	101	39	51, 51, 55	0.91	3 (5%)	$59,\!59,\!63$	1.07	<mark>5 (8%)</mark>
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.17	4 (7%)
26	SQD	В	621	_	53,54,54	1.04	3 (5%)	$62,\!65,\!65$	1.45	8 (12%)
23	CLA	b	601	41	59,73,73	2.06	12 (20%)	67,113,113	2.12	20 (29%)
36	HTG	В	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.60	1 (4%)
23	CLA	В	615	2	59,73,73	1.96	13 (22%)	67,113,113	2.24	21 (31%)
34	LMG	С	501	-	51, 51, 55	0.95	2 (3%)	$59,\!59,\!63$	1.26	6(10%)
23	CLA	d	403	4	59,73,73	2.02	12 (20%)	67,113,113	2.18	22 (32%)
23	CLA	С	506	3	59,73,73	1.96	13 (22%)	67,113,113	2.18	20 (29%)
34	LMG	m	101	-	$51,\!51,\!55$	0.89	2 (3%)	$59,\!59,\!63$	1.17	6 (10%)
36	HTG	V	203	_	11,11,19	0.28	0	$15,\!15,\!24$	1.35	1(6%)
35	LMT	В	623	-	36,36,36	0.42	0	47,47,47	1.14	4 (8%)
23	CLA	В	612	2	59,73,73	2.02	12 (20%)	67,113,113	2.25	23 (34%)
25	BCR	D	406	-	41,41,41	1.03	1 (2%)	$56,\!56,\!56$	1.77	13 (23%)
23	CLA	с	504	41	59,73,73	2.07	14 (23%)	67,113,113	<mark>2.13</mark>	23 (34%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56, 56, 56	1.39	6 (10%)

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.



5G ⁻	ГΙ

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	с	520	-	-	8/46/66/70	0/1/1/1
25	BCR	d	404	_	-	8/29/63/63	0/2/2/2
36	HTG	b	623	-	-	2/10/30/30	0/1/1/1
27	GOL	А	410	-	-	4/4/4/4	-
29	PL9	d	405	-	-	$\frac{6}{53}$	0/1/1/1
23	CLA	с	502	3	3/3/20/25	8/37/135/135	-
37	DGD	С	517	-	-	15/51/91/95	0/2/2/2
24	PHO	a	408	_	-	3/53/103/103	0/5/6/6
23	CLA	В	608	41	3/3/20/25	3/37/135/135	-
27	GOL	a	412	_	-	2/4/4/4	-
23	CLA	b	605	2	3/3/20/25	13/37/135/135	-
23	CLA	b	611	2	3/3/20/25	10/37/135/135	-
25	BCR	Н	101	_	-	4/29/63/63	0/2/2/2
23	CLA	В	606	2	3/3/20/25	11/37/135/135	-
25	BCR	Т	101	-	-	5/29/63/63	0/2/2/2
25	BCR	у	101	-	-	4/29/63/63	0/2/2/2
29	PL9	a	415	-	-	16/53/73/73	0/1/1/1
24	PHO	a	407	-	-	4/53/103/103	0/5/6/6
23	CLA	А	405	41	2/2/20/25	8/37/135/135	-
35	LMT	D	403	-	-	8/21/61/61	0/2/2/2
23	CLA	с	508	3	3/3/20/25	6/37/135/135	-
26	SQD	L	102	_	-	22/49/69/69	0/1/1/1
27	GOL	b	624	-	-	2/4/4/4	-
27	GOL	Ο	302	-	-	2/4/4/4	-
25	BCR	А	408	-	-	1/29/63/63	0/2/2/2
23	CLA	D	404	4	1/1/20/25	2/37/135/135	-
35	LMT	М	101	-	-	2/21/61/61	0/2/2/2
38	HEM	E	103	5,6	-	0/6/54/54	-
34	LMG	Z	101	-	-	15/34/54/70	0/1/1/1
31	LHG	d	406	-	-	12/53/53/53	-
23	CLA	c	511	3	3/3/20/25	5/37/135/135	-
$\frac{36}{36}$	HTG HTC	C B	524 620	-	-	$\frac{1/6/6/30}{1/10/30/30}$	-
23	CLA	а Ь	403		$\frac{-}{3/3/20/25}$	6/37/135/135	
20	CLA	C	504	3	3/3/20/25	3/37/135/135	_
$\boxed{\begin{array}{c} 20\\ 25\end{array}}$	BCR	C	516	-	-	1/29/63/63	0/2/2/2



$5 \mathrm{GTI}$

Mol	Type	Chain	$\frac{10 \text{ page}}{\text{Res}}$	Link	Chirals	Torsions	Rings
27	GOL	В	627	-	_	$\frac{4}{4}/\frac{4}{4}$	-
35	LMT	b	628	-	_	9/17/37/61	0/1/1/2
23	CLA	a	406	41	2/2/20/25	8/37/135/135	-
23	CLA	В	602	41	3/3/20/25	13/37/135/135	-
23	CLA	С	507	3	3/3/20/25	14/37/135/135	-
23	CLA	С	502	3	3/3/20/25	5/37/135/135	-
38	HEM	е	103	5,6	-	0/6/54/54	-
23	CLA	a	404	1	3/3/20/25	5/37/135/135	-
34	LMG	a	417	-	-	14/46/66/70	0/1/1/1
36	HTG	В	630	-	-	1/10/30/30	0/1/1/1
34	LMG	j	101	39	-	8/46/66/70	0/1/1/1
40	HEC	V	202	16	-	0/6/54/54	-
23	CLA	D	401	41	3/3/20/25	8/37/135/135	-
23	CLA	с	509	3	3/3/20/25	15/37/135/135	-
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
23	CLA	с	512	3	3/3/20/25	9/37/135/135	-
26	SQD	А	411	-	-	14/49/69/69	0/1/1/1
23	CLA	d	402	4	1/1/20/25	3/37/135/135	-
24	PHO	D	402	-	-	6/53/103/103	0/5/6/6
23	CLA	с	506	3	3/3/20/25	12/37/135/135	-
23	CLA	с	503	3	3/3/20/25	3/37/135/135	-
35	LMT	Е	102	-	-	10/21/61/61	0/2/2/2
23	CLA	В	609	2	3/3/20/25	4/37/135/135	-
23	CLA	А	407	1	3/3/20/25	8/37/135/135	-
37	DGD	С	519	-	-	7/51/91/95	0/2/2/2
29	PL9	А	413	-	_	11/53/73/73	0/1/1/1
31	LHG	D	408	-	-	18/53/53/53	-
24	PHO	А	406	-	-	4/53/103/103	0/5/6/6
23	CLA	С	510	3	3/3/20/25	14/37/135/135	-
23	CLA	С	514	3	2/2/20/25	8/37/135/135	-
25	BCR	С	515	-	-	1/29/63/63	0/2/2/2
34	LMG	с	519	-	-	13/46/66/70	0/1/1/1
31	LHG	b	630	-	-	19/53/53/53	-
27	GOL	C	525	-	_	2/4/4/4	-
23	CLA	В	604	2	3/3/20/25	6/37/135/135	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
23	CLA	В	605	2	3/3/20/25	13/37/135/135	-
35	LMT	В	633	-	-	5/21/61/61	0/2/2/2
23	CLA	с	505	3	1/1/20/25	7/37/135/135	-
23	CLA	b	615	2	3/3/20/25	7/37/135/135	-
36	HTG	b	621	-	-	2/10/30/30	0/1/1/1
25	BCR	В	618	-	-	2/29/63/63	0/2/2/2
36	HTG	В	624	-	-	4/10/30/30	0/1/1/1
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
23	CLA	b	602	2	2/2/20/25	4/37/135/135	-
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
23	CLA	b	607	41	3/3/20/25	9/37/135/135	-
31	LHG	е	101	-	-	14/46/46/53	-
23	CLA	b	612	2	3/3/20/25	5/37/135/135	-
29	PL9	D	407	-	-	7/53/73/73	0/1/1/1
23	CLA	с	501	3	3/3/20/25	8/37/135/135	-
25	BCR	h	102	_	-	0/29/63/63	0/2/2/2
27	GOL	В	628	-	-	4/4/4/4	-
37	DGD	с	517	-	-	14/51/91/95	0/2/2/2
36	HTG	h	101	-	-	3/7/27/30	0/1/1/1
31	LHG	Е	101	-	-	17/46/46/53	-
23	CLA	b	608	2	2/2/20/25	5/37/135/135	-
36	HTG	с	522	-	-	2/10/30/30	0/1/1/1
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
36	HTG	С	523	-	-	0/10/30/30	0/1/1/1
23	CLA	b	606	2	3/3/20/25	10/37/135/135	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	С	508	41	3/3/20/25	7/37/135/135	-
36	HTG	В	626	-	-	4/10/30/30	0/1/1/1
23	CLA	b	604	2	3/3/20/25	9/37/135/135	-
23	CLA	С	505	41	3/3/20/25	6/37/135/135	-
34	LMG	С	520	_	-	16/46/66/70	0/1/1/1
25	BCR	b	618	_	-	2/29/63/63	0/2/2/2
23	CLA	С	511	3	3/3/20/25	13/37/135/135	-
35	LMT	B	632	_	-	7/17/37/61	0/1/1/2



$5 \mathrm{GTI}$

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	a	418	-	_	3/21/61/61	0/2/2/2
26	SQD	f	101	-	_	16/38/58/69	0/1/1/1
26	SQD	А	409	-	-	14/49/69/69	0/1/1/1
37	DGD	С	518	-	_	15/51/91/95	0/2/2/2
36	HTG	D	412	-	-	1/7/27/30	0/1/1/1
23	CLA	b	610	41	3/3/20/25	7/37/135/135	-
36	HTG	с	521	-	-	3/10/30/30	0/1/1/1
23	CLA	с	510	3	3/3/20/25	8/37/135/135	-
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
23	CLA	В	613	2	3/3/20/25	4/37/135/135	-
25	BCR	В	619	-	-	0/29/63/63	0/2/2/2
23	CLA	А	404	1	3/3/20/25	3/37/135/135	-
35	LMT	М	103	-	-	14/21/61/61	0/2/2/2
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
23	CLA	В	616	2	3/3/20/25	10/37/135/135	-
23	CLA	С	509	3	3/3/20/25	6/37/135/135	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
27	GOL	d	401	-	-	2/4/4/4	-
23	CLA	С	512	3	3/3/20/25	6/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
23	CLA	С	503	3	3/3/20/25	9/37/135/135	-
23	CLA	В	607	2	3/3/20/25	5/37/135/135	-
35	LMT	m	103	-	-	8/21/61/61	0/2/2/2
23	CLA	b	603	2	2/2/20/25	4/37/135/135	-
23	CLA	b	609	2	3/3/20/25	8/37/135/135	-
36	HTG	b	622	_	-	1/10/30/30	0/1/1/1
34	LMG	m	101	-	-	16/46/66/70	0/1/1/1
25	BCR	с	514	-	-	2/29/63/63	0/2/2/2
34	LMG	С	521	-	-	9/46/66/70	0/1/1/1
23	CLA	с	507	41	3/3/20/25	8/37/135/135	-
31	LHG	А	415	-	-	11/53/53/53	-
23	CLA	b	614	2	3/3/20/25	15/37/135/135	-
35	LMT	b	620	-	-	5/17/37/61	0/1/1/2
25	BCR	В	620	_	-	0/29/63/63	0/2/2/2



Mol	Type	Chain	$\overline{\mathbf{Res}}$	Link	Chirals	Torsions	Rings
23	CLA	В	603	2	3/3/20/25	8/37/135/135	-
23	CLA	C	513	3	3/3/20/25	7/37/135/135	_
35	LMT	C	522			9/21/61/61	0/2/2/2
31	LHG	d	408	-	_	17/53/53/53	-
37	DGD	с	518	_	_	6/51/91/95	0/2/2/2
23	CLA	В	614	2	3/3/20/25	5/37/135/135	_
25	BCR	С	527	_	-	1/29/63/63	0/2/2/2
23	CLA	b	613	2	3/3/20/25	7/37/135/135	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
35	LMT	е	102	-	-	8/21/61/61	0/2/2/2
31	LHG	D	409	-	-	14/53/53/53	_
23	CLA	с	513	3	2/2/20/25	6/37/135/135	-
23	CLA	b	616	2	3/3/20/25	12/37/135/135	-
23	CLA	a	409	1	3/3/20/25	7/37/135/135	-
23	CLA	В	611	41	3/3/20/25	7/37/135/135	-
23	CLA	D	405	4	3/3/20/25	7/37/135/135	-
31	LHG	d	407	-	-	23/53/53/53	-
37	DGD	с	516	_	-	15/51/91/95	0/2/2/2
35	LMT	В	634	-	-	6/17/38/61	0/1/1/2
37	DGD	Н	102	-	-	10/51/91/95	0/2/2/2
23	CLA	a	405	41	3/3/20/25	5/37/135/135	-
25	BCR	с	515	-	-	0/29/63/63	0/2/2/2
23	CLA	В	617	2	3/3/20/25	7/37/135/135	-
34	LMG	В	622	-	-	12/46/66/70	0/1/1/1
37	DGD	h	103	-	-	11/51/91/95	0/2/2/2
34	LMG	J	101	39	-	10/46/66/70	0/1/1/1
31	LHG	L	101	-	-	16/53/53/53	-
26	SQD	В	621	-	-	21/49/69/69	0/1/1/1
23	CLA	b	601	41	2/2/20/25	19/37/135/135	-
36	HTG	В	625	-	-	5/10/30/30	0/1/1/1
23	CLA	В	615	2	3/3/20/25	12/37/135/135	-
34	LMG	С	501	-	-	11/46/66/70	0/1/1/1
23	CLA	С	506	3	1/1/20/25	7/37/135/135	-
23	CLA	В	610	2	3/3/20/25	9/37/135/135	-
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	В	623	-	-	8/21/61/61	0/2/2/2
23	CLA	В	612	2	3/3/20/25	4/37/135/135	-
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
23	CLA	с	504	41	3/3/20/25	12/37/135/135	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2

All (1130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
23	с	502	CLA	C3B-C2B	6.96	1.50	1.40
23	В	614	CLA	C3B-C2B	6.74	1.49	1.40
23	А	404	CLA	C3B-C2B	6.65	1.49	1.40
23	С	509	CLA	C3B-C2B	6.56	1.49	1.40
23	b	613	CLA	C3B-C2B	6.54	1.49	1.40
23	D	404	CLA	C3B-C2B	6.49	1.49	1.40
23	с	504	CLA	C3B-C2B	6.48	1.49	1.40
23	b	612	CLA	C3B-C2B	6.45	1.49	1.40
23	b	611	CLA	C3B-C2B	6.44	1.49	1.40
23	С	505	CLA	C3B-C2B	6.41	1.49	1.40
23	b	614	CLA	C3B-C2B	6.37	1.49	1.40
23	С	512	CLA	C3B-C2B	6.36	1.49	1.40
23	В	613	CLA	C3B-C2B	6.31	1.49	1.40
23	С	502	CLA	C3B-C2B	6.31	1.49	1.40
23	b	602	CLA	C3B-C2B	6.29	1.49	1.40
23	В	616	CLA	C3D-C2D	6.28	1.50	1.39
23	а	404	CLA	C3B-C2B	6.28	1.49	1.40
23	b	608	CLA	C3B-C2B	6.26	1.49	1.40
23	b	610	CLA	C3B-C2B	6.24	1.49	1.40
23	В	612	CLA	C3B-C2B	6.22	1.49	1.40
23	с	508	CLA	C3B-C2B	6.22	1.49	1.40
23	а	405	CLA	C3D-C2D	6.21	1.50	1.39
23	b	616	CLA	C3D-C2D	6.17	1.50	1.39
23	а	405	CLA	C3B-C2B	6.15	1.48	1.40
23	С	510	CLA	C3B-C2B	6.14	1.48	1.40
24	а	407	PHO	C3B-C2B	6.12	1.49	1.37
23	с	511	CLA	C3B-C2B	6.12	1.48	1.40
24	A	406	PHO	C3B-C2B	6.10	1.49	1.37
23	В	604	CLA	$C3B-C2\overline{B}$	6.09	1.48	1.40
23	a	406	CLA	C3B-C2B	6.07	1.48	1.40
24	a	408	PHO	C3B-C2B	6.06	1.49	1.37
23	В	617	CLA	C3B-C2B	6.06	1.48	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3D-C2D	6.05	1.50	1.39
23	с	509	CLA	C3B-C2B	6.05	1.48	1.40
23	b	616	CLA	C3B-C2B	6.04	1.48	1.40
23	с	512	CLA	C3D-C2D	5.98	1.50	1.39
23	с	508	CLA	C3D-C2D	5.97	1.50	1.39
23	В	603	CLA	C3D-C2D	5.95	1.50	1.39
23	В	602	CLA	C3B-C2B	5.94	1.48	1.40
23	b	601	CLA	C3B-C2B	5.93	1.48	1.40
23	с	501	CLA	C3B-C2B	5.93	1.48	1.40
23	В	613	CLA	C3D-C2D	5.92	1.50	1.39
23	В	617	CLA	C3D-C2D	5.91	1.50	1.39
23	С	509	CLA	C3D-C2D	5.91	1.50	1.39
23	В	611	CLA	C3B-C2B	5.90	1.48	1.40
23	d	403	CLA	C3B-C2B	5.90	1.48	1.40
23	d	403	CLA	C3D-C2D	5.89	1.50	1.39
23	С	508	CLA	C3D-C2D	5.89	1.50	1.39
23	В	606	CLA	C3D-C2D	5.88	1.50	1.39
23	С	513	CLA	C3B-C2B	5.88	1.48	1.40
23	a	406	CLA	C3D-C2D	5.88	1.50	1.39
23	В	610	CLA	C3D-C2D	5.88	1.50	1.39
23	с	501	CLA	C3D-C2D	5.87	1.50	1.39
23	С	512	CLA	C3D-C2D	5.87	1.50	1.39
23	С	514	CLA	C3D-C2D	5.87	1.50	1.39
23	b	609	CLA	C3B-C2B	5.86	1.48	1.40
23	В	603	CLA	C3B-C2B	5.84	1.48	1.40
24	a	407	PHO	C3C-C2C	5.84	1.49	1.36
24	a	408	PHO	C3C-C2C	5.83	1.49	1.36
23	A	407	CLA	C3B-C2B	5.82	1.48	1.40
23	b	601	CLA	C3D-C2D	5.81	1.49	1.39
23	В	614	CLA	C3D-C2D	5.81	1.49	1.39
23	С	509	CLA	C3C-C2C	5.80	1.49	1.36
23	с	504	CLA	C3D-C2D	5.80	1.49	1.39
23	В	611	CLA	C3D-C2D	5.80	1.49	1.39
23	В	607	CLA	C3D-C2D	5.78	1.49	1.39
23	с	510	CLA	C3B-C2B	5.77	1.48	1.40
23	C	514	CLA	C3B-C2B	5.77	1.48	1.40
23	b	605	CLA	C3B-C2B	5.77	1.48	1.40
23	В	615	CLA	C3D-C2D	5.76	1.49	1.39
23	С	513	CLA	C3B-C2B	5.75	1.48	1.40
23	b	605	CLA	C3D-C2D	5.75	1.49	1.39
23	B	605	CLA	C3B-C2B	5.74	1.48	1.40
23	В	602	CLA	C3D-C2D	5.73	1.49	1.39



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3D-C2D	5.72	1.49	1.39
23	b	602	CLA	C3D-C2D	5.71	1.49	1.39
23	В	604	CLA	C3D-C2D	5.70	1.49	1.39
23	с	503	CLA	C3D-C2D	5.70	1.49	1.39
23	С	511	CLA	C3D-C2D	5.70	1.49	1.39
23	D	404	CLA	C3C-C2C	5.69	1.48	1.36
23	с	506	CLA	C3D-C2D	5.69	1.49	1.39
23	А	404	CLA	C3D-C2D	5.67	1.49	1.39
23	d	402	CLA	C3B-C2B	5.67	1.48	1.40
23	С	506	CLA	C3B-C2B	5.67	1.48	1.40
23	С	507	CLA	C3D-C2D	5.67	1.49	1.39
23	b	608	CLA	C3D-C2D	5.67	1.49	1.39
23	А	405	CLA	CHC-C1C	5.65	1.49	1.35
23	с	507	CLA	C3D-C2D	5.65	1.49	1.39
23	b	604	CLA	C3B-C2B	5.65	1.48	1.40
23	b	610	CLA	C3C-C2C	5.65	1.48	1.36
23	с	513	CLA	C3D-C2D	5.65	1.49	1.39
23	b	609	CLA	C3D-C2D	5.64	1.49	1.39
23	А	405	CLA	C3D-C2D	5.64	1.49	1.39
23	a	409	CLA	C3D-C2D	5.64	1.49	1.39
23	D	401	CLA	C3D-C2D	5.63	1.49	1.39
23	С	505	CLA	C3D-C2D	5.62	1.49	1.39
23	b	610	CLA	C3D-C2D	5.62	1.49	1.39
23	А	407	CLA	C3D-C2D	5.62	1.49	1.39
23	a	404	CLA	C3D-C2D	5.60	1.49	1.39
23	С	502	CLA	C3D-C2D	5.59	1.49	1.39
23	В	617	CLA	C3C-C2C	5.59	1.48	1.36
23	С	513	CLA	C3D-C2D	5.59	1.49	1.39
23	с	503	CLA	C3B-C2B	5.59	1.48	1.40
23	С	507	CLA	C3B-C2B	5.58	1.48	1.40
23	В	612	CLA	C3D-C2D	5.58	1.49	1.39
23	В	602	CLA	C3C-C2C	5.58	1.48	1.36
23	b	612	CLA	C3D-C2D	5.57	1.49	1.39
23	С	503	CLA	C3D-C2D	5.57	1.49	1.39
23	d	402	CLA	C3D-C2D	5.56	1.49	1.39
23	С	510	CLA	C3D-C2D	5.56	1.49	1.39
23	b	607	CLA	C3D-C2D	5.55	1.49	1.39
23	C	508	CLA	C3C-C2C	5.54	1.48	1.36
24	D	402	PHO	C3B-C2B	5.54	1.48	1.37
23	b	613	CLA	C3C-C2C	5.54	1.48	1.36
23	B	608	CLA	C3B-C2B	5.53	1.48	1.40
23	C	511	CLA	C3B-C2B	5.53	1.48	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3C-C2C	5.53	1.48	1.36
23	с	508	CLA	C3C-C2C	5.53	1.48	1.36
23	В	603	CLA	C3C-C2C	5.53	1.48	1.36
23	В	609	CLA	C3D-C2D	5.52	1.49	1.39
25	d	404	BCR	C23-C22	-5.52	1.34	1.45
23	с	512	CLA	C3C-C2C	5.51	1.48	1.36
23	b	606	CLA	C3B-C2B	5.50	1.48	1.40
23	А	407	CLA	C3C-C2C	5.50	1.48	1.36
23	с	502	CLA	C3D-C2D	5.50	1.49	1.39
23	a	406	CLA	C3C-C2C	5.49	1.48	1.36
23	b	615	CLA	C3D-C2D	5.49	1.49	1.39
24	А	406	PHO	CHC-C1C	5.49	1.49	1.38
23	a	405	CLA	C3C-C2C	5.48	1.48	1.36
23	В	608	CLA	C3D-C2D	5.48	1.49	1.39
24	a	408	PHO	CHB-C1B	5.47	1.49	1.38
23	с	509	CLA	C3D-C2D	5.47	1.49	1.39
23	a	409	CLA	C3B-C2B	5.46	1.47	1.40
23	d	403	CLA	CHC-C1C	5.46	1.49	1.35
23	А	404	CLA	CHC-C1C	5.44	1.48	1.35
23	В	611	CLA	C3C-C2C	5.44	1.48	1.36
23	с	511	CLA	C3C-C2C	5.43	1.48	1.36
24	А	406	PHO	CHB-C1B	5.43	1.49	1.38
23	D	405	CLA	C3C-C2C	5.43	1.48	1.36
23	b	616	CLA	C3C-C2C	5.43	1.48	1.36
23	С	504	CLA	C3D-C2D	5.42	1.49	1.39
23	С	504	CLA	C3C-C2C	5.42	1.48	1.36
23	В	609	CLA	C3B-C2B	5.42	1.47	1.40
23	В	615	CLA	C3B-C2B	5.41	1.47	1.40
23	С	513	CLA	CHC-C1C	5.41	1.48	1.35
23	С	504	CLA	C3B-C2B	5.41	1.47	1.40
23	b	612	CLA	C3C-C2C	5.41	1.48	1.36
23	с	501	CLA	C3C-C2C	5.40	1.48	1.36
23	b	611	CLA	C3C-C2C	5.40	1.48	1.36
24	D	402	PHO	C3C-C2C	5.40	1.48	1.36
23	D	405	CLA	CHC-C1C	5.39	1.48	1.35
23	b	603	CLA	C3C-C2C	5.39	1.48	1.36
24	a	408	PHO	CHC-C1C	5.39	1.49	1.38
23	b	606	CLA	C3C-C2C	5.39	1.48	1.36
23	D	404	CLA	C3D-C2D	5.38	1.49	1.39
23	с	505	CLA	C3C-C2C	5.37	1.48	1.36
23	C	505	CLA	C3C-C2C	5.37	1.48	1.36
23	с	513	CLA	C3C-C2C	5.36	1.48	1.36



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C3D-C2D	5.36	1.49	1.39
23	с	507	CLA	C3B-C2B	5.36	1.47	1.40
23	b	609	CLA	CHC-C1C	5.36	1.48	1.35
23	с	507	CLA	CHC-C1C	5.35	1.48	1.35
23	В	605	CLA	CHC-C1C	5.35	1.48	1.35
23	с	506	CLA	C3B-C2B	5.35	1.47	1.40
23	с	502	CLA	C3C-C2C	5.34	1.48	1.36
23	А	405	CLA	C3B-C2B	5.34	1.47	1.40
23	С	514	CLA	CHC-C1C	5.34	1.48	1.35
23	b	603	CLA	C3B-C2B	5.33	1.47	1.40
23	b	606	CLA	C3D-C2D	5.33	1.49	1.39
23	А	407	CLA	CHC-C1C	5.33	1.48	1.35
23	В	611	CLA	CHC-C1C	5.32	1.48	1.35
23	b	614	CLA	C3D-C2D	5.32	1.49	1.39
23	с	505	CLA	C3B-C2B	5.32	1.47	1.40
23	a	409	CLA	CHC-C1C	5.31	1.48	1.35
23	D	401	CLA	CHC-C1C	5.31	1.48	1.35
23	С	512	CLA	CHC-C1C	5.31	1.48	1.35
23	В	604	CLA	C3C-C2C	5.31	1.48	1.36
23	В	612	CLA	O2D-CGD	5.31	1.46	1.33
23	b	615	CLA	C3B-C2B	5.31	1.47	1.40
23	В	607	CLA	C3C-C2C	5.30	1.48	1.36
23	d	403	CLA	C3C-C2C	5.29	1.48	1.36
23	В	608	CLA	C3C-C2C	5.29	1.48	1.36
23	b	614	CLA	C3C-C2C	5.28	1.48	1.36
23	С	513	CLA	C3C-C2C	5.28	1.48	1.36
23	b	601	CLA	C3C-C2C	5.28	1.48	1.36
23	с	510	CLA	O2D-CGD	5.28	1.46	1.33
23	D	405	CLA	C3D-C2D	5.28	1.48	1.39
23	В	609	CLA	C3C-C2C	5.27	1.47	1.36
23	С	511	CLA	C3C-C2C	5.26	1.47	1.36
23	С	503	CLA	CHC-C1C	5.26	1.48	1.35
23	D	405	CLA	C3B-C2B	5.26	1.47	1.40
23	В	608	CLA	CHC-C1C	5.26	1.48	1.35
23	D	401	CLA	C3C-C2C	5.26	1.47	1.36
23	С	503	CLA	C3B-C2B	5.26	1.47	1.40
24	a	408	PHO	O2D-CGD	5.26	1.46	1.33
23	с	512	CLA	C3B-C2B	5.25	1.47	1.40
23	В	606	CLA	CHC-C1C	5.25	1.48	1.35
23	b	605	CLA	C3C-C2C	5.25	1.47	1.36
23	b	602	CLA	CHC-C1C	5.24	1.48	1.35
25	У	101	BCR	C23-C22	-5.24	1.34	1.45



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	603	CLA	CHC-C1C	5.24	1.48	1.35
23	а	409	CLA	C3C-C2C	5.23	1.47	1.36
23	с	509	CLA	C3C-C2C	5.23	1.47	1.36
23	b	602	CLA	C3C-C2C	5.23	1.47	1.36
23	с	505	CLA	CHC-C1C	5.23	1.48	1.35
23	В	615	CLA	C3C-C2C	5.23	1.47	1.36
23	В	606	CLA	C3C-C2C	5.23	1.47	1.36
23	b	608	CLA	C3C-C2C	5.23	1.47	1.36
23	с	511	CLA	C3D-C2D	5.22	1.48	1.39
23	с	507	CLA	C3C-C2C	5.22	1.47	1.36
23	с	504	CLA	O2D-CGD	5.21	1.45	1.33
23	С	507	CLA	O2D-CGD	5.21	1.45	1.33
23	b	601	CLA	CHC-C1C	5.20	1.48	1.35
23	b	610	CLA	CHC-C1C	5.20	1.48	1.35
24	a	407	PHO	CHB-C1B	5.20	1.48	1.38
23	С	502	CLA	C3C-C2C	5.20	1.47	1.36
23	А	404	CLA	C3C-C2C	5.20	1.47	1.36
23	с	512	CLA	CHC-C1C	5.19	1.48	1.35
23	с	508	CLA	CHC-C1C	5.19	1.48	1.35
23	В	604	CLA	CHC-C1C	5.19	1.48	1.35
24	D	402	PHO	CHC-C1C	5.19	1.48	1.38
23	В	607	CLA	C3B-C2B	5.19	1.47	1.40
23	С	506	CLA	CHC-C1C	5.19	1.48	1.35
23	b	607	CLA	C3B-C2B	5.19	1.47	1.40
23	А	405	CLA	C3C-C2C	5.18	1.47	1.36
23	С	506	CLA	C3C-C2C	5.18	1.47	1.36
24	А	406	PHO	C3C-C2C	5.18	1.47	1.36
25	b	619	BCR	C23-C22	-5.17	1.34	1.45
23	С	507	CLA	C3C-C2C	5.17	1.47	1.36
25	k	101	BCR	C23-C22	-5.16	1.34	1.45
23	В	616	CLA	OBD-CAD	5.16	1.29	1.22
23	b	612	CLA	CHC-C1C	5.16	1.48	1.35
24	А	406	PHO	CHD-C1D	5.16	1.48	1.38
23	С	510	CLA	C3C-C2C	5.15	1.47	1.36
23	b	604	CLA	CHC-C1C	5.15	1.48	1.35
23	В	616	CLA	C3B-C2B	5.15	1.47	1.40
23	b	$60\overline{2}$	CLA	O2D-CGD	$5.1\overline{4}$	1.45	1.33
23	a	404	CLA	C3C-C2C	5.14	1.47	1.36
23	В	610	CLA	C3B-C2B	5.14	1.47	1.40
23	В	613	CLA	C3C-C2C	5.14	1.47	1.36
23	с	509	CLA	O2D-CGD	5.14	1.45	1.33
23	с	506	CLA	O2D-CGD	5.14	1.45	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	610	CLA	C3C-C2C	5.13	1.47	1.36
23	b	614	CLA	CHC-C1C	5.13	1.48	1.35
23	С	502	CLA	CHC-C1C	5.13	1.48	1.35
23	D	401	CLA	C3B-C2B	5.13	1.47	1.40
23	D	401	CLA	O2D-CGD	5.13	1.45	1.33
23	С	508	CLA	CHC-C1C	5.13	1.48	1.35
23	b	601	CLA	O2D-CGD	5.13	1.45	1.33
23	с	511	CLA	CHC-C1C	5.13	1.48	1.35
23	В	614	CLA	O2D-CGD	5.13	1.45	1.33
23	В	610	CLA	O2D-CGD	5.12	1.45	1.33
23	с	502	CLA	CHC-C1C	5.11	1.48	1.35
23	С	503	CLA	C3C-C2C	5.11	1.47	1.36
23	С	514	CLA	C3C-C2C	5.11	1.47	1.36
23	С	512	CLA	O2D-CGD	5.10	1.45	1.33
23	В	611	CLA	OBD-CAD	5.10	1.29	1.22
23	d	402	CLA	CHC-C1C	5.10	1.48	1.35
24	D	402	PHO	CHB-C1B	5.10	1.48	1.38
23	В	616	CLA	O2D-CGD	5.09	1.45	1.33
23	с	513	CLA	CHC-C1C	5.09	1.48	1.35
23	с	505	CLA	C3D-C2D	5.09	1.48	1.39
23	В	605	CLA	C3C-C2C	5.09	1.47	1.36
23	В	610	CLA	CHC-C1C	5.09	1.48	1.35
23	С	504	CLA	CHC-C1C	5.08	1.48	1.35
23	a	404	CLA	CHC-C1C	5.08	1.48	1.35
23	b	603	CLA	CHC-C1C	5.08	1.48	1.35
23	С	508	CLA	C3B-C2B	5.08	1.47	1.40
23	b	604	CLA	C3C-C2C	5.08	1.47	1.36
23	b	616	CLA	O2D-CGD	5.08	1.45	1.33
23	с	503	CLA	C3C-C2C	5.07	1.47	1.36
23	с	503	CLA	CHC-C1C	5.07	1.48	1.35
23	А	407	CLA	O2D-CGD	5.07	1.45	1.33
23	В	617	CLA	CHC-C1C	5.07	1.48	1.35
23	с	504	CLA	C3C-C2C	5.06	1.47	1.36
23	В	614	CLA	C3C-C2C	5.05	1.47	1.36
25	В	620	BCR	C23-C22	-5.04	1.35	1.45
23	С	507	CLA	CHC-C1C	5.04	1.47	1.35
25	Т	101	BCR	C23-C22	-5.03	1.35	1.45
23	В	616	CLA	C3C-C2C	5.03	1.47	1.36
23	С	510	CLA	CHC-C1C	5.03	1.47	1.35
23	с	501	CLA	CHC-C1C	5.03	1.47	1.35
25	Н	101	BCR	C23-C22	-5.02	1.35	1.45
23	a	406	CLA	$\overline{\mathrm{CH}}\overline{\mathrm{C-C1C}}$	5.02	1.47	1.35



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	O2D-CGD	5.02	1.45	1.33
23	В	602	CLA	O2D-CGD	5.01	1.45	1.33
23	с	510	CLA	C3C-C2C	5.01	1.47	1.36
23	b	613	CLA	CHC-C1C	5.01	1.47	1.35
23	В	602	CLA	CHC-C1C	5.01	1.47	1.35
23	с	509	CLA	CHC-C1C	5.01	1.47	1.35
25	С	527	BCR	C23-C22	-5.01	1.35	1.45
23	b	609	CLA	O2D-CGD	5.01	1.45	1.33
23	D	404	CLA	O2D-CGD	5.01	1.45	1.33
23	В	606	CLA	O2D-CGD	5.00	1.45	1.33
23	с	511	CLA	OBD-CAD	5.00	1.29	1.22
23	С	509	CLA	OBD-CAD	5.00	1.29	1.22
23	с	510	CLA	C3D-C2D	5.00	1.48	1.39
23	b	603	CLA	O2D-CGD	5.00	1.45	1.33
23	b	608	CLA	CHC-C1C	4.99	1.47	1.35
23	В	608	CLA	O2D-CGD	4.99	1.45	1.33
25	С	516	BCR	C23-C22	-4.99	1.35	1.45
23	b	609	CLA	C3C-C2C	4.99	1.47	1.36
23	В	607	CLA	CHC-C1C	4.99	1.47	1.35
23	D	405	CLA	O2D-CGD	4.99	1.45	1.33
23	В	605	CLA	OBD-CAD	4.99	1.29	1.22
23	С	505	CLA	O2D-CGD	4.99	1.45	1.33
23	а	405	CLA	CHC-C1C	4.98	1.47	1.35
23	b	606	CLA	CHC-C1C	4.98	1.47	1.35
23	b	604	CLA	C3D-C2D	4.97	1.48	1.39
23	С	510	CLA	O2D-CGD	4.97	1.45	1.33
23	С	511	CLA	OBD-CAD	4.97	1.29	1.22
23	В	612	CLA	CHC-C1C	4.96	1.47	1.35
23	С	511	CLA	CHC-C1C	4.96	1.47	1.35
23	с	502	CLA	O2D-CGD	4.95	1.45	1.33
23	В	605	CLA	C3D-C2D	4.95	1.48	1.39
23	В	603	CLA	O2D-CGD	4.95	1.45	1.33
23	В	606	CLA	C3B-C2B	4.94	1.47	1.40
23	с	506	CLA	C3C-C2C	4.94	1.47	1.36
23	B	615	CLA	CHC-C1C	4.93	1.47	1.35
23	В	613	CLA	CHC-C1C	4.93	1.47	1.35
23	a	405	CLA	O2D-CGD	4.93	1.45	1.33
24	A	406	PHO	O2D-CGD	$4.9\overline{2}$	1.45	1.33
23	В	616	CLA	CHC-C1C	4.92	1.47	1.35
23	с	505	CLA	O2D-CGD	4.92	1.45	1.33
23	b	603	CLA	OBD-CAD	4.92	1.29	1.22
23	b	601	CLA	OBD-CAD	4.91	1.29	1.22



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	605	CLA	O2D-CGD	4.91	1.45	1.33
23	D	404	CLA	CHC-C1C	4.91	1.47	1.35
23	b	613	CLA	O2D-CGD	4.90	1.45	1.33
23	b	616	CLA	CHC-C1C	4.90	1.47	1.35
23	b	614	CLA	OBD-CAD	4.90	1.29	1.22
23	В	613	CLA	O2D-CGD	4.90	1.45	1.33
23	В	615	CLA	O2D-CGD	4.90	1.45	1.33
23	С	512	CLA	C3C-C2C	4.89	1.47	1.36
23	С	505	CLA	CHC-C1C	4.89	1.47	1.35
23	a	409	CLA	O2D-CGD	4.89	1.45	1.33
23	b	612	CLA	O2D-CGD	4.89	1.45	1.33
25	С	515	BCR	C23-C22	-4.88	1.35	1.45
23	В	612	CLA	C3C-C2C	4.88	1.47	1.36
23	b	615	CLA	CHC-C1C	4.88	1.47	1.35
23	b	604	CLA	O2D-CGD	4.87	1.45	1.33
23	С	503	CLA	O2D-CGD	4.87	1.45	1.33
23	b	607	CLA	O2D-CGD	4.87	1.45	1.33
23	В	612	CLA	OBD-CAD	4.87	1.29	1.22
23	b	615	CLA	O2D-CGD	4.86	1.45	1.33
23	С	509	CLA	CHC-C1C	4.86	1.47	1.35
23	с	510	CLA	CHC-C1C	4.86	1.47	1.35
25	D	406	BCR	C23-C22	-4.85	1.35	1.45
23	b	605	CLA	O2D-CGD	4.85	1.45	1.33
24	a	407	PHO	O2D-CGD	4.84	1.45	1.33
23	b	607	CLA	C3C-C2C	4.84	1.47	1.36
23	b	610	CLA	O2D-CGD	4.84	1.45	1.33
23	В	602	CLA	OBD-CAD	4.84	1.29	1.22
23	с	513	CLA	O2D-CGD	4.83	1.45	1.33
23	А	405	CLA	O2D-CGD	4.83	1.45	1.33
24	а	408	PHO	CHD-C1D	4.83	1.48	1.38
23	В	609	CLA	O2D-CGD	4.83	1.45	1.33
23	С	509	CLA	O2D-CGD	4.83	1.45	1.33
25	с	514	BCR	C23-C22	-4.83	1.35	1.45
23	b	607	CLA	CHC-C1C	4.83	1.47	1.35
23	b	608	CLA	O2D-CGD	4.82	1.45	1.33
25	В	618	BCR	C23-C22	-4.82	1.35	1.45
23	d	402	CLA	$\overline{\text{C3C-C2C}}$	4.82	1.47	1.36
23	В	603	CLA	OBD-CAD	4.82	1.29	1.22
23	В	617	CLA	O2D-CGD	4.82	1.45	1.33
23	b	609	CLA	OBD-CAD	4.81	1.29	1.22
23	с	512	CLA	O2D-CGD	4.81	1.44	1.33
23	В	611	CLA	O2D-CGD	4.81	1.44	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	O2D-CGD	4.80	1.44	1.33
${23}$	B	604	CLA	O2D-CGD	4.80	1.44	1.33
23	a	404	CLA	O2D-CGD	4.80	1.44	1.33
23	D	405	CLA	OBD-CAD	4.80	1.29	1.22
23	b	605	CLA	OBD-CAD	4.80	1.29	1.22
23	С	512	CLA	OBD-CAD	4.79	1.29	1.22
25	A	408	BCR	C23-C22	-4.79	1.35	1.45
25	h	102	BCR	C23-C22	-4.79	1.35	1.45
23	С	510	CLA	OBD-CAD	4.79	1.29	1.22
24	a	407	PHO	CHC-C1C	4.78	1.48	1.38
23	С	511	CLA	O2D-CGD	4.78	1.44	1.33
23	с	507	CLA	O2D-CGD	4.77	1.44	1.33
25	t	101	BCR	C23-C22	-4.77	1.35	1.45
23	b	608	CLA	OBD-CAD	4.76	1.29	1.22
23	a	406	CLA	O2D-CGD	4.76	1.44	1.33
23	с	501	CLA	O2D-CGD	4.75	1.44	1.33
23	с	506	CLA	CHC-C1C	4.74	1.47	1.35
23	b	605	CLA	CHC-C1C	4.74	1.47	1.35
23	В	614	CLA	CHC-C1C	4.74	1.47	1.35
23	В	609	CLA	CHC-C1C	4.73	1.47	1.35
23	с	509	CLA	OBD-CAD	4.73	1.28	1.22
23	С	506	CLA	O2D-CGD	4.72	1.44	1.33
23	С	508	CLA	O2D-CGD	4.72	1.44	1.33
25	b	617	BCR	C23-C22	-4.72	1.35	1.45
23	с	508	CLA	O2D-CGD	4.72	1.44	1.33
23	с	504	CLA	CHC-C1C	4.71	1.47	1.35
23	С	506	CLA	C3D-C2D	4.70	1.47	1.39
23	В	614	CLA	OBD-CAD	4.69	1.28	1.22
23	a	405	CLA	OBD-CAD	4.69	1.28	1.22
23	С	513	CLA	O2D-CGD	4.69	1.44	1.33
23	b	610	CLA	OBD-CAD	4.68	1.28	1.22
23	с	503	CLA	OBD-CAD	4.67	1.28	1.22
24	a	407	PHO	CHD-C1D	4.67	1.47	1.38
23	C	506	CLA	OBD-CAD	4.67	1.28	1.22
25	a	410	BCR	C23-C22	-4.67	1.35	1.45
23	d	402	CLA	O2D-CGD	4.67	1.44	1.33
23	c	504	CLA	OBD-CAD	4.67	1.28	1.22
23	C	503	CLA	OBD-CAD	4.66	1.28	1.22
23	с	507	CLA	OBD-CAD	4.64	1.28	1.22
26	a	413	SQD	048-C23	4.64	1.46	1.33
23	a	404	CLA	OBD-CAD	4.64	1.28	1.22
23	b	611	CLA	O2D-CGD	4.63	1.44	1.33



Mol	Chain	Res		Atoms	Z	Observed(Å)	Ideal(Å)
23	С	505	CLA	OBD-CAD	4.62	1.28	1.22
23	с	506	CLA	OBD-CAD	4.62	1.28	1.22
23	А	405	CLA	OBD-CAD	4.62	1.28	1.22
23	В	607	CLA	O2D-CGD	4.62	1.44	1.33
23	b	616	CLA	OBD-CAD	4.61	1.28	1.22
23	D	401	CLA	OBD-CAD	4.61	1.28	1.22
23	А	404	CLA	O2D-CGD	4.61	1.44	1.33
25	b	618	BCR	C23-C22	-4.61	1.36	1.45
23	С	502	CLA	O2D-CGD	4.61	1.44	1.33
23	С	513	CLA	OBD-CAD	4.59	1.28	1.22
23	d	402	CLA	OBD-CAD	4.59	1.28	1.22
23	с	513	CLA	OBD-CAD	4.59	1.28	1.22
23	А	407	CLA	OBD-CAD	4.58	1.28	1.22
36	b	621	HTG	C1'-S1	-4.57	1.75	1.81
23	D	404	CLA	OBD-CAD	4.55	1.28	1.22
25	с	515	BCR	C23-C22	-4.55	1.36	1.45
23	с	508	CLA	OBD-CAD	4.55	1.28	1.22
23	С	514	CLA	O2D-CGD	4.54	1.44	1.33
23	с	503	CLA	O2D-CGD	4.54	1.44	1.33
23	с	511	CLA	O2D-CGD	4.54	1.44	1.33
34	Z	101	LMG	O8-C28	4.53	1.46	1.33
23	В	617	CLA	OBD-CAD	4.53	1.28	1.22
23	с	510	CLA	OBD-CAD	4.52	1.28	1.22
24	D	402	PHO	CHD-C1D	4.52	1.47	1.38
23	с	512	CLA	OBD-CAD	4.51	1.28	1.22
23	b	601	CLA	O2A-CGA	4.50	1.46	1.33
23	b	613	CLA	OBD-CAD	4.49	1.28	1.22
23	В	602	CLA	O2A-CGA	4.48	1.46	1.33
23	b	602	CLA	OBD-CAD	4.48	1.28	1.22
23	a	406	CLA	OBD-CAD	4.47	1.28	1.22
23	A	404	CLA	OBD-CAD	4.47	1.28	1.22
23	В	608	CLA	OBD-CAD	4.47	1.28	1.22
23	b	608	CLA	O2A-CGA	4.47	1.46	1.33
23	d	403	CLA	O2D-CGD	4.46	1.44	1.33
23	b	604	CLA	OBD-CAD	4.45	1.28	1.22
23	С	504	CLA	O2D-CGD	4.45	1.44	1.33
26	D	413	SQD	O47-C7	4.45	1.46	1.34
23	d	402	CLA	O2A-CGA	4.44	1.46	1.33
23	В	608	CLA	O2A-CGA	4.44	1.46	1.33
23	b	606	CLA	O2D-CGD	4.44	1.44	1.33
23	b	611	CLA	CHC-C1C	4.44	1.46	1.35
23	с	505	CLA	OBD-CAD	4.43	1.28	1.22



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	610	CLA	OBD-CAD	4.43	1.28	1.22
23	В	613	CLA	OBD-CAD	4.43	1.28	1.22
23	с	502	CLA	OBD-CAD	4.42	1.28	1.22
23	b	615	CLA	OBD-CAD	4.41	1.28	1.22
23	С	507	CLA	OBD-CAD	4.41	1.28	1.22
26	f	101	SQD	O47-C7	4.40	1.46	1.34
23	С	504	CLA	OBD-CAD	4.40	1.28	1.22
23	b	611	CLA	O2A-CGA	4.40	1.46	1.33
31	d	408	LHG	O7-C7	4.39	1.46	1.34
26	А	411	SQD	O48-C23	4.39	1.46	1.33
23	В	604	CLA	OBD-CAD	4.38	1.28	1.22
23	с	507	CLA	O2A-CGA	4.38	1.46	1.33
23	С	503	CLA	O2A-CGA	4.38	1.46	1.33
26	В	621	SQD	O47-C7	4.38	1.46	1.34
23	С	508	CLA	O2A-CGA	4.37	1.46	1.33
25	Y	101	BCR	C23-C22	-4.37	1.36	1.45
23	a	405	CLA	O2A-CGA	4.37	1.46	1.33
23	В	610	CLA	O2A-CGA	4.36	1.46	1.33
34	С	521	LMG	O8-C28	4.36	1.46	1.33
23	b	612	CLA	OBD-CAD	4.36	1.28	1.22
26	a	413	SQD	O47-C7	4.36	1.46	1.34
23	с	513	CLA	O2A-CGA	4.35	1.46	1.33
23	с	512	CLA	O2A-CGA	4.35	1.46	1.33
23	b	615	CLA	O2A-CGA	4.35	1.46	1.33
34	с	520	LMG	O7-C10	4.34	1.46	1.34
23	А	405	CLA	O2A-CGA	4.34	1.46	1.33
24	a	408	PHO	O2A-CGA	4.34	1.46	1.33
23	с	509	CLA	O2A-CGA	4.34	1.46	1.33
31	Ε	101	LHG	O8-C23	4.33	1.46	1.33
37	Н	102	DGD	O1G-C1A	4.33	1.46	1.33
34	С	521	LMG	O7-C10	4.33	1.46	1.34
23	b	611	CLA	OBD-CAD	4.33	1.28	1.22
23	с	508	CLA	O2A-CGA	4.33	1.46	1.33
31	е	101	LHG	O8-C23	4.32	1.46	1.33
23	С	504	CLA	O2A-CGA	4.32	1.46	1.33
23	В	607	CLA	O2A-CGA	4.32	1.46	1.33
26	В	621	SQD	O48-C23	4.32	1.46	1.33
26	L	102	SQD	O47-C7	4.31	1.46	1.34
34	с	519	LMG	O8-C28	4.30	1.45	1.33
23	С	512	CLA	O2A-CGA	4.30	1.45	1.33
23	d	403	CLA	O2A-CGA	4.30	1.45	1.33
23	C	505	CLA	O2A-CGA	4.30	1.45	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	с	517	DGD	O1G-C1A	4.29	1.45	1.33
23	С	514	CLA	O2A-CGA	4.29	1.45	1.33
23	С	508	CLA	OBD-CAD	4.28	1.28	1.22
23	В	603	CLA	O2A-CGA	4.28	1.45	1.33
23	d	403	CLA	OBD-CAD	4.27	1.28	1.22
23	b	612	CLA	O2A-CGA	4.27	1.45	1.33
23	В	614	CLA	O2A-CGA	4.26	1.45	1.33
34	j	101	LMG	O8-C28	4.26	1.45	1.33
31	L	101	LHG	O8-C23	4.26	1.45	1.33
34	С	501	LMG	O7-C10	4.26	1.46	1.34
23	D	401	CLA	O2A-CGA	4.25	1.45	1.33
34	С	501	LMG	O8-C28	4.25	1.45	1.33
23	a	409	CLA	OBD-CAD	4.25	1.28	1.22
26	L	102	SQD	O48-C23	4.25	1.45	1.33
23	с	502	CLA	O2A-CGA	4.24	1.45	1.33
26	f	101	SQD	O48-C23	4.24	1.45	1.33
34	с	520	LMG	O8-C28	4.24	1.45	1.33
23	С	513	CLA	O2A-CGA	4.24	1.45	1.33
37	С	517	DGD	O2G-C1B	4.23	1.46	1.34
26	А	409	SQD	O48-C23	4.23	1.45	1.33
23	с	511	CLA	O2A-CGA	4.22	1.45	1.33
34	а	417	LMG	O7-C10	4.22	1.46	1.34
23	В	609	CLA	OBD-CAD	4.22	1.28	1.22
34	С	520	LMG	O8-C28	4.22	1.45	1.33
23	b	607	CLA	OBD-CAD	4.22	1.28	1.22
26	А	411	SQD	O47-C7	4.22	1.46	1.34
23	с	506	CLA	O2A-CGA	4.21	1.45	1.33
40	V	202	HEC	CBB-CAB	-4.21	1.33	1.49
40	V	202	HEC	CBC-CAC	-4.21	1.33	1.49
34	m	101	LMG	O8-C28	4.21	1.45	1.33
34	В	622	LMG	O8-C28	4.20	1.45	1.33
23	С	507	CLA	O2A-CGA	4.20	1.45	1.33
23	с	503	CLA	O2A-CGA	4.19	1.45	1.33
40	V	201	HEC	CBC-CAC	-4.19	1.33	1.49
23	b	614	CLA	O2A-CGA	4.19	1.45	1.33
23	В	605	CLA	O2A-CGA	4.19	1.45	1.33
23	а	409	CLA	O2A-CGA	4.19	1.45	1.33
23	С	511	CLA	O2A-CGA	4.18	1.45	1.33
25	В	619	BCR	C23-C22	-4.18	1.37	1.45
37	с	516	DGD	O1G-C1A	4.18	1.45	1.33
31	b	630	LHG	O8-C23	4.18	1.45	1.33
23	C	514	CLA	OBD-CAD	4.17	1.28	1.22


Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	е	101	LHG	O7-C7	4.17	1.46	1.34
23	b	606	CLA	OBD-CAD	4.16	1.28	1.22
31	D	409	LHG	O7-C7	4.16	1.46	1.34
23	В	616	CLA	O2A-CGA	4.16	1.45	1.33
34	J	101	LMG	O8-C28	4.16	1.45	1.33
40	V	201	HEC	CBB-CAB	-4.16	1.33	1.49
34	a	417	LMG	O8-C28	4.15	1.45	1.33
26	a	411	SQD	O48-C23	4.15	1.45	1.33
23	В	606	CLA	OBD-CAD	4.14	1.28	1.22
23	С	502	CLA	O2A-CGA	4.14	1.45	1.33
23	В	606	CLA	O2A-CGA	4.13	1.45	1.33
23	В	612	CLA	O2A-CGA	4.13	1.45	1.33
24	А	406	PHO	O2A-CGA	4.13	1.45	1.33
23	D	405	CLA	O2A-CGA	4.13	1.45	1.33
23	b	609	CLA	O2A-CGA	4.13	1.45	1.33
34	Ζ	101	LMG	O7-C10	4.13	1.46	1.34
23	В	615	CLA	OBD-CAD	4.12	1.28	1.22
31	Е	101	LHG	O7-C7	4.12	1.45	1.34
23	В	607	CLA	OBD-CAD	4.12	1.28	1.22
23	b	613	CLA	O2A-CGA	4.12	1.45	1.33
31	d	408	LHG	O8-C23	4.12	1.45	1.33
23	В	617	CLA	O2A-CGA	4.12	1.45	1.33
23	с	505	CLA	O2A-CGA	4.11	1.45	1.33
31	D	409	LHG	O8-C23	4.11	1.45	1.33
23	b	602	CLA	O2A-CGA	4.11	1.45	1.33
23	С	502	CLA	OBD-CAD	4.10	1.28	1.22
24	D	402	PHO	OBD-CAD	4.10	1.29	1.22
34	С	520	LMG	O7-C10	4.10	1.45	1.34
31	b	630	LHG	O7-C7	4.09	1.45	1.34
34	с	519	LMG	O7-C10	4.08	1.45	1.34
23	b	606	CLA	O2A-CGA	4.08	1.45	1.33
24	a	408	PHO	CHC-C4B	4.08	1.50	1.40
26	a	411	SQD	O47-C7	4.07	1.45	1.34
37	С	518	DGD	O1G-C1A	4.07	1.45	1.33
23	A	407	CLA	O2A-CGA	4.07	1.45	1.33
37	Н	102	DGD	O2G-C1B	4.06	1.45	1.34
23	В	615	CLA	O2A-CGA	4.06	1.45	1.33
23	b	607	CLA	O2A-CGA	4.05	1.45	1.33
23	В	611	CLA	O2A-CGA	4.05	1.45	1.33
23	С	506	CLA	O2A-CGA	4.05	1.45	1.33
31	D	408	LHG	O7-C7	4.05	1.45	1.34
31	d	407^{-}	LHG	O7-C7	4.04	1.45	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	с	518	DGD	O1G-C1A	4.04	1.45	1.33
23	b	616	CLA	O2A-CGA	4.04	1.45	1.33
23	В	609	CLA	O2A-CGA	4.04	1.45	1.33
23	С	510	CLA	O2A-CGA	4.04	1.45	1.33
23	С	509	CLA	O2A-CGA	4.03	1.45	1.33
23	с	501	CLA	OBD-CAD	4.03	1.27	1.22
37	h	103	DGD	O2G-C1B	4.02	1.45	1.34
23	с	504	CLA	O2A-CGA	4.02	1.45	1.33
34	Z	101	LMG	O7-C10	4.02	1.45	1.34
24	a	408	PHO	OBD-CAD	4.01	1.29	1.22
23	b	605	CLA	O2A-CGA	4.00	1.45	1.33
37	С	519	DGD	O1G-C1A	4.00	1.45	1.33
23	В	613	CLA	O2A-CGA	3.99	1.45	1.33
23	a	406	CLA	O2A-CGA	3.97	1.45	1.33
26	D	413	SQD	O48-C23	3.95	1.44	1.33
23	с	510	CLA	O2A-CGA	3.94	1.44	1.33
23	с	501	CLA	O2A-CGA	3.93	1.44	1.33
37	с	516	DGD	O2G-C1B	3.93	1.45	1.34
23	В	604	CLA	O2A-CGA	3.91	1.44	1.33
37	С	519	DGD	O2G-C1B	3.90	1.45	1.34
34	В	622	LMG	O7-C10	3.89	1.45	1.34
23	D	404	CLA	O2A-CGA	3.87	1.44	1.33
34	m	101	LMG	O7-C10	3.86	1.45	1.34
23	b	604	CLA	O2A-CGA	3.86	1.44	1.33
24	А	406	PHO	CHD-C4C	3.85	1.49	1.40
37	с	518	DGD	O2G-C1B	3.85	1.45	1.34
37	С	518	DGD	O2G-C1B	3.85	1.45	1.34
37	h	103	DGD	O1G-C1A	3.85	1.44	1.33
37	с	517	DGD	O2G-C1B	3.83	1.45	1.34
36	b	623	HTG	C1'-S1	-3.83	1.76	1.81
31	d	407	LHG	O8-C23	3.82	1.44	1.33
23	b	603	CLA	O2A-CGA	3.80	1.44	1.33
36	b	626	HTG	C1'-S1	-3.79	1.76	1.81
26	A	409	SQD	O47-C7	3.78	1.45	1.34
36	В	624	HTG	C1'-S1	-3.76	1.76	1.81
24	A	406	PHO	C3D-C2D	3.76	1.49	1.39
24	a	407	PHO	C3D-C2D	3.75	1.49	1.39
24	a	407	PHO	OBD-CAD	3.75	1.28	1.22
24	a	408	PHO	C3D-C2D	3.75	1.49	1.39
31	L	101	LHG	07-C7	3.73	1.44	1.34
31	d	406	LHG	O8-C23	3.73	1.44	1.33
24	D	402	PHO	CHC-C4B	3.72	1.49	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C3D-C2D	3.72	1.49	1.39
34	j	101	LMG	O7-C10	3.69	1.44	1.34
31	Ă	415	LHG	O7-C7	3.68	1.44	1.34
24	D	402	PHO	C4A-NA	-3.68	1.26	1.35
37	С	517	DGD	O1G-C1A	3.67	1.44	1.33
23	b	610	CLA	O2A-CGA	3.66	1.44	1.33
24	a	407	PHO	O2A-CGA	3.65	1.44	1.33
31	D	408	LHG	O8-C23	3.62	1.43	1.33
36	b	622	HTG	C1'-S1	-3.58	1.76	1.81
31	А	415	LHG	O8-C23	3.58	1.43	1.33
24	D	402	PHO	O2A-CGA	3.56	1.43	1.33
24	D	402	PHO	CHD-C4C	3.56	1.48	1.40
36	В	630	HTG	C1'-S1	-3.53	1.76	1.81
23	а	404	CLA	O2A-CGA	3.52	1.43	1.33
24	А	406	PHO	C4A-NA	-3.51	1.26	1.35
36	h	101	HTG	C1'-S1	-3.49	1.77	1.81
34	J	101	LMG	O7-C10	3.49	1.44	1.34
36	с	522	HTG	C1'-S1	-3.48	1.77	1.81
31	d	406	LHG	O7-C7	3.47	1.44	1.34
40	V	201	HEC	C3B-C2B	-3.44	1.37	1.40
36	b	625	HTG	C1'-S1	-3.44	1.77	1.81
24	A	406	PHO	OBD-CAD	3.42	1.28	1.22
24	a	407	PHO	CHC-C4B	3.41	1.48	1.40
24	A	406	PHO	CHC-C4B	3.37	1.48	1.40
23	A	404	CLA	O2A-CGA	3.35	1.43	1.33
36	С	523	HTG	C1'-S1	-3.34	1.77	1.81
24	а	408	PHO	CHD-C4C	3.33	1.48	1.40
36	В	626	HTG	C1'-S1	-3.32	1.77	1.81
24	a	407	PHO	CHB-C4A	3.32	1.48	1.40
36	В	629	HTG	C1'-S1	-3.29	1.77	1.81
24	a	408	PHO	C4A-NA	-3.27	1.27	1.35
24	D	402	PHO	C3B-C4B	3.23	1.50	1.43
23	D	401	CLA	C1C-C2C	3.21	1.50	1.44
24	a	408	PHO	CHB-C4A	3.21	1.48	1.40
23	С	507	CLA	C1D-C2D	3.20	1.49	1.42
40	V .	202	HEC	C3B-C2B	-3.20	1.37	1.40
23		510	CLA	CIC-C2C	3.16	1.50	1.44
36	D	412	HTG	C1'-S1	-3.12	1.77	1.81
23	C	507	CLA	CID-C2D	3.11	1.49	1.42
36	С	521	HTG	C1'-S1	-3.10	1.77	1.81
24	a	408	PHO	C3B-C4B	3.07	1.49	1.43
23	D	404	CLA	C1C-C2C	3.05	1.50	1.44



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	С	514	CLA	C1D-C2D	3.05	1.49	1.42
23	В	608	CLA	C1C-C2C	3.04	1.50	1.44
24	a	407	PHO	CHD-C4C	3.03	1.47	1.40
23	b	601	CLA	C1D-C2D	3.02	1.49	1.42
23	В	610	CLA	C1D-C2D	3.02	1.49	1.42
23	b	609	CLA	C1D-C2D	3.02	1.49	1.42
23	с	513	CLA	C1D-C2D	3.01	1.49	1.42
23	А	407	CLA	C1D-C2D	3.01	1.49	1.42
23	с	504	CLA	C1D-C2D	3.01	1.49	1.42
23	с	505	CLA	C1B-CHB	2.99	1.49	1.41
23	D	401	CLA	C1D-C2D	2.99	1.49	1.42
24	a	407	PHO	C4A-NA	-2.99	1.28	1.35
23	с	501	CLA	C1D-C2D	2.98	1.49	1.42
23	В	603	CLA	C1D-C2D	2.98	1.49	1.42
24	А	406	PHO	CHB-C4A	2.98	1.47	1.40
23	D	405	CLA	C1C-C2C	2.98	1.50	1.44
36	В	625	HTG	C1'-S1	-2.97	1.77	1.81
23	d	403	CLA	C1D-C2D	2.97	1.49	1.42
23	b	605	CLA	C1D-C2D	2.97	1.49	1.42
23	С	511	CLA	C4C-C3C	2.97	1.50	1.45
23	С	514	CLA	C1C-C2C	2.97	1.50	1.44
23	В	602	CLA	C1D-C2D	2.95	1.49	1.42
23	а	406	CLA	C1D-C2D	2.93	1.49	1.42
40	V	201	HEC	C3B-C4B	2.92	1.48	1.43
23	с	508	CLA	C1C-C2C	2.88	1.50	1.44
23	а	405	CLA	C1D-C2D	2.87	1.49	1.42
23	с	511	CLA	C1B-CHB	2.87	1.49	1.41
23	b	611	CLA	C1B-CHB	2.87	1.49	1.41
23	a	409	CLA	C1D-C2D	2.87	1.49	1.42
23	с	503	CLA	C4C-C3C	2.84	1.49	1.45
23	b	613	CLA	C1C-C2C	2.84	1.50	1.44
23	a	409	CLA	CHD-C4C	2.84	1.49	1.41
23	D	405	CLA	C1D-C2D	2.84	1.49	1.42
23	D	405	CLA	C4B-CHC	2.84	1.48	1.41
23	C	511	CLA	C1D-C2D	2.83	1.49	1.42
23	С	513	CLA	C1C-C2C	2.83	1.50	1.44
29	a	415	PL9	C6-C5	2.82	1.50	1.35
26	f	101	SQD	C6-S	-2.82	1.67	1.77
23	С	510	CLA	C1D-C2D	2.82	1.48	1.42
23	В	607	CLA	C1D-C2D	2.81	1.48	1.42
23	С	503	CLA	C1D-C2D	2.81	1.48	1.42
23	с	511	CLA	C1D-C2D	2.80	1.48	1.42



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C1C-C2C	2.80	1.50	1.44
23	В	606	CLA	C1D-C2D	2.80	1.48	1.42
23	b	611	CLA	C1D-C2D	2.80	1.48	1.42
23	D	401	CLA	C4B-CHC	2.80	1.48	1.41
23	b	602	CLA	C1D-C2D	2.80	1.48	1.42
23	с	504	CLA	C4C-C3C	2.79	1.49	1.45
23	b	603	CLA	C1C-C2C	2.79	1.50	1.44
26	D	413	SQD	C6-S	-2.79	1.67	1.77
23	В	613	CLA	C1C-C2C	2.79	1.50	1.44
23	b	615	CLA	C1D-C2D	2.79	1.48	1.42
26	А	411	SQD	C6-S	-2.79	1.67	1.77
23	d	403	CLA	C4B-CHC	2.79	1.48	1.41
38	е	103	HEM	C3B-C2B	-2.78	1.36	1.40
23	В	615	CLA	C1D-C2D	2.78	1.48	1.42
23	В	612	CLA	C1C-C2C	2.78	1.49	1.44
23	b	613	CLA	C4B-CHC	2.78	1.48	1.41
23	В	608	CLA	C4B-CHC	2.78	1.48	1.41
23	В	615	CLA	C4C-C3C	2.78	1.49	1.45
23	с	509	CLA	C1D-C2D	2.77	1.48	1.42
23	с	507	CLA	C1C-C2C	2.77	1.49	1.44
23	D	404	CLA	C4C-C3C	2.77	1.49	1.45
23	с	513	CLA	CHD-C4C	2.77	1.49	1.41
23	a	409	CLA	C4C-C3C	2.75	1.49	1.45
23	В	608	CLA	C1B-NB	-2.75	1.32	1.35
23	b	610	CLA	C1D-C2D	2.75	1.48	1.42
23	с	505	CLA	C1C-C2C	2.75	1.49	1.44
23	b	610	CLA	C4B-CHC	2.75	1.48	1.41
23	С	512	CLA	C1C-C2C	2.74	1.49	1.44
29	А	413	PL9	C6-C5	2.74	1.49	1.35
23	с	503	CLA	C1D-C2D	2.74	1.48	1.42
23	A	404	CLA	C1C-C2C	2.73	1.49	1.44
23	A	404	CLA	C4B-CHC	2.73	1.48	1.41
23	b	610	CLA	C4C-C3C	2.73	1.49	1.45
26	L	102	SQD	C6-S	-2.72	1.67	1.77
23	В	611	CLA	C4B-CHC	2.72	1.48	1.41
23	В	605	CLA	C1C-C2C	2.72	1.49	1.44
23	b	607	CLA	C1C-C2C	2.72	1.49	1.44
23	C	504	CLA	C4C-C3C	2.71	1.49	1.45
23	В	606	CLA	C1C-C2C	2.71	1.49	1.44
23	С	506	CLA	C1C-C2C	2.71	1.49	1.44
23	C	512	CLA	C1D-C2D	2.71	1.48	1.42
23	A	405	CLA	C1D-C2D	2.70	1.48	1.42



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	с	506	CLA	C1D-C2D	2.70	1.48	1.42
23	С	508	CLA	C1C-C2C	2.70	1.49	1.44
23	С	511	CLA	CHD-C4C	2.69	1.48	1.41
23	b	609	CLA	CHD-C4C	2.69	1.48	1.41
23	С	513	CLA	C1D-C2D	2.68	1.48	1.42
23	с	502	CLA	C1D-C2D	2.68	1.48	1.42
23	b	603	CLA	C1D-C2D	2.68	1.48	1.42
23	В	616	CLA	C1D-C2D	2.68	1.48	1.42
26	А	409	SQD	C6-S	-2.68	1.67	1.77
23	b	601	CLA	CHD-C4C	2.67	1.48	1.41
23	с	507	CLA	CHD-C4C	2.67	1.48	1.41
23	С	505	CLA	C1B-CHB	2.67	1.48	1.41
23	с	512	CLA	C4B-CHC	2.66	1.48	1.41
23	с	510	CLA	CHD-C4C	2.66	1.48	1.41
23	С	506	CLA	C1B-CHB	2.66	1.48	1.41
23	С	504	CLA	C1D-C2D	2.65	1.48	1.42
23	С	505	CLA	C1C-C2C	2.65	1.49	1.44
26	В	621	SQD	C6-S	-2.65	1.67	1.77
24	a	408	PHO	C1A-NA	-2.65	1.32	1.37
23	a	404	CLA	C1C-C2C	2.64	1.49	1.44
40	V	202	HEC	C3B-C4B	2.64	1.47	1.43
24	a	407	PHO	C3B-C4B	2.64	1.48	1.43
23	С	508	CLA	CHD-C4C	2.63	1.48	1.41
23	В	603	CLA	C4C-C3C	2.63	1.49	1.45
23	a	404	CLA	C1D-C2D	2.62	1.48	1.42
23	В	614	CLA	C1C-C2C	2.62	1.49	1.44
23	b	602	CLA	C1C-C2C	2.62	1.49	1.44
26	a	413	SQD	C6-S	-2.62	1.67	1.77
23	с	513	CLA	C1C-C2C	2.61	1.49	1.44
23	С	509	CLA	C1B-CHB	2.61	1.48	1.41
23	В	611	CLA	C1D-C2D	2.61	1.48	1.42
23	В	612	CLA	C1B-CHB	2.61	1.48	1.41
23	В	603	CLA	CHD-C4C	2.61	1.48	1.41
23	a	409	CLA	C1C-C2C	2.60	1.49	1.44
23	В	615	CLA	CHD-C4C	2.60	1.48	1.41
23	с	510	CLA	C1D-C2D	2.60	1.48	1.42
23	C _	510	CLA	CHD-C4C	2.60	1.48	1.41
23	В	608	CLA	C1D-C2D	2.59	1.48	1.42
26	a	411	SQD	C6-S	-2.59	1.67	1.77
23	С	513	CLA	C4B-CHC	2.59	1.48	1.41
23	C	508	CLA	C1D-C2D	2.59	1.48	1.42
34	Z	101	LMG	O8-C28	2.59	1.46	1.33



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	608	CLA	C4C-C3C	2.58	1.49	1.45
23	b	610	CLA	C1C-C2C	2.58	1.49	1.44
23	c	509	CLA	C1B-CHB	2.58	1.48	1.41
23	с	509	CLA	C1C-C2C	2.58	1.49	1.44
23	В	602	CLA	C1C-C2C	2.58	1.49	1.44
23	b	613	CLA	C1B-CHB	2.58	1.48	1.41
23	В	613	CLA	C1B-NB	-2.58	1.32	1.35
23	В	617	CLA	C1D-C2D	2.57	1.48	1.42
23	С	504	CLA	CHD-C4C	2.57	1.48	1.41
23	с	510	CLA	C1B-CHB	2.57	1.48	1.41
23	b	609	CLA	C1B-CHB	2.57	1.48	1.41
23	с	501	CLA	CHD-C4C	2.57	1.48	1.41
23	b	614	CLA	C1D-C2D	2.57	1.48	1.42
23	b	612	CLA	C1D-C2D	2.57	1.48	1.42
23	С	503	CLA	C1B-CHB	2.57	1.48	1.41
23	с	507	CLA	C4B-CHC	2.57	1.48	1.41
35	D	403	LMT	O1'-C1'	2.56	1.44	1.40
23	В	614	CLA	C4C-C3C	2.56	1.49	1.45
23	с	503	CLA	CHD-C4C	2.56	1.48	1.41
23	b	610	CLA	C1B-CHB	2.56	1.48	1.41
23	b	607	CLA	C1B-CHB	2.56	1.48	1.41
23	с	501	CLA	C4C-C3C	2.56	1.49	1.45
24	D	402	PHO	CHB-C4A	2.55	1.46	1.40
23	В	604	CLA	C4C-C3C	2.55	1.49	1.45
23	С	506	CLA	C1D-C2D	2.55	1.48	1.42
23	с	508	CLA	C1B-CHB	2.55	1.48	1.41
23	b	608	CLA	C1D-C2D	2.55	1.48	1.42
23	b	602	CLA	C4B-CHC	2.55	1.48	1.41
23	С	507	CLA	CHD-C4C	2.55	1.48	1.41
23	D	404	CLA	C1B-CHB	2.54	1.48	1.41
23	С	502	CLA	C1D-C2D	2.54	1.48	1.42
23	A	404	CLA	C1D-C2D	2.53	1.48	1.42
23	В	606	CLA	C1B-CHB	2.53	1.48	1.41
29	D	407	PL9	C6-C5	2.53	1.48	1.35
23	с	511	CLA	C1C-C2C	2.53	1.49	1.44
23	с	502	CLA	C1B-CHB	2.53	1.48	1.41
23	В	610	CLA	C1C-C2C	2.53	1.49	1.44
23	В	604	CLA	C4B-CHC	2.53	1.48	1.41
23	С	503	CLA	CHD-C4C	2.52	1.48	1.41
23	В	611	CLA	C1B-CHB	2.52	1.48	1.41
23	b	612	CLA	C1C-C2C	2.52	1.49	1.44
23	b	606	CLA	C1C-C2C	2.51	1.49	1.44



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
23	A	404	CLA	CHD-C4C	2.51	1.48	1.41
29	d	405	PL9	C6-C5	2.51	1.48	1.35
23	с	506	CLA	CHD-C4C	2.51	1.48	1.41
23	b	605	CLA	C1B-CHB	2.51	1.48	1.41
23	С	512	CLA	CHD-C4C	2.51	1.48	1.41
24	D	402	PHO	C1A-NA	-2.51	1.32	1.37
23	d	402	CLA	C1C-C2C	2.51	1.49	1.44
23	С	509	CLA	C1C-C2C	2.50	1.49	1.44
23	А	407	CLA	C4B-CHC	2.50	1.48	1.41
23	В	614	CLA	C1D-C2D	2.50	1.48	1.42
23	с	505	CLA	C4B-CHC	2.50	1.47	1.41
23	b	616	CLA	C1D-C2D	2.50	1.48	1.42
23	А	407	CLA	CHD-C4C	2.50	1.48	1.41
23	С	505	CLA	C1D-C2D	2.50	1.48	1.42
23	b	611	CLA	C4C-C3C	2.50	1.49	1.45
23	С	509	CLA	C4C-C3C	2.50	1.49	1.45
23	D	404	CLA	CHD-C4C	2.50	1.48	1.41
23	С	514	CLA	CHD-C4C	2.50	1.48	1.41
23	d	403	CLA	C1C-C2C	2.49	1.49	1.44
23	В	609	CLA	C1B-CHB	2.49	1.47	1.41
23	D	405	CLA	C1B-CHB	2.49	1.47	1.41
23	b	602	CLA	CHD-C4C	2.49	1.48	1.41
23	А	404	CLA	C4C-C3C	2.49	1.49	1.45
23	a	404	CLA	CHD-C4C	2.49	1.48	1.41
23	b	614	CLA	C1B-CHB	2.49	1.47	1.41
23	В	610	CLA	C4B-CHC	2.49	1.47	1.41
23	С	506	CLA	CHD-C4C	2.48	1.48	1.41
23	b	610	CLA	CHD-C4C	2.48	1.48	1.41
23	b	604	CLA	C1D-C2D	2.48	1.48	1.42
23	D	404	CLA	C1D-C2D	2.48	1.48	1.42
23	C	502	CLA	C1C-C2C	2.48	1.49	1.44
23	с	503	CLA	C4B-CHC	$2.\overline{48}$	1.47	1.41
23	В	606	CLA	C4B-CHC	2.48	1.47	1.41
23	В	604	CLA	C1D-C2D	2.47	1.48	1.42
23	В	607	CLA	C1C-C2C	2.47	1.49	1.44
23	b	614	CLA	C1C-C2C	2.47	1.49	1.44
23	С	503	CLA	C4B-CHC	2.47	1.47	1.41
23	В	608	CLA	CHD-C4C	2.46	1.48	1.41
23	C	505	CLA	$\overline{\mathrm{CHD}}$ -C4C	2.46	1.48	1.41
23	b	609	CLA	$\overline{\text{C1C-C2C}}$	2.46	1.49	1.44
24	A	406	PHO	C4C-C3C	2.46	1.49	1.45
23	В	607	CLA	CHD-C4C	2.46	1.48	1.41



Mol	Chain	Res	Tvpe	Atoms	Z	Observed(Å)	Ideal(Å)
23	С	502	CLA	CHD-C4C	$\frac{-}{246}$	1 48	1 41
23	C	513	CLA	CHD-C4C	2.10 2.45	1.10	1.11
23	C	514	CLA	C1B-CHB	2.10 2.45	1.10	1 41
23	d	403	CLA	CHD-C4C	2.10 2.45	1.11	1 41
23	c	501	CLA	C1B-CHB	2.13 2.44	1.10	1 41
23	c	512	CLA	C1C-C2C	2.44	1.49	1.44
23	c	505	CLA	C1D-C2D	2.44	1.48	1.42
23	C	507	CLA	C1C-C2C	2.44	1.49	1.44
23	b	606	CLA	C1D-C2D	2.44	1.48	1.42
23	В	617	CLA	C4B-CHC	2.44	1.47	1.41
23	b	615	CLA	CHD-C4C	2.44	1.48	1.41
23	b	615	CLA	C1B-CHB	2.44	1.47	1.41
23	В	615	CLA	C1B-CHB	2.44	1.47	1.41
23	с	504	CLA	C1C-C2C	2.44	1.49	1.44
37	с	518	DGD	O2G-C2G	-2.44	1.40	1.46
23	С	504	CLA	C4B-CHC	2.44	1.47	1.41
23	В	617	CLA	C1B-CHB	2.43	1.47	1.41
23	d	402	CLA	C1D-C2D	2.43	1.48	1.42
23	b	609	CLA	C4B-CHC	2.43	1.47	1.41
23	С	502	CLA	C4B-CHC	2.43	1.47	1.41
23	b	616	CLA	C4C-C3C	2.43	1.49	1.45
23	С	508	CLA	C4B-CHC	2.43	1.47	1.41
23	С	507	CLA	C4B-CHC	2.42	1.47	1.41
23	b	613	CLA	C1D-C2D	2.42	1.48	1.42
23	В	605	CLA	C1B-CHB	2.42	1.47	1.41
23	b	606	CLA	CHD-C4C	2.42	1.48	1.41
23	с	509	CLA	CHD-C4C	2.42	1.48	1.41
23	b	608	CLA	C1C-C2C	2.42	1.49	1.44
23	с	511	CLA	CHD-C4C	2.42	1.48	1.41
24	A	406	PHO	C3B-C4B	2.42	1.48	1.43
23	b	612	CLA	C4B-CHC	2.42	1.47	1.41
23	B	609	CLA	C1C-NC	-2.41	1.34	1.37
23	b	614	CLA	C4B-CHC	2.41	1.47	1.41
23	b	608	CLA	CHD-C4C	2.41	1.48	1.41
23	с	512	CLA	CHD-C4C	2.41	1.48	1.41
23	b	607	CLA	C1D-C2D	2.41	1.48	1.42
24	A	406	PHO	CIA-NA	-2.41	1.32	1.37
23	B	604	CLA	CIB-CHB	2.41	1.47	1.41
23		512	CLA	CIB-CHB	2.40	1.47	1.41
23	В	615	CLA	C4B-CHC	2.40	1.47	1.41
23	В	613	CLA	CIB-CHB	2.40	1.47	1.41
23	с	513	CLA	C4B-CHC	2.40	1.47	1.41



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C4C-C3C	2.40	1.49	1.45
23	A	405	CLA	CHD-C4C	2.40	1.48	1.41
23	с	512	CLA	C1D-C2D	2.40	1.48	1.42
23	В	603	CLA	C1C-C2C	2.40	1.49	1.44
23	С	502	CLA	C1B-CHB	2.40	1.47	1.41
23	a	406	CLA	CHD-C4C	2.40	1.48	1.41
23	a	404	CLA	C1B-CHB	2.40	1.47	1.41
23	А	405	CLA	C4C-C3C	2.40	1.49	1.45
23	В	617	CLA	C1C-C2C	2.40	1.49	1.44
23	b	606	CLA	C1B-CHB	2.40	1.47	1.41
23	В	611	CLA	C1C-C2C	2.40	1.49	1.44
23	В	612	CLA	C1D-C2D	2.39	1.48	1.42
23	b	603	CLA	CHD-C4C	2.39	1.48	1.41
23	a	409	CLA	C4B-CHC	2.39	1.47	1.41
23	b	612	CLA	C4C-C3C	2.39	1.49	1.45
23	В	610	CLA	CHD-C4C	2.39	1.48	1.41
23	с	506	CLA	C1B-NB	-2.39	1.33	1.35
23	В	604	CLA	C1C-C2C	2.39	1.49	1.44
23	b	601	CLA	C4B-CHC	2.39	1.47	1.41
23	С	510	CLA	C1B-CHB	2.39	1.47	1.41
23	С	506	CLA	C4C-C3C	2.39	1.49	1.45
23	b	616	CLA	C1B-CHB	2.39	1.47	1.41
23	с	510	CLA	C4C-C3C	2.39	1.49	1.45
23	a	405	CLA	CHD-C4C	2.39	1.47	1.41
23	b	608	CLA	C4B-CHC	2.38	1.47	1.41
35	В	633	LMT	O1'-C1'	2.38	1.44	1.40
23	В	612	CLA	C4B-CHC	2.38	1.47	1.41
23	с	504	CLA	CHD-C4C	2.38	1.47	1.41
23	В	604	CLA	CHD-C4C	2.38	1.47	1.41
23	b	605	CLA	CHD-C4C	2.37	1.47	1.41
23	В	610	CLA	C1B-CHB	2.37	1.47	1.41
23	с	505	CLA	CHD-C4C	2.37	1.47	1.41
23	с	504	CLA	C4B-NB	-2.37	1.33	1.35
23	d	402	CLA	C4B-CHC	2.37	1.47	1.41
23	D	401	CLA	CHD-C4C	2.37	1.47	1.41
23	d	402	CLA	C1B-CHB	2.36	1.47	1.41
23	с	503	CLA	C1B-CHB	2.36	1.47	1.41
36	b	621	HTG	C1-S1	-2.36	1.77	1.80
23	b	606	CLA	C4B-CHC	2.36	1.47	1.41
23	с	510	CLA	C1C-C2C	2.36	1.49	1.44
23	b	614	CLA	CHD-C4C	2.36	1.47	1.41
23	b	603	CLA	C4C-C3C	2.36	1.49	1.45



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	С	512	CLA	C4C-C3C	2.35	1.49	1.45
23	В	613	CLA	C4C-C3C	2.35	1.49	1.45
23	с	510	CLA	C4B-CHC	2.35	1.47	1.41
23	b	611	CLA	CHD-C4C	2.35	1.47	1.41
23	b	607	CLA	C4C-C3C	2.35	1.49	1.45
23	с	502	CLA	CHD-C4C	2.34	1.47	1.41
23	d	402	CLA	CHD-C4C	2.34	1.47	1.41
23	с	511	CLA	C4B-CHC	2.34	1.47	1.41
23	с	509	CLA	C4C-C3C	2.34	1.49	1.45
23	С	514	CLA	C4B-CHC	2.34	1.47	1.41
23	С	511	CLA	C1B-CHB	2.34	1.47	1.41
23	В	606	CLA	C1C-NC	-2.34	1.34	1.37
23	с	508	CLA	C4B-CHC	2.34	1.47	1.41
23	В	616	CLA	C1C-C2C	2.34	1.49	1.44
23	А	405	CLA	C1C-C2C	2.34	1.49	1.44
23	В	605	CLA	C4B-CHC	2.34	1.47	1.41
23	b	613	CLA	CHD-C4C	2.34	1.47	1.41
23	В	602	CLA	C4B-CHC	2.33	1.47	1.41
23	с	504	CLA	C1B-CHB	2.33	1.47	1.41
23	С	505	CLA	C4C-C3C	2.33	1.49	1.45
23	В	603	CLA	C1B-CHB	2.33	1.47	1.41
23	В	607	CLA	C4B-CHC	2.33	1.47	1.41
23	В	605	CLA	C1D-C2D	2.33	1.47	1.42
23	D	405	CLA	CHD-C4C	2.33	1.47	1.41
23	с	503	CLA	C1C-C2C	2.33	1.49	1.44
24	a	407	PHO	C4D-CHA	2.33	1.50	1.43
23	с	508	CLA	C1D-C2D	2.33	1.47	1.42
35	С	522	LMT	O1'-C1'	2.33	1.44	1.40
23	с	501	CLA	C4B-CHC	2.33	1.47	1.41
23	С	505	CLA	C4B-CHC	2.32	1.47	1.41
23	С	510	CLA	C4B-CHC	2.32	1.47	1.41
23	С	513	CLA	C1B-CHB	2.32	1.47	1.41
36	B	629	HTG	C1-S1	-2.32	1.77	1.80
23	A	405	CLA	C4B-CHC	2.32	1.47	1.41
23	B	606	CLA	CHD-C4C	2.32	1.47	1.41
23		502	CLA	C4C-C3C	2.32	1.49	1.45
23	В	602	CLA	CHD-C4C	2.32	1.47	
23	b	612	CLA	CHD-C4C	2.31	1.47	1.41
23		504	UTC	CIB-CHB	2.31	1.47	1.41
36	b	626	HIG	CI-SI	-2.31		1.80
23	b	607	CLA	CHD-C4C	2.31	1.47	1.41
23	b	016	CLA	UHD-C4C	2.31	1.47	1.41



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	C4B-CHC	2.31	1.47	1.41
23	b	603	CLA	C4B-CHC	2.31	1.47	1.41
23	b	602	CLA	C1B-CHB	2.31	1.47	1.41
23	В	609	CLA	C1C-C2C	2.30	1.49	1.44
23	В	603	CLA	C4B-CHC	2.30	1.47	1.41
23	a	406	CLA	C1C-NC	-2.30	1.34	1.37
23	D	401	CLA	C1B-CHB	2.30	1.47	1.41
23	b	605	CLA	C1C-C2C	2.30	1.49	1.44
23	с	502	CLA	C1C-C2C	2.30	1.49	1.44
36	D	412	HTG	C1-S1	-2.29	1.77	1.80
23	с	506	CLA	C1B-CHB	2.29	1.47	1.41
23	С	507	CLA	C4C-C3C	2.29	1.49	1.45
23	В	616	CLA	CHD-C4C	2.29	1.47	1.41
23	А	405	CLA	C1B-CHB	2.29	1.47	1.41
23	с	505	CLA	C4C-C3C	2.29	1.49	1.45
23	А	405	CLA	C1B-NB	-2.28	1.33	1.35
24	А	406	PHO	C4D-CHA	2.28	1.49	1.43
23	a	405	CLA	C1B-NB	-2.28	1.33	1.35
23	А	407	CLA	C1C-C2C	2.28	1.49	1.44
23	b	601	CLA	C1C-C2C	2.28	1.49	1.44
23	с	508	CLA	CHD-C4C	2.27	1.47	1.41
23	b	605	CLA	C4C-C3C	2.27	1.49	1.45
23	b	601	CLA	C1B-CHB	2.27	1.47	1.41
23	b	604	CLA	C4B-CHC	2.27	1.47	1.41
23	b	614	CLA	C4C-C3C	2.27	1.49	1.45
23	В	614	CLA	C1B-CHB	2.27	1.47	1.41
23	В	614	CLA	C4B-CHC	2.27	1.47	1.41
23	с	501	CLA	C1C-C2C	2.27	1.49	1.44
23	b	604	CLA	CHD-C4C	2.27	1.47	1.41
23	d	403	CLA	C1B-CHB	2.27	1.47	1.41
23	b	604	CLA	C1B-CHB	2.26	1.47	1.41
23	b	615	CLA	C4C-C3C	2.26	1.48	1.45
24	a	407	PHO	C4C-C3C	2.26	1.49	1.45
23	В	612	CLA	CHD-C4C	2.26	1.47	1.41
23	b	605	CLA	C4B-CHC	2.26	1.47	1.41
23	с	513	CLA	C4C-C3C	2.26	1.48	1.45
23	В	614	CLA	CHD-C4C	2.25	1.47	1.41
23	с	512	CLA	C1B-CHB	2.25	1.47	1.41
23	с	506	CLA	C4C-C3C	2.25	1.48	1.45
23	С	503	CLA	C1C-C2C	2.25	1.48	1.44
23	D	404	CLA	C4B-CHC	2.25	1.47	1.41
23	с	509	CLA	C4B-CHC	2.25	1.47	1.41



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	611	CLA	CHD-C4C	2.24	1.47	1.41
23	В	608	CLA	C1B-CHB	2.24	1.47	1.41
23	С	509	CLA	C4B-CHC	2.24	1.47	1.41
23	b	607	CLA	C1B-NB	-2.23	1.33	1.35
23	В	613	CLA	C4B-CHC	2.23	1.47	1.41
23	a	409	CLA	C1B-CHB	2.23	1.47	1.41
23	В	602	CLA	C1B-CHB	2.23	1.47	1.41
36	с	522	HTG	C1-S1	-2.23	1.77	1.80
37	h	103	DGD	O5D-C1E	2.22	1.44	1.40
23	В	609	CLA	C1D-C2D	2.22	1.47	1.42
23	В	602	CLA	C4C-C3C	2.22	1.48	1.45
23	с	502	CLA	C4B-CHC	2.22	1.47	1.41
23	В	617	CLA	CHD-C4C	2.22	1.47	1.41
23	В	613	CLA	CHD-C4C	2.22	1.47	1.41
23	b	612	CLA	C1B-CHB	2.21	1.47	1.41
23	а	405	CLA	C1C-C2C	2.21	1.48	1.44
23	В	613	CLA	C1D-C2D	2.21	1.47	1.42
23	с	507	CLA	C4C-C3C	2.21	1.48	1.45
24	D	402	PHO	C4C-C3C	2.21	1.49	1.45
36	b	623	HTG	C1-S1	-2.20	1.77	1.80
23	с	508	CLA	C4C-C3C	2.20	1.48	1.45
38	Ε	103	HEM	C3B-C2B	-2.20	1.37	1.40
23	А	407	CLA	C1B-NB	-2.19	1.33	1.35
23	с	509	CLA	C4B-NB	-2.19	1.33	1.35
23	с	504	CLA	C4B-CHC	2.19	1.47	1.41
23	b	608	CLA	C1B-CHB	2.18	1.47	1.41
23	с	511	CLA	C4C-C3C	2.18	1.48	1.45
23	С	509	CLA	C1C-NC	-2.18	1.34	1.37
34	Z	101	LMG	O1-C1	2.18	1.43	1.40
23	b	616	CLA	C4B-CHC	2.18	1.47	1.41
36	В	630	HTG	C1-S1	-2.17	1.77	1.80
23	A	407	CLA	C1B-CHB	2.17	1.47	1.41
23	d	402	CLA	C1B-NB	-2.17	1.33	1.35
24	D	402	PHO	C4D-CHA	2.17	1.49	1.43
23	В	615	CLA	C1C-C2C	2.15	1.48	1.44
23	b	607	CLA	C4B-CHC	2.15	1.47	1.41
36	b	625	HTG	C1-S1	-2.15	1.77	1.80
23	C	512	CLA	C4C-C3C	2.15	1.48	1.45
23	C	507	CLA	C1B-CHB	2.15	1.47	1.41
23	С	513	CLA	C1B-CHB	2.14	1.47	1.41
23	с	507	CLA	C1B-CHB	2.14	1.46	1.41
34	a	417	LMG	O1-C1	2.14	1.43	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	В	617	CLA	C1C-NC	-2.13	1.34	1.37
23	В	607	CLA	C1B-CHB	2.13	1.46	1.41
23	b	602	CLA	C4C-C3C	2.13	1.48	1.45
23	С	506	CLA	C4B-CHC	2.12	1.46	1.41
23	с	506	CLA	C4B-CHC	2.12	1.46	1.41
23	В	616	CLA	C1B-CHB	2.12	1.46	1.41
23	С	512	CLA	C4B-CHC	2.12	1.46	1.41
37	с	517	DGD	O3G-C1D	2.11	1.43	1.40
23	В	605	CLA	CHD-C4C	2.11	1.47	1.41
23	b	608	CLA	C1C-NC	-2.10	1.34	1.37
23	С	508	CLA	C4C-C3C	2.10	1.48	1.45
23	с	506	CLA	C1C-NC	-2.10	1.34	1.37
23	С	510	CLA	C4C-C3C	2.09	1.48	1.45
23	В	606	CLA	C4C-C3C	2.09	1.48	1.45
23	а	409	CLA	C1B-NB	-2.09	1.33	1.35
36	h	101	HTG	C1-S1	-2.08	1.77	1.80
34	с	519	LMG	O1-C1	2.08	1.43	1.40
26	а	413	SQD	O6-C1	2.08	1.43	1.40
23	С	512	CLA	C1C-NC	-2.07	1.34	1.37
35	Ε	102	LMT	O1'-C1'	2.07	1.43	1.40
23	b	615	CLA	C4B-CHC	2.07	1.46	1.41
23	С	509	CLA	C1D-C2D	2.07	1.47	1.42
23	С	504	CLA	C1C-C2C	2.06	1.48	1.44
23	В	611	CLA	C4C-C3C	2.06	1.48	1.45
23	а	405	CLA	C4B-CHC	2.06	1.46	1.41
29	D	407	PL9	C2-C1	-2.06	1.39	1.44
23	В	609	CLA	C4B-CHC	2.05	1.46	1.41
34	С	521	LMG	O1-C1	2.05	1.43	1.40
29	A	413	PL9	C2-C3	2.05	1.40	1.34
35	b	628	LMT	O1'-C1'	2.04	1.43	1.40
25	b	619	BCR	C30-C25	-2.04	1.51	1.53
36	b	622	HTG	C1-S1	-2.04	1.77	1.80
23	b	609	CLA	C4C-C3C	2.04	1.48	1.45
23	В	610	CLA	C1B-NB	-2.03	1.33	1.35
24	a	407	PHO	C1A-NA	-2.03	1.33	1.37
23	В	609	CLA	CHD-C4C	2.03	1.46	1.41
23	b	615	CLA	C1C-NC	-2.03	1.34	1.37
23	b	616	CLA	C1C-C2C	2.03	1.48	1.44
23	b	611	CLA	C4B-CHC	2.03	1.46	1.41
29	d	405	PL9	C2-C3	2.02	1.40	1.34
34	J	101	LMG	O1-C1	2.02	1.43	1.40
35	a	418	LMT	O1'-C1'	2.02	1.43	1.40



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
31	d	406	LHG	O7-C5	-2.02	1.41	1.46
23	b	613	CLA	C4C-C3C	2.02	1.48	1.45
23	С	510	CLA	C1C-NC	-2.02	1.34	1.37
23	b	606	CLA	C4C-C3C	2.01	1.48	1.45
23	С	514	CLA	C4C-C3C	2.00	1.48	1.45
23	С	503	CLA	C4C-C3C	2.00	1.48	1.45

All (2292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
24	А	406	PHO	CMD-C2D-C1D	8.02	137.41	125.06
23	В	608	CLA	C4A-NA-C1A	-7.32	103.41	106.71
23	В	612	CLA	CHD-C4C-C3C	-6.98	114.58	124.84
23	В	609	CLA	CHD-C4C-C3C	-6.93	114.66	124.84
24	a	407	PHO	CMD-C2D-C1D	6.91	135.70	125.06
24	D	402	PHO	CMD-C2D-C1D	6.88	135.66	125.06
23	С	507	CLA	C4A-NA-C1A	-6.77	103.66	106.71
23	b	609	CLA	C4A-NA-C1A	-6.77	103.66	106.71
23	с	507	CLA	O2D-CGD-CBD	6.75	123.27	111.27
23	b	611	CLA	C2C-C1C-NC	6.68	116.23	109.97
23	В	617	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
38	Е	103	HEM	CAD-CBD-CGD	6.67	123.86	112.67
23	В	611	CLA	CHD-C4C-C3C	-6.67	115.04	124.84
23	D	405	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	b	602	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	В	617	CLA	O2D-CGD-CBD	6.52	122.85	111.27
23	b	616	CLA	C4A-NA-C1A	-6.51	103.78	106.71
23	b	613	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
24	a	408	PHO	CMD-C2D-C1D	6.47	135.03	125.06
23	с	513	CLA	C4A-NA-C1A	-6.47	103.80	106.71
23	с	507	CLA	C4A-NA-C1A	-6.46	103.80	106.71
23	В	606	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
23	А	404	CLA	C4A-NA-C1A	-6.38	103.84	106.71
23	D	401	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
25	D	406	BCR	C7-C8-C9	-6.34	116.66	126.23
29	a	415	PL9	C7-C3-C4	6.31	122.01	116.88
23	В	603	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	C	505	CLA	C2C-C1C-NC	6.31	115.88	109.97
23	с	512	CLA	O2D-CGD-CBD	$6.\overline{30}$	122.47	111.27
23	В	610	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
36	В	625	HTG	C1'-S1-C1	$6.\overline{25}$	111.79	100.09
23	a	409	CLA	C4A-NA-C1A	-6.25	103.90	106.71



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal(o) $ $
23	b	604	CLA	O2D-CGD-CBD	6.25	122.37	111.27
23	C	510	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
23	d	402	CLA	C2C-C1C-NC	6.23	115.81	109.97
23	с	502	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
23	с	505	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	В	617	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	В	613	CLA	O2D-CGD-CBD	6.21	122.31	111.27
23	С	513	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
36	В	626	HTG	C1'-S1-C1	6.19	111.68	100.09
23	d	403	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
23	С	508	CLA	O2D-CGD-CBD	6.17	122.24	111.27
23	С	513	CLA	C4A-NA-C1A	-6.15	103.94	106.71
23	a	406	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	b	608	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	В	605	CLA	O2D-CGD-CBD	6.14	122.17	111.27
23	с	503	CLA	C4A-NA-C1A	-6.11	103.96	106.71
23	В	603	CLA	O2D-CGD-CBD	6.11	122.13	111.27
23	b	606	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	b	611	CLA	O2D-CGD-CBD	6.10	122.11	111.27
23	С	509	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
36	b	623	HTG	C1'-S1-C1	6.08	111.47	100.09
23	a	405	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	с	512	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	А	407	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	С	506	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	В	615	CLA	O2D-CGD-CBD	6.06	122.05	111.27
23	с	508	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	с	511	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
23	С	514	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	b	604	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	b	615	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	b	602	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	В	605	CLA	CHD-C4C-C3C	-6.02	115.98	124.84
23	b	610	CLA	C4A-NA-C1A	-6.01	104.00	106.71
23	b	605	CLA	CHD-C4C-C3C	-6.00	116.01	124.84
23	В	613	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	b	614	CLA	O2D-CGD-CBD	5.97	121.87	111.27
23	a	404	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	В	607	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	b	607	CLA	C2C-C1C-NC	5.93	115.53	109.97
23	D	404	CLA	C2C-C1C-NC	5.92	$1\overline{15.52}$	109.97



Mol	Chain	\mathbf{Res}	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
36	с	521	HTG	C1'-S1-C1	5.92	111.16	100.09
24	a	407	PHO	O2D-CGD-CBD	5.91	121.77	111.27
23	b	610	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	С	511	CLA	C2C-C1C-NC	5.91	115.50	109.97
23	В	616	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
36	b	621	HTG	C1'-S1-C1	5.87	111.08	100.09
23	С	508	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	b	603	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	с	504	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	с	510	CLA	C4A-NA-C1A	-5.85	104.08	106.71
23	с	508	CLA	O2D-CGD-CBD	5.84	121.65	111.27
23	В	602	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
29	А	413	PL9	C7-C3-C4	5.83	121.62	116.88
23	В	604	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
23	В	604	CLA	O2D-CGD-CBD	5.82	121.61	111.27
36	D	412	HTG	C1'-S1-C1	5.82	110.98	100.09
23	С	502	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	b	609	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	В	607	CLA	C4A-NA-C1A	-5.81	104.09	106.71
23	b	601	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	D	404	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	с	501	CLA	C4A-NA-C1A	-5.80	104.10	106.71
23	b	607	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	В	611	CLA	O2D-CGD-CBD	5.77	121.52	111.27
23	С	504	CLA	C4A-NA-C1A	-5.77	104.11	106.71
23	В	615	CLA	C2C-C1C-NC	5.76	115.37	109.97
23	b	601	CLA	O2D-CGD-CBD	5.76	121.50	111.27
26	А	409	SQD	O6-C1-C2	5.76	117.29	108.30
23	В	614	CLA	C2C-C1C-NC	5.75	115.36	109.97
38	е	103	HEM	CAD-CBD-CGD	5.75	122.32	112.67
26	D	413	SQD	O47-C7-C8	5.74	123.88	111.50
25	Т	101	BCR	C15-C16-C17	-5.72	111.75	123.47
23	С	502	CLA	O2D-CGD-CBD	5.72	121.43	111.27
23	b	612	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	b	614	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	b	601	CLA	C4A-NA-C1A	-5.71	104.14	106.71
23	b	616	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
23	с	509	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	С	509	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	В	604	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	В	602	CLA	O2D-CGD-CBD	5.69	121.37	111.27
23	d	403	CLA	C4A-NA-C1A	-5.68	104.15	106.71



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	Uhain	Kes	Type	Atoms		Ubserved(°)	100.0 ⁻			
23	c	508	CLA	C2C-C1C-NC	5.68	115.29	109.97			
23	A	404	CLA	CHD-C4C-C3C	-5.68	116.49	124.84			
23	С	501	CLA	O2D-CGD-CBD	5.67	121.35	111.27			
23	b	616	CLA	O2D-CGD-CBD	5.67	121.34	111.27			
23	В	608	CLA	CHD-C4C-C3C	-5.67	116.51	124.84			
23	с	503	CLA	C2C-C1C-NC	5.67	115.28	109.97			
23	С	511	CLA	O2D-CGD-CBD	5.65	121.31	111.27			
23	В	611	CLA	C4A-NA-C1A	-5.65	104.17	106.71			
23	С	503	CLA	CHD-C4C-C3C	-5.65	116.54	124.84			
23	a	405	CLA	CHD-C4C-C3C	-5.64	116.54	124.84			
23	С	506	CLA	O2D-CGD-CBD	5.64	121.29	111.27			
24	А	406	PHO	C3D-C2D-C1D	-5.62	97.68	105.87			
23	b	616	CLA	C2C-C1C-NC	5.61	115.23	109.97			
23	b	612	CLA	C4A-NA-C1A	-5.61	104.19	106.71			
23	а	404	CLA	CHD-C4C-C3C	-5.59	116.62	124.84			
23	с	506	CLA	C2C-C1C-NC	5.58	115.20	109.97			
23	С	502	CLA	C2C-C1C-NC	5.57	115.19	109.97			
24	a	407	PHO	C3D-C2D-C1D	-5.57	97.76	105.87			
23	В	614	CLA	CHD-C4C-C3C	-5.56	116.66	124.84			
23	b	611	CLA	CHD-C4C-C3C	-5.56	116.66	124.84			
23	В	610	CLA	C4A-NA-C1A	-5.55	104.21	106.71			
23	С	509	CLA	O2D-CGD-CBD	5.55	121.13	111.27			
25	Y	101	BCR	C33-C5-C6	-5.54	118.30	124.53			
23	b	603	CLA	O2D-CGD-CBD	5.54	121.11	111.27			
23	с	510	CLA	C1-C2-C3	-5.54	116.46	126.04			
23	С	512	CLA	CHD-C4C-C3C	-5.54	116.70	124.84			
23	b	605	CLA	C2C-C1C-NC	5.54	115.16	109.97			
24	А	406	PHO	O2D-CGD-CBD	5.53	121.10	111.27			
23	b	615	CLA	C4A-NA-C1A	-5.53	104.22	106.71			
23	с	507	CLA	CHD-C4C-C3C	-5.53	116.71	124.84			
23	с	505	CLA	O2D-CGD-CBD	5.52	121.07	111.27			
23	A	405	CLA	C4A-NA-C1A	-5.51	104.23	106.71			
23	С	514	CLA	C4A-NA-C1A	-5.51	104.23	106.71			
23	С	503	CLA	O2D-CGD-CBD	5.51	121.05	111.27			
23	С	504	CLA	CHD-C4C-C3C	-5.50	116.75	124.84			
23	с	506	CLA	CHD-C4C-C3C	-5.49	116.76	124.84			
23	С	506	CLA	C4A-NA-C1A	-5.49	104.24	106.71			
23	C	506	CLA	C2C-C1C-NC	5.49	115.11	109.97			
23	C	504	CLA	C2C-C1C-NC	5.48	115.10	109.97			
-						110.00	100.00			
36	В	630	HTG	C1'-S1-C1	5.47	110.32	100.09			
$\frac{36}{36}$	B C	$\begin{array}{c} 630\\ 523\end{array}$	HTG HTG	C1'-S1-C1 C1'-S1-C1	5.47 5.47	110.32	$\frac{100.09}{100.09}$			

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	Choin	<i>i previ</i>	Turna	Atoma	7	Observed(0)	Ideal(0)
	Unain	res 519				Observed(*)	10ear(*)
23	C C	513	CLA	$\begin{array}{c} \text{CHD-C4C-C3C} \\ \text{CHD-C4C-C3C} \end{array}$	-5.40	116.81	124.84
23	L L	507 COF	CLA	$\frac{\text{CHD-C4C-C3C}}{\text{CHD-C4C-C3C}}$	-5.40	110.81	124.84
23		000 C10	CLA CLA	O2D-CGD-CBD	5.40	120.97	111.27
23	D	610	CLA	02D-CGD-CBD	5.45	120.95	111.27
23	D	604	CLA	C4A-NA-CIA	-5.45	104.26	106.71
23	d	402	CLA	C4A-NA-CIA	-5.43	104.26	106.71
23	a	404	CLA	C2C-CIC-NC	5.43	115.06	109.97
23	b	603	CLA	C4A-NA-CIA	-5.42	104.27	106.71
23	С	502	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	b	606	CLA	O2D-CGD-CBD	5.41	120.89	111.27
23	D	404	CLA	C4A-NA-C1A	-5.41	104.27	106.71
23	C	505	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	В	603	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	D	402	PHO	C2D-C1D-ND	5.39	117.93	109.79
24	D	402	PHO	C3D-C2D-C1D	-5.39	98.02	105.87
23	b	608	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	с	502	CLA	O2D-CGD-CBD	5.38	120.83	111.27
23	В	607	CLA	O2D-CGD-CBD	5.37	120.82	111.27
24	a	407	PHO	C2D-C1D-ND	5.37	117.90	109.79
23	A	404	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	b	613	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	В	616	CLA	C2C-C1C-NC	5.35	114.98	109.97
23	с	504	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
25	У	101	BCR	C33-C5-C6	-5.35	118.52	124.53
23	В	615	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	С	502	CLA	C4A-NA-C1A	-5.34	104.30	106.71
23	с	501	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	a	406	CLA	C4A-NA-C1A	-5.30	104.32	106.71
23	с	509	CLA	C2C-C1C-NC	5.30	114.94	109.97
26	a	411	SQD	O6-C1-C2	5.29	116.56	108.30
23	В	616	CLA	C4A-NA-C1A	-5.29	104.33	106.71
23	В	608	CLA	C2C-C1C-NC	5.29	114.92	109.97
25	с	514	BCR	C15-C14-C13	-5.28	119.77	127.31
23	с	510	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
23	С	511	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	b	612	CLA	O2D-CGD-CBD	5.25	120.59	111.27
26	f	101	SQD	O47-C7-C8	5.24	122.78	111.50
23	b	603	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	d	403	CLA	O2D-CGD-CBD	5.22	120.55	111.27
23	В	603	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
23	С	505	CLA	O2D-CGD-CBD	5.20	120.52	111.27
23	С	509	CLA	C3C-C4C-NC	5.20	116.40	110.57



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	d	402	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
23	С	508	CLA	C4A-NA-C1A	-5.18	104.38	106.71
23	В	610	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	С	507	CLA	C2C-C1C-NC	5.18	114.82	109.97
23	С	513	CLA	O2D-CGD-CBD	5.17	120.46	111.27
23	b	602	CLA	O2D-CGD-CBD	5.17	120.45	111.27
23	В	613	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	D	405	CLA	O2D-CGD-CBD	5.16	120.44	111.27
23	с	505	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	С	510	CLA	O2D-CGD-CBD	5.15	120.43	111.27
23	b	604	CLA	C2C-C1C-NC	5.15	114.80	109.97
23	с	510	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	с	501	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
23	с	513	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	с	509	CLA	C4A-NA-C1A	-5.13	104.40	106.71
23	В	609	CLA	C2C-C1C-NC	5.13	114.78	109.97
26	В	621	SQD	O6-C1-C2	5.13	116.31	108.30
23	с	512	CLA	C2C-C1C-NC	5.13	114.77	109.97
23	С	508	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	a	409	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
23	b	610	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	В	605	CLA	C2C-C1C-NC	5.11	114.75	109.97
23	В	612	CLA	C2C-C1C-NC	5.10	114.75	109.97
25	b	619	BCR	C3-C4-C5	-5.10	104.97	114.08
23	С	503	CLA	C2C-C1C-NC	5.09	114.75	109.97
23	A	407	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	b	615	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
23	с	503	CLA	CHD-C4C-C3C	-5.07	117.38	124.84
23	b	609	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	A	405	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
23	b	611	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	b	602	CLA	C2C-C1C-NC	5.04	114.70	109.97
23	b	601	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	b	613	CLA	C2C-C1C-NC	5.03	114.68	109.97
23	С	510	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	a	405	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
23	c	513	CLA	O2D-CGD-CBD	5.01	120.18	111.27
23	B	607	CLA	C2C-C1C-NC	5.01	114.67	109.97
26	L	102	SQD	047-C7-C8	5.01	122.29	111.50
23	b	606	CLA	C2C-C1C-NC	4.99	114.65	109.97
29	d	405	PL9	C42-C43-C44	-4.98	115.66	127.66
23	b	612	CLA	C2C-C1C-NC	4.98	114 64	109.97
$\begin{array}{c} 23\\ 23\\ 23\\ 23\\ 23\\ 23\\ 23\\ 23\\ 23\\ 23\\$	B B C a b B B B C A b C A b C b C A b C A b C B C a c B L b d b	$\begin{array}{c} 509\\ 609\\ 621\\ 512\\ 508\\ 409\\ 610\\ 605\\ 612\\ 619\\ 503\\ 407\\ 615\\ 503\\ 407\\ 615\\ 503\\ 609\\ 405\\ 611\\ 602\\ 601\\ 613\\ 510\\ 405\\ 513\\ 607\\ 102\\ 606\\ 405\\ 612\\ \end{array}$	CLA CLA CLA CLA CLA CLA CLA CLA	C2C-C1C-NC O6-C1-C2 C2C-C1C-NC C4A-NA-C1A CHD-C4C-C3C O2D-CGD-CBD CHD-C4C-C3C C4A-NA-C1A C2C-C1C-NC C2C-C1C-NC C2C-C1C-NC C2C-C1C-NC C4A-NA-C1A C1C-C2C-C3C O2D-CGD-CBD C2C-C1C-NC C4A-NA-C1A C1C-C2C-C3C O2D-CGD-CBD C2C-C1C-NC O47-C7-C8 C2C-C1C-NC O47-C7-C8 C2C-C1C-NC C42-C43-C44 C2C-C1C-NC	$\begin{array}{r} -5.13\\ \overline{5.13}\\ \overline{5.13}\\ \overline{5.13}\\ \overline{5.13}\\ \overline{5.13}\\ \overline{5.12}\\ -5.12\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.11}\\ \overline{5.01}\\ \overline{5.04}\\ \overline{5.02}\\ -\overline{5.02}\\ \overline{5.01}\\ \overline{5.01}\\ \overline{5.01}\\ \overline{5.01}\\ \overline{4.99}\\ -4.98\\ \overline{4.98}\\ \overline{4.98}\end{array}$	$\begin{array}{c} 114.78 \\ 114.78 \\ 116.31 \\ 114.77 \\ 114.77 \\ 117.32 \\ 114.76 \\ 114.75 \\ 104.97 \\ 114.75 \\ 104.97 \\ 114.75 \\ 104.42 \\ 117.37 \\ 117.38 \\ 120.28 \\ 117.30 \\ 104.44 \\ 114.70 \\ 104.44 \\ 114.70 \\ 114.68 \\ 104.45 \\ 101.68 \\ 120.18 \\ 114.67 \\ 122.29 \\ 114.65 \\ 115.66 \\ 114.64 \\ \end{array}$	$\begin{array}{r} 100.11\\ 109.97\\ 108.30\\ 109.97\\ 109.97\\ 109.97\\ 124.84\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 106.71\\ 124.84\\ 124.84\\ 124.84\\ 111.27\\ 124.84\\ 106.71\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 109.97\\ 111.50\\ 109.97\\ 111.50\\ 109.97\\ 127.66\\ 109.97\\ \end{array}$

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
25	В	618	BCR	C33-C5-C6	-4.98	118.94	124.53
23	В	602	CLA	C2C-C1C-NC	4.96	114.61	109.97
23	с	512	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	С	512	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	с	511	CLA	C2C-C1C-NC	4.94	114.60	109.97
24	a	408	PHO	O2D-CGD-CBD	4.94	120.04	111.27
23	с	509	CLA	O2D-CGD-CBD	4.93	120.03	111.27
23	a	409	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	а	409	CLA	O2D-CGD-CBD	4.93	120.02	111.27
23	В	605	CLA	C3C-C4C-NC	4.92	116.09	110.57
23	В	606	CLA	C4A-NA-C1A	-4.92	104.49	106.71
34	С	501	LMG	O7-C10-C11	4.92	122.11	111.50
23	В	604	CLA	C2C-C1C-NC	4.92	114.58	109.97
23	В	613	CLA	C3C-C4C-NC	4.91	116.07	110.57
23	С	503	CLA	C4A-NA-C1A	-4.90	104.50	106.71
26	А	409	SQD	O47-C7-C8	4.90	122.06	111.50
24	a	408	PHO	C3D-C2D-C1D	-4.89	98.74	105.87
24	a	408	PHO	C1-C2-C3	-4.89	117.59	126.04
23	a	406	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	с	505	CLA	C3C-C4C-NC	4.87	116.04	110.57
23	С	512	CLA	C2C-C1C-NC	4.87	114.53	109.97
23	b	608	CLA	C2C-C1C-NC	4.86	114.52	109.97
23	с	504	CLA	O2D-CGD-CBD	4.85	119.89	111.27
23	А	407	CLA	C2C-C1C-NC	4.84	114.51	109.97
24	А	406	PHO	C2D-C1D-ND	4.84	117.09	109.79
23	А	405	CLA	O2D-CGD-CBD	4.83	119.86	111.27
23	b	607	CLA	C3C-C4C-NC	4.83	115.99	110.57
23	А	405	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	В	612	CLA	O2D-CGD-CBD	4.80	119.80	111.27
25	Т	101	BCR	С7-С8-С9	-4.80	118.98	126.23
23	b	607	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	В	606	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	a	406	CLA	C2C-C1C-NC	4.78	114.45	109.97
23	В	610	CLA	C3C-C4C-NC	4.77	115.92	110.57
23	b	614	CLA	C2C-C1C-NC	4.75	114.42	109.97
23	В	606	CLA	C2C-C1C-NC	4.75	114.42	109.97
23	В	615	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	С	511	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
23	с	508	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	a	408	PHO	C2D-C1D-ND	4.71	116.90	109.79
23	D	401	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	В	613	CLA	C4A-NA-C1A	-4.70	104.59	106.71

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Mol	Chain	\mathbf{Res}	Tvpe	Atoms	Z	Observed(^o)	Ideal(°)
23	B	608	CLA	O2D-CGD-CBD	4 70	119.63	111 27
$\frac{20}{25}$	c c	515	BCR	C7-C8-C9	-4.70	119.14	126.23
$\frac{-3}{24}$	D	402	PHO	O2D-CGD-CBD	4.68	119.59	111.27
36	с	522	HTG	C1'-S1-C1	4.68	108.85	100.09
36	b	622	HTG	C1'-S1-C1	4.67	108.83	100.09
26	L	102	SQD	O6-C1-C2	4.67	115.59	108.30
23	В	611	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	с	507	CLA	C2C-C1C-NC	4.67	114.34	109.97
25	Y	101	BCR	C16-C17-C18	-4.66	120.66	127.31
23	В	611	CLA	C2C-C1C-NC	4.66	114.33	109.97
23	b	608	CLA	O2D-CGD-CBD	4.64	119.52	111.27
23	В	609	CLA	C3C-C4C-NC	4.64	115.78	110.57
36	h	101	HTG	C1'-S1-C1	4.64	108.76	100.09
23	с	508	CLA	C3C-C4C-NC	4.63	115.76	110.57
25	С	515	BCR	C15-C14-C13	-4.61	120.73	127.31
23	D	404	CLA	C3C-C4C-NC	4.61	115.74	110.57
25	t	101	BCR	C33-C5-C6	-4.60	119.36	124.53
23	d	402	CLA	O2D-CGD-CBD	4.59	119.42	111.27
23	С	502	CLA	C1D-CHD-C4C	-4.59	116.51	122.56
23	b	613	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	С	507	CLA	O2D-CGD-CBD	4.58	119.41	111.27
23	b	609	CLA	C2C-C1C-NC	4.58	114.26	109.97
37	С	517	DGD	O2G-C1B-C2B	4.58	121.37	111.50
23	С	514	CLA	C2C-C1C-NC	4.57	114.25	109.97
23	С	510	CLA	C1-C2-C3	-4.56	118.15	126.04
23	b	611	CLA	O2D-CGD-O1D	-4.56	114.93	123.84
23	С	511	CLA	C1-C2-C3	-4.55	118.17	126.04
23	С	510	CLA	C2C-C1C-NC	4.54	114.23	109.97
23	С	505	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
23	C	513	CLA	C2C-C1C-NC	4.54	114.22	109.97
23	D	405	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	В	605	CLA	C1-C2-C3	-4.53	118.22	126.04
23	D	404	CLA	O2D-CGD-CBD	4.52	119.30	111.27
23	В	614	CLA	C4A-NA-C1A	-4.52	104.68	106.71
26	a	411	SQD	047-C7-C8	4.51	121.23	111.50
23	В	617	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	D	401	CLA	O2D-CGD-CBD	4.50	119.26	111.27
23	с	509	CLA	C1-C2-C3	-4.50	118.27	126.04
23	В	612	CLA	C4A-NA-C1A	-4.50	104.69	106.71
23	b	604	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	b	603	CLA	C1D-CHD-C4C	-4.48	116.65	122.56
23	В	617	CLA	C3C-C4C-NC	4.48	115.59	110.57

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
23	a	404	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	С	506	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	D	405	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	В	609	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	d	402	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
25	с	514	BCR	C20-C21-C22	-4.45	120.96	127.31
23	В	612	CLA	C3C-C4C-NC	4.43	115.54	110.57
25	Т	101	BCR	C33-C5-C6	-4.43	119.56	124.53
29	d	405	PL9	C10-C9-C11	4.42	122.71	115.27
26	В	621	SQD	O47-C7-C8	4.42	121.03	111.50
23	В	606	CLA	C3C-C4C-NC	4.41	115.52	110.57
36	b	625	HTG	C1'-S1-C1	4.41	108.33	100.09
23	с	505	CLA	C4A-NA-C1A	-4.39	104.73	106.71
25	b	617	BCR	C7-C8-C9	-4.39	119.60	126.23
23	С	510	CLA	C3C-C4C-NC	4.39	115.49	110.57
26	f	101	SQD	O7-S-C6	4.39	112.15	106.94
23	С	508	CLA	C3C-C4C-NC	4.38	115.49	110.57
23	В	616	CLA	C1D-CHD-C4C	-4.38	116.78	122.56
38	Е	103	HEM	CBD-CAD-C3D	-4.38	104.42	112.48
23	с	502	CLA	C4A-NA-C1A	-4.36	104.75	106.71
23	b	614	CLA	C4A-NA-C1A	-4.36	104.75	106.71
23	b	615	CLA	O2D-CGD-CBD	4.35	119.00	111.27
29	a	415	PL9	C7-C3-C2	-4.34	117.60	123.30
23	с	511	CLA	O2D-CGD-CBD	4.33	118.97	111.27
25	d	404	BCR	C7-C8-C9	-4.33	119.70	126.23
23	с	502	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
23	b	616	CLA	C1D-CHD-C4C	-4.32	116.86	122.56
23	В	606	CLA	C1D-CHD-C4C	-4.31	116.86	122.56
29	А	413	PL9	C7-C3-C2	-4.31	117.63	123.30
26	f	101	SQD	C1-O5-C5	4.30	122.13	113.69
25	В	619	BCR	C15-C14-C13	-4.30	121.17	127.31
25	t	101	BCR	C15-C16-C17	-4.29	114.69	123.47
23	a	404	CLA	C1D-CHD-C4C	-4.28	116.90	122.56
23	d	403	CLA	C2C-C1C-NC	4.28	113.98	109.97
25	В	618	BCR	C7-C8-C9	-4.27	119.78	126.23
31	Е	101	LHG	O7-C7-C8	4.27	120.70	111.50
23	b	607	CLA	C4A-NA-C1A	-4.27	104.79	106.71
26	А	411	SQD	O8-S-C6	4.26	112.54	105.74
23	b	611	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	С	514	CLA	O2D-CGD-CBD	4.26	118.84	111.27
23	С	514	CLA	C3C-C4C-NC	4.26	115.34	110.57
23	b	606	CLA	O2D-CGD-O1D	-4.25	115.52	123.84

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Mol Chain Res Type Atoms Z Observe	$\operatorname{Pd}(^{o}) \mid \operatorname{Ideal}(^{o})$
26 A 409 SQD C1-C2-C3 -4.25 101.1	5 110.00
23 b 611 CLA C3B-C4B-NB 4.25 114.7	0 109.21
23 D 404 CLA C1C-C2C-C3C -4.25 102.49	9 106.96
23 D 401 CLA C2C-C1C-NC 4.24 113.94	4 109.97
23 b 616 CLA C3C-C4C-NC 4.24 115.3	2 110.57
23 B 602 CLA C4A-NA-C1A -4.22 104.8	1 106.71
23 c 506 CLA C4A-NA-C1A -4.22 104.8	1 106.71
26 A 409 SQD C1-O5-C5 -4.22 105.4	1 113.69
23 B 616 CLA O2D-CGD-CBD 4.22 118.70	6 111.27
23 c 508 CLA C1C-C2C-C3C -4.21 102.53	3 106.96
23 b 611 CLA C1C-C2C-C3C -4.21 102.53	3 106.96
34 J 101 LMG O7-C10-C11 4.21 120.53	8 111.50
34 Z 101 LMG O7-C10-C11 4.21 120.5	7 111.50
23 B 614 CLA C1C-C2C-C3C -4.20 102.54	4 106.96
23 d 402 CLA C3C-C4C-NC 4.20 115.24	8 110.57
23 B 605 CLA C4A-NA-C1A -4.20 104.8	2 106.71
23 c 509 CLA C3C-C4C-NC 4.18 115.20	6 110.57
23 B 612 CLA C1C-C2C-C3C -4.17 102.54	8 106.96
37 c 516 DGD O2G-C1B-C2B 4.16 120.4	7 111.50
36 b 626 HTG C1'-S1-C1 4.16 107.8	7 100.09
31 D 409 LHG 07-C7-C8 4.15 120.4	5 111.50
23 b 614 CLA C3C-C4C-NC 4.15 115.2	2 110.57
24 A 406 PHO CAC-C3C-C4C 4.14 129.74	4 125.22
23 C 505 CLA C3C-C4C-NC 4.13 115.2	1 110.57
23 B 609 CLA C1D-CHD-C4C -4.13 117.10	0 122.56
23 D 401 CLA C1C-C2C-C3C -4.13 102.6	2 106.96
23 a 405 CLA C3B-C4B-NB 4.13 114.5	5 109.21
29 a 415 PL9 C32-C33-C34 -4.12 117.74	3 127.66
25 T 101 BCR C11-C10-C9 -4.11 121.44	4 127.31
23 C 502 CLA O2D-CGD-O1D -4.10 115.8	1 123.84
23 c 512 CLA C3C-C4C-NC 4.10 115.1	7 110.57
23 A 407 CLA C3C-C4C-NC 4.10 115.1	7 110.57
23 B 608 CLA C1C-C2C-C3C -4.10 102.6	5 106.96
36 B 629 HTG C1'-S1-C1 4.09 107.74	4 100.09
23 C 502 CLA C3C-C4C-NC 4.09 115.14	6 110.57
23 B 610 CLA O2D-CGD-CBD 4.09 118.55	3 111.27
23 C 513 CLA C3C-C4C-NC 4.09 115.14	6 110.57
25 b 619 BCR C7-C8-C9 -4.08 120.0	7 126.23
23 B 607 CLA C3C-C4C-NC 4.08 115.1	5 110.57
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4 110.57
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\frac{10.57}{3}$
23 B 615 CLA C1C-C2C-C3C -4.07 102.65	8 106.96

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	D	405	CLA	C2C-C1C-NC	4.06	113.77	109.97
23	С	505	CLA	C3B-C4B-NB	4.06	114.45	109.21
26	D	413	SQD	O6-C1-C2	4.05	114.63	108.30
23	В	617	CLA	C1D-CHD-C4C	-4.04	117.22	122.56
23	b	605	CLA	C4A-NA-C1A	-4.04	104.89	106.71
24	D	402	PHO	C1-C2-C3	-4.03	119.06	126.04
23	В	608	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	b	610	CLA	C3C-C4C-NC	4.02	115.08	110.57
23	В	613	CLA	C1-C2-C3	-4.00	119.12	126.04
34	с	519	LMG	O7-C10-C11	4.00	120.12	111.50
23	a	405	CLA	O2D-CGD-CBD	4.00	118.38	111.27
23	С	505	CLA	C1D-CHD-C4C	-4.00	117.28	122.56
23	С	512	CLA	O2D-CGD-CBD	3.99	118.37	111.27
23	d	403	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
23	А	404	CLA	O2A-CGA-CBA	3.99	124.43	111.91
23	D	404	CLA	C1-C2-C3	-3.99	119.15	126.04
23	с	506	CLA	O2D-CGD-CBD	3.99	118.35	111.27
23	с	511	CLA	C3C-C4C-NC	3.98	115.04	110.57
23	с	503	CLA	C1D-CHD-C4C	-3.98	117.31	122.56
23	b	603	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	A	404	CLA	C1D-CHD-C4C	-3.97	117.32	122.56
23	b	615	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	с	504	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	с	507	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	b	606	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	d	403	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	С	512	CLA	CAC-C3C-C4C	3.96	129.94	124.81
23	с	510	CLA	O2D-CGD-CBD	3.95	118.29	111.27
23	b	606	CLA	C1D-CHD-C4C	-3.95	117.34	122.56
23	С	511	CLA	C3B-C4B-NB	3.95	114.32	109.21
23	С	504	CLA	O2D-CGD-CBD	3.95	118.29	111.27
24	a	407	PHO	C4C-C3C-C2C	-3.94	102.42	106.78
23	С	502	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
25	b	619	BCR	C15-C14-C13	-3.94	121.69	127.31
23	b	607	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	с	511	CLA	C1-C2-C3	-3.93	119.24	126.04
34	с	520	LMG	O6-C5-C4	3.93	116.84	109.69
25	C	515	BCR	C16-C17-C18	-3.93	121.70	127.31
34	C	521	LMG	07-C10-C11	3.93	119.98	111.50
23	C	509	CLA	C4C-C3C-C2C	-3.93	101.17	106.90
23	Ā	405	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	C	503	CLA	C3C-C4C-NC	3.93	114.97	110.57



5G	ΤI
90	ΤT

Mal	nucu 11011	Previ	Tuno	Atoms	7	Observed ⁽⁰⁾	Ideal(0)
10101		1105 E 19	туре		2.00	117.20	100 FC
25 21		013 101		070702	-3.92	110.05	
<u>31</u> 02		101		$\begin{array}{c} 01-01-08 \\ 020,040,000 \\ \end{array}$	3.92	119.90	111.00
 	D c	406		CID CUD CAC	3.92	114.97	110.07
23	a D	400	CLA CLA	CID-CHD-C4C	-3.92	117.39	122.30
23	B	616	ULA LUC	$\begin{array}{c} 010-020-030 \\ \hline \end{array}$	-3.91	102.84	100.90
31	b	630	LHG	07-07-08	3.91	119.92	111.50
23	С	504	CLA	C3B-C4B-NB	3.91	114.26	109.21
25	d	404	BCR	C38-C26-C25	-3.90	120.14	124.53
23	C	509	CLA	C3B-C4B-NB	3.90	114.26	109.21
23	C	512	CLA	C3C-C4C-NC	3.90	114.95	110.57
23	С	506	CLA	C3C-C4C-NC	3.90	114.95	110.57
25	С	514	BCR	C16-C17-C18	-3.90	121.74	127.31
23	с	513	CLA	C3C-C4C-NC	3.90	114.94	110.57
26	В	621	SQD	07-S-C6	3.90	111.57	106.94
23	b	602	CLA	C3C-C4C-NC	3.89	114.94	110.57
25	k	101	BCR	C11-C10-C9	-3.89	121.75	127.31
23	b	605	CLA	C1D-CHD-C4C	-3.89	117.42	122.56
23	В	604	CLA	C1D-CHD-C4C	-3.89	117.43	122.56
29	D	407	PL9	C42-C43-C44	-3.89	118.30	127.66
23	b	609	CLA	C1-C2-C3	-3.88	119.33	126.04
25	k	101	BCR	C24-C23-C22	-3.88	120.37	126.23
23	А	407	CLA	O2D-CGD-CBD	3.88	118.16	111.27
29	a	415	PL9	C27-C28-C29	-3.88	118.32	127.66
23	b	605	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	с	503	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	В	602	CLA	C3C-C4C-NC	3.87	114.92	110.57
23	с	510	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
23	D	405	CLA	C1D-CHD-C4C	-3.87	117.46	122.56
25	С	527	BCR	C7-C8-C9	-3.86	120.40	126.23
25	Н	101	BCR	C7-C8-C9	-3.86	120.40	126.23
23	с	502	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	b	612	CLA	C1-C2-C3	-3.86	119.37	126.04
23	b	611	CLA	C1-C2-C3	-3.85	119.38	126.04
23	с	504	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	A	407	CLA	C4-C3-C5	3.85	121.74	115.27
23	b	603	CLA	C3C-C4C-NC	3.84	114.88	110.57
23	С	504	CLA	C3C-C4C-NC	3.84	114.88	110.57
25	t	101	BCR	C35-C13-C12	3.84	124.12	118.08
23	b	610	CLA	C1-C2-C3	-3.83	119.42	126.04
23	С	509	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	A	404	CLA	C3C-C4C-NC	3.82	114.86	110.57
23	b	602	CLA	C1C-C2C-C3C	-3.82	102.94	106.96

Contin $d f_{a}$



5G	ΤI
90	ΤT

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
23	С	507	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	В	615	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
25	Н	101	BCR	C16-C17-C18	-3.82	121.86	127.31
23	b	607	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
25	d	404	BCR	C33-C5-C6	-3.81	120.25	124.53
23	b	602	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
23	с	502	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
23	В	604	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	b	609	CLA	C3C-C4C-NC	3.80	114.83	110.57
25	D	406	BCR	C38-C26-C25	-3.80	120.27	124.53
25	k	101	BCR	C15-C14-C13	-3.79	121.91	127.31
23	С	511	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
23	В	603	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	А	404	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
34	a	417	LMG	O7-C10-C11	3.77	119.63	111.50
25	b	617	BCR	C33-C5-C6	-3.77	120.29	124.53
35	D	403	LMT	O5'-C5'-C4'	3.77	117.70	109.75
23	с	512	CLA	C1D-CHD-C4C	-3.77	117.59	122.56
23	С	509	CLA	C4D-C3D-CAD	-3.77	106.37	108.47
23	В	609	CLA	C4A-NA-C1A	-3.77	105.01	106.71
23	С	508	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
23	b	605	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	В	616	CLA	C3C-C4C-NC	3.76	114.78	110.57
25	А	408	BCR	C15-C14-C13	-3.75	121.95	127.31
23	b	604	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	a	405	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
23	С	504	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
23	В	612	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
23	с	506	CLA	C3B-C4B-NB	3.74	114.04	109.21
25	С	516	BCR	C11-C10-C9	-3.74	121.98	127.31
23	С	506	CLA	C1D-CHD-C4C	-3.74	117.63	122.56
23	с	503	CLA	CAC-C3C-C4C	3.74	129.66	124.81
23	В	603	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	В	611	CLA	C1-C2-C3	-3.74	119.58	126.04
23	с	501	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
25	Н	101	BCR	C24-C23-C22	-3.73	120.60	126.23
23	с	512	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	В	605	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	с	513	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	b	610	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
24	a	408	PHO	C4-C3-C5	3.72	121.54	115.27
23	b	615	CLA	C3B-C4B-NB	3.72	114.02	109.21



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
23	с	501	CLA	CAC-C3C-C4C	3.72	129.64	124.81	
23	В	607	CLA	C1C-C2C-C3C	-3.72	103.05	106.96	
23	В	614	CLA	C1-C2-C3	-3.72	119.61	126.04	
23	с	501	CLA	C3C-C4C-NC	3.72	114.74	110.57	
23	b	608	CLA	C1C-C2C-C3C	-3.72	103.05	106.96	
31	А	415	LHG	O7-C7-C8	3.72	119.51	111.50	
23	В	611	CLA	C1D-CHD-C4C	-3.72	117.65	122.56	
26	А	409	SQD	C44-O6-C1	-3.71	106.49	113.74	
23	С	510	CLA	CMC-C2C-C1C	3.71	130.69	125.04	
40	V	201	HEC	CAD-CBD-CGD	3.70	118.89	112.67	
34	В	622	LMG	O7-C10-C11	3.70	119.48	111.50	
23	В	606	CLA	O2D-CGD-O1D	-3.70	116.60	123.84	
29	D	407	PL9	C10-C9-C11	3.70	121.50	115.27	
23	D	401	CLA	CHD-C4C-NC	3.70	130.03	124.20	
25	t	101	BCR	С11-С10-С9	-3.69	122.04	127.31	
23	В	610	CLA	C1C-C2C-C3C	-3.69	103.08	106.96	
23	А	407	CLA	C1C-C2C-C3C	-3.69	103.08	106.96	
23	a	404	CLA	CMB-C2B-C3B	3.69	131.58	124.68	
23	a	406	CLA	C3C-C4C-NC	3.69	114.70	110.57	
23	С	508	CLA	C1C-C2C-C3C	-3.68	103.09	106.96	
23	С	503	CLA	C1C-C2C-C3C	-3.68	103.09	106.96	
23	С	511	CLA	C4-C3-C5	3.67	121.45	115.27	
23	a	405	CLA	C1D-CHD-C4C	-3.67	117.72	122.56	
23	С	502	CLA	C1-C2-C3	-3.66	119.70	126.04	
23	b	609	CLA	O2D-CGD-O1D	-3.66	116.67	123.84	
34	с	520	LMG	O7-C10-C11	3.66	119.38	111.50	
23	b	615	CLA	C3C-C4C-NC	3.66	114.67	110.57	
25	D	406	BCR	C33-C5-C6	-3.66	120.42	124.53	
23	С	508	CLA	O2D-CGD-O1D	-3.65	116.69	123.84	
29	d	405	PL9	C25-C24-C26	3.65	121.42	115.27	
23	b	614	CLA	C1D-CHD-C4C	-3.65	117.74	122.56	
23	с	512	CLA	C1-C2-C3	-3.65	119.73	126.04	
23	С	509	CLA	C4A-NA-C1A	-3.65	105.07	106.71	
37	С	518	DGD	O2G-C1B-C2B	3.64	119.36	111.50	
35	М	101	LMT	O1'-C1'-C2'	3.64	113.99	108.30	
23	В	613	CLA	C3B-C4B-NB	3.64	113.92	109.21	
23	b	615	CLA	C1D-CHD-C4C	-3.64	117.75	122.56	
26	L	102	SQD	07-S-C6	3.63	111.26	106.94	
23	b	601	CLA	C3C-C4C-NC	3.63	114.64	110.57	
35	В	623	LMT	O5'-C5'-C4'	3.63	117.40	109.75	
23	b	601	CLA	C1C-C2C-C3C	-3.62	103.15	106.96	
23	с	504	CLA	C4A-NA-C1A	-3.62	105.08	106.71	

a... .1 L.



Mol	Chain	Res	Tvne	Atoms	Z	Observed(^o)	Ideal(°)
23	D	401	-JPC	CMC-C2C-C1C	3.62	130.56	125.04
35	C	522	LMT	C1'-05'-C5'	3.02	120.80	120.04 113.69
$\frac{36}{26}$	A	411	SOD	047-C7-C8	3.62	119.30	110.00 111.50
23	2	404	CLA	C3B-C4B-NB	3.62	113.89	109.21
$\frac{28}{23}$	h	616	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	b	606	CLA	C1C-C2C-C3C	-3.62	103 15	106.96
29	a	415	PL9	C15-C14-C16	3.62	121.35	100.00 115.27
23	B	602	CLA	<u>C1C-C2C-C3C</u>	-3.61	103 16	106.96
$\frac{23}{24}$	D	402	PHO	$\frac{C4C-C3C-C2C}{C4C-C3C-C2C}$	-3 61	102.78	106.78
23	b	601	CLA	C1D-CHD-C4C	-3.61	117.79	122.56
23	b	614	CLA	C1-C2-C3	-3 61	119.80	126.04
31	d	408	LHG	07-C7-C8	3.61	119.28	111.50
37	Н	102	DGD	O2G-C1B-C2B	3.61	119.28	111.50
23	B	612	CLA	CMC-C2C-C1C	3.61	130.53	125.04
23	С	506	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	С	507	CLA	C3C-C4C-NC	3.61	114.62	110.57
34	C	501	LMG	C7-O1-C1	-3.61	106.69	113.74
23	В	609	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
26	a	411	SQD	C1-C2-C3	-3.61	102.49	110.00
23	С	512	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	В	612	CLA	OBD-CAD-C3D	-3.60	122.00	127.98
34	Ζ	101	LMG	C1-C2-C3	3.59	117.48	110.00
25	с	514	BCR	С11-С10-С9	-3.59	122.19	127.31
23	a	404	CLA	C3C-C4C-NC	3.59	114.59	110.57
23	В	617	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
23	В	612	CLA	CHD-C4C-NC	3.59	129.85	124.20
25	С	515	BCR	C33-C5-C6	-3.59	120.50	124.53
25	Y	101	BCR	C15-C14-C13	-3.58	122.20	127.31
23	А	404	CLA	CAA-C2A-C3A	-3.58	102.98	112.78
23	a	409	CLA	C3B-C4B-NB	3.58	113.83	109.21
23	В	614	CLA	CMB-C2B-C3B	3.58	131.37	124.68
23	a	404	CLA	CAA-C2A-C3A	-3.57	102.99	112.78
23	с	501	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
23	b	613	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
23	В	613	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
23	b	614	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
26	А	409	SQD	O7-S-C6	3.56	111.17	106.94
23	В	613	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	с	507	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
23	С	507	CLA	C1-C2-C3	-3.55	119.90	126.04
23	с	509	CLA	$\overline{\text{C1C-C2C-C3C}}$	-3.55	103.22	106.96
23	b	605	CLA	O2D-CGD-O1D	-3.55	116.89	123.84



$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Mol	Chain	Res	Tvne	Atoms	7	Observed ^(o)	Ideal(°)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23	R	603	CLA		_3 55		119.78
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{23}{23}$	D a	409		C3C-C4C-NC	-3.55	105.05 114.55	112.70 110.57
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{20}{23}$		508		02D-CGD-01D	-3.55	114.90	123.84
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{20}{23}$	h	607		C1D-CHD-C4C	-3.55	117.87	120.04 122.56
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	20	h	612		C1C-C2C-C3C	-3.55	103.23	106.96
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	20	0	409		$C_{10}^{-0.20}$	-3.00	105.25	100.90 115.97
34 C 344 Decrete 3 3.55 110.31 110.48 25 B 619 BCR C29-C30-C25 3.55 115.94 110.48 23 b 612 CLA C1D-CHD-C4C -3.54 117.89 122.56 23 c 511 CLA CMC-C2C-C1C 3.53 105.12 106.71 23 c 509 CLA C1D-CHD-C4C -3.53 117.90 122.56 23 b 604 CLA C1D-CHD-C4C -3.53 117.90 122.56 23 b 614 CLA C1D-CHD-C4C -3.53 117.90 122.56 25 b 619 BCR C24-C23-C22 -3.53 112.27 127.31 35 D 403 LMT C1'-O5'-C5' 3.52 112.60 113.69 23 d 406 LHG O'-C7-C8 3.52 119.08 111.50 23 c 510	20		40 <i>3</i> 591	LMG	$C_{4} C_{2} C_{4} C_{5}$	3.55	121.24	110.27 110.24
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	- 04 - 25	B	610	BCB	$C_{20} C_{30} C_{25}$	3.55	115.97	110.24 110.48
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{20}{23}$	b	612		C1D CHD C4C	3.50	117.89	110.40 122.56
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	B	614		$\frac{\text{CHC}-\text{CHD}-\text{C4C}}{\text{CMC}-\text{C2C}-\text{C1C}}$	-0.04	117.09	122.00 125.04
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20		511		$\frac{\text{C4A NA C1A}}{\text{C4A NA C1A}}$	3.53	105.42	125.04 106 71
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	R B	607		$O^{2}D$ CCD O1D	-0.00	116.03	100.71 123.84
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20		500		C1D CHD C4C	-0.00	117.90	120.04 122.56
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20 	L b	604		CID-CID-C4C	-0.00	117.90	122.50 122.56
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	25	b b	610	BCB	$\begin{array}{c} \text{C1D-C1D-C4C} \\ \text{C24 C23 C22} \end{array}$	-0.00	117.90	122.00 126.23
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		d d	402		C2R C4R NR	-0.00	120.90 113.77	120.23 100.21
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	25	u P	618	BCB	$\frac{\text{C3D-C4D-IND}}{\text{C16}\text{ C17}\text{ C18}}$	2.52	110.77	109.21 127.21
35D405DM1C1+05+C5 3.52 1120.00 113.09 23B615CLAC3B-C4B-NB 3.52 113.76 109.21 31d406LHGO7-C7-C8 3.52 119.08 111.50 23c510CLAC1D-CHD-C4C -3.52 117.92 122.56 23A405CLAC3C-C4C-NC 3.51 114.51 110.57 36V203HTGC1-C2-C3 3.51 113.99 109.67 25T101BCRC12-C13-C14 -3.51 113.55 118.94 23b611CLAC1D-CHD-C4C -3.51 117.92 122.56 23D405CLAO2D-CGD-O1D -3.51 116.98 123.84 29A413PL9C37-C38-C39 -3.51 119.21 127.66 23C513CLAC1C-C2C-C3C -3.51 103.27 106.96 23c506CLACAC-C3C-C4C 3.50 112.936 124.81 23B611CLAC3C-C4C-NC 3.50 113.74 109.21 23D401CLAC3C-C4C-NC 3.50 117.94 122.56 23D401CLAC3C-C4C-NC 3.50 117.94 122.56 23D613CLAC1D-CHD-C4C -3.50 117.94 122.56 23b613CLAC1D-CHD-C4C	25		402		C10-C17-C10	-0.00 2 50	122.27	127.31
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	- <u>0</u> 0 - <u>0</u> 2	D B	403 615		C1-03-03	3.02	112.00	110.09
314400EIRC $O_{1}-C_{1}-C_{3}$ 3.52 119.08 111.30 23c510CLAC1D-CHD-C4C -3.52 117.92 122.56 23A405CLAC3C-C4C-NC 3.51 114.51 110.57 36V203HTGC1-C2-C3 3.51 113.99 109.67 25T101BCRC12-C13-C14 -3.51 113.55 118.94 23b611CLAC1D-CHD-C4C -3.51 117.92 122.56 23D405CLAO2D-CGD-O1D -3.51 116.98 123.84 29A413PL9C37-C38-C39 -3.51 119.21 127.66 23C513CLAC1C-C2C-C3C -3.51 103.27 106.96 23c506CLACAC-C3C-C4C 3.50 1129.36 124.81 23B611CLAC4C-C3C-C2C -3.50 101.79 106.90 23B612CLAC3B-C4B-NB 3.50 113.74 109.21 23D401CLAC3C-C4C-NC 3.50 117.94 122.56 23b613CLAC1D-CHD-C4C -3.50 117.94 122.56 23b613CLAC1D-CHD-C4C -3.50 117.94 122.56 24a407PHO $02D-CGD-O1D$ -3.49 117.01 123.84 34z101BCR	20 21	D d	406	ULA IHC	$\frac{0.00-0.40-0.00}{0.07-0.02}$	$\frac{0.02}{2.52}$	113.70	109.21 111.50
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	01 02	u	400 510		$\frac{07-07-06}{010}$	2.52	117.00	111.50
23A 403 CLA $C3C-C4C-NC$ 3.51 114.51 110.57 36 V 203 HTG $C1-C2-C3$ 3.51 113.99 109.67 25 T 101 BCR $C12-C13-C14$ -3.51 113.55 118.94 23 b 611 CLA $C1D-CHD-C4C$ -3.51 117.92 122.56 23 D 405 CLA $O2D-CGD-O1D$ -3.51 116.98 123.84 29 A 413 PL9 $C37-C38-C39$ -3.51 119.21 127.66 23 C 513 CLA $C1C-C2C-C3C$ -3.51 103.27 106.96 23 c 506 CLACAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLAC4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLAC3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLAC3C-C4C-NC 3.50 114.50 110.57 23 B 607 CLAC1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLAC1D-CHD-C4C -3.50 117.94 1	20 		405		C1D-C1D-C4C	-5.02	117.92	122.50 110.57
36 V 203 1116 $C1-C2-C3$ 3.51 113.39 109.07 25 T101BCR $C12-C13-C14$ -3.51 113.55 118.94 23 b 611 CLA $C1D-CHD-C4C$ -3.51 117.92 122.56 23 D 405 CLA $O2D-CGD-O1D$ -3.51 116.98 123.84 29 A 413 PL9 $C37-C38-C39$ -3.51 119.21 127.66 23 C 513 CLA $C1C-C2C-C3C$ -3.51 103.27 106.96 23 c 506 CLACAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLAC4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLAC3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLAC3C-C4C-NC 3.50 117.94 122.56 23 b 613 CLAC1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLAC1D-CHD-C4C -3.50 117.94 122.56 24 a 407 PHO $02D-CGD-O1D$ -3.49 117.01 123.84 34 z 101 BCR $C12-C13-C14$ -3.50 113.58 118.94 24 a 407 PHO $02D-CGD-O1D$ -3.49 117.01 123.84 34 z 101 LMG $07-C10-C11$ 3.49 119.03 <td>20</td> <td>A V</td> <td>403</td> <td>ULA UTC</td> <td>$\begin{array}{c} 0.00-0.40-0.00\\ \hline 0.100002\\ \hline 0.00002\\ \hline 0.00002\\ \hline 0.0002\\ \hline 0.0002\\$</td> <td>2.51</td> <td>114.01</td> <td>100.67</td>	20	A V	403	ULA UTC	$\begin{array}{c} 0.00-0.40-0.00\\ \hline 0.100002\\ \hline 0.00002\\ \hline 0.00002\\ \hline 0.0002\\ \hline 0.0002\\$	2.51	114.01	100.67
25 1 101 Berr C12-C13-C14 -3.51 113.55 116.54 23 b 611 CLA C1D-CHD-C4C -3.51 117.92 122.56 23 D 405 CLA O2D-CGD-O1D -3.51 116.98 123.84 29 A 413 PL9 C37-C38-C39 -3.51 119.21 127.66 23 C 513 CLA C1C-C2C-C3C -3.51 103.27 106.96 23 c 506 CLA CAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLA C4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLA C3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLA C3C-C4C-NC 3.50 114.50 110.57 23 D 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b	25		203	BCB	C12 C13 C14	3.51	113.99	109.07
23 b 611 CLA $CHD-CHD-C4C$ -3.51 117.92 1122.50 23 D 405 CLA $O2D-CGD-O1D$ -3.51 116.98 123.84 29 A 413 $PL9$ $C37-C38-C39$ -3.51 119.21 127.66 23 C 513 CLA $C1C-C2C-C3C$ -3.51 103.27 106.96 23 c 506 CLA $CAC-C3C-C4C$ 3.50 129.36 124.81 23 B 611 CLA $C4C-C3C-C2C$ -3.50 101.79 106.90 23 B 612 CLA $C3B-C4B-NB$ 3.50 113.74 109.21 23 D 401 CLA $C3C-C4C-NC$ 3.50 114.50 110.57 23 B 607 CLA $C1D-CHD-C4C$ -3.50 117.94 122.56 23 b 613 CLA $C1D-CHD-C4C$ -3.50 117.94 122.56 23 b 613 CLA $C1D-CHD-C4C$ -3.50 117.94 122.56 24 a 407 PHO $O2D-CGD-O1D$ -3.49 117.01 123.84 34 z 101 LMG $O7-C10-C11$ 3.49 117.07 126.72 23 b 615 CLA $CHC-C1C-C2C$ -3.48 117.09 126.72 23 b 615 CLA $CHC-C1C-C2C$ -3.48 117.09 126.72 23 b	20 02	L b	611		$\frac{\text{C12-C13-C14}}{\text{C1D-C4C}}$	-0.01	117.00	110.94 122.56
23 D 403 CLA O2D-CGD-O1D -3.51 110.33 123.34 29 A 413 PL9 C37-C38-C39 -3.51 119.21 127.66 23 C 513 CLA C1C-C2C-C3C -3.51 103.27 106.96 23 c 506 CLA CAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLA CAC-C3C-C2C -3.50 101.79 106.90 23 B 612 CLA C3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLA C3C-C4C-NC 3.50 114.50 110.57 23 B 607 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-C13-C14 -3.50 113.58 118.94 24 a	20 		405		O2D CCD O1D	-0.01	117.92	122.00 122.84
29 A 413 1 L9 C37-C38-C39 -3.51 113.21 127.00 23 C 513 CLA C1C-C2C-C3C -3.51 103.27 106.96 23 c 506 CLA CAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLA C4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLA C3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLA C3C-C4C-NC 3.50 114.50 110.57 23 B 607 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 24 a 407 PHO 02D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG 07-C10-C11 3.49 119.03 111.50 23 b	20		400	DIO	$C_{2D}^{-}C_{3D}^{-}C_{-$	-3.51	110.90	125.04 127.66
23 C 513 CHA CHC-C2C-C3C -3.51 105.21 106.90 23 c 506 CLA CAC-C3C-C4C 3.50 129.36 124.81 23 B 611 CLA C4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLA C3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLA C3C-C4C-NC 3.50 114.50 110.57 23 B 607 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 113.58 118.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 <t< td=""><td>29</td><td>A C</td><td>413 513</td><td></td><td>$\frac{0.01 - 0.03}{0.000}$</td><td>-3.51</td><td>119.21</td><td>106.06</td></t<>	29	A C	413 513		$\frac{0.01 - 0.03}{0.000}$	-3.51	119.21	106.06
25 C 500 CHA CACCOSCC4C 5.00 125.00 124.31 23 B 611 CLA C4C-C3C-C2C -3.50 101.79 106.90 23 B 612 CLA C3B-C4B-NB 3.50 113.74 109.21 23 D 401 CLA C3C-C4C-NC 3.50 114.50 110.57 23 B 607 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 25 t 101 BCR C12-C13-C14 -3.50 113.58 118.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b	23	C C	506		$\frac{C1C-C2C-C3C}{CAC}$	-3.51	100.27	100.90
23B611CHAC4C-C3C-C2C-3.30101.19100.9023B612CLAC3B-C4B-NB3.50113.74109.2123D401CLAC3C-C4C-NC3.50114.50110.5723B607CLAC1D-CHD-C4C-3.50117.94122.5623b613CLAC1D-CHD-C4C-3.50117.94122.5625t101BCRC12-C13-C14-3.50113.58118.9424a407PHOO2D-CGD-O1D-3.49117.01123.8434z101LMGO7-C10-C113.49119.03111.5023b611CLACHC-C1C-C2C-3.49117.07126.7223b615CLACHC-C1C-C2C-3.48117.09126.7237c517DGDO2G-C1B-C2B3.48119.00111.5023C506CLAC3B-C4B-NB3.48113.71109.21	20	B	611		$\frac{C4C}{C4C} \frac{C3C}{C2C} \frac{C2C}{C2C}$	3.50	123.30	106.00
25D012CHAC3D-C4D-ND3.50113.14103.2123D401CLAC3C-C4C-NC3.50114.50110.5723B607CLAC1D-CHD-C4C-3.50117.94122.5623b613CLAC1D-CHD-C4C-3.50117.94122.5625t101BCRC12-C13-C14-3.50113.58118.9424a407PHOO2D-CGD-O1D-3.49117.01123.8434z101LMGO7-C10-C113.49119.03111.5023b611CLACHC-C1C-C2C-3.49117.07126.7223b615CLACHC-C1C-C2C-3.48117.09126.7237c517DGDO2G-C1B-C2B3.48119.00111.5023C506CLAC3B-C4B-NB3.48113.71109.21	20	B	612		C3B C4B NB	-3.50	101.75	100.50
23 B 607 CLA C1D-CHD-C4C -3.50 114.56 116.57 23 B 607 CLA C1D-CHD-C4C -3.50 117.94 122.56 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 25 t 101 BCR C12-C13-C14 -3.50 113.58 118.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21 <td>$\frac{20}{23}$</td> <td></td> <td>401</td> <td></td> <td>C3C-C4C-NC</td> <td>3.50</td> <td>110.74</td> <td>109.21 110.57</td>	$\frac{20}{23}$		401		C3C-C4C-NC	3.50	110.74	109.21 110.57
23 B 607 CHA CHD-CHD-C4C -3.50 111.54 122.50 23 b 613 CLA C1D-CHD-C4C -3.50 117.94 122.56 25 t 101 BCR C12-C13-C14 -3.50 113.58 118.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	20	B	607		C1D CHD C/C	3.50	117.94	122 56
25 b 615 CHA CHD+CHD+C4C -3.50 111.54 122.50 25 t 101 BCR C12-C13-C14 -3.50 113.58 118.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	$\frac{20}{23}$	b b	613		C1D-CHD-C4C	-3.50	117.94	122.00 122.56
23 0 101 BCR C12-C13-C14 -3.30 115.36 116.94 24 a 407 PHO O2D-CGD-O1D -3.49 117.01 123.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	$\frac{20}{25}$	t b	1013	BCB	C12 C13 C14	-3.50	117.54	118.94
24 a 407 110 02D-CGD-C1D -3.49 111.01 125.84 34 z 101 LMG O7-C10-C11 3.49 119.03 111.50 23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	$\frac{20}{24}$	U 9	407	DUR PHO	$\frac{012-013-014}{020}$	-3.00	117.01	110.94 193.84
23 b 611 CLA CHC-C1C-C2C -3.49 117.07 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	24	a	101	LMC	02D-03D-01D 07-010 011	3 /0	110.03	111 50
23 b 615 CLA CHC-C1C-C2C -3.49 117.07 120.72 23 b 615 CLA CHC-C1C-C2C -3.48 117.09 126.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	- 04 	b L	611	CLA	CHC_C1C_C2C	-3 40	117.07	126 72
25 0 013 014 010-010-020 -3.48 117.09 120.72 37 c 517 DGD O2G-C1B-C2B 3.48 119.00 111.50 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21		b h	615		CHC C1C C2C	-3.49		120.72
37 C 317 DGD O2G-C1B-C2B 3.48 119.00 111.30 23 C 506 CLA C3B-C4B-NB 3.48 113.71 109.21	$\frac{20}{37}$	C D	517		010-010-020	2 / 2	110.00	111 50
25 0 000 0 A 0 0 - 0 - 0 - 0 - 0 - 0 - 0 -	- 01 	C	506	CLA	C3B-C4B NR	3.40	112.00	100.91
25 T 101 BCB C15 C14 C13 2 49 122 27 127 21	20 95		101	BCP	$\begin{array}{c} 03D - 04D - ND \\ \hline 015 \ 014 \ 012 \end{array}$	3.40	129.97	109.21



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26.23
26.23
26.04
0.57
9.21
1.91
6.90
6.96
6.96
27.31
4.08
22.56
6.78
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22.56
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1.27
22.56
1.27
1.86
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	В	616	CLA	C3B-C4B-NB	3.42	113.63	109.21
26	a	411	SQD	O8-S-C6	3.42	111.19	105.74
23	a	406	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	a	405	CLA	C3C-C4C-NC	3.42	114.40	110.57
23	С	511	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
25	t	101	BCR	C37-C22-C23	3.41	123.46	118.08
23	d	402	CLA	C1-C2-C3	-3.41	120.14	126.04
23	С	512	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	b	603	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
23	В	609	CLA	C3B-C4B-NB	3.40	113.61	109.21
23	В	614	CLA	C3B-C4B-NB	3.40	113.61	109.21
25	у	101	BCR	C15-C14-C13	-3.40	122.45	127.31
23	В	609	CLA	CHD-C4C-NC	3.40	129.56	124.20
23	с	502	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
24	a	407	PHO	O2A-CGA-CBA	3.40	122.58	111.91
23	С	511	CLA	CHC-C1C-C2C	-3.40	117.32	126.72
23	В	604	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	a	409	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
23	с	504	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	b	615	CLA	C11-C10-C8	-3.39	104.97	115.92
23	В	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
25	a	410	BCR	C20-C21-C22	-3.39	122.48	127.31
25	С	527	BCR	С11-С10-С9	-3.39	122.48	127.31
23	b	609	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	с	508	CLA	C3B-C4B-NB	3.38	113.58	109.21
34	С	520	LMG	O7-C10-C11	3.38	118.78	111.50
23	b	616	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	С	509	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
23	В	615	CLA	CHC-C1C-C2C	-3.37	117.39	126.72
29	a	415	PL9	C22-C23-C24	-3.37	119.54	127.66
23	С	503	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
23	В	604	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
23	D	401	CLA	C1D-CHD-C4C	-3.37	118.12	122.56
34	m	101	LMG	O7-C10-C11	3.37	118.75	111.50
23	b	604	CLA	CMC-C2C-C1C	3.37	130.16	125.04
23	b	614	CLA	C3B-C4B-NB	3.36	113.56	109.21
23	с	508	CLA	CMB-C2B-C3B	3.36	130.97	124.68
23	С	505	CLA	C4A-NA-C1A	-3.36	105.19	106.71
23	А	404	CLA	O2A-CGA-O1A	-3.36	115.11	123.59
23	a	406	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	В	608	CLA	CMC-C2C-C1C	3.36	130.15	125.04
23	С	511	CLA	C3C-C4C-NC	3.35	114.33	110.57



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Conti	Continued from previous page							
Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$	
23	b	612	CLA	C3B-C4B-NB	3.35	113.54	109.21	
23	b	612	CLA	O2A-CGA-CBA	3.35	122.42	111.91	
23	A	407	CLA	C3B-C4B-NB	3.35	113.54	109.21	
23	С	512	CLA	C4-C3-C5	3.34	120.89	115.27	
25	b	618	BCR	C37-C22-C21	-3.34	118.24	122.92	
23	В	616	CLA	CED-O2D-CGD	3.34	123.49	115.94	
23	А	404	CLA	O2D-CGD-CBD	3.33	117.19	111.27	
23	с	510	CLA	CBC-CAC-C3C	-3.33	103.25	112.43	
26	a	413	SQD	O48-C23-C24	3.33	122.36	111.91	
23	с	509	CLA	C1-O2A-CGA	3.33	125.18	116.44	
26	А	409	SQD	C45-O47-C7	-3.33	109.60	117.79	
25	h	102	BCR	C38-C26-C25	-3.33	120.79	124.53	
23	С	504	CLA	C4-C3-C5	3.32	120.85	115.27	
23	d	403	CLA	C1D-CHD-C4C	-3.32	118.18	122.56	
25	А	408	BCR	C38-C26-C25	-3.32	120.80	124.53	
23	с	512	CLA	CMA-C3A-C4A	-3.32	102.86	111.77	
23	С	509	CLA	C1C-C2C-C3C	-3.31	103.47	106.96	
23	с	506	CLA	C1D-CHD-C4C	-3.31	118.19	122.56	
23	С	502	CLA	C3B-C4B-NB	3.31	113.49	109.21	
29	А	413	PL9	C30-C29-C31	3.31	120.84	115.27	
23	с	502	CLA	C3B-C4B-NB	3.31	113.49	109.21	
38	Е	103	HEM	CBA-CAA-C2A	-3.31	106.39	112.49	
23	с	501	CLA	C1D-CHD-C4C	-3.31	118.19	122.56	
23	С	506	CLA	C1-C2-C3	-3.30	120.33	126.04	
23	с	502	CLA	CHD-C4C-NC	3.30	129.41	124.20	
23	b	604	CLA	C1-C2-C3	-3.30	120.34	126.04	
23	С	514	CLA	C1C-C2C-C3C	-3.30	103.49	106.96	
23	В	609	CLA	C4C-C3C-C2C	-3.30	102.09	106.90	
23	с	510	CLA	C3B-C4B-NB	3.29	113.46	109.21	
23	b	607	CLA	CAA-C2A-C3A	-3.29	103.78	112.78	
23	b	609	CLA	C1D-CHD-C4C	-3.29	118.22	122.56	
23	b	609	CLA	O2A-CGA-CBA	3.29	122.22	111.91	
23	В	617	CLA	CHD-C4C-NC	3.28	129.38	124.20	
23	с	509	CLA	C3B-C4B-NB	3.28	113.45	109.21	
23	с	505	CLA	C1D-CHD-C4C	-3.28	118.22	122.56	
23	с	506	CLA	C1-C2-C3	-3.28	120.37	126.04	
23	В	615	CLA	CBC-CAC-C3C	-3.28	103.39	112.43	
23	D	405	CLA	C4C-C3C-C2C	-3.28	102.12	106.90	
29	A	413	PL9	C15-C14-C16	3.27	120.78	115.27	
23	b	608	CLA	C1D-CHD-C4C	-3.27	118.24	122.56	
23	С	504	CLA	C3B-C4B-NB	3.27	113.44	109.21	
23	С	510	CLA	C1C-C2C-C3C	-3.27	103.52	106.96	

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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
23	с	501	CLA	C1-C2-C3	-3.26	120.40	126.04	
23	В	605	CLA	C3B-C4B-NB	3.26	113.43	109.21	
36	b	625	HTG	C1-O5-C5	3.26	118.59	112.58	
38	е	103	HEM	CBD-CAD-C3D	-3.26	106.47	112.48	
23	b	606	CLA	C3B-C4B-NB	3.26	113.42	109.21	
23	В	603	CLA	O2D-CGD-O1D	-3.26	117.47	123.84	
23	А	404	CLA	CMB-C2B-C3B	3.26	130.77	124.68	
25	b	618	BCR	C38-C26-C25	-3.26	120.87	124.53	
23	с	510	CLA	CMC-C2C-C1C	3.26	130.00	125.04	
23	В	613	CLA	C1C-C2C-C3C	-3.26	103.53	106.96	
23	d	403	CLA	CMC-C2C-C1C	3.25	130.00	125.04	
25	В	619	BCR	C37-C22-C21	-3.25	118.36	122.92	
23	С	510	CLA	C1D-CHD-C4C	-3.25	118.27	122.56	
23	С	502	CLA	CBC-CAC-C3C	-3.25	103.47	112.43	
23	D	405	CLA	CHD-C4C-NC	3.25	129.33	124.20	
25	В	620	BCR	C38-C26-C25	-3.25	120.88	124.53	
25	А	408	BCR	C24-C23-C22	-3.25	121.33	126.23	
23	b	616	CLA	C1C-C2C-C3C	-3.24	103.55	106.96	
23	А	405	CLA	C3B-C4B-NB	3.24	113.40	109.21	
23	с	505	CLA	C1C-C2C-C3C	-3.24	103.55	106.96	
23	В	617	CLA	C3B-C4B-NB	3.24	113.39	109.21	
23	с	503	CLA	C1-C2-C3	-3.23	120.45	126.04	
23	с	504	CLA	C1D-CHD-C4C	-3.23	118.29	122.56	
23	В	602	CLA	C1-C2-C3	-3.23	120.46	126.04	
23	с	510	CLA	C3C-C4C-NC	3.23	114.19	110.57	
24	a	407	PHO	C4D-CHA-C1A	-3.23	118.10	125.37	
23	С	504	CLA	CHC-C1C-C2C	-3.23	117.79	126.72	
23	с	512	CLA	O2D-CGD-O1D	-3.23	117.53	123.84	
23	С	513	CLA	O2A-CGA-CBA	3.23	122.03	111.91	
23	a	409	CLA	CAC-C3C-C4C	3.22	128.99	124.81	
23	с	503	CLA	O2D-CGD-O1D	-3.22	117.54	123.84	
29	D	407	PL9	C53-C6-C1	3.22	121.57	114.99	
23	b	601	CLA	C4-C3-C5	3.22	120.68	115.27	
23	b	612	CLA	O2D-CGD-O1D	-3.22	117.55	123.84	
31	е	101	LHG	O7-C7-C8	3.22	118.43	111.50	
31	d	407	LHG	O7-C7-C8	3.22	118.43	111.50	
23	В	611	CLA	O2A-CGA-CBA	3.22	122.00	111.91	
23	С	511	CLA	O2D-CGD-O1D	-3.22	117.55	123.84	
23	с	507	CLA	O2D-CGD-O1D	-3.22	117.55	123.84	
23	с	512	CLA	C4-C3-C5	3.21	120.67	115.27	
35	b	628	LMT	C1'-O5'-C5'	3.21	119.99	113.69	
23	В	605	CLA	O2A-CGA-CBA	3.21	121.98	111.91	
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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
23	В	602	CLA	C1D-CHD-C4C	-3.21	118.33	122.56
23	В	609	CLA	C1-C2-C3	-3.21	120.50	126.04
23	b	604	CLA	O2A-CGA-CBA	3.21	121.97	111.91
23	с	510	CLA	CAC-C3C-C4C	3.20	128.97	124.81
23	D	404	CLA	O2A-CGA-CBA	3.20	121.96	111.91
23	a	405	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
23	b	610	CLA	O2A-CGA-CBA	3.20	121.95	111.91
23	с	503	CLA	C3B-C4B-NB	3.20	113.35	109.21
23	b	607	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	a	409	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	d	403	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
35	b	628	LMT	O5'-C1'-C2'	3.20	117.12	110.35
23	d	403	CLA	CHD-C4C-NC	3.20	129.24	124.20
23	D	404	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	В	602	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	В	603	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	с	505	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
23	В	615	CLA	C4-C3-C5	3.19	120.64	115.27
29	А	413	PL9	C27-C28-C29	-3.19	119.97	127.66
23	С	503	CLA	C3B-C4B-NB	3.19	113.34	109.21
23	b	616	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
23	b	608	CLA	CHD-C4C-NC	3.19	129.23	124.20
23	b	614	CLA	O2A-CGA-CBA	3.19	121.91	111.91
25	t	101	BCR	C3-C4-C5	-3.19	108.39	114.08
23	b	603	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
23	D	405	CLA	CMC-C2C-C1C	3.18	129.89	125.04
29	А	413	PL9	C22-C23-C24	-3.18	120.01	127.66
23	В	615	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	С	507	CLA	C4-C3-C5	3.17	120.61	115.27
23	b	605	CLA	CAC-C3C-C4C	3.17	128.92	124.81
23	В	617	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
34	Z	101	LMG	C4-C3-C2	3.17	116.35	110.82
23	b	607	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	В	610	CLA	C4C-C3C-C2C	-3.16	102.28	106.90
29	a	415	PL9	C37-C38-C39	-3.16	120.04	127.66
23	с	502	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
23	D	401	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
23	b	613	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	С	510	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	В	604	CLA	O2A-CGA-CBA	3.15	121.80	111.91
23	b	608	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	с	508	CLA	C1D-CHD-C4C	-3.15	118.40	122.56



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Mol	Chain	Kes	Type	Atoms	Z	Ubserved(^o)	Ideal(°)
25	k	101	BCR	C29-C30-C25	3.15	115.33	110.48
23	C	514	CLA	C2A-C1A-CHA	-3.15	118.36	123.86
23	b	614	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
23	a	405	CLA	C4A-NA-C1A	-3.14	105.29	106.71
23	В	614	CLA	CAC-C3C-C4C	3.14	128.89	124.81
23	В	611	CLA	CHD-C4C-NC	3.14	129.15	124.20
23	С	507	CLA	CAC-C3C-C4C	3.14	128.88	124.81
26	А	409	SQD	O48-C23-C24	3.14	121.75	111.91
23	с	501	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
23	a	406	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
23	В	604	CLA	C4-C3-C5	3.13	120.54	115.27
25	Y	101	BCR	C16-C15-C14	-3.13	117.06	123.47
23	b	609	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
23	С	506	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
23	С	503	CLA	C1D-CHD-C4C	-3.12	118.44	122.56
23	В	615	CLA	O2A-CGA-CBA	3.12	121.71	111.91
26	a	413	SQD	O47-C7-C8	3.12	118.23	111.50
23	b	613	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	с	511	CLA	C4-C3-C5	3.12	120.52	115.27
23	С	508	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
26	a	411	SQD	C45-O47-C7	-3.12	110.11	117.79
34	Ζ	101	LMG	C3-C4-C5	3.12	115.80	110.24
25	у	101	BCR	C40-C30-C25	-3.12	105.25	110.30
23	a	409	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
23	С	513	CLA	CHD-C4C-NC	3.11	129.11	124.20
25	Н	101	BCR	C38-C26-C25	-3.11	121.03	124.53
23	В	611	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
34	m	101	LMG	O8-C28-C29	3.11	121.68	111.91
40	V	202	HEC	CBA-CAA-C2A	-3.11	106.74	112.48
23	В	616	CLA	CMC-C2C-C1C	3.11	129.78	125.04
23	b	610	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
23	В	613	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	a	404	CLA	O2D-CGD-CBD	3.11	116.79	111.27
23	В	607	CLA	C3B-C4B-NB	3.11	113.23	109.21
29	A	413	PL9	C20-C19-C21	3.11	120.50	115.27
23	D	405	CLA	C3B-C4B-NB	3.11	113.22	109.21
23	с	513	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
23	b	602	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	B	606	CLA	CHD-C4C-NC	3.10	129.09	124.20
$\frac{-3}{23}$	C C	501	CLA	C3B-C4B-NB	3.10	113.22	109.21
$\frac{-3}{23}$	Č	512	CLA	CMC-C2C-C1C	3.10	129.76	125.04
$\frac{-5}{25}$	C	527	BCR	C24-C23-C22	-3 10	121.55	126.23
$ \begin{array}{r} 23 \\ 23 \\ 23 \\ 23 \\ 23 \\ 23 \\ 25 \\ 25 \\ \end{array} $	D c B C C C	$ \begin{array}{r} 405 \\ 513 \\ 602 \\ 606 \\ 501 \\ 512 \\ 527 \\ \end{array} $	CLA CLA CLA CLA CLA CLA BCR	C3B-C4B-NB CAA-C2A-C3A CHD-C4C-NC CHD-C4C-NC C3B-C4B-NB CMC-C2C-C1C C24-C23-C22	$\begin{array}{r} 3.11 \\ -3.11 \\ 3.11 \\ 3.10 \\ 3.10 \\ 3.10 \\ -3.10 \end{array}$	$ \begin{array}{r} 113.22\\ 104.27\\ 129.10\\ 129.09\\ 113.22\\ 129.76\\ 121.55\\ \end{array} $	$ \begin{array}{r} 109.21 \\ 112.78 \\ 124.20 \\ 124.20 \\ 109.21 \\ 125.04 \\ 126.23 \\ \end{array} $

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	с	505	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	b	608	CLA	C3B-C4B-NB	3.10	113.21	109.21
31	А	415	LHG	O8-C23-O10	-3.09	115.79	123.59
23	b	616	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	b	613	CLA	O2A-CGA-CBA	3.09	121.61	111.91
23	С	514	CLA	C1-C2-C3	-3.09	120.70	126.04
23	с	506	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
23	b	606	CLA	CHD-C4C-NC	3.09	129.07	124.20
23	с	504	CLA	CMB-C2B-C3B	3.09	130.46	124.68
23	b	616	CLA	OBD-CAD-C3D	-3.09	122.86	127.98
23	с	507	CLA	CMC-C2C-C1C	3.09	129.74	125.04
23	b	602	CLA	C3B-C4B-NB	3.09	113.20	109.21
23	В	605	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
23	b	605	CLA	CHD-C4C-NC	3.08	129.06	124.20
23	С	502	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
23	А	404	CLA	C3B-C4B-NB	3.08	113.19	109.21
23	b	614	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	b	601	CLA	CHD-C4C-NC	3.08	129.06	124.20
25	с	515	BCR	С11-С10-С9	-3.08	122.92	127.31
23	a	405	CLA	CHD-C4C-NC	3.07	129.05	124.20
23	b	603	CLA	O2A-CGA-CBA	3.07	121.55	111.91
23	С	510	CLA	CAC-C3C-C4C	3.07	128.80	124.81
23	В	615	CLA	CAC-C3C-C4C	3.07	128.80	124.81
24	D	402	PHO	C2B-C1B-NB	3.07	114.43	109.79
23	d	402	CLA	O2A-CGA-CBA	3.07	121.55	111.91
26	L	102	SQD	C3-C4-C5	3.07	115.72	110.24
23	С	509	CLA	C4-C3-C5	3.07	120.43	115.27
36	b	622	HTG	O5-C1-C2	3.07	114.17	110.31
23	с	509	CLA	O2A-CGA-CBA	3.07	121.53	111.91
23	В	605	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	В	610	CLA	C3B-C4B-NB	3.07	113.17	109.21
23	D	404	CLA	C2A-C1A-CHA	-3.07	118.50	123.86
23	С	507	CLA	CMC-C2C-C1C	3.07	129.71	125.04
23	В	606	CLA	C1C-C2C-C3C	-3.06	103.73	106.96
23	b	612	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	С	514	CLA	CMC-C2C-C1C	3.06	129.70	125.04
25	Y	101	BCR	C37-C22-C23	3.06	122.90	118.08
23	С	504	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	А	406	PHO	C1-O2A-CGA	3.06	124.47	116.44
23	В	616	CLA	CHD-C4C-NC	3.06	129.02	124.20
26	a	413	SQD	C3-C4-C5	3.06	115.69	110.24
23	с	511	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
29	A	413	PL9	C42-C43-C44	-3.06	120.30	127.66
23	С	507	CLA	CBC-CAC-C3C	-3.06	104.00	112.43
25	a	410	BCR	C24-C23-C22	-3.05	121.62	126.23
23	с	509	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	с	506	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	С	512	CLA	C1D-CHD-C4C	-3.05	118.53	122.56
23	с	511	CLA	CHD-C4C-NC	3.05	129.01	124.20
23	с	513	CLA	CAC-C3C-C4C	3.05	128.77	124.81
29	d	405	PL9	C35-C34-C36	3.05	120.40	115.27
23	с	513	CLA	CMC-C2C-C1C	3.05	129.68	125.04
25	с	515	BCR	C38-C26-C25	-3.05	121.10	124.53
23	b	606	CLA	C4-C3-C5	3.05	120.40	115.27
23	b	612	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	В	603	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
23	С	512	CLA	CMB-C2B-C3B	3.05	130.38	124.68
36	b	621	HTG	C1-O5-C5	3.04	118.19	112.58
23	С	505	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	D	401	CLA	C4-C3-C5	3.04	120.39	115.27
23	b	613	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	b	602	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
34	С	520	LMG	O8-C28-C29	3.03	121.42	111.91
23	В	612	CLA	C1-C2-C3	-3.03	120.80	126.04
23	b	613	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	С	514	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	А	404	CLA	CAA-C2A-C1A	-3.03	102.05	111.97
26	a	413	SQD	O9-S-C6	3.03	110.54	106.94
23	В	604	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	a	404	CLA	O2A-CGA-CBA	3.03	121.41	111.91
23	b	616	CLA	O2A-CGA-CBA	3.03	121.41	111.91
23	С	503	CLA	C1-C2-C3	-3.03	120.81	126.04
23	d	402	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
23	А	407	CLA	CMB-C2B-C3B	3.02	130.33	124.68
23	b	601	CLA	C3B-C4B-NB	3.02	113.11	109.21
23	с	504	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
25	Т	101	BCR	C35-C13-C12	3.02	122.83	118.08
25	d	404	BCR	C15-C14-C13	-3.02	123.01	127.31
23	a	404	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
23	a	405	CLA	C1-C2-C3	-3.01	120.83	126.04
23	C	509	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
25	b	618	BCR	C20-C21-C22	-3.01	123.01	127.31
23	С	511	CLA	O2A-CGA-CBA	3.01	121.36	111.91
23	b	602	CLA	CMC-C2C-C1C	3.01	129.62	125.04

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Mol	Chain	Kes	Type	Atoms		Ubserved(°)	Ideal(")	
23	В	608	CLA	CAA-C2A-C3A	-3.01	104.55	112.78	
23	c	501	CLA	C4D-C3D-CAD	-3.01	106.79	108.47	
25	B	620	BCR	C15-C14-C13	-3.00	123.02	127.31	
23	В	605	CLA	C1D-CHD-C4C	-3.00	118.59	122.56	
23	с	502	CLA	CMB-C2B-C3B	3.00	130.30	124.68	
23	с	506	CLA	C4-C3-C5	3.00	120.32	115.27	
34	с	519	LMG	O8-C28-C29	3.00	121.32	111.91	
23	a	406	CLA	CHC-C1C-C2C	-3.00	118.43	126.72	
25	В	620	BCR	C7-C8-C9	-3.00	121.70	126.23	
23	В	604	CLA	CAA-C2A-C3A	-3.00	104.57	112.78	
23	С	513	CLA	CMC-C2C-C1C	2.99	129.60	125.04	
23	b	604	CLA	C3B-C4B-NB	2.99	113.08	109.21	
23	с	512	CLA	CHD-C4C-NC	2.99	128.92	124.20	
23	В	604	CLA	C3B-C4B-NB	2.99	113.08	109.21	
23	В	614	CLA	C1D-CHD-C4C	-2.99	118.61	122.56	
23	D	404	CLA	C4C-C3C-C2C	-2.99	102.54	106.90	
23	b	603	CLA	CHD-C4C-NC	2.99	128.91	124.20	
23	b	605	CLA	O2A-CGA-CBA	2.98	121.27	111.91	
23	А	407	CLA	CHD-C4C-NC	2.98	128.91	124.20	
31	D	408	LHG	O8-C23-O10	-2.98	116.07	123.59	
23	с	506	CLA	O2D-CGD-O1D	-2.98	118.01	123.84	
23	b	616	CLA	O2D-CGD-O1D	-2.98	118.01	123.84	
25	с	515	BCR	C3-C4-C5	-2.98	108.75	114.08	
23	В	607	CLA	O2A-CGA-CBA	2.98	121.26	111.91	
37	С	517	DGD	O6D-C1D-O3G	-2.98	102.92	109.97	
23	В	611	CLA	CAA-C2A-C3A	-2.98	104.62	112.78	
24	D	402	PHO	O2D-CGD-O1D	-2.98	118.02	123.84	
23	b	611	CLA	C4C-C3C-C2C	-2.98	102.56	106.90	
23	В	616	CLA	CHC-C1C-C2C	-2.98	118.49	126.72	
23	с	513	CLA	C3B-C4B-NB	2.98	113.06	109.21	
36	В	624	HTG	C1'-S1-C1	2.98	105.66	100.09	
23	В	604	CLA	CHD-C4C-NC	2.97	128.89	124.20	
23	В	616	CLA	CAC-C3C-C4C	2.97	128.67	124.81	
23	С	502	CLA	C4-C3-C5	2.97	120.27	115.27	
23	D	404	CLA	CMC-C2C-C1C	2.97	129.56	125.04	
25	A	408	BCR	C11-C10-C9	-2.97	123.07	127.31	
23	b	610	CLA	C4-C3-C5	2.97	120.27	115.27	
$\frac{-3}{23}$	B	605	CLA	02A-CGA-01A	-2.97	116.10	123.59	
$\frac{-3}{23}$	B	603	CLA	C4C-C3C-C2C	-2.97	102 57	106.90	
$\frac{-20}{35}$	M	101	LMT	C1-O1'-C1'	-2.97	108.92	113.84	
24	D	402	PHO	C4D-ND-C1D	-2.97	101.42	106 76	
29	2	415	PLO	C25-C24-C26	2.01 2.97	120.26	115 27	
29	a	410	PL9	023-024-026	2.97	120.20	110.27	

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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	Ideal(°)	
23	b	601	CLA	O2D-CGD-O1D	-2.97	118.04	123.84	
23	D	405	CLA	C1C-C2C-C3C	-2.97	103.84	106.96	
34	m	101	LMG	C7-O1-C1	-2.96	107.95	113.74	
25	Т	101	BCR	C16-C15-C14	2.96	129.54	123.47	
23	b	609	CLA	CHD-C4C-NC	2.96	128.87	124.20	
24	D	402	PHO	CAC-C3C-C4C	2.96	128.45	125.22	
23	d	403	CLA	C4C-C3C-C2C	-2.96	102.58	106.90	
24	D	402	PHO	C6-C5-C3	-2.96	105.69	113.45	
23	d	403	CLA	O2A-CGA-CBA	2.96	121.19	111.91	
23	с	503	CLA	C4C-C3C-C2C	-2.96	102.58	106.90	
25	h	102	BCR	C7-C8-C9	-2.96	121.77	126.23	
23	А	405	CLA	C1D-CHD-C4C	-2.96	118.66	122.56	
23	с	501	CLA	C4C-C3C-C2C	-2.95	102.59	106.90	
23	D	404	CLA	C4-C3-C5	2.95	120.24	115.27	
23	с	508	CLA	C4C-C3C-C2C	-2.95	102.60	106.90	
23	В	613	CLA	C4-C3-C5	2.95	120.23	115.27	
23	С	512	CLA	C4C-C3C-C2C	-2.95	102.60	106.90	
25	с	515	BCR	C2-C1-C6	2.95	115.02	110.48	
23	с	508	CLA	O2A-CGA-CBA	2.95	121.16	111.91	
23	с	504	CLA	C4C-C3C-C2C	-2.95	102.60	106.90	
23	В	614	CLA	C4-C3-C5	2.95	120.23	115.27	
23	a	406	CLA	CAA-C2A-C3A	-2.94	104.71	112.78	
25	a	410	BCR	C37-C22-C21	-2.94	118.80	122.92	
23	С	510	CLA	CHD-C4C-NC	2.94	128.84	124.20	
23	D	404	CLA	O2D-CGD-O1D	-2.94	118.08	123.84	
23	b	610	CLA	CAA-C2A-C3A	-2.94	104.72	112.78	
23	b	605	CLA	CHC-C1C-C2C	-2.94	118.58	126.72	
23	В	602	CLA	C4C-C3C-C2C	-2.94	102.61	106.90	
23	с	510	CLA	O2A-CGA-CBA	2.94	121.13	111.91	
23	В	616	CLA	CBC-CAC-C3C	-2.94	104.33	112.43	
23	b	603	CLA	O2A-CGA-O1A	-2.94	116.18	123.59	
23	В	602	CLA	CHD-C4C-NC	2.94	128.83	124.20	
23	A	407	CLA	C4C-C3C-C2C	-2.94	102.62	106.90	
23	b	615	CLA	C4C-C3C-C2C	-2.94	102.62	106.90	
23	b	607	CLA	CHC-C1C-C2C	-2.94	118.60	126.72	
25	С	527	BCR	C20-C21-C22	-2.94	123.12	127.31	
23	A	405	CLA	O2A-CGA-O1A	-2.93	116.19	123.59	
23	b	605	CLA	CMC-C2C-C1C	2.93	129.51	125.04	
23	С	514	CLA	CAC-C3C-C4C	2.93	128.61	124.81	
23	B	603	CLA	C1D-CHD-C4C	-2.93	118.69	122.56	
23	D	404	CLA	O2A-CGA-O1A	-2.93	116.20	123.59	
23	b	602	CLA	C1-C2-C3	-2.93	120.98	126.04	

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		res		Atoms		Ubserved(°)	10eai(°)
23		505	CLA	UHU-UIU-U2U	-2.93	118.62	120.72
31	D	409	LHG	08-C23-C24	2.93	121.10	111.91
23	B	608	CLA	CID-CHD-C4C	-2.93	118.69	122.56
23	В	610	CLA	O2A-CGA-CBA	2.93	121.09	111.91
23	В	607	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	b	605	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
23	С	510	CLA	C4-C3-C5	2.92	120.19	115.27
23	d	403	CLA	CAC-C3C-C4C	2.92	128.60	124.81
37	h	103	DGD	O1G-C1A-O1A	-2.92	116.22	123.59
23	d	402	CLA	C1D-CHD-C4C	-2.92	118.71	122.56
23	A	405	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
23	В	604	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
23	С	504	CLA	O2A-CGA-CBA	2.91	121.05	111.91
25	С	516	BCR	C33-C5-C6	-2.91	121.26	124.53
23	с	512	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
23	b	611	CLA	O2A-CGA-CBA	2.91	121.04	111.91
23	b	613	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	с	510	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
23	В	602	CLA	O2A-CGA-CBA	2.91	121.03	111.91
34	Z	101	LMG	O8-C28-C29	2.91	121.03	111.91
23	с	507	CLA	C1-C2-C3	-2.91	121.01	126.04
23	b	609	CLA	CAC-C3C-C4C	2.91	128.58	124.81
23	А	407	CLA	C1D-CHD-C4C	-2.91	118.72	122.56
23	В	603	CLA	CAC-C3C-C4C	2.91	128.58	124.81
23	b	608	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
23	b	604	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
23	С	509	CLA	CMB-C2B-C3B	2.90	130.11	124.68
23	с	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	603	CLA	CMC-C2C-C1C	2.90	129.46	125.04
23	b	605	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	614	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
24	А	406	PHO	C4C-C3C-C2C	-2.90	103.57	106.78
23	с	503	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
31	b	630	LHG	O8-C23-C24	2.90	121.01	111.91
23	a	404	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	b	605	CLA	C4-C3-C5	2.90	120.15	115.27
25	y	101	BCR	C23-C24-C25	-2.90	119.06	127.20
23	b	610	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	с	507	CLA	CAC-C3C-C4C	2.89	128.57	124.81
23	A	405	CLA	O2A-CGA-CBA	2.89	120.99	111.91
23	С	510	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	b	612	CLA	C4-C3-C5	2.89	120.14	115.27

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	nucu 11011 Chain	i previ	Type	Atoms	7	Observed ⁽⁰⁾	Ideal(0)
10101		105	туре		<u> </u>		111 00
29		400		$\begin{array}{c} 0.00 \\ 0.012 \\ 0.012 \\ 0.014 \\ $	-2.89	102.38	111.88
29		407	PL9 CLA	C12-C13-C14	-2.89	120.70	127.00
23		003 007	CLA CLA	CBC-CAC-C3C	-2.89	104.47	112.43
23	d D	<u>607</u>	DCD	C4D-C3D-CAD	-2.89	100.80	108.47
25		527	BCR	C3-C4-C5	-2.88	108.93	114.08
23	D	401	CLA	C1-C2-C3	-2.88	121.06	126.04
36	b	621	HIG	05-C1-C2	2.88	113.94	110.31
23	A	405	CLA	O2D-CGD-OID	-2.88	118.21	123.84
29	D	407	PL9	<u>C7-C3-C4</u>	2.88	119.22	116.88
34	J	101	LMG	08-C28-C29	2.88	120.94	111.91
23	В	607	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	C	507	CLA	C2A-C1A-CHA	-2.88	118.83	123.86
37	с	516	DGD	C2G-O2G-C1B	-2.88	110.70	117.79
23	b	604	CLA	CAC-C3C-C4C	2.87	128.54	124.81
23	с	512	CLA	CHB-C4A-NA	2.87	128.49	124.51
23	b	614	CLA	CAC-C3C-C4C	2.87	128.54	124.81
36	В	626	HTG	O5-C1-C2	2.87	113.92	110.31
23	b	609	CLA	CMC-C2C-C1C	2.87	129.41	125.04
23	С	507	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	А	404	CLA	CAA-CBA-CGA	-2.87	104.88	113.25
31	А	415	LHG	C5-O7-C7	-2.87	110.73	117.79
23	С	512	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
23	b	612	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
40	V	201	HEC	CBA-CAA-C2A	-2.86	107.20	112.48
23	С	514	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	с	510	CLA	CHD-C4C-NC	2.86	128.71	124.20
25	b	619	BCR	C39-C30-C25	-2.86	105.66	110.30
23	С	502	CLA	C4D-C3D-CAD	-2.86	106.88	108.47
23	С	508	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	С	502	CLA	CAC-C3C-C4C	2.86	128.52	124.81
23	В	617	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
36	С	524	HTG	C1-S1-C1'	2.85	110.19	100.40
37	с	518	DGD	O2G-C1B-C2B	2.85	117.65	111.50
23	с	512	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
29	A	413	PL9	C17-C18-C19	-2.85	120.80	127.66
24	D	402	PHO	CHC-C1C-C2C	-2.85	118.56	125.73
23	В	602	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
25	D	406	BCR	C40-C30-C25	-2.85	105.68	110.30
23	с	511	CLA	O2A-CGA-CBA	2.85	120.84	111.91
25	В	620	BCR	C20-C21-C22	-2.85	123.25	127.31
23	b	604	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	С	509	CLA	C1-C2-C3	-2.84	121.12	126.04

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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$		
23	В	604	CLA	CBC-CAC-C3C	-2.84	104.59	112.43		
34	В	622	LMG	O8-C28-C29	2.84	120.83	111.91		
24	a	407	PHO	CBD-CHA-C1A	2.84	132.99	126.40		
23	С	507	CLA	C3B-C4B-NB	2.84	112.88	109.21		
23	a	404	CLA	CHC-C1C-C2C	-2.84	118.86	126.72		
25	Н	101	BCR	C11-C10-C9	-2.84	123.26	127.31		
23	с	513	CLA	C4C-C3C-C2C	-2.84	102.76	106.90		
23	a	409	CLA	C4C-C3C-C2C	-2.84	102.76	106.90		
23	b	608	CLA	CMB-C2B-C3B	2.84	129.99	124.68		
23	В	605	CLA	C4-C3-C5	2.84	120.04	115.27		
26	А	411	SQD	O48-C23-C24	2.84	120.81	111.91		
29	D	407	PL9	C37-C38-C39	-2.84	120.83	127.66		
25	А	408	BCR	C20-C21-C22	-2.83	123.26	127.31		
34	с	520	LMG	O8-C28-C29	2.83	120.80	111.91		
23	с	505	CLA	C1-C2-C3	-2.83	121.14	126.04		
23	А	405	CLA	CBC-CAC-C3C	-2.83	104.62	112.43		
25	t	101	BCR	C21-C20-C19	-2.83	114.38	123.22		
25	с	514	BCR	C37-C22-C21	-2.83	118.96	122.92		
23	С	511	CLA	C4C-C3C-C2C	-2.83	102.78	106.90		
23	b	616	CLA	C4-C3-C5	2.83	120.03	115.27		
26	A	409	SQD	O9-S-C6	2.83	110.30	106.94		
23	В	605	CLA	CMC-C2C-C1C	2.83	129.34	125.04		
23	С	508	CLA	C1-C2-C3	-2.83	121.16	126.04		
23	с	501	CLA	C4-C3-C5	2.82	120.02	115.27		
36	b	625	HTG	O5-C5-C4	2.82	114.82	109.69		
23	b	601	CLA	CHC-C1C-C2C	-2.82	118.91	126.72		
34	a	417	LMG	O6-C5-C4	2.82	114.82	109.69		
25	D	406	BCR	C28-C27-C26	-2.82	109.04	114.08		
23	с	504	CLA	C4-C3-C5	2.82	120.02	115.27		
23	В	612	CLA	CBC-CAC-C3C	-2.82	104.65	112.43		
23	b	608	CLA	CMC-C2C-C1C	2.82	129.34	125.04		
24	D	402	PHO	C4D-CHA-C1A	-2.82	119.02	125.37		
23	b	605	CLA	CED-O2D-CGD	2.82	122.32	115.94		
25	t	101	BCR	C1-C6-C7	2.82	123.76	115.78		
24	A	406	PHO	C1C-C2C-C3C	-2.82	103.27	106.51		
23	c	506	CLA	CGD-CBD-CAD	-2.82	101.60	110.73		
23	c	512	CLA	C3B-C4B-NB	2.82	112.85	109.21		
37	c	516	DGD	03G-C3G-C2G	-2.82	104.10	110.90		
23	Ā	404	CLA	CHD-C4C-NC	2.82	128.64	124.20		
$\frac{-3}{23}$	b	606	CLA	C4C-C3C-C2C	-2.82	102.79	106.90		
35	Č	522	LMT	01B-C4'-C3'	2.82	114.78	107.28		
23	h	605	CLA	<u>C1-C2-C3</u>	-2.82	121.17	126.04		
$ \begin{array}{r} 23\\ 25\\ 24\\ 23\\ 23\\ 37\\ 23\\ 23\\ 35\\ 23\\ 23\\ \end{array} $	t A c c c A b C b	$ \begin{array}{r} 101 \\ 406 \\ 506 \\ 512 \\ 516 \\ 404 \\ 606 \\ 522 \\ 605 \\ \end{array} $	BCR PHO CLA CLA DGD CLA CLA LMT CLA	C1-C6-C7 C1C-C2C-C3C CGD-CBD-CAD C3B-C4B-NB O3G-C3G-C2G CHD-C4C-NC C4C-C3C-C2C O1B-C4'-C3' C1-C2-C3	$\begin{array}{c} 2.82 \\ \hline 2.82 \\ \hline -2.82 \\ \hline 2.82 \\ \hline -2.82 \\ \hline 2.82 \\ \hline 2.82 \\ \hline -2.82 \\ \hline 2.82 \\ \hline 2.82 \\ \hline -2.82 \\ \hline -2.82 \end{array}$	$\begin{array}{r} 122.52 \\ \hline 123.76 \\ \hline 103.27 \\ \hline 101.60 \\ \hline 112.85 \\ \hline 104.10 \\ \hline 128.64 \\ \hline 102.79 \\ \hline 114.78 \\ \hline 121.17 \end{array}$	$\begin{array}{r} 115.74 \\ 115.78 \\ 106.51 \\ 110.73 \\ 109.21 \\ 110.90 \\ 124.20 \\ 106.90 \\ 107.28 \\ 126.04 \end{array}$		



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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
23	С	507	CLA	C1D-CHD-C4C	-2.81	118.84	122.56
23	A	404	CLA	CAC-C3C-C4C	2.81	128.46	124.81
25	с	514	BCR	C38-C26-C25	-2.81	121.37	124.53
23	В	609	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
23	С	503	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	с	502	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	С	507	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	В	614	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
23	b	602	CLA	C11-C10-C8	-2.80	106.86	115.92
23	d	403	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
23	b	610	CLA	CMB-C2B-C3B	2.80	129.92	124.68
23	b	605	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
25	у	101	BCR	C28-C27-C26	-2.80	109.08	114.08
25	k	101	BCR	C3-C4-C5	-2.80	109.08	114.08
23	В	613	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	с	507	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	b	608	CLA	C1-C2-C3	-2.80	121.21	126.04
23	с	506	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
23	В	609	CLA	O2A-CGA-CBA	2.79	120.68	111.91
23	с	506	CLA	O2A-CGA-CBA	2.79	120.67	111.91
25	А	408	BCR	C7-C8-C9	-2.79	122.02	126.23
23	С	507	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	В	617	CLA	O2A-CGA-CBA	2.79	120.67	111.91
23	В	606	CLA	C3B-C4B-NB	2.79	112.82	109.21
23	В	607	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
36	В	629	HTG	C1-O5-C5	2.79	117.72	112.58
31	d	406	LHG	O8-C23-O10	-2.78	116.56	123.59
23	b	612	CLA	O2A-CGA-O1A	-2.78	116.56	123.59
25	A	408	BCR	C8-C7-C6	-2.78	119.39	127.20
25	b	618	BCR	C29-C30-C25	2.78	114.76	110.48
25	с	514	BCR	C28-C27-C26	-2.78	109.11	114.08
36	b	623	HTG	O5-C1-C2	2.78	113.81	110.31
25	С	515	BCR	C7-C8-C9	-2.78	122.04	126.23
23	В	610	CLA	C1-C2-C3	-2.78	121.24	126.04
23	В	608	CLA	CED-O2D-CGD	2.78	122.22	115.94
23	С	514	CLA	C3B-C4B-NB	2.78	112.80	109.21
26	В	621	SQD	O48-C23-C24	2.78	120.62	111.91
23	b	606	CLA	CMC-C2C-C1C	2.78	129.27	125.04
31	D	408	LHG	07-C7-C8	2.77	117.48	111.50
23	C	513	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
23	C	511	CLA	CAC-C3C-C4C	2.77	128.41	124.81
23	C	503	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
23 23 23	C C C	513 511 503	CLA CLA CLA	C4C-C3C-C2C CAC-C3C-C4C C4C-C3C-C2C	$ \begin{array}{r} -2.77\\ 2.77\\ -2.77\\ -2.77\end{array} $	102.85 128.41 102.86	$ \begin{array}{r} 111.00 \\ 106.90 \\ 124.81 \\ 106.90 \\ \end{array} $

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	Chain	l preui	Uus puye	Atoms	Z	Observed $(^{o})$	Ideal(°)
23	С	507		CHD C4C NC	2 77	128 57	124.20
$\frac{23}{23}$	B	615		CHD-C4C-NC	2.11 2.77	128.57 128.57	124.20 124.20
$\frac{20}{26}$	D D	413	SOD	0.17-0.40-100	-2.11	117.01	124.20 123.70
$\frac{20}{25}$	t D	101	BCB	$C_{20} C_{21} C_{22}$	2.11 2.77	193.36	125.70 197.31
$\frac{20}{24}$		402	PHO	$\begin{array}{c} 020 - 021 - 022 \\ \hline 010 \ 020 \ 021 - 022 \\ \hline \end{array}$	-2.11 2.77	103 33	127.51 106 51
24	B	613		$\frac{010-020-030}{020}$	-2.11 9.77	100.50	100.01
20	D	405		$\frac{O2A-CGA-CDA}{C2A-CTA-CHA}$	2.11 9.77	120.09	111.91
20 	d	400		CHC C1C C2C	-2.11 2.77	119.02	125.00 126.72
$\frac{20}{23}$	u B	616		$\frac{C4D}{C4D} \frac{C3D}{C4D} \frac{C4D}{C4D}$	-2.11 9.77	106.03	120.72 108.47
20	D	502		CHD CAC NC	-2.11 2.76	100.95	100.47
20	b	600		C2R C4R NR	2.10	112.30	124.20 100.21
25	D	618	BCB	$\frac{\text{C3D-C4D-IND}}{\text{C3D-C3D-C35}}$	2.70	112.70	109.21 110.48
20 02	D	604		CUC C1C C20	2.10	114.75	110.40 126.72
20 02	D	606		000000000000000000000000000000000000	-2.70	119.09	120.72
23	B D	606		OBD-CAD-C3D	-2.70	123.40	127.98
23	B	500	CLA CLA	CZA-CIA-CHA	-2.70	119.04	123.80
23		503	DLO	$\begin{array}{c} CAC-C3C-C4C \\ \hline CAC-C3C-C4C \\ \hline \end{array}$	2.75	128.38	124.81
29	<u>a</u>	405	PL9 CLA	C40-C39-C41	2.75	119.90	115.27
23	D	604	CLA	02A-CGA-OIA	-2.75	110.04	123.59
23	B	608	CLA	C3B-C4B-NB	2.75	112.77	109.21
23	b	609	CLA	$\begin{array}{c} C4C-C3C-C2C \\ \hline C4C-C3C-C2C \\ \hline \end{array}$	-2.75	102.89	106.90
23	A	405	CLA	CAC-C3C-C4C	2.75	128.38	124.81
25	b	619	BCR	C4-C5-C6	-2.75	118.74	122.73
23	В	610	CLA	CMC-C2C-CIC	2.75	129.22	125.04
23	d	403	CLA	C2A-CIA-CHA	-2.75	119.06	123.86
23	B	610	CLA	C1D-CHD-C4C	-2.75	118.94	122.56
23	C	506	CLA	C4-C3-C5	2.75	119.89	115.27
26	f	101	SQD	C4-C3-C2	-2.74	106.03	110.82
23	В	609	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
25	С	514	BCR	C35-C13-C14	-2.74	119.08	122.92
23	B	611	CLA	C3B-C4B-NB	2.74	112.75	109.21
25	A	408	BCR	C37-C22-C21	-2.74	119.08	122.92
24	a	407	PHO	C2B-C1B-NB	2.74	113.92	109.79
24	D	402	PHO	C2A-C1A-NA	2.74	115.00	111.86
23	b	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	b	603	CLA	C4-C3-C5	2.74	119.88	115.27
23	с	511	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
23	d	403	CLA	C3B-C4B-NB	2.74	112.75	109.21
31	А	415	LHG	O8-C23-C24	2.74	120.49	111.91
31	E	101	LHG	O8-C23-C24	$2.7\overline{4}$	120.49	111.91
23	a	409	CLA	$C1-C2-\overline{C3}$	-2.74	121.31	126.04
23	b	603	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
29	d	405	PL9	C7-C8-C9	-2.73	122.24	126.79

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		res		Atoms			10eai(°)
23	C	506	CLA	CHD-C4C-NC	2.73	128.51	124.20
29	D	407	PL9	C51-C49-C50	2.73	120.64	114.60
23	C	512	CLA	O2A-CGA-CBA	2.73	120.48	111.91
35	В	633	LMT	05'-C5'-C4'	2.73	115.51	109.75
25	d	404	BCR	C23-C24-C25	-2.73	119.55	127.20
31	d	408	LHG	O8-C23-C24	2.73	120.46	111.91
25	A	408	BCR	C33-C5-C6	-2.72	121.47	124.53
23	D	401	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
29	d	405	PL9	C37-C38-C39	-2.72	121.11	127.66
23	b	611	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
25	с	514	BCR	C2-C1-C6	2.72	114.67	110.48
23	a	409	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
23	b	611	CLA	CAC-C3C-C4C	2.72	128.34	124.81
29	a	415	PL9	C35-C34-C36	2.72	119.84	115.27
23	С	503	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	С	506	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	d	402	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
23	b	602	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
29	А	413	PL9	C35-C34-C36	2.71	119.83	115.27
23	b	607	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
23	В	608	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
23	В	606	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
24	a	407	PHO	C2C-C1C-NC	2.71	113.88	109.79
29	a	415	PL9	C20-C19-C21	2.71	119.83	115.27
23	b	601	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	D	402	PHO	C3C-C4C-NC	2.71	114.48	110.28
23	D	404	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
23	с	504	CLA	CMC-C2C-C1C	2.71	129.16	125.04
25	a	410	BCR	C38-C26-C25	-2.71	121.49	124.53
37	С	517	DGD	C4E-C3E-C2E	-2.70	106.10	110.82
23	b	604	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	С	506	CLA	CMC-C2C-C1C	2.70	129.16	125.04
25	В	619	BCR	C36-C18-C19	2.70	122.33	118.08
23	с	508	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
23	b	606	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
29	A	413	PL9	C25-C24-C26	2.70	119.81	115.27
23	В	610	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	b	603	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	c	502	CLA	O2A-CGA-CBA	2.70	120.37	111.91
26	D	413	SOD	O5-C5-C4	2.70	114.59	109.69
23	A	404	CLA	C4-C3-C5	2.70	119.81	115.27
23	A	405	CLA	CAA-C2A-C3A	-2.70	105.39	112.78

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
23	С	506	CLA	CHC-C1C-C2C	-2.70	119.27	126.72
23	b	610	CLA	C2A-C1A-CHA	-2.70	119.15	123.86
23	b	616	CLA	C4D-C3D-CAD	-2.70	106.97	108.47
23	a	404	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	a	406	CLA	C4-C3-C5	2.69	119.80	115.27
23	с	506	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
23	В	602	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	b	607	CLA	C4-C3-C5	2.69	119.80	115.27
23	В	607	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
29	а	415	PL9	C10-C9-C11	2.69	119.80	115.27
23	В	617	CLA	CBC-CAC-C3C	-2.69	105.01	112.43
23	В	603	CLA	O2A-CGA-CBA	2.69	120.35	111.91
23	b	610	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
23	b	608	CLA	O2A-CGA-CBA	2.69	120.34	111.91
29	D	407	PL9	C15-C14-C16	2.69	119.79	115.27
25	t	101	BCR	C7-C6-C5	-2.69	114.95	121.46
24	А	406	PHO	C1-C2-C3	-2.69	121.40	126.04
23	a	409	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	b	610	CLA	C3B-C4B-NB	2.68	112.68	109.21
23	с	513	CLA	O2A-CGA-CBA	2.68	120.33	111.91
23	А	407	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
23	D	405	CLA	CAC-C3C-C4C	2.68	128.29	124.81
31	L	101	LHG	O8-C23-C24	2.68	120.33	111.91
24	А	406	PHO	CHC-C1C-C2C	-2.68	118.98	125.73
25	Н	101	BCR	C29-C30-C25	2.68	114.61	110.48
23	В	604	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
23	С	502	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
23	b	608	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
29	d	405	PL9	C53-C6-C1	2.68	120.47	114.99
23	b	612	CLA	CHD-C4C-NC	2.68	128.42	124.20
25	t	101	BCR	C37-C22-C21	-2.68	119.17	122.92
24	A	406	PHO	C4D-CHA-C1A	-2.67	119.35	125.37
23	В	613	CLA	CMC-C2C-C1C	2.67	129.11	125.04
23	a	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	С	505	CLA	C1-C2-C3	-2.67	121.42	126.04
23	b	614	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	В	610	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
23	В	611	CLA	CAC-C3C-C4C	2.67	128.27	124.81
25	b	618	BCR	C37-C22-C23	2.67	122.28	118.08
23	С	505	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
37	C	519	DGD	O1G-C1A-C2A	2.67	120.28	111.91
37	с	518	DGD	O1G-C1A-C2A	2.67	120.28	111.91

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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$	
23	b	613	CLA	O2A-CGA-O1A	-2.67	116.86	123.59	
25	В	620	BCR	C24-C23-C22	-2.67	122.21	126.23	
23	С	513	CLA	C3B-C4B-NB	2.67	112.66	109.21	
25	у	101	BCR	C10-C11-C12	-2.66	114.90	123.22	
23	D	401	CLA	C2A-C1A-CHA	-2.66	119.20	123.86	
23	А	404	CLA	C4C-C3C-C2C	-2.66	103.01	106.90	
23	В	608	CLA	CHD-C4C-NC	2.66	128.40	124.20	
26	a	411	SQD	C1-O5-C5	-2.66	108.46	113.69	
23	с	513	CLA	C4-C3-C5	2.66	119.75	115.27	
25	В	620	BCR	C37-C22-C21	-2.66	119.20	122.92	
23	В	606	CLA	O2A-CGA-CBA	2.66	120.25	111.91	
31	d	407	LHG	O8-C23-C24	2.66	120.25	111.91	
23	b	608	CLA	CHC-C1C-C2C	-2.66	119.37	126.72	
29	А	413	PL9	C10-C9-C11	2.66	119.74	115.27	
23	b	612	CLA	CHC-C1C-C2C	-2.66	119.37	126.72	
26	a	411	SQD	C44-O6-C1	-2.66	108.55	113.74	
23	b	609	CLA	CHC-C1C-C2C	-2.66	119.38	126.72	
29	d	405	PL9	C17-C18-C19	-2.65	121.27	127.66	
23	В	617	CLA	CHC-C1C-C2C	-2.65	119.39	126.72	
23	С	508	CLA	C3B-C4B-NB	2.65	112.64	109.21	
23	В	616	CLA	C1-C2-C3	-2.65	121.46	126.04	
23	a	409	CLA	OBD-CAD-C3D	-2.65	123.58	127.98	
23	с	511	CLA	CMB-C2B-C3B	2.65	129.64	124.68	
37	h	103	DGD	O2G-C1B-C2B	2.65	117.21	111.50	
24	a	407	РНО	CMB-C2B-C1B	2.65	129.14	125.06	
23	b	610	CLA	CHC-C1C-C2C	-2.65	119.40	126.72	
23	с	508	CLA	C4D-C3D-CAD	-2.65	106.99	108.47	
23	В	613	CLA	C4D-C3D-CAD	-2.65	106.99	108.47	
25	b	618	BCR	C28-C27-C26	-2.65	109.35	114.08	
23	В	602	CLA	C2A-C1A-CHA	-2.65	119.23	123.86	
23	В	606	CLA	CAC-C3C-C4C	2.65	128.24	124.81	
23	С	507	CLA	C4C-C3C-C2C	-2.65	103.04	106.90	
23	D	401	CLA	O2A-CGA-O1A	-2.65	116.91	123.59	
23	с	513	CLA	O2D-CGD-O1D	-2.65	118.67	123.84	
23	с	513	CLA	C1-C2-C3	-2.64	121.47	126.04	
23	b	615	CLA	C4-C3-C5	2.64	119.72	115.27	
23	a	406	CLA	O2D-CGD-O1D	-2.64	118.67	123.84	
23	C	504	CLA	CHD-C4C-NC	2.64	128.37	124.20	
$\frac{-3}{25}$	Č	516	BCR	C15-C14-C13	-2.64	123.54	127.31	
$\frac{-3}{23}$	B	608	CLA	C2A-C1A-CHA	-2.64	119.24	123.86	
$\frac{-3}{23}$	b	602	CLA	O2A-CGA-CBA	2.64	120.19	111.91	
$\frac{-3}{23}$		510	CLA	02D-CGD-01D	-2.64	118 68	123.84	
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	С	510	CLA	C1-O2A-CGA	2.64	123.36	116.44
29	A	413	PL9	C53-C6-C1	2.64	120.38	114.99
29	d	405	PL9	C31-C32-C33	-2.64	103.22	111.88
23	С	505	CLA	CMC-C2C-C1C	2.63	129.05	125.04
23	D	404	CLA	OBD-CAD-C3D	-2.63	123.61	127.98
23	D	405	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
23	b	602	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
24	D	402	PHO	C2C-C1C-NC	2.63	113.77	109.79
23	С	512	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	D	401	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	с	512	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
23	С	503	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	a	407	PHO	C4D-ND-C1D	-2.63	102.03	106.76
23	D	401	CLA	CMA-C3A-C2A	-2.63	103.21	113.83
34	с	520	LMG	C3-C4-C5	2.63	114.93	110.24
23	С	508	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	b	601	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	В	617	CLA	C4-C3-C5	2.63	119.69	115.27
23	с	505	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	b	614	CLA	CHD-C4C-NC	2.63	128.34	124.20
23	b	602	CLA	CMB-C2B-C3B	2.63	129.59	124.68
23	с	507	CLA	C3B-C4B-NB	2.62	112.60	109.21
25	А	408	BCR	C16-C17-C18	-2.62	123.56	127.31
26	L	102	SQD	O48-C23-C24	2.62	120.14	111.91
23	b	604	CLA	CHC-C1C-C2C	-2.62	119.46	126.72
23	b	602	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
23	с	503	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	С	504	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	с	508	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
23	a	409	CLA	CMA-C3A-C2A	-2.62	103.26	113.83
23	b	615	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	В	613	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
24	a	407	PHO	CHD-C1D-C2D	-2.62	119.14	125.73
36	С	523	HTG	C1-O5-C5	2.62	117.41	112.58
23	с	509	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
23	b	615	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
23	С	511	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
23	C	506	CLA	CAC-C3C-C4C	2.62	128.20	124.81
26	D	413	SQD	O48-C23-C24	2.61	120.11	111.91
23	C	514	CLA	O2A-CGA-CBA	2.61	120.11	111.91
23	В	604	CLA	CAC-C3C-C4C	2.61	128.20	124.81
25	d	404	BCR	C28-C27-C26	-2.61	109.41	114.08

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	Chain	Res	Type	Atoms	<u>L</u>	Observed(°)	Ideal(°)
37	C	518	DGD	C2G-O2G-C1B	-2.61	111.36	117.79
24	A	406	PHO	CMC-C2C-CIC	2.61	129.09	125.06
23	С	505	CLA	CHC-CIC-C2C	-2.61	119.50	126.72
23	с	507	CLA	OID-CGD-CBD	-2.61	119.15	124.48
29	D	407	PL9	C20-C19-C21	2.61	119.66	115.27
23	В	611	CLA	CMC-C2C-C1C	2.61	129.01	125.04
23	A	407	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
29	A	413	PL9	C40-C39-C41	2.61	119.65	115.27
23	С	509	CLA	O2A-CGA-CBA	2.61	120.08	111.91
26	D	413	SQD	C3-C4-C5	2.60	114.89	110.24
23	с	508	CLA	CHD-C4C-NC	2.60	128.31	124.20
23	В	603	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	с	501	CLA	CMB-C2B-C3B	2.60	129.54	124.68
23	С	513	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
23	a	406	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
23	В	606	CLA	CMC-C2C-C1C	2.60	129.00	125.04
23	С	504	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
23	В	609	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
34	j	101	LMG	O8-C28-C29	2.60	120.06	111.91
23	С	513	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
25	В	619	BCR	C38-C26-C25	-2.60	121.61	124.53
23	А	405	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
23	a	405	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	А	405	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
23	с	507	CLA	C1D-CHD-C4C	-2.59	119.14	122.56
23	a	409	CLA	CMC-C2C-C1C	2.59	128.99	125.04
26	А	409	SQD	O47-C7-O49	-2.59	117.44	123.70
31	d	408	LHG	O8-C23-O10	-2.59	117.05	123.59
23	с	506	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	с	509	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	С	508	CLA	CHD-C4C-NC	2.59	128.28	124.20
26	a	413	SQD	O5-C5-C4	2.59	114.39	109.69
23	с	510	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
34	Z	101	LMG	O6-C1-C2	2.58	115.81	110.35
23	b	602	CLA	C11-C12-C13	-2.58	107.58	115.92
23	В	608	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
23	b	614	CLA	CMC-C2C-C1C	2.58	128.96	125.04
25	Т	101	BCR	C16-C17-C18	-2.58	123.63	127.31
23	с	505	CLA	CHD-C4C-NC	2.58	128.26	124.20
23	с	507	CLA	CHD-C4C-NC	2.58	128.26	124.20
24	a	408	PHO	C2B-C1B-NB	2.58	113.68	109.79
23	С	514	CLA	CAA-C2A-C3A	-2.57	105.73	112.78

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\mathbf{Mol}	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$ $ Ideal(o)
23	А	404	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
29	А	413	PL9	C12-C13-C14	-2.57	121.46	127.66
23	b	605	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
23	В	611	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
23	с	507	CLA	C4-C3-C5	2.57	119.60	115.27
25	D	406	BCR	C3-C4-C5	-2.57	109.48	114.08
23	В	616	CLA	O2A-CGA-CBA	2.57	119.98	111.91
34	J	101	LMG	C8-O7-C10	-2.57	111.46	117.79
23	с	513	CLA	CMB-C2B-C3B	2.57	129.49	124.68
25	с	515	BCR	C33-C5-C6	-2.57	121.64	124.53
23	с	502	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
23	В	615	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	В	612	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
23	с	502	CLA	CMC-C2C-C1C	2.57	128.95	125.04
24	a	408	PHO	C1C-C2C-C3C	-2.57	103.56	106.51
35	D	403	LMT	O5B-C5B-C4B	2.57	114.36	109.69
23	с	502	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
23	С	505	CLA	C4-C3-C5	2.57	119.59	115.27
23	В	616	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
23	С	504	CLA	C1-C2-C3	-2.56	121.61	126.04
23	В	606	CLA	CMB-C2B-C1B	2.56	132.41	128.46
31	d	406	LHG	O8-C23-C24	2.56	119.95	111.91
24	a	407	PHO	CHC-C1C-C2C	-2.56	119.28	125.73
29	D	407	PL9	C22-C23-C24	-2.56	121.49	127.66
23	В	614	CLA	O2A-CGA-CBA	2.56	119.95	111.91
23	с	513	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	с	513	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
23	с	501	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
24	a	407	PHO	CAC-C3C-C4C	2.56	128.01	125.22
24	D	402	PHO	C4-C3-C5	2.56	119.58	115.27
23	b	604	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
24	a	407	PHO	C1C-C2C-C3C	-2.56	103.57	106.51
23	b	616	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	С	509	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
25	С	527	BCR	C38-C26-C25	-2.56	121.66	124.53
23	с	509	CLA	CAC-C3C-C4C	2.56	128.13	124.81
23	A	407	CLA	C1-C2-C3	-2.56	121.62	126.04
23	С	513	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
23	В	615	CLA	CMC-C2C-C1C	2.55	128.93	125.04
25	С	527	BCR	C10-C11-C12	-2.55	115.25	123.22
23	b	601	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
23	С	513	CLA	C4-C3-C5	2.55	119.56	115.27



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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$	
25	b	618	BCR	C24-C23-C22	-2.55	122.38	126.23	
23	В	611	CLA	O2D-CGD-O1D	-2.55	118.85	123.84	
23	В	615	CLA	C2A-C1A-CHA	-2.55	119.40	123.86	
23	b	602	CLA	C4-C3-C5	2.55	119.56	115.27	
23	b	615	CLA	C11-C12-C13	-2.55	107.68	115.92	
24	a	408	PHO	CAC-C3C-C4C	2.55	128.00	125.22	
34	с	520	LMG	C1-O6-C5	2.55	118.69	113.69	
23	с	510	CLA	O1D-CGD-CBD	-2.55	119.27	124.48	
23	В	605	CLA	CHC-C1C-C2C	-2.55	119.68	126.72	
23	с	508	CLA	CMC-C2C-C1C	2.55	128.92	125.04	
26	В	621	SQD	C1-C2-C3	-2.55	104.69	110.00	
24	a	408	PHO	C4D-ND-C1D	-2.54	102.19	106.76	
23	В	614	CLA	CHD-C4C-NC	2.54	128.21	124.20	
25	В	620	BCR	C21-C20-C19	-2.54	115.28	123.22	
23	С	508	CLA	CHC-C1C-C2C	-2.54	119.69	126.72	
23	В	614	CLA	C4C-C3C-C2C	-2.54	103.19	106.90	
23	С	507	CLA	CAA-C2A-C3A	-2.54	105.82	112.78	
23	с	513	CLA	C2A-C1A-CHA	-2.54	119.42	123.86	
25	b	618	BCR	C3-C4-C5	-2.54	109.54	114.08	
36	b	626	HTG	C1-O5-C5	2.54	117.26	112.58	
24	a	407	PHO	O2A-CGA-O1A	-2.54	117.19	123.59	
37	с	517	DGD	O1G-C1A-C2A	2.53	119.86	111.91	
23	b	611	CLA	CBC-CAC-C3C	-2.53	105.45	112.43	
23	В	607	CLA	O2A-CGA-O1A	-2.53	117.20	123.59	
25	d	404	BCR	C37-C22-C23	2.53	122.06	118.08	
23	В	606	CLA	C1-C2-C3	-2.53	121.67	126.04	
23	с	501	CLA	O2A-CGA-CBA	2.52	119.83	111.91	
29	a	415	PL9	C53-C6-C1	2.52	120.15	114.99	
23	с	511	CLA	CMC-C2C-C1C	2.52	128.88	125.04	
25	у	101	BCR	C16-C17-C18	-2.52	123.71	127.31	
23	с	503	CLA	C4-C3-C5	2.52	119.51	115.27	
25	С	516	BCR	C7-C8-C9	-2.52	122.43	126.23	
23	с	502	CLA	C2A-C1A-CHA	-2.52	119.45	123.86	
25	В	618	BCR	C15-C14-C13	-2.52	123.72	127.31	
23	b	608	CLA	OBD-CAD-C3D	-2.52	123.80	127.98	
24	a	408	PHO	CBA-CAA-C2A	-2.52	106.43	113.86	
29	a	415	PL9	C17-C18-C19	-2.52	121.60	127.66	
23	с	507	CLA	C6-C7-C8	-2.52	107.78	115.92	
25	k	101	BCR	C10-C11-C12	-2.52	115.36	123.22	
23	С	502	CLA	OBD-CAD-C3D	-2.52	123.81	127.98	
23	B	612	CLA	C4C-C3C-C2C	-2.51	103.23	106.90	
23	В	616	CLA	CMB-C2B-C1B	2.51	132.33	128.46	



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Mol	Chain	Res	Type	Atoms		Observed(^o)	Ideal(°)
23	C	505	CLA	CAC-C3C-C4C	2.51	128.07	124.81
23	b	608	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	b	616	CLA	C1-C2-C3	-2.51	121.70	126.04
24	a	408	PHO	CHC-C1C-C2C	-2.51	119.41	125.73
23	b	603	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	d	403	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
23	С	502	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	a	409	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	d	405	PL9	C12-C13-C14	-2.51	121.62	127.66
23	с	507	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
23	b	616	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	В	615	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
29	a	415	PL9	C51-C49-C50	2.51	120.14	114.60
23	d	402	CLA	C4-C3-C5	2.51	119.49	115.27
23	В	602	CLA	CAC-C3C-C4C	2.51	128.06	124.81
23	С	502	CLA	CMB-C2B-C3B	2.51	129.37	124.68
25	С	527	BCR	C15-C14-C13	-2.50	123.73	127.31
23	a	406	CLA	O2A-CGA-CBA	2.50	119.77	111.91
26	f	101	SQD	O5-C5-C4	2.50	114.24	109.69
23	с	509	CLA	CMC-C2C-C1C	2.50	128.85	125.04
23	D	401	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
29	D	407	PL9	C7-C8-C9	-2.50	122.63	126.79
23	с	505	CLA	C4-C3-C5	2.50	119.48	115.27
25	d	404	BCR	C16-C17-C18	-2.50	123.74	127.31
23	В	608	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
23	В	603	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	b	610	CLA	CAC-C3C-C4C	2.50	128.05	124.81
26	A	409	SQD	O9-S-O7	-2.50	105.30	113.95
23	A	404	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
23	В	602	CLA	C4-C3-C5	2.50	119.47	115.27
26	a	413	SQD	C1-O5-C5	2.50	118.59	113.69
23	D	401	CLA	C3B-C4B-NB	2.50	112.44	109.21
23	С	510	CLA	O2A-CGA-CBA	2.50	119.74	111.91
34	i	101	LMG	C8-O7-C10	-2.50	111.65	117.79
23	D	401	CLA	O2A-CGA-CBA	2.49	119.74	111.91
25	B	618	BCR	C11-C10-C9	-2.49	123.75	127.31
25	C	516	BCR	C34-C9-C10	-2.49	119.43	122.92
26	a	411	SOD	047-C7-049	-2.49	117.68	123.70
23	a	409	CLA	CHD-C4C-NC	2.49	128.13	124.20
23	R	612	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
29	D	407	PL9	C30-C29-C31	2.10 2.49	119.46	115.72
23	h	604		C4-C3-C5	2.10 2.49	119.46	115.27
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Mol	Chain	Res	Type	Δtoms	7	Observed ⁽⁰⁾	Ideal(0)
22	Chain	507			2.48	110 70	$\frac{11101}{11101}$
20		101	I MC	OZA-CGA-CDA	2.40	119.70	111.91
04 95	ј Ц	101	BCB	C7 C6 C5	-2.40	117.70	123.70
20	D II	101 612	CLA	0.00000000000000000000000000000000000	2.40	127.40	121.40 192.50
20 	D	607		C4 C2 C5	-2.40	117.33	125.09 115.97
20	D L	610		$\frac{04-05-05}{04-010}$	2.40	119.44	115.27
23		010	CLA CLA		2.48	128.81	125.04
23	D	405	DUO	$\begin{array}{c} C4-C3-C5 \\ \hline C2C C4C NC \end{array}$	2.48	119.44	115.27
24	a	407	PHO	C3C-C4C-NC	2.48	114.12	110.28
23	D	404	CLA	CID-CHD-C4C	-2.48	119.29	122.56
24	a	408	PHO	C4D-CHA-CIA	-2.47	119.80	125.37
25	С	515	BCR	C36-C18-C19	2.47	121.97	118.08
23	d	402	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
23	C	506	CLA	O2A-CGA-CBA	2.47	119.67	111.91
25	a	410	BCR	C33-C5-C6	-2.47	121.75	124.53
23	В	607	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	с	504	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
25	с	514	BCR	C34-C9-C10	-2.47	119.46	122.92
23	a	404	CLA	C1-C2-C3	-2.47	121.77	126.04
23	В	617	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
31	е	101	LHG	O8-C23-C24	2.47	119.66	111.91
25	С	515	BCR	C38-C26-C25	-2.47	121.76	124.53
23	с	504	CLA	C1-O2A-CGA	2.47	122.92	116.44
29	d	405	PL9	C51-C49-C50	2.47	120.05	114.60
37	С	519	DGD	C3G-C2G-C1G	-2.47	105.96	111.79
29	D	407	PL9	C7-C3-C2	-2.46	120.06	123.30
23	В	607	CLA	CMC-C2C-C1C	2.46	128.79	125.04
23	В	606	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
23	С	511	CLA	C4-C3-C2	-2.46	117.36	123.68
37	С	518	DGD	O1G-C1A-C2A	2.46	119.63	111.91
24	А	406	PHO	O1D-CGD-CBD	-2.46	119.45	124.48
26	f	101	SQD	O48-C23-C24	2.46	119.63	111.91
23	b	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	с	515	BCR	C15-C14-C13	-2.46	123.80	127.31
31	d	406	LHG	C5-O7-C7	-2.46	111.74	117.79
23	a	404	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	b	618	BCR	C15-C14-C13	-2.46	123.80	127.31
26	D	413	SQD	07-S-C6	2.46	109.86	106.94
23	С	505	CLA	C1-O2A-CGA	2.46	122.89	116.44
29	a	415	PL9	C40-C39-C41	2.46	119.40	115.27
35	В	623	LMT	C1'-O5'-C5'	2.46	118.51	113.69
34	В	622	LMG	O1-C1-C2	-2.45	104.47	108.30
23	A	405	CLA	CHD-C4C-NC	2.45	128.07	124.20

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
25	у	101	BCR	C21-C20-C19	-2.45	115.56	123.22
26	f	101	SQD	O47-C7-O49	-2.45	117.78	123.70
26	L	102	SQD	O8-S-C6	2.45	109.64	105.74
23	С	513	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
23	с	505	CLA	O2A-CGA-CBA	2.45	119.59	111.91
37	с	517	DGD	O5D-C1E-C2E	2.45	112.12	108.30
23	b	601	CLA	O2A-CGA-CBA	2.45	119.59	111.91
23	a	406	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
37	С	517	DGD	C3G-C2G-C1G	-2.45	106.00	111.79
36	В	624	HTG	C1-O5-C5	2.44	117.09	112.58
23	a	405	CLA	CAA-CBA-CGA	2.44	120.40	113.25
23	С	513	CLA	CBA-CAA-C2A	-2.44	106.65	113.86
23	a	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	с	511	CLA	CAC-C3C-C4C	2.44	127.98	124.81
26	D	413	SQD	C44-O6-C1	-2.44	108.97	113.74
25	a	410	BCR	C2-C1-C6	2.44	114.23	110.48
23	d	403	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
25	Y	101	BCR	C29-C28-C27	-2.44	105.93	111.38
24	А	406	PHO	C2C-C1C-NC	2.44	113.47	109.79
23	В	616	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	с	506	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	h	102	BCR	C16-C15-C14	-2.43	118.49	123.47
24	a	407	PHO	CMC-C2C-C1C	2.43	128.81	125.06
23	С	513	CLA	CMA-C3A-C4A	-2.43	105.24	111.77
23	В	617	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
23	С	507	CLA	CMB-C2B-C3B	2.43	129.22	124.68
23	b	613	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
29	D	407	PL9	C25-C24-C26	2.42	119.35	115.27
25	А	408	BCR	C3-C4-C5	-2.42	109.75	114.08
23	b	603	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	С	507	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
23	a	405	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	b	602	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
23	В	613	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
25	Y	101	BCR	C36-C18-C19	2.42	121.89	118.08
25	Н	101	BCR	C15-C14-C13	-2.42	123.86	127.31
23	В	607	CLA	C11-C10-C8	-2.42	108.10	115.92
23	b	607	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	В	603	CLA	CHD-C4C-NC	2.42	128.01	124.20
34	m	101	LMG	C8-O7-C10	-2.42	111.84	117.79
26	L	102	SQD	C44-O6-C1	-2.42	109.02	113.74
25	С	516	BCR	C21-C20-C19	-2.41	115.69	123.22



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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	с	509	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
23	с	504	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	b	613	CLA	CED-O2D-CGD	2.41	121.39	115.94
36	b	623	HTG	C1-O5-C5	2.41	117.02	112.58
25	b	617	BCR	C3-C4-C5	-2.41	109.78	114.08
23	d	402	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
36	С	523	HTG	O5-C1-C2	2.41	113.34	110.31
25	a	410	BCR	C11-C10-C9	-2.41	123.88	127.31
23	С	513	CLA	CMB-C2B-C3B	2.41	129.18	124.68
24	а	408	PHO	O2D-CGD-O1D	-2.41	119.14	123.84
23	с	509	CLA	CED-O2D-CGD	2.40	121.38	115.94
29	D	407	PL9	C40-C39-C41	2.40	119.31	115.27
26	D	413	SQD	C1-C2-C3	-2.40	104.99	110.00
23	А	405	CLA	C4-C3-C5	2.40	119.31	115.27
23	В	608	CLA	C1-O2A-CGA	2.40	122.75	116.44
23	с	509	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	b	603	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
23	В	604	CLA	CMC-C2C-C1C	2.40	128.70	125.04
26	a	411	SQD	O48-C23-C24	2.40	119.44	111.91
23	a	405	CLA	O2A-CGA-CBA	2.40	119.44	111.91
23	b	605	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
23	b	611	CLA	CHD-C4C-NC	2.40	127.98	124.20
23	С	512	CLA	O2A-CGA-CBA	2.40	119.44	111.91
23	b	614	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	с	508	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
23	b	606	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
23	с	509	CLA	C4-C3-C5	2.40	119.30	115.27
23	С	514	CLA	C4-C3-C5	2.40	119.30	115.27
23	с	501	CLA	CHD-C4C-NC	2.40	127.98	124.20
24	D	402	PHO	CHD-C1D-C2D	-2.39	119.71	125.73
23	d	402	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	В	608	CLA	O2A-CGA-CBA	2.39	119.40	111.91
23	D	404	CLA	CHD-C4C-NC	2.39	127.96	124.20
23	b	615	CLA	CHD-C4C-NC	2.38	127.96	124.20
23	с	506	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
34	a	417	LMG	O8-C28-C29	2.38	119.38	111.91
25	h	102	BCR	C29-C30-C25	2.38	114.14	110.48
23	a	404	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
25	В	619	BCR	C2-C1-C6	2.38	114.14	110.48
31	D	408	LHG	O8-C23-C24	2.38	119.37	111.91
23	b	614	CLA	C2A-C1A-CHA	-2.38	119.70	123.86

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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
23	С	510	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
25	d	404	BCR	C23-C22-C21	-2.38	115.29	118.94
25	С	515	BCR	C23-C24-C25	-2.38	120.53	127.20
29	D	407	PL9	C36-C37-C38	-2.38	104.07	111.88
23	b	614	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
40	V	201	HEC	CBD-CAD-C3D	-2.38	108.10	112.49
29	А	413	PL9	C45-C44-C46	2.37	119.27	115.27
23	В	611	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
29	d	405	PL9	C27-C28-C29	-2.37	121.94	127.66
34	J	101	LMG	O8-C28-O10	-2.37	117.60	123.59
25	В	620	BCR	C10-C11-C12	-2.37	115.82	123.22
23	В	612	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	А	406	PHO	C4A-NA-C1A	-2.37	106.22	108.14
23	a	405	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	h	102	BCR	C37-C22-C21	-2.37	119.61	122.92
26	a	411	SQD	O9-S-C6	2.37	109.75	106.94
34	С	521	LMG	O8-C28-C29	2.37	119.33	111.91
25	В	618	BCR	C36-C18-C17	-2.37	119.61	122.92
35	В	634	LMT	O1'-C1'-C2'	2.36	112.00	108.30
34	m	101	LMG	O8-C28-O10	-2.36	117.63	123.59
35	В	623	LMT	C3'-C4'-C5'	2.36	116.34	110.93
23	b	612	CLA	CMC-C2C-C1C	2.36	128.64	125.04
23	b	602	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	A	407	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
25	k	101	BCR	C34-C9-C8	2.36	121.80	118.08
23	a	405	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
23	a	406	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
25	Y	101	BCR	C37-C22-C21	-2.36	119.62	122.92
25	b	619	BCR	C21-C20-C19	-2.36	115.86	123.22
36	В	629	HTG	O5-C5-C4	2.36	113.98	109.69
29	a	415	PL9	C45-C44-C46	2.36	119.24	115.27
36	c	522	HTG	O5-C5-C4	2.36	113.97	109.69
34	Z	101	LMG	C8-O7-C10	-2.36	111.99	117.79
23	b	613	CLA	C4-C3-C5	2.36	119.23	115.27
24	A	406	PHO	C4D-ND-C1D	-2.36	102 53	106.76
25	A	408	BCR	C31-C1-C6	-2.36	106.48	110.30
23	B	605	CLA	CHD-C4C-NC	2.35	127.91	124 20
23	R	612	CLA	CMA-C3A-C4A	-2.35	105 45	111 77
35	h	628	LMT	<u>C1'-C2'-C3'</u>	2.00 2.35	114.89	110.00
37	с С	516	DGD	0.02 G - 0.01 R	-2.35	118.09	123 70
25		406	BCB	C21_C20_C10	-2.35	115.88	123.10
25		597	BCR	$\begin{array}{c} 021 \\ 020 \\ 010 \\$	2.00	11/ 10	110.48
20		021	DON	02-01-00	⊿.00	114.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
23	d	403	CLA	C4-C3-C5	2.35	119.22	115.27		
23	С	503	CLA	C4-C3-C5	2.35	119.22	115.27		
23	А	404	CLA	C16-C15-C13	-2.35	108.33	115.92		
23	С	505	CLA	CHD-C4C-NC	2.35	127.90	124.20		
23	D	404	CLA	CAC-C3C-C4C	2.35	127.85	124.81		
23	В	602	CLA	CHB-C4A-NA	2.35	127.75	124.51		
23	С	512	CLA	C11-C10-C8	-2.34	108.34	115.92		
37	с	518	DGD	C3G-C2G-C1G	-2.34	106.25	111.79		
23	В	613	CLA	CHD-C4C-NC	2.34	127.89	124.20		
40	V	202	HEC	CAD-CBD-CGD	2.34	116.60	112.67		
23	b	613	CLA	C4D-C3D-CAD	-2.34	107.17	108.47		
25	Y	101	BCR	C34-C9-C8	2.34	121.76	118.08		
23	d	403	CLA	CAA-C2A-C3A	-2.34	106.38	112.78		
23	С	508	CLA	С11-С10-С8	-2.34	108.36	115.92		
25	h	102	BCR	C10-C11-C12	-2.33	115.94	123.22		
23	d	402	CLA	CAA-C2A-C3A	-2.33	106.39	112.78		
23	С	505	CLA	CHB-C4A-NA	2.33	127.74	124.51		
25	D	406	BCR	C16-C17-C18	-2.33	123.98	127.31		
23	D	405	CLA	OBD-CAD-C3D	-2.33	124.11	127.98		
24	А	406	PHO	C2B-C1B-NB	2.33	113.31	109.79		
37	С	519	DGD	O2G-C1B-C2B	2.33	116.52	111.50		
23	С	510	CLA	CMB-C2B-C3B	2.33	129.04	124.68		
37	С	517	DGD	C2G-O2G-C1B	-2.33	112.05	117.79		
23	D	405	CLA	CHC-C1C-C2C	-2.33	120.28	126.72		
23	С	514	CLA	CHC-C1C-C2C	-2.33	120.28	126.72		
23	b	606	CLA	O2A-CGA-CBA	2.33	119.21	111.91		
37	с	516	DGD	C3G-C2G-C1G	-2.33	106.29	111.79		
23	с	504	CLA	C2A-C1A-CHA	-2.33	119.79	123.86		
26	f	101	SQD	O5-C1-C2	2.32	115.27	110.35		
31	A	415	LHG	O7-C7-O9	-2.32	118.09	123.70		
31	d	406	LHG	O7-C7-O9	-2.32	118.09	123.70		
23	С	511	CLA	O2A-CGA-O1A	-2.32	117.73	123.59		
24	a	408	PHO	C4-C3-C2	-2.32	117.72	123.68		
34	j	101	LMG	O8-C28-O10	-2.32	117.73	123.59		
34	Z	101	LMG	C9-C8-C7	-2.32	106.30	111.79		
23	b	601	CLA	CBC-CAC-C3C	-2.32	106.04	112.43		
26	L	102	SQD	C1-C2-C3	-2.32	105.17	110.00		
25	a	410	BCR	C32-C1-C6	-2.32	106.54	110.30		
23	b	615	CLA	O2D-CGD-O1D	-2.31	119.31	123.84		
25	Y	101	BCR	C21-C20-C19	-2.31	116.00	123.22		
23	с	506	CLA	CBC-CAC-C3C	-2.31	106.05	112.43		
23	b	607	CLA	O2A-CGA-CBA	2.31	119.17	111.91		

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Mol	Chain	\mathbf{Res}	Tvpe	Atoms	Z	Observed(^o)	Ideal(°)
23	B	610	CLA	02D-CGD-01D	-2.31	119.32	123.84
$\frac{23}{23}$	b	601	CLA	CMC-C2C-C1C	2.01 2.31	128.56	125.04
$\frac{23}{23}$	C	505	CLA	CMB-C2B-C3B	2.31	129.00	124.68
23	C	508	CLA	CAC-C3C-C4C	2.31	127.81	124.81
25	k	101	BCR	C2-C1-C6	2.31	114.04	110.48
23	В	612	CLA	CMB-C2B-C3B	2.31	129.00	124.68
23	С	503	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
34	С	501	LMG	O1-C1-C2	2.31	111.90	108.30
25	h	102	BCR	C36-C18-C17	-2.31	119.69	122.92
23	с	510	CLA	C4-C3-C2	-2.31	117.76	123.68
26	a	411	SQD	O5-C1-C2	-2.30	105.47	110.35
23	b	611	CLA	OBD-CAD-C3D	-2.30	124.16	127.98
23	В	616	CLA	C6-C7-C8	-2.30	108.47	115.92
23	С	511	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	с	508	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
34	С	520	LMG	O8-C28-O10	-2.30	117.78	123.59
23	a	409	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	В	611	CLA	C6-C7-C8	-2.30	108.49	115.92
23	с	506	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	С	514	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
26	В	621	SQD	C3-C4-C5	2.30	114.33	110.24
23	с	507	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
25	В	620	BCR	C3-C4-C5	-2.29	109.98	114.08
23	b	612	CLA	CAC-C3C-C4C	2.29	127.79	124.81
23	С	509	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	b	619	BCR	C33-C5-C4	2.29	118.02	113.62
23	С	514	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
35	m	103	LMT	O5B-C5B-C4B	2.29	113.85	109.69
25	b	618	BCR	C21-C20-C19	-2.29	116.07	123.22
23	a	404	CLA	CMC-C2C-C1C	2.29	128.53	125.04
23	С	510	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
25	с	514	BCR	C3-C4-C5	-2.28	110.00	114.08
31	А	415	LHG	O8-C6-C5	-2.28	101.79	108.43
23	С	506	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
25	Y	101	BCR	C28-C27-C26	-2.28	110.00	114.08
23	b	606	CLA	$CAC-C\overline{3C-C4}C$	2.28	127.77	124.81
26	A	409	SQD	O48-C23-O10	-2.28	117.84	123.59
23	B	608	CLA	$CAC-C\overline{3C-C4C}$	2.28	127.77	124.81
23	с	510	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
23	C	511	CLA	CHD-C4C-NC	2.28	127.79	124.20
23	B	607	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
23	b	616	CLA	CMB-C2B-C3B	2.28	128.94	124.68

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Conti	Continued from previous page								
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
23	а	404	CLA	C4-C3-C5	2.28	119.10	115.27		
23	В	609	CLA	C4-C3-C5	2.28	119.10	115.27		
25	В	620	BCR	C2-C3-C4	-2.28	106.29	111.38		
23	В	609	CLA	CMC-C2C-C1C	2.28	128.51	125.04		
25	Y	101	BCR	C10-C11-C12	-2.28	116.11	123.22		
23	с	504	CLA	CHB-C4A-NA	2.28	127.66	124.51		
23	D	401	CLA	C4D-C3D-CAD	-2.28	107.20	108.47		
23	b	615	CLA	C4D-C3D-CAD	-2.28	107.20	108.47		
23	С	506	CLA	CBC-CAC-C3C	-2.28	106.16	112.43		
23	В	602	CLA	CBC-CAC-C3C	-2.28	106.16	112.43		
40	V	202	HEC	CMB-C2B-C3B	2.27	128.50	125.82		
25	b	619	BCR	C16-C17-C18	-2.27	124.06	127.31		
29	А	413	PL9	C51-C49-C50	2.27	119.63	114.60		
23	А	405	CLA	CMA-C3A-C4A	-2.27	105.66	111.77		
25	А	408	BCR	C35-C13-C12	2.27	121.66	118.08		
37	Н	102	DGD	O1G-C1A-C2A	2.27	119.04	111.91		
23	b	613	CLA	O2D-CGD-O1D	-2.27	119.40	123.84		
23	b	609	CLA	C2A-C1A-CHA	-2.27	119.89	123.86		
23	В	617	CLA	C2A-C1A-CHA	-2.27	119.89	123.86		
23	С	510	CLA	C2A-C1A-CHA	-2.27	119.89	123.86		
36	В	624	HTG	O5-C1-C2	2.27	113.17	110.31		
23	В	608	CLA	O2D-CGD-O1D	-2.27	119.41	123.84		
23	с	505	CLA	CMC-C2C-C1C	2.27	128.49	125.04		
25	у	101	BCR	C37-C22-C23	2.27	121.65	118.08		
34	Ζ	101	LMG	C1-O6-C5	2.27	118.13	113.69		
29	d	405	PL9	C16-C17-C18	-2.26	104.44	111.88		
23	С	502	CLA	O2A-CGA-CBA	2.26	119.01	111.91		
35	С	522	LMT	O1'-C1'-C2'	2.26	111.83	108.30		
25	с	514	BCR	C7-C8-C9	-2.26	122.82	126.23		
23	a	406	CLA	OBD-CAD-C3D	-2.26	124.23	127.98		
23	С	508	CLA	C4D-C3D-CAD	-2.26	107.21	108.47		
23	b	607	CLA	C1-O2A-CGA	2.26	122.37	116.44		
23	С	508	CLA	C4-C3-C5	2.26	119.07	115.27		
26	L	102	SQD	C1-O5-C5	-2.26	109.26	113.69		
23	с	503	CLA	CMC-C2C-C1C	2.26	128.48	125.04		
36	b	621	HTG	O5-C5-C4	2.26	113.79	109.69		
23	b	611	CLA	CMB-C2B-C3B	2.25	128.90	124.68		
34	Ζ	101	LMG	O6-C5-C4	2.25	113.78	109.69		
25	k	101	BCR	C20-C21-C22	-2.25	124.10	127.31		
25	С	516	BCR	C2-C1-C6	2.25	113.95	110.48		
23	D	405	CLA	CBC-CAC-C3C	-2.25	106.23	112.43		
25	c	515	BCR	C37-C22-C21	-2.25	119.77	122.92		
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	D	413	SQD	O9-S-C6	2.25	109.61	106.94
23	b	602	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
23	с	504	CLA	O2A-CGA-CBA	2.25	118.96	111.91
37	с	517	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
23	с	512	CLA	OBD-CAD-C3D	-2.25	124.25	127.98
36	В	624	HTG	O2-C2-C3	-2.25	105.16	110.35
23	В	609	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	В	609	CLA	CBC-CAC-C3C	-2.24	106.24	112.43
24	a	407	PHO	CBA-CAA-C2A	-2.24	107.24	113.86
25	В	620	BCR	C37-C22-C23	2.24	121.61	118.08
24	А	406	PHO	O2D-CGD-O1D	-2.24	119.45	123.84
25	В	619	BCR	C33-C5-C6	-2.24	122.01	124.53
23	a	405	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	В	605	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	с	510	CLA	CMB-C2B-C3B	2.24	128.87	124.68
23	С	503	CLA	O2A-CGA-CBA	2.24	118.93	111.91
23	А	407	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
23	С	508	CLA	OBD-CAD-C3D	-2.24	124.27	127.98
25	В	619	BCR	C16-C17-C18	-2.24	124.12	127.31
23	С	509	CLA	CHD-C4C-NC	2.24	127.73	124.20
23	с	504	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
23	С	504	CLA	OBD-CAD-C3D	-2.23	124.27	127.98
25	b	619	BCR	C37-C22-C23	2.23	121.59	118.08
23	D	401	CLA	C4C-C3C-C2C	-2.23	103.64	106.90
25	t	101	BCR	C16-C17-C18	-2.23	124.13	127.31
25	У	101	BCR	C1-C6-C7	2.23	122.09	115.78
37	с	516	DGD	C6D-O5D-C1E	-2.23	109.38	113.74
23	с	511	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
34	С	501	LMG	O7-C10-O9	-2.23	118.32	123.70
29	d	405	PL9	C25-C24-C23	-2.23	117.97	123.68
29	d	405	PL9	C45-C44-C43	-2.22	117.97	123.68
23	С	509	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
23	В	602	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
23	С	505	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
23	с	503	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
23	A	407	CLA	O2A-CGA-CBA	$2.2\overline{2}$	118.87	111.91
26	D	413	SQD	O48-C23-O10	-2.22	117.99	123.59
23	В	607	CLA	CAC-C3C-C4C	2.22	127.69	124.81
23	b	605	CLA	C1-O2A-CGA	2.22	122.26	116.44
23	C	502	CLA	C3D-CAD-CBD	2.22	110.52	107.61
29	A	413	PL9	C47-C48-C49	-2.22	120.17	127.75
23	b	613	CLA	CHB-C4A-NA	2.22	127.58	124.51



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
25	d	404	BCR	C11-C10-C9	-2.22	124.15	127.31
23	с	503	CLA	CHD-C4C-NC	2.22	127.70	124.20
25	Y	101	BCR	C40-C30-C25	-2.22	106.70	110.30
25	Н	101	BCR	C2-C1-C6	2.22	113.89	110.48
23	A	407	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
23	С	508	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
31	L	101	LHG	O4-P-O5	2.22	123.19	112.24
23	a	406	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	с	505	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
25	k	101	BCR	C28-C27-C26	-2.21	110.13	114.08
23	a	409	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	a	407	PHO	C3A-C4A-CHB	-2.21	118.01	121.83
26	А	409	SQD	O8-S-C6	2.21	109.26	105.74
23	С	507	CLA	OBD-CAD-C3D	-2.21	124.31	127.98
29	d	405	PL9	C36-C34-C33	-2.20	116.66	121.12
23	В	611	CLA	OBD-CAD-C3D	-2.20	124.32	127.98
23	А	407	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
23	b	610	CLA	CMA-C3A-C2A	-2.20	104.95	113.83
23	С	513	CLA	CHB-C4A-NA	2.20	127.55	124.51
25	с	515	BCR	C37-C22-C23	2.20	121.54	118.08
23	В	606	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	D	409	LHG	O8-C23-O10	-2.20	118.05	123.59
23	b	604	CLA	CHA-C1A-NA	-2.20	121.37	126.40
23	С	513	CLA	C1-C2-C3	-2.20	122.24	126.04
23	b	607	CLA	CHD-C4C-NC	2.20	127.66	124.20
24	a	408	PHO	C2A-C1A-NA	2.20	114.38	111.86
34	j	101	LMG	O7-C10-O9	-2.20	118.40	123.70
25	D	406	BCR	C29-C30-C25	2.19	113.86	110.48
29	a	415	PL9	C47-C48-C49	-2.19	120.25	127.75
23	В	612	CLA	O2A-CGA-CBA	2.19	118.79	111.91
25	В	618	BCR	C31-C1-C6	-2.19	106.75	110.30
23	с	501	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	b	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	В	617	CLA	C1-C2-C3	-2.19	122.25	126.04
23	с	512	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
23	B	613	CLA	C11-C12-C13	-2.18	108.86	115.92
29	A	413	PL9	C37-C36-C34	-2.18	105.80	112.98
$\frac{-3}{23}$	D	405	CLA	C1-C2-C3	-2.18	122.27	126.04
25	C C	515	BCR	C15-C16-C17	-2.18	119.01	123.01 123.47
$\frac{-20}{34}$	7	101	LMG	C7-01-C1	-2.18	109.48	113 74
23	h h	602	CLA	C4D-C3D-CAD	-2.18	107.10	108 47
20	h	602		C4D-C3D-CAD	_2.10	107.25	108.47
$\begin{array}{r} 25\\ 34\\ 23\\ 23\end{array}$	c z b b	$ 515 \\ 101 \\ 602 \\ 608 $	BCR LMG CLA CLA	C15-C16-C17 C7-O1-C1 C4D-C3D-CAD C4D-C3D-CAD	-2.18 -2.18 -2.18 -2.18	$ 119.01 \\ 109.48 \\ 107.25 \\ 107.25 $	123.47 113.74 108.47 108.47

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		res		Atoms		Ubserved(°)	100.47
23	d	403	CLA	C4D-C3D-CAD	-2.18	107.26	108.47
23	C	504	CLA	CMB-C2B-C3B	2.18	128.75	124.68
23	a	405	CLA	C4-C3-C5	2.18	118.93	115.27
23	C	509	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	C	513	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	a	404	CLA	CED-O2D-CGD	2.17	120.85	115.94
23	с	501	CLA	CMC-C2C-C1C	2.17	128.34	125.04
25	C	527	BCR	C37-C22-C21	-2.17	119.88	122.92
26	L	102	SQD	O47-C7-O49	-2.17	118.46	123.70
25	В	620	BCR	C29-C30-C25	2.17	113.82	110.48
23	b	603	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	с	511	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
25	с	515	BCR	C21-C20-C19	-2.17	116.45	123.22
25	С	516	BCR	C24-C23-C22	-2.17	122.96	126.23
23	В	602	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
25	k	101	BCR	C7-C8-C9	-2.16	122.97	126.23
23	a	405	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
23	b	613	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
23	В	606	CLA	C4D-C3D-CAD	-2.16	107.26	108.47
25	С	527	BCR	C36-C18-C19	2.16	121.48	118.08
23	С	508	CLA	C6-C7-C8	-2.16	108.93	115.92
25	d	404	BCR	C21-C20-C19	-2.16	116.47	123.22
25	a	410	BCR	C36-C18-C19	2.16	121.48	118.08
24	a	408	PHO	CBD-CHA-C1A	2.16	131.41	126.40
23	D	404	CLA	CMB-C2B-C3B	2.16	128.72	124.68
24	a	407	PHO	C4-C3-C5	2.16	118.91	115.27
40	V	202	HEC	C3B-C4B-NB	-2.16	106.86	110.94
23	С	502	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
23	a	404	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
23	с	513	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
25	h	102	BCR	C35-C13-C12	2.16	121.48	118.08
23	с	504	CLA	CED-O2D-CGD	2.16	120.82	115.94
37	С	518	DGD	O1G-C1A-O1A	-2.16	118.14	123.59
24	D	402	PHO	O2A-CGA-CBA	2.16	118.68	111.91
23	В	605	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	b	615	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	b	616	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
23	В	614	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	d	404	BCR	C40-C30-C25	-2.16	106.80	110.30
23	B	609	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
23	B	611	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
23	b	607	CLA	CBC-CAC-C3C	-2.15	106.49	112.43

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Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
23	В	617	CLA	CMB-C2B-C3B	2.15	128.71	124.68
38	е	103	HEM	C3C-C4C-NC	-2.15	106.88	110.94
40	v	201	HEC	C3B-C4B-NB	-2.15	106.88	110.94
23	В	611	CLA	CMB-C2B-C3B	2.15	128.70	124.68
23	с	513	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	d	403	CLA	C1-C2-C3	-2.15	122.33	126.04
25	k	101	BCR	C34-C9-C10	-2.15	119.92	122.92
23	В	608	CLA	C4-C3-C5	2.15	118.88	115.27
31	L	101	LHG	C5-O7-C7	-2.15	112.51	117.79
23	с	509	CLA	CMB-C2B-C3B	2.15	128.69	124.68
23	b	601	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
23	a	409	CLA	CBC-CAC-C3C	-2.15	106.52	112.43
23	В	605	CLA	CMB-C2B-C3B	2.14	128.69	124.68
25	Н	101	BCR	C31-C1-C6	-2.14	106.82	110.30
23	D	405	CLA	CHB-C4A-NA	2.14	127.48	124.51
25	А	408	BCR	C36-C18-C19	2.14	121.45	118.08
23	С	504	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
23	С	509	CLA	CAC-C3C-C2C	2.14	131.19	127.53
23	С	505	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
34	m	101	LMG	C1-C2-C3	-2.14	105.54	110.00
29	d	405	PL9	C42-C41-C39	-2.14	105.94	112.98
23	В	614	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
23	b	608	CLA	C11-C10-C8	-2.14	109.01	115.92
25	b	617	BCR	C16-C17-C18	-2.14	124.26	127.31
23	b	611	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
23	В	609	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
23	b	614	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
23	В	614	CLA	C7-C6-C5	-2.13	107.56	113.36
25	В	619	BCR	C37-C22-C23	2.13	121.44	118.08
23	В	609	CLA	CAC-C3C-C2C	2.13	131.18	127.53
23	a	405	CLA	C4C-C3C-C2C	-2.13	103.79	106.90
23	a	409	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
23	a	404	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
31	Е	101	LHG	O8-C23-O10	-2.13	118.22	123.59
23	В	611	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
23	В	607	CLA	CMB-C2B-C3B	2.13	128.66	124.68
23	с	509	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
23	D	401	CLA	CAA-CBA-CGA	2.12	119.46	113.25
23	с	502	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	с	512	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
23	В	603	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
23	a	404	CLA	C4C-C3C-C2C	-2.12	103.81	106.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
24	a	408	PHO	CHD-C1D-C2D	-2.12	120.40	125.73
23	В	603	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	с	504	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
26	a	413	SQD	O7-S-C6	2.12	109.46	106.94
34	с	519	LMG	O7-C10-O9	-2.12	118.58	123.70
23	с	501	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
23	С	502	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	b	615	CLA	C6-C7-C8	-2.12	109.08	115.92
23	В	604	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
23	a	406	CLA	CMB-C2B-C3B	2.12	128.64	124.68
23	С	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	b	608	CLA	C4-C3-C5	2.12	118.83	115.27
25	b	617	BCR	C37-C22-C21	-2.11	119.96	122.92
23	В	606	CLA	C4-C3-C5	2.11	118.83	115.27
23	b	602	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	С	506	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
23	В	616	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	k	101	BCR	C36-C18-C19	2.11	121.40	118.08
24	a	407	PHO	C1-C2-C3	-2.11	122.40	126.04
25	Y	101	BCR	C36-C18-C17	-2.11	119.97	122.92
23	с	510	CLA	C6-C7-C8	-2.11	109.11	115.92
24	А	406	PHO	CBA-CAA-C2A	-2.11	107.64	113.86
25	с	514	BCR	C15-C16-C17	-2.11	119.16	123.47
24	a	407	PHO	OBD-CAD-C3D	-2.11	123.45	128.52
23	В	616	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
35	b	628	LMT	C3'-C4'-C5'	-2.11	106.10	110.93
23	b	604	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
23	с	512	CLA	CMC-C2C-C1C	2.10	128.24	125.04
23	b	613	CLA	C1-C2-C3	-2.10	122.41	126.04
23	b	607	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
23	С	505	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
23	В	604	CLA	C1-C2-C3	-2.10	122.41	126.04
23	b	606	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	b	615	CLA	C1-O2A-CGA	2.10	121.95	116.44
25	Y	101	BCR	C38-C26-C25	-2.10	122.17	124.53
25	A	408	BCR	C37-C22-C23	2.10	121.38	118.08
34	с	519	LMG	O8-C28-O10	-2.10	118.30	123.59
23	a	404	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
26	a	413	SQD	O8-S-C6	2.10	109.08	105.74
23	В	602	CLA	CMC-C2C-C1C	2.10	128.23	125.04
25	Y	101	BCR	C11-C10-C9	-2.10	124.32	127.31
34	с	520	LMG	C9-C8-C7	-2.09	106.83	111.79

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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	В	614	CLA	CED-O2D-CGD	2.09	120.67	115.94
23	с	510	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
37	С	517	DGD	O2G-C1B-O1B	-2.09	118.64	123.70
31	d	407	LHG	O8-C23-O10	-2.09	118.31	123.59
23	b	611	CLA	C7-C6-C5	-2.09	107.67	113.36
23	d	402	CLA	CHD-C4C-NC	2.09	127.50	124.20
23	А	405	CLA	CMC-C2C-C1C	2.09	128.22	125.04
26	А	411	SQD	O48-C23-O10	-2.09	118.31	123.59
23	В	612	CLA	C1-O2A-CGA	2.09	121.93	116.44
23	В	617	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	С	505	CLA	O2A-CGA-CBA	2.09	118.47	111.91
23	С	512	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
23	В	604	CLA	C5-C3-C2	-2.09	116.89	121.12
23	С	508	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
35	е	102	LMT	O1B-C1B-C2B	2.09	113.51	108.10
23	В	612	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	с	515	BCR	C29-C30-C25	2.09	113.69	110.48
26	D	413	SQD	C46-C45-C44	-2.09	106.85	111.79
23	С	514	CLA	CMB-C2B-C3B	2.09	128.58	124.68
40	V	202	HEC	CMB-C2B-C1B	-2.09	125.26	128.46
35	е	102	LMT	C1B-C2B-C3B	2.08	114.34	110.00
34	с	520	LMG	O8-C28-O10	-2.08	118.33	123.59
25	h	102	BCR	C20-C21-C22	-2.08	124.34	127.31
25	с	515	BCR	C16-C17-C18	-2.08	124.34	127.31
25	В	618	BCR	C33-C5-C4	2.08	117.62	113.62
23	b	604	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
23	D	404	CLA	C11-C12-C13	-2.08	109.19	115.92
23	С	512	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
25	Т	101	BCR	C7-C6-C5	-2.08	116.43	121.46
24	a	408	PHO	C2C-C1C-NC	2.08	112.93	109.79
35	М	101	LMT	O1B-C1B-C2B	2.08	113.48	108.10
26	В	621	SQD	O48-C23-O10	-2.08	118.35	123.59
29	D	407	PL9	C42-C41-C39	-2.08	106.15	112.98
24	D	402	PHO	CMB-C2B-C1B	2.08	128.26	125.06
34	j	101	LMG	C7-O1-C1	-2.07	109.69	113.74
37	Н	102	DGD	C3G-O3G-C1D	-2.07	109.69	113.74
24	D	402	PHO	CBD-CHA-C1A	2.07	131.21	126.40
23	b	602	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
23	b	615	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
23	a	405	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
25	Y	101	BCR	C33-C5-C4	2.07	117.59	113.62
29	d	405	PL9	C7-C3-C4	2.07	118.56	116.88



Mol	Chain	Res		Atoms	Z	$Observed(^{o})$	Ideal(°)
23	с	512	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	D	406	BCR	C32-C1-C6	-2.07	106.95	110.30
24	A	406	PHO	C7-C6-C5	-2.07	107.75	113.36
24	a	408	PHO	O2A-CGA-CBA	2.07	118.39	111.91
25	у	101	BCR	C7-C6-C5	-2.07	116.46	121.46
23	D	401	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
23	А	407	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
25	С	516	BCR	C15-C16-C17	-2.06	119.25	123.47
25	а	410	BCR	C3-C4-C5	-2.06	110.40	114.08
23	с	503	CLA	C1-O2A-CGA	2.06	121.85	116.44
25	D	406	BCR	C37-C22-C23	2.06	121.32	118.08
23	с	505	CLA	C1-O2A-CGA	2.06	121.85	116.44
24	А	406	PHO	CBD-CHA-C1A	2.06	131.18	126.40
23	a	406	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
25	a	410	BCR	C15-C16-C17	-2.06	119.26	123.47
38	Е	103	HEM	C3C-C4C-NC	-2.06	107.06	110.94
34	В	622	LMG	C8-O7-C10	-2.06	112.72	117.79
23	С	510	CLA	C16-C15-C13	-2.06	109.27	115.92
40	V	201	HEC	CMB-C2B-C1B	-2.06	125.30	128.46
23	d	402	CLA	CAC-C3C-C4C	2.06	127.48	124.81
23	b	601	CLA	CAC-C3C-C4C	2.05	127.48	124.81
25	А	408	BCR	C35-C13-C14	-2.05	120.05	122.92
23	С	512	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
37	С	517	DGD	O1G-C1A-O1A	-2.05	118.42	123.59
25	С	516	BCR	C38-C26-C25	-2.05	122.22	124.53
23	с	510	CLA	CED-O2D-CGD	2.05	120.58	115.94
26	В	621	SQD	O9-S-C6	2.05	109.38	106.94
23	В	612	CLA	CED-O2D-CGD	2.05	120.57	115.94
25	а	410	BCR	C10-C11-C12	-2.05	116.82	123.22
23	С	509	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
35	С	522	LMT	O5'-C5'-C4'	2.05	114.06	109.75
23	с	508	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
23	с	507	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	b	607	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
23	D	405	CLA	CMB-C2B-C1B	2.04	131.60	128.46
23	b	613	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
35	М	103	LMT	O5'-C5'-C4'	2.04	114.06	109.75
25	D	406	BCR	C10-C11-C12	-2.04	116.84	123.22
36	b	621	HTG	C3-C4-C5	2.04	113.88	110.24
23	В	616	CLA	CHB-C4A-NA	2.04	127.33	124.51
35	a	418	LMT	C1B-O1B-C4'	-2.04	112.92	117.96
23	b	602	CLA	CMA-C3A-C2A	-2.04	105.60	113.83



MolChainResTypeAtomsZObserved(o)Ideal23c501CLAC3D-CAD-CBD2.04110.29107.623b616CLACED-O2D-CGD2.04120.55115.923B603CLAC11-C10-C8-2.04109.34115.929A413PL9C7-C8-C9-2.04123.40126.723b608CLAC11-C12-C13-2.04109.34115.924c519LMGC8-O7-C10-2.04112.78117.735e102LMTO5'-C5'-C4'2.03114.04109.725d404BCRC29-C30-C252.03113.61110.423b608CLACAC-C3C-C4C2.03127.45124.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
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$\begin{array}{c cccccccccccc} 23 & B & 603 & CLA & C11-C10-C8 & -2.04 & 109.34 & 115.9 \\ \hline 29 & A & 413 & PL9 & C7-C8-C9 & -2.04 & 123.40 & 126.7 \\ \hline 23 & b & 608 & CLA & C11-C12-C13 & -2.04 & 109.34 & 115.9 \\ \hline 34 & c & 519 & LMG & C8-O7-C10 & -2.04 & 112.78 & 117.7 \\ \hline 35 & e & 102 & LMT & O5'-C5'-C4' & 2.03 & 114.04 & 109.7 \\ \hline 25 & d & 404 & BCR & C29-C30-C25 & 2.03 & 113.61 & 110.4 \\ \hline 23 & b & 608 & CLA & CAC-C3C-C4C & 2.03 & 127.45 & 124.8 \\ \hline \end{array}$
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34 c 519 LMG C8-O7-C10 -2.04 112.78 117.7 35 e 102 LMT O5'-C5'-C4' 2.03 114.04 109.7 25 d 404 BCR C29-C30-C25 2.03 113.61 110.4 23 b 608 CLA CAC-C3C-C4C 2.03 127.45 124.8
35 e 102 LMT O5'-C5'-C4' 2.03 114.04 109.7 25 d 404 BCR C29-C30-C25 2.03 113.61 110.4 23 b 608 CLA CAC-C3C-C4C 2.03 127.45 124.8
25 d 404 BCR C29-C30-C25 2.03 113.61 110.4 23 b 608 CLA CAC-C3C-C4C 2.03 127.45 124.8
23 b 608 CLA CAC-C3C-C4C 2.03 127.45 124.8 20 415 PLO 606 <td< td=""></td<>
29 a 415 PL9 C7-C8-C9 -2.03 123.41 126.7
23 B 611 CLA O2A-CGA-O1A -2.03 118.47 123.5
23 B 605 CLA C6-C7-C8 -2.03 109.36 115.9
23 b 615 CLA CHC-C1C-NC 2.03 127.28 124.2
23 C 514 CLA CMA-C3A-C2A -2.03 105.64 113.8
23 c 507 CLA C11-C10-C8 -2.03 109.36 115.9
34 B 622 LMG C12-C11-C10 -2.03 106.25 113.6
23 a 405 CLA CMC-C2C-C1C 2.03 128.13 125.0
23 B 608 CLA O2A-CGA-O1A -2.03 118.47 123.5
25 B 619 BCR C10-C11-C12 -2.03 116.89 123.2
37 C 519 DGD O1G-C1A-O1A -2.03 118.48 123.5
25 B 619 BCR C28-C27-C26 -2.03 110.46 114.0
35 D 403 LMT O1B-C1B-C2B 2.02 113.34 108.1
24 a 408 PHO C3C-C4C-NC 2.02 113.42 110.2
23 b 616 CLA CBC-CAC-C3C -2.02 106.85 112.4
23 a 409 CLA CMA-C3A-C4A -2.02 106.33 111.7
23 b 612 CLA C6-C7-C8 -2.02 109.38 115.9
25 B 619 BCR C35-C13-C14 -2.02 120.09 122.9
34 C 501 LMG O8-C28-C29 2.02 118.25 111.9
23 B 610 CLA C1-O2A-CGA 2.02 121.75 116.4
23 C 512 CLA C1-C2-C3 -2.02 122.55 126.0
25 B 619 BCR C36-C18-C17 -2.02 120.09 122.9
23 C 514 CLA OBD-CAD-C3D -2.02 124.63 127.9
23 A 404 CLA OBD-CAD-C3D -2.02 124.63 127.9
23 a 409 CLA CHB-C4A-NA 2.02 127.31 124.5
23 a 405 CLA CMA-C3A-C2A -2.02 105.68 113.8
37 c 518 DGD O6E-C1E-O5D -2.02 105.19 109.9
34 a 417 LMG 01-C1-C2 2.02 111.45 108.3
23 B 617 CLA CAC-C3C-C4C 2.02 127.43 124.8
34 C 501 LMG C30-C29-C28 -2.02 106.29 113.6
23 c 503 CLA O2A-CGA-O1A -2.02 118.50 123 5
25 b 617 BCR C38-C26-C25 -2.02 122.27 124 5
25 H 101 BCR C39-C30-C25 -2.01 107.03 110.2

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	Chain	Res	Type	Δtoms	7	Observed $(^{o})$	Ideal(°)
- 1 1101 		405			2.01	105 71	112.82
25	A C	400 516	BCB	$\begin{array}{c} \text{CMA-CJA-CJA} \\ \text{C27 C22 C22} \end{array}$	-2.01	105.71	119.00
20	C	510	CLA	$\begin{array}{c} 0.37 + 0.22 + 0.23 \\ \hline 0.1 \\ 0.24 \\ \hline 0.2$	2.01	121.20 101.70	116.00
20	C	101		CI-OZA-CGA	2.01	121.72	110.44 102.47
20	У	101	BUR I MT	010-010-014	-2.01	119.30	123.47
- <u>3</u> 5 - 99	B	023		UIB-04-03	2.01	112.04	107.28
23	A	405	CLA	CMB-C2B-C3B	2.01	128.44	124.08
23	b	609	CLA	<u> </u>	-2.01	107.89	113.36
29	D	407	PL9	C47-C48-C49	-2.01	120.88	127.75
37	C	518	DGD	C3G-O3G-C1D	-2.01	109.81	113.74
40	V	202	HEC	CBD-CAD-C3D	-2.01	108.78	112.49
23	A	404	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	В	608	CLA	CMB-C2B-C3B	2.01	128.44	124.68
23	В	610	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
23	b	606	CLA	C1-C2-C3	-2.01	122.57	126.04
23	b	616	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	D	407	PL9	C17-C18-C19	-2.01	122.82	127.66
23	С	509	CLA	CMD-C2D-C3D	2.01	128.43	124.68
25	С	527	BCR	C33-C5-C6	-2.01	122.27	124.53
23	В	613	CLA	C6-C5-C3	-2.01	108.19	113.45
25	с	514	BCR	C29-C28-C27	-2.01	106.89	111.38
23	с	510	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
23	В	602	CLA	CMB-C2B-C3B	2.00	128.43	124.68
25	С	515	BCR	C21-C20-C19	-2.00	116.96	123.22
25	b	618	BCR	C8-C7-C6	-2.00	121.57	127.20
23	d	402	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	с	503	CLA	C2A-C1A-CHA	-2.00	120.35	123.86
24	D	402	PHO	CAA-CBA-CGA	-2.00	107.40	113.25
25	с	514	BCR	C37-C22-C23	2.00	121.23	118.08
24	А	406	PHO	C4-C3-C5	2.00	118.64	115.27
23	В	603	CLA	C11-C12-C13	-2.00	109.45	115.92
23	В	605	CLA	C11-C10-C8	-2.00	109.45	115.92
23	В	615	CLA	CHC-C1C-NC	2.00	127.24	124.20
23	В	606	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
23	b	611	CLA	C11-C12-C13	-2.00	109.45	115.92

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All (194) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	с	502	CLA	NC
23	с	502	CLA	ND
23	с	502	CLA	NA
23	В	608	CLA	NC



Mol	Chain	Res	Type	Atom
23	В	608	CLA	ND
23	В	608	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	В	606	CLA	NC
23	В	606	CLA	ND
23	В	606	CLA	NA
23	А	405	CLA	NC
23	А	405	CLA	NA
23	с	508	CLA	NC
23	с	508	CLA	ND
23	с	508	CLA	NA
23	D	404	CLA	ND
23	с	511	CLA	NC
23	с	511	CLA	ND
23	с	511	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	С	504	CLA	NC
23	С	504	CLA	ND
23	С	504	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	NA
23	В	602	CLA	NC
23	В	602	CLA	ND
23	В	602	CLA	NA
23	С	507	CLA	NC
23	С	507	CLA	ND
23	С	507	CLA	NA
23	C	502	CLA	NC
23	С	502	CLA	ND
23	С	502	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA
23	D	401	CLA	NC
23	D	401	CLA	ND

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Mol	Chain	Res	Type	Atom
23	D	401	CLA	NA
23	с	509	CLA	NC
23	с	509	CLA	ND
23	с	509	CLA	NA
23	с	512	CLA	NC
23	с	512	CLA	ND
23	с	512	CLA	NA
23	d	402	CLA	ND
23	с	506	CLA	NC
23	с	506	CLA	ND
23	с	506	CLA	NA
23	с	503	CLA	NC
23	с	503	CLA	ND
23	с	503	CLA	NA
23	В	609	CLA	NC
23	В	609	CLA	ND
23	В	609	CLA	NA
23	А	407	CLA	NC
23	А	407	CLA	ND
23	А	407	CLA	NA
23	С	510	CLA	NC
23	С	510	CLA	ND
23	С	510	CLA	NA
23	С	514	CLA	NC
23	С	514	CLA	NA
23	В	604	CLA	NC
23	В	604	CLA	ND
23	В	604	CLA	NA
23	В	605	CLA	NC
23	В	605	CLA	ND
23	В	605	CLA	NA
23	с	505	CLA	ND
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND

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Mol	Chain	Res		Atom
	h	619		NA
$\frac{20}{23}$	0	501		NC NC
20 	C	501		ND
	C	501		ND NA
<u></u> 	C b	608	CLA	NA NC
20 	D L	008 C08		NO NA
23	D	608	CLA	NA
23	D	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	C	505	CLA	NC
23	С	505	CLA	ND
23	С	505	CLA	NA
23	С	511	CLA	NC
23	С	511	CLA	ND
23	С	511	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	с	510	CLA	NC
23	с	510	CLA	ND
23	с	510	CLA	NA
23	В	613	CLA	NC
23	В	613	CLA	ND
23	В	613	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	В	616	CLA	NA
23	В	616	CLA	NC
23	В	616	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
20				1111

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$5 \mathrm{GTI}$

Mol	Chain	Res	Type	Atom
23	С	503	CLA	NC
23	С	503	CLA	ND
23	С	503	CLA	NA
23	В	607	CLA	NC
23	В	607	CLA	ND
23	В	607	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	с	507	CLA	NC
23	с	507	CLA	ND
23	с	507	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	В	603	CLA	NC
23	В	603	CLA	ND
23	В	603	CLA	NA
23	С	513	CLA	NC
23	С	513	CLA	ND
23	С	513	CLA	NA
23	В	614	CLA	NC
23	В	614	CLA	ND
23	В	614	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	с	513	CLA	NC
23	с	513	CLA	NA
23	b	616	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	В	611	CLA	NC
23	В	611	CLA	ND
23	В	611	CLA	NA
23	D	405	CLA	NC
23	D	405	CLA	ND

Continued from previous page...



Mol	Chain	Res	Type	Atom
23	D	405	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	В	617	CLA	NA
23	В	617	CLA	NC
23	В	617	CLA	ND
23	b	601	CLA	ND
23	b	601	CLA	NA
23	В	615	CLA	NC
23	В	615	CLA	ND
23	В	615	CLA	NA
23	С	506	CLA	ND
23	В	610	CLA	NC
23	В	610	CLA	ND
23	В	610	CLA	NA
23	В	612	CLA	NC
23	В	612	CLA	ND
23	В	612	CLA	NA
23	с	504	CLA	NC
23	с	504	CLA	ND
23	с	504	CLA	NA

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All (1339) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	с	520	LMG	O9-C10-O7-C8
34	с	520	LMG	C11-C10-O7-C8
23	с	502	CLA	C14-C13-C15-C16
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C34
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
25	d	404	BCR	C23-C24-C25-C30
27	a	412	GOL	O1-C1-C2-O2
27	а	412	GOL	O1-C1-C2-C3
25	Н	101	BCR	C5-C6-C7-C8
25	Н	101	BCR	C7-C8-C9-C34
25	Т	101	BCR	C7-C8-C9-C10
25	Т	101	BCR	C7-C8-C9-C34
25	Т	101	BCR	C13-C14-C15-C16
25	у	101	BCR	C1-C6-C7-C8



Mol	Chain	Res	Type	Atoms
25	v	101	BCR	C5-C6-C7-C8
29	a	415	PL9	C14-C16-C17-C18
29	a	415	PL9	C28-C29-C31-C32
29	а	415	PL9	C30-C29-C31-C32
35	D	403	LMT	C2'-C1'-O1'-C1
35	D	403	LMT	O5'-C1'-O1'-C1
23	с	508	CLA	CHA-CBD-CGD-O1D
23	с	508	CLA	CHA-CBD-CGD-O2D
26	L	102	SQD	O49-C7-O47-C45
26	L	102	SQD	C8-C7-O47-C45
26	L	102	SQD	C5-C6-S-O7
26	L	102	SQD	C5-C6-S-O8
26	L	102	SQD	C5-C6-S-O9
27	0	302	GOL	O1-C1-C2-C3
36	В	626	HTG	O5-C1-S1-C1'
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
31	d	406	LHG	C3-O3-P-O4
23	d	403	CLA	C4-C3-C5-C6
23	С	504	CLA	CBD-CGD-O2D-CED
27	В	627	GOL	O1-C1-C2-C3
35	b	628	LMT	O5'-C1'-O1'-C1
23	С	507	CLA	C2-C3-C5-C6
23	С	507	CLA	C4-C3-C5-C6
23	D	401	CLA	CHA-CBD-CGD-O2D
23	с	509	CLA	C2-C1-O2A-CGA
26	А	411	SQD	C5-C6-S-O7
26	А	411	SQD	C5-C6-S-O8
35	Ε	102	LMT	C2'-C1'-O1'-C1
$\overline{35}$	Е	102	LMT	O5'-C1'-O1'-C1
29	А	413	PL9	C15-C14-C16-C17
29	A	413	PL9	C23-C24-C26-C27
29	А	413	PL9	C25-C24-C26-C27
31	D	408	LHG	C4-O6-P-O4
31	D	408	LHG	C4-O6-P-O5
23	С	510	CLA	C2-C1-O2A-CGA
23	С	510	CLA	C6-C7-C8-C9
31	b	630	LHG	C4-O6-P-O3
31	b	630	LHG	C4-O6-P-O4
31	b	630	LHG	C4-O6-P-O5
27	С	525	GOL	O1-C1-C2-O2

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001000	<u></u>	<u> </u>	<u> </u>	
Mol	Chain	Res	Type	Atoms
27	С	525	GOL	O1-C1-C2-C3
23	В	604	CLA	C2-C3-C5-C6
23	В	604	CLA	C4-C3-C5-C6
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
35	В	633	LMT	C2'-C1'-O1'-C1
35	В	633	LMT	O5'-C1'-O1'-C1
36	В	624	HTG	C2'-C1'-S1-C1
34	Z	101	LMG	C2-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
31	е	101	LHG	C3-O3-P-O5
31	е	101	LHG	O10-C23-O8-C6
31	е	101	LHG	C24-C23-O8-C6
27	b	624	GOL	O1-C1-C2-C3
27	В	628	GOL	C1-C2-C3-O3
27	В	628	GOL	O2-C2-C3-O3
31	Е	101	LHG	C3-O3-P-O4
31	Е	101	LHG	C3-O3-P-O5
31	Е	101	LHG	C3-O3-P-O6
31	Е	101	LHG	O10-C23-O8-C6
31	Е	101	LHG	C24-C23-O8-C6
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	С	505	CLA	C2-C3-C5-C6
23	С	505	CLA	C4-C3-C5-C6
35	В	632	LMT	C2'-C1'-O1'-C1
35	В	632	LMT	O5'-C1'-O1'-C1
35	a	418	LMT	C2'-C1'-O1'-C1
35	a	418	LMT	O5'-C1'-O1'-C1
26	f	101	SQD	O49-C7-O47-C45
26	f	101	SQD	C8-C7-O47-C45
26	f	101	SQD	C5-C6-S-O7
26	f	101	SQD	C5-C6-S-O8
26	f	101	SQD	C5-C6-S-O9
31	d	408	LHG	C4-O6-P-O4
23	b	610	CLA	C11-C12-C13-C14
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
35	М	103	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
35	М	103	LMT	O5'-C1'-O1'-C1
26	D	413	SQD	O49-C7-O47-C45
26	D	413	SQD	C8-C7-O47-C45
26	D	413	SQD	C5-C6-S-O7
26	D	413	SQD	C5-C6-S-O8
26	D	413	SQD	C5-C6-S-O9
27	d	401	GOL	O1-C1-C2-O2
27	d	401	GOL	O1-C1-C2-C3
23	В	607	CLA	CHA-CBD-CGD-O1D
23	В	607	CLA	CHA-CBD-CGD-O2D
35	m	103	LMT	C2'-C1'-O1'-C1
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	C4-C3-C5-C6
35	b	620	LMT	C2'-C1'-O1'-C1
35	b	620	LMT	O5'-C1'-O1'-C1
35	С	522	LMT	O5'-C1'-O1'-C1
35	е	102	LMT	C2'-C1'-O1'-C1
35	е	102	LMT	O5'-C1'-O1'-C1
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O5
31	d	407	LHG	C4-O6-P-O4
31	d	407	LHG	C4-O6-P-O5
35	В	634	LMT	O5'-C1'-O1'-C1
35	В	634	LMT	C2-C1-O1'-C1'
31	L	101	LHG	C4-O6-P-O4
26	В	621	SQD	O49-C7-O47-C45
26	В	621	SQD	C8-C7-O47-C45
26	В	621	SQD	C5-C6-S-O7
36	В	625	HTG	C2'-C1'-S1-C1
23	В	615	CLA	CAD-CBD-CGD-O1D
23	В	615	CLA	CAD-CBD-CGD-O2D
23	В	615	CLA	C2-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
34	C	501	LMG	O9-C10-O7-C8
25	D	406	BCR	C7-C8-C9-C10
25	D	406	BCR	C7-C8-C9-C34
25	D	406	BCR	C21-C22-C23-C24
25	D	406	BCR	C37-C22-C23-C24
25	b	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	O1D-CGD-O2D-CED
35	С	522	LMT	C3'-C4'-O1B-C1B
23	с	501	CLA	CBD-CGD-O2D-CED
23	С	504	CLA	O1D-CGD-O2D-CED
23	d	403	CLA	C3-C5-C6-C7
23	b	614	CLA	C3-C5-C6-C7
23	В	615	CLA	C3-C5-C6-C7
34	С	501	LMG	C11-C10-O7-C8
23	с	509	CLA	CBD-CGD-O2D-CED
29	a	415	PL9	C25-C24-C26-C27
23	с	507	CLA	C4-C3-C5-C6
29	А	413	PL9	C13-C14-C16-C17
23	b	603	CLA	C2-C3-C5-C6
23	с	507	CLA	C2A-CAA-CBA-CGA
23	с	506	CLA	C3-C5-C6-C7
23	А	407	CLA	C3-C5-C6-C7
23	А	405	CLA	CBD-CGD-O2D-CED
23	С	514	CLA	CBD-CGD-O2D-CED
34	С	521	LMG	O6-C5-C6-O5
35	М	103	LMT	C4B-C5B-C6B-O6B
31	А	415	LHG	O2-C2-C3-O3
23	С	513	CLA	C3-C5-C6-C7
23	В	617	CLA	C3-C5-C6-C7
35	В	623	LMT	O5B-C5B-C6B-O6B
35	С	522	LMT	O5B-C5B-C6B-O6B
36	В	626	HTG	O5-C5-C6-O6
36	b	625	HTG	O5-C5-C6-O6
35	М	103	LMT	O5'-C5'-C6'-O6'
34	с	519	LMG	C4-C5-C6-O5
36	h	101	HTG	C4-C5-C6-O6
23	b	614	CLA	CBD-CGD-O2D-CED
34	с	520	LMG	O6-C5-C6-O5
35	E	102	LMT	O5'-C5'-C6 ['] -O6'
23	b	605	CLA	C4-C3-C5-C6
29	a	415	PL9	C15-C14-C16-C17
23	C	508	CLA	C4-C3-C5-C6
23	с	504	CLA	C4-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
29	a	415	PL9	C13-C14-C16-C17
23	d	403	CLA	C2-C3-C5-C6
23	C	508	CLA	$C2-\overline{C3}-\overline{C5}-\overline{C6}$
23	с	507	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C2-C3-C5-C6
23	с	504	CLA	C2-C3-C5-C6
23	В	607	CLA	C2A-CAA-CBA-CGA
34	с	519	LMG	O6-C5-C6-O5
35	m	103	LMT	O5'-C1'-O1'-C1
26	В	621	SQD	O5-C1-O6-C44
29	d	405	PL9	C39-C41-C42-C43
29	А	413	PL9	C14-C16-C17-C18
29	D	407	PL9	C39-C41-C42-C43
31	d	408	LHG	C33-C34-C35-C36
36	h	101	HTG	O5-C5-C6-O6
31	А	415	LHG	C1-C2-C3-O3
31	d	407	LHG	C1-C2-C3-O3
23	с	509	CLA	C3-C5-C6-C7
23	В	602	CLA	CBA-CGA-O2A-C1
23	А	407	CLA	CBA-CGA-O2A-C1
23	С	510	CLA	CBA-CGA-O2A-C1
25	t	101	BCR	C13-C14-C15-C16
23	В	615	CLA	C5-C6-C7-C8
35	В	623	LMT	C4B-C5B-C6B-O6B
31	D	408	LHG	O2-C2-C3-O3
35	В	634	LMT	C2'-C1'-O1'-C1
26	А	411	SQD	O6-C44-C45-O47
26	a	413	SQD	O6-C44-C45-O47
35	М	103	LMT	O5B-C5B-C6B-O6B
23	В	606	CLA	C6-C7-C8-C9
23	с	512	CLA	C6-C7-C8-C9
23	с	506	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	В	603	CLA	C6-C7-C8-C9
23	С	513	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	с	504	CLA	C11-C12-C13-C14
23	a	404	CLA	C15-C16-C17-C18
23	В	617	CLA	C10-C11-C12-C13
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
25	Н	101	BCR	C7-C8-C9-C10
26	А	409	SQD	C8-C7-O47-C45
34	Z	101	LMG	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18
23	В	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	С	514	CLA	C13-C15-C16-C17
23	b	616	CLA	C5-C6-C7-C8
23	В	615	CLA	C8-C10-C11-C12
34	Z	101	LMG	O6-C5-C6-O5
35	Е	102	LMT	C4'-C5'-C6'-O6'
23	С	511	CLA	CBA-CGA-O2A-C1
23	В	602	CLA	C15-C16-C17-C18
23	с	509	CLA	C5-C6-C7-C8
23	b	607	CLA	C13-C15-C16-C17
23	с	507	CLA	C8-C10-C11-C12
23	В	615	CLA	C10-C11-C12-C13
36	с	522	HTG	O5-C5-C6-O6
23	В	606	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C13-C15-C16-C17
23	с	513	CLA	C15-C16-C17-C18
23	С	506	CLA	C8-C10-C11-C12
23	С	510	CLA	O1A-CGA-O2A-C1
34	с	519	LMG	C28-C29-C30-C31
37	С	518	DGD	C1A-C2A-C3A-C4A
23	с	502	CLA	C13-C15-C16-C17
23	с	502	CLA	C15-C16-C17-C18
23	с	511	CLA	C3-C5-C6-C7
23	d	403	CLA	CBA-CGA-O2A-C1
31	d	408	LHG	C24-C23-O8-C6
23	a	409	CLA	CBA-CGA-O2A-C1
36	b	623	HTG	O5-C5-C6-O6
23	b	601	CLA	C2-C1-O2A-CGA
23	b	605	CLA	C5-C6-C7-C8
37	с	517	DGD	C1B-C2B-C3B-C4B
23	b	602	CLA	C15-C16-C17-C18
23	С	509	CLA	C10-C11-C12-C13
23	С	507	CLA	C6-C7-C8-C10
23	С	511	CLA	C6-C7-C8-C10
23	В	616	CLA	C11-C12-C13-C15
23	В	603	CLA	C11-C12-C13-C15
23	b	605	CLA	C8-C10-C11-C12
23	b	604	CLA	C15-C16-C17-C18
23	В	607	CLA	C13-C15-C16-C17
23	b	601	CLA	C8-C10-C11-C12
23	с	504	CLA	C5-C6-C7-C8
36	В	624	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C32-C33-C34-C35
35	В	623	LMT	C3'-C4'-O1B-C1B
23	А	407	CLA	O1A-CGA-O2A-C1
23	С	503	CLA	CBD-CGD-O2D-CED
23	с	513	CLA	C13-C15-C16-C17
29	a	415	PL9	C24-C26-C27-C28
29	a	415	PL9	C39-C41-C42-C43
37	с	516	DGD	O6D-C5D-C6D-O5D
26	А	409	SQD	O49-C7-O47-C45
23	b	616	CLA	C3-C5-C6-C7
23	С	502	CLA	C15-C16-C17-C18
35	В	623	LMT	C5'-C4'-O1B-C1B
23	d	403	CLA	O1A-CGA-O2A-C1
23	В	602	CLA	O1A-CGA-O2A-C1
34	с	520	LMG	C4-C5-C6-O5
23	С	507	CLA	C8-C10-C11-C12
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C15-C16-C17-C18
35	В	634	LMT	O1'-C1-C2-C3
35	М	103	LMT	C4'-C5'-C6'-O6'
23	с	509	CLA	O1A-CGA-O2A-C1
23	С	511	CLA	O1A-CGA-O2A-C1
23	a	409	CLA	O1A-CGA-O2A-C1
26	L	102	SQD	C18-C19-C20-C21
31	е	101	LHG	C11-C12-C13-C14
26	В	621	SQD	C30-C31-C32-C33
23	В	616	CLA	C8-C10-C11-C12
31	d	406	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	е	101	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O3
35	b	628	LMT	O1'-C1-C2-C3
23	В	606	CLA	CBA-CGA-O2A-C1
23	с	509	CLA	CBA-CGA-O2A-C1
23	с	510	CLA	C10-C11-C12-C13
34	j	101	LMG	C10-C11-C12-C13
34	a	417	LMG	O9-C10-O7-C8
23	В	605	CLA	C4-C3-C5-C6
23	с	509	CLA	O1D-CGD-O2D-CED
23	В	611	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	С	517	DGD	O6D-C5D-C6D-O5D
23	b	611	CLA	C8-C10-C11-C12
23	b	604	CLA	C8-C10-C11-C12
34	a	417	LMG	C11-C10-O7-C8
23	В	603	CLA	C15-C16-C17-C18
26	L	102	SQD	C27-C28-C29-C30
34	j	101	LMG	C21-C22-C23-C24
26	a	411	SQD	C9-C10-C11-C12
26	a	411	SQD	C15-C16-C17-C18
26	А	409	SQD	C9-C10-C11-C12
31	d	408	LHG	C32-C33-C34-C35
34	m	101	LMG	C35-C36-C37-C38
37	Н	102	DGD	C6A-C7A-C8A-C9A
23	В	616	CLA	C16-C17-C18-C20
34	m	101	LMG	C38-C39-C40-C41
34	a	417	LMG	C31-C32-C33-C34
34	С	521	LMG	C16-C17-C18-C19
31	L	101	LHG	C25-C26-C27-C28
23	с	501	CLA	O1D-CGD-O2D-CED
26	a	411	SQD	C11-C12-C13-C14
26	A	409	SQD	C11-C10-C9-C8
23	с	508	CLA	C5-C6-C7-C8
35	m	103	LMT	C7-C8-C9-C10
34	В	622	LMG	C36-C37-C38-C39
23	С	508	CLA	CBD-CGD-O2D-CED
37	С	518	DGD	C2E-C1E-O5D-C6D
37	с	516	DGD	C2E-C1E-O5D-C6D
26	а	413	SQD	C24-C25-C26-C27
31	Е	101	LHG	C24-C25-C26-C27
34	С	501	LMG	C14-C15-C16-C17
31	d	408	LHG	O10-C23-O8-C6
23	В	609	CLA	C16-C17-C18-C20
23	С	514	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	C4-C3-C5-C6
37	С	517	DGD	C5B-C6B-C7B-C8B
34	a	417	LMG	C30-C31-C32-C33
34	C	520	LMG	C16-C17-C18-C19
31	A	415	LHG	C32-C33-C34-C35
34	J	101	LMG	C30-C31-C32-C33
23	C	506	CLA	C2-C3-C5-C6
23	a	406	CLA	C11-C12-C13-C14
23	A	407	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	с	505	CLA	C11-C12-C13-C14
23	С	511	CLA	C14-C13-C15-C16
23	В	617	CLA	C6-C7-C8-C9
37	С	517	DGD	C9A-CAA-CBA-CCA
26	A	411	SQD	C16-C17-C18-C19
31	D	408	LHG	C13-C14-C15-C16
34	Ζ	101	LMG	C17-C18-C19-C20
23	a	404	CLA	C2A-CAA-CBA-CGA
35	С	522	LMT	C4B-C5B-C6B-O6B
37	С	517	DGD	C4D-C5D-C6D-O5D
37	с	516	DGD	C4D-C5D-C6D-O5D
34	с	519	LMG	C33-C34-C35-C36
27	А	410	GOL	O1-C1-C2-C3
27	А	410	GOL	C1-C2-C3-O3
27	В	627	GOL	C1-C2-C3-O3
31	А	415	LHG	O1-C1-C2-C3
31	D	409	LHG	O1-C1-C2-C3
23	с	506	CLA	C10-C11-C12-C13
37	С	519	DGD	CBA-CCA-CDA-CEA
37	с	517	DGD	C4B-C5B-C6B-C7B
34	С	521	LMG	C37-C38-C39-C40
34	J	101	LMG	C19-C20-C21-C22
26	А	411	SQD	C18-C19-C20-C21
31	е	101	LHG	C26-C27-C28-C29
34	С	520	LMG	C12-C13-C14-C15
26	А	409	SQD	C15-C16-C17-C18
34	m	101	LMG	C39-C40-C41-C42
37	Н	102	DGD	C5B-C6B-C7B-C8B
23	b	615	CLA	C16-C17-C18-C20
23	В	616	CLA	C16-C17-C18-C19
23	В	611	CLA	C16-C17-C18-C19
34	Z	101	LMG	O6-C1-O1-C7
37	с	516	DGD	O6E-C1E-O5D-C6D
23	В	602	CLA	C10-C11-C12-C13
23	a	404	CLA	C13-C15-C16-C17
29	d	405	PL9	C34-C36-C37-C38
37	с	516	DGD	C5A-C6A-C7A-C8A
35	В	634	LMT	C6-C7-C8-C9
31	b	630	LHG	C12-C13-C14-C15
26	D	413	SQD	C30-C31-C32-C33
34	С	521	LMG	C17-C18-C19-C20
31	D	409	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
37	Н	102	DGD	CBA-CCA-CDA-CEA
34	В	622	LMG	C28-C29-C30-C31
23	b	615	CLA	C13-C15-C16-C17
23	В	606	CLA	O1A-CGA-O2A-C1
26	a	413	SQD	C25-C26-C27-C28
35	В	633	LMT	C2-C3-C4-C5
34	m	101	LMG	C14-C15-C16-C17
34	В	622	LMG	C17-C18-C19-C20
36	В	629	HTG	O5-C5-C6-O6
37	С	517	DGD	C7B-C8B-C9B-CAB
37	С	518	DGD	CAB-CBB-CCB-CDB
23	с	506	CLA	C13-C15-C16-C17
23	С	508	CLA	C5-C6-C7-C8
23	b	603	CLA	C13-C15-C16-C17
26	А	409	SQD	C12-C13-C14-C15
23	с	502	CLA	C16-C17-C18-C20
26	L	102	SQD	C24-C25-C26-C27
36	В	626	HTG	C3'-C4'-C5'-C6'
26	f	101	SQD	C29-C30-C31-C32
31	D	409	LHG	C26-C27-C28-C29
37	с	517	DGD	C9A-CAA-CBA-CCA
23	А	405	CLA	O1D-CGD-O2D-CED
23	В	605	CLA	C3-C5-C6-C7
23	D	401	CLA	C15-C16-C17-C18
23	b	611	CLA	C4-C3-C5-C6
24	a	407	PHO	C4-C3-C5-C6
23	с	505	CLA	C4-C3-C5-C6
29	D	407	PL9	C30-C29-C31-C32
23	В	616	CLA	C4-C3-C5-C6
24	а	407	PHO	C2-C3-C5-C6
23	с	505	CLA	C2-C3-C5-C6
29	D	407	PL9	C28-C29-C31-C32
23	b	609	CLA	C2-C3-C5-C6
34	m	101	LMG	C11-C10-O7-C8
37	C	517	DGD	C8A-C9A-CAA-CBA
31	d	406	LHG	C25-C26-C27-C28
27	0	302	GOL	O1-C1-C2-O2
27	В	627	GOL	O2-C2-C3-O3
27	b	624	GOL	O1-C1-C2-O2
36	В	626	HTG	C4-C5-C6-O6
35	b	628	LMT	C4'-C5'-C6'-O6'
26	D	413	SQD	C24-C25-C26-C27

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\mathbf{Mol}	Chain	\mathbf{Res}	Type	Atoms
34	m	101	LMG	O9-C10-O7-C8
31	D	408	LHG	C14-C15-C16-C17
23	С	511	CLA	C5-C6-C7-C8
26	L	102	SQD	C13-C14-C15-C16
31	Е	101	LHG	C27-C28-C29-C30
37	h	103	DGD	CAA-CBA-CCA-CDA
26	В	621	SQD	C24-C25-C26-C27
25	d	404	BCR	C23-C24-C25-C26
25	Н	101	BCR	C1-C6-C7-C8
25	Т	101	BCR	C1-C6-C7-C8
25	Т	101	BCR	C5-C6-C7-C8
25	В	618	BCR	C1-C6-C7-C8
25	D	406	BCR	C23-C24-C25-C26
25	D	406	BCR	C23-C24-C25-C30
25	b	617	BCR	C5-C6-C7-C8
35	b	628	LMT	C4-C5-C6-C7
26	D	413	SQD	C32-C33-C34-C35
31	D	409	LHG	C24-C23-O8-C6
36	b	625	HTG	C3'-C4'-C5'-C6'
31	D	408	LHG	C16-C17-C18-C19
35	m	103	LMT	C11-C10-C9-C8
35	М	101	LMT	C2-C3-C4-C5
26	D	413	SQD	C7-C8-C9-C10
26	D	413	SQD	C23-C24-C25-C26
35	b	620	LMT	C1-C2-C3-C4
23	b	601	CLA	C10-C11-C12-C13
37	С	519	DGD	C8B-C9B-CAB-CBB
29	D	407	PL9	C15-C14-C16-C17
23	b	609	CLA	C4-C3-C5-C6
23	b	611	CLA	C2-C3-C5-C6
23	a	406	CLA	C6-C7-C8-C10
23	с	509	CLA	C12-C13-C15-C16
23	A	407	CLA	C11-C10-C8-C7
23	с	505	CLA	C11-C12-C13-C15
29	D	407	PL9	C13-C14-C16-C17
23	b	606	CLA	C11-C10-C8-C7
23	С	511	CLA	C12-C13-C15-C16
23	В	616	CLA	C2-C3-C5-C6
23	D	405	CLA	C11-C10-C8-C7
23	с	504	CLA	C11-C12-C13-C15
23	с	504	CLA	C12-C13-C15-C16
36	h	101	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C3-C5-C6-C7
31	D	409	LHG	O10-C23-O8-C6
26	L	102	SQD	C14-C15-C16-C17
37	с	517	DGD	C3B-C4B-C5B-C6B
31	L	101	LHG	C17-C18-C19-C20
36	В	625	HTG	C4-C5-C6-O6
23	С	507	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
23	В	611	CLA	C13-C15-C16-C17
23	D	405	CLA	C10-C11-C12-C13
26	А	411	SQD	C15-C16-C17-C18
35	М	103	LMT	O1'-C1-C2-C3
34	С	520	LMG	C37-C38-C39-C40
26	a	411	SQD	C27-C28-C29-C30
37	с	517	DGD	C5A-C6A-C7A-C8A
37	С	518	DGD	C7B-C8B-C9B-CAB
34	С	521	LMG	C15-C16-C17-C18
26	а	413	SQD	C27-C28-C29-C30
23	В	605	CLA	C2C-C3C-CAC-CBC
34	J	101	LMG	C35-C36-C37-C38
31	L	101	LHG	C34-C35-C36-C37
23	С	512	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	C16-C17-C18-C19
37	с	517	DGD	O6E-C1E-O5D-C6D
37	С	518	DGD	O6E-C1E-O5D-C6D
26	а	413	SQD	C33-C34-C35-C36
26	А	411	SQD	C8-C7-O47-C45
26	a	413	SQD	C8-C7-O47-C45
31	Ε	101	LHG	C8-C7-O7-C5
26	L	102	SQD	C10-C11-C12-C13
23	В	610	CLA	CBD-CGD-O2D-CED
31	L	101	LHG	C12-C13-C14-C15
26	A	411	SQD	O49-C7-O47-C45
23	b	601	CLA	C3-C5-C6-C7
35	b	628	LMT	C2'-C1'-O1'-C1
26	A	409	SQD	O6-C44-C45-O47
23	В	612	CLA	C8-C10-C11-C12
29	a	415	PL9	C23-C24-C26-C27
29	a	415	PL9	C4-C3-C7-C8
29	A	413	PL9	C4-C3-C7-C8
23	a	406	CLA	C6-C7-C8-C9
23	с	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C11-C10-C8-C9
23	С	511	CLA	C6-C7-C8-C9
23	В	603	CLA	C11-C12-C13-C14
23	D	405	CLA	C11-C10-C8-C9
23	с	504	CLA	C14-C13-C15-C16
34	j	101	LMG	C29-C30-C31-C32
23	c	510	CLA	C3-C5-C6-C7
35	D	403	LMT	O1'-C1-C2-C3
34	Z	101	LMG	O6-C5-C6-O5
35	В	623	LMT	O5'-C5'-C6'-O6'
26	a	413	SQD	C7-C8-C9-C10
23	С	510	CLA	C8-C10-C11-C12
35	b	628	LMT	C3-C4-C5-C6
24	D	402	PHO	C2C-C3C-CAC-CBC
23	a	406	CLA	C1A-C2A-CAA-CBA
23	С	502	CLA	C1A-C2A-CAA-CBA
23	с	512	CLA	C1A-C2A-CAA-CBA
23	с	501	CLA	C1A-C2A-CAA-CBA
23	С	512	CLA	C1A-C2A-CAA-CBA
23	В	610	CLA	C1A-C2A-CAA-CBA
23	с	502	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	В	611	CLA	C16-C17-C18-C20
26	a	413	SQD	O49-C7-O47-C45
31	Е	101	LHG	O9-C7-O7-C5
34	В	622	LMG	O9-C10-O7-C8
35	Е	102	LMT	C2B-C1B-O1B-C4'
34	В	622	LMG	C11-C10-O7-C8
31	d	407	LHG	C3-O3-P-O6
37	Н	102	DGD	C4A-C5A-C6A-C7A
31	D	408	LHG	C7-C8-C9-C10
34	С	501	LMG	C10-C11-C12-C13
35	С	522	LMT	O5'-C5'-C6'-O6'
35	e	102	LMT	C4'-C5'-C6'-O6'
35	e	102	LMT	C4-C5-C6-C7
23	b	615	CLA	C5-C6-C7-C8
31	b	630	LHG	O6-C4-C5-C6
35	E	102	LMT	O5B-C1B-O1B-C4'
34	J	101	LMG	C12-C13-C14-C15
37	C	518	DGD	C9B-CAB-CBB-CCB
37	Н	102	DGD	CDB-CEB-CFB-CGB
23	В	606	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	В	612	CLA	C16-C17-C18-C20
34	с	519	LMG	C35-C36-C37-C38
37	с	518	DGD	CAB-CBB-CCB-CDB
31	d	408	LHG	C27-C28-C29-C30
31	А	415	LHG	C25-C26-C27-C28
23	b	612	CLA	C10-C11-C12-C13
37	h	103	DGD	C5B-C6B-C7B-C8B
37	с	516	DGD	O6E-C5E-C6E-O5E
29	d	405	PL9	C15-C14-C16-C17
23	С	511	CLA	C4-C3-C5-C6
31	L	101	LHG	C30-C31-C32-C33
31	е	101	LHG	C9-C10-C11-C12
23	В	609	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C20
35	b	628	LMT	O5'-C5'-C6'-O6'
26	L	102	SQD	C44-C45-C46-O48
35	е	102	LMT	C3-C4-C5-C6
26	В	621	SQD	C44-C45-C46-O48
34	j	101	LMG	C38-C39-C40-C41
37	с	517	DGD	C5D-C6D-O5D-C1E
37	С	518	DGD	C5D-C6D-O5D-C1E
31	А	415	LHG	C9-C10-C11-C12
23	b	609	CLA	C13-C15-C16-C17
36	b	623	HTG	S1-C1'-C2'-C3'
37	С	518	DGD	CDA-CEA-CFA-CGA
31	d	407	LHG	C34-C35-C36-C37
31	L	101	LHG	C24-C25-C26-C27
27	А	410	GOL	O1-C1-C2-O2
27	В	627	GOL	O1-C1-C2-O2
34	С	521	LMG	C4-C5-C6-O5
37	с	517	DGD	CBA-CCA-CDA-CEA
35	С	522	LMT	C1-C2-C3-C4
23	В	603	CLA	C13-C15-C16-C17
23	a	405	CLA	C15-C16-C17-C18
37	C	517	DGD	O6E-C5E-C6E-O5E
$\overline{34}$	J	101	LMG	O6-C5-C6-O5
$\overline{37}$	C	518	DGD	CCB-CDB-CEB-CFB
31	A	415	LHG	C11-C10-C9-C8
37	с	518	DGD	CBA-CCA-CDA-CEA
23	С	512	CLA	CBA-CGA-O2A-C1
37	С	516	DGD	C2A-C1A-O1G-C1G
23	b	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	B os		Atoms
25	Chain	102	туре	
<u>30</u> 20	III I	103		$\begin{array}{c} 09-010-011-012 \\ 01-012-02-022 \\ \end{array}$
<u>- 30</u> - 21		621	HIG	$\begin{array}{c} SI-UT-U2-U3 \\ \hline \\ C00, C00, C20, C21 \\ \hline \end{array}$
31		408	LHG	C28-C29-C30-C31
26	Ŀ	102	SQD	C46-C45-O47-C7
34	J	101	LMG	06-C5-C6-O5
	C	502	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C15-C16-C17-C18
34	a	417	LMG	C35-C36-C37-C38
36	b	625	HTG	C4'-C5'-C6'-C7'
23	С	503	CLA	O1D-CGD-O2D-CED
26	f	101	SQD	C26-C27-C28-C29
26	f	101	SQD	C31-C32-C33-C34
23	b	611	CLA	CBA-CGA-O2A-C1
23	В	612	CLA	C16-C17-C18-C19
37	с	516	DGD	CDA-CEA-CFA-CGA
34	С	501	LMG	C37-C38-C39-C40
23	b	605	CLA	CBD-CGD-O2D-CED
23	С	510	CLA	C10-C11-C12-C13
23	В	613	CLA	C10-C11-C12-C13
37	С	517	DGD	C2E-C1E-O5D-C6D
37	с	517	DGD	C2E-C1E-O5D-C6D
35	С	522	LMT	C2'-C1'-O1'-C1
34	m	101	LMG	C2-C1-O1-C7
37	h	103	DGD	C9B-CAB-CBB-CCB
37	h	103	DGD	O2G-C1B-C2B-C3B
23	b	601	CLA	CAA-CBA-CGA-O2A
26	f	101	SQD	O6-C44-C45-O47
23	с	502	CLA	C10-C11-C12-C13
23	b	611	CLA	O1A-CGA-O2A-C1
31	b	630	LHG	C32-C33-C34-C35
26	А	409	SQD	C16-C17-C18-C19
31	d	407	LHG	C13-C14-C15-C16
34	с	519	LMG	C10-C11-C12-C13
29	d	405	PL9	C13-C14-C16-C17
23	A	405	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C15
23	с	506	CLA	C6-C7-C8-C10
23	В	605	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C10-C8-C7
23	- Č	511	CLA	C2-C3-C5-C6
23	b	601	CLA	C6-C7-C8-C10
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Mol	Chain	Res	Type	Atoms
37	Н	102	DGD	O2G-C1B-C2B-C3B
23	С	507	CLA	C6-C7-C8-C9
23	С	514	CLA	C11-C10-C8-C9
23	В	605	CLA	C6-C7-C8-C9
23	С	505	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C10-C8-C9
23	В	615	CLA	C14-C13-C15-C16
23	С	502	CLA	CBD-CGD-O2D-CED
34	С	520	LMG	C17-C18-C19-C20
35	m	103	LMT	C3-C4-C5-C6
35	m	103	LMT	C6-C7-C8-C9
26	В	621	SQD	C24-C23-O48-C46
37	с	518	DGD	C2A-C1A-O1G-C1G
34	Z	101	LMG	C15-C16-C17-C18
37	с	516	DGD	O1A-C1A-O1G-C1G
34	С	520	LMG	C11-C10-O7-C8
35	Е	102	LMT	C5-C6-C7-C8
36	В	624	HTG	C4'-C5'-C6'-C7'
26	L	102	SQD	C24-C23-O48-C46
23	b	616	CLA	C8-C10-C11-C12
34	Z	101	LMG	C16-C17-C18-C19
35	a	418	LMT	C4-C5-C6-C7
23	В	610	CLA	O1D-CGD-O2D-CED
23	В	604	CLA	C3-C5-C6-C7
34	a	417	LMG	C10-C11-C12-C13
31	b	630	LHG	C14-C15-C16-C17
31	D	409	LHG	C17-C18-C19-C20
31	е	101	LHG	C24-C25-C26-C27
23	b	601	CLA	C4-C3-C5-C6
34	с	520	LMG	C21-C22-C23-C24
23	b	601	CLA	O1A-CGA-O2A-C1
23	с	512	CLA	C3-C5-C6-C7
36	В	625	HTG	C2'-C3'-C4'-C5'
23	с	511	CLA	CBA-CGA-O2A-C1
34	С	520	LMG	C36-C37-C38-C39
35	В	632	LMT	C7-C8-C9-C10
23	С	507	CLA	C3A-C2A-CAA-CBA
23	с	512	CLA	C3A-C2A-CAA-CBA
23	В	610	CLA	C3A-C2A-CAA-CBA
26	f	101	SQD	C27-C28-C29-C30
26	A	411	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
37	С	518	DGD	C9A-CAA-CBA-CCA
31	d	407	LHG	C26-C27-C28-C29
31	d	406	LHG	C32-C33-C34-C35
23	b	605	CLA	CBA-CGA-O2A-C1
31	d	407	LHG	C32-C33-C34-C35
23	D	401	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
34	a	417	LMG	C7-C8-C9-O8
26	А	411	SQD	O6-C44-C45-C46
26	a	413	SQD	O6-C44-C45-C46
31	е	101	LHG	C4-C5-C6-O8
31	Е	101	LHG	C4-C5-C6-O8
26	А	409	SQD	O6-C44-C45-C46
37	h	103	DGD	O1G-C1G-C2G-C3G
37	С	517	DGD	C6B-C7B-C8B-C9B
26	a	411	SQD	C30-C31-C32-C33
37	С	517	DGD	CAB-CBB-CCB-CDB
23	В	603	CLA	O2A-C1-C2-C3
34	с	519	LMG	C29-C30-C31-C32
37	с	517	DGD	CAA-CBA-CCA-CDA
34	С	520	LMG	C28-C29-C30-C31
37	с	518	DGD	O1A-C1A-O1G-C1G
23	b	614	CLA	O1D-CGD-O2D-CED
31	D	409	LHG	O1-C1-C2-O2
31	d	406	LHG	C33-C34-C35-C36
26	А	411	SQD	C30-C31-C32-C33
23	В	605	CLA	CBA-CGA-O2A-C1
31	b	630	LHG	C35-C36-C37-C38
23	b	605	CLA	O1A-CGA-O2A-C1
23	с	512	CLA	O1A-CGA-O2A-C1
26	В	621	SQD	O10-C23-O48-C46
23	D	401	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C19
$3\overline{1}$	E	101	LHG	C25-C26-C27-C28
34	с	520	LMG	O1-C7-C8-O7
26	a	411	SQD	O6-C44-C45-O47
31	е	101	LHG	O7-C5-C6-O8
$\overline{37}$	C	517	DGD	C3B-C4B-C5B-C6B
$3\overline{1}$	d	408	LHG	C9-C10-C11-C12
31	d	407	LHG	C14-C15-C16-C17
23	с	509	CLA	C13-C15-C16-C17
23	с	506	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	А	404	CLA	C13-C15-C16-C17
31	D	408	LHG	C1-C2-C3-O3
35	b	620	LMT	C6-C7-C8-C9
34	С	520	LMG	O9-C10-O7-C8
23	d	402	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C3-C5-C6
35	М	103	LMT	C2B-C1B-O1B-C4'
23	В	616	CLA	C14-C13-C15-C16
23	b	609	CLA	C6-C7-C8-C9
31	d	408	LHG	C2-C3-O3-P
31	D	409	LHG	C2-C3-O3-P
34	J	101	LMG	C34-C35-C36-C37
25	d	404	BCR	C1-C6-C7-C8
23	D	405	CLA	C3-C5-C6-C7
23	с	501	CLA	C10-C11-C12-C13
34	Z	101	LMG	C19-C20-C21-C22
35	С	522	LMT	O1'-C1-C2-C3
37	С	517	DGD	C7A-C8A-C9A-CAA
31	b	630	LHG	C34-C35-C36-C37
37	с	516	DGD	C4B-C5B-C6B-C7B
34	с	520	LMG	C28-C29-C30-C31
26	D	413	SQD	C29-C30-C31-C32
35	е	102	LMT	C2B-C1B-O1B-C4'
23	b	614	CLA	C15-C16-C17-C18
23	с	511	CLA	O1A-CGA-O2A-C1
34	с	519	LMG	C21-C22-C23-C24
23	b	615	CLA	C15-C16-C17-C18
31	d	407	LHG	O6-C4-C5-C6
23	с	502	CLA	C12-C13-C15-C16
23	b	611	CLA	C6-C7-C8-C10
23	А	405	CLA	C11-C10-C8-C7
23	d	402	CLA	C11-C12-C13-C15
23	С	510	CLA	C6-C7-C8-C10
23	С	514	CLA	C11-C10-C8-C7
23	С	505	CLA	C12-C13-C15-C16
23	В	616	CLA	C12-C13-C15-C16
23	В	603	CLA	C6-C7-C8-C10
23	В	615	CLA	C12-C13-C15-C16
36	С	524	HTG	S1-C1'-C2'-C3'
23	С	513	CLA	C10-C11-C12-C13
23	b	607	CLA	C16-C17-C18-C20
34	В	622	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	D	413	SQD	C27-C28-C29-C30
36	с	521	HTG	O5-C1-S1-C1'
34	m	101	LMG	C22-C23-C24-C25
23	с	512	CLA	C13-C15-C16-C17
23	С	512	CLA	CBA-CGA-O2A-C1
31	d	407	LHG	C24-C23-O8-C6
34	В	622	LMG	C32-C33-C34-C35
31	d	407	LHG	C29-C30-C31-C32
23	В	607	CLA	C10-C11-C12-C13
24	a	407	PHO	CAD-CBD-CGD-O2D
24	А	406	PHO	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	с	501	CLA	CAD-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	В	617	CLA	CAD-CBD-CGD-O2D
35	М	103	LMT	O5B-C1B-O1B-C4'
26	L	102	SQD	O10-C23-O48-C46
23	b	605	CLA	O1D-CGD-O2D-CED
37	С	517	DGD	O6E-C1E-O5D-C6D
26	a	413	SQD	O5-C1-O6-C44
34	m	101	LMG	O6-C1-O1-C7
23	В	606	CLA	C13-C15-C16-C17
35	В	623	LMT	C6-C7-C8-C9
34	с	520	LMG	O1-C7-C8-C9
34	Z	101	LMG	O1-C7-C8-C9
26	a	411	SQD	O6-C44-C45-C46
34	m	101	LMG	O1-C7-C8-C9
36	b	625	HTG	C4-C5-C6-O6
31	b	630	LHG	C27-C28-C29-C30
$2\overline{3}$	C	514	CLA	C3-C5-C6-C7
23	B	$60\overline{2}$	CLA	CAA-CBA-CGA-O2A
31	D	408	LHG	C17-C18-C19-C20
23	В	605	CLA	C4C-C3C-CAC-CBC
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	B	$60\overline{2}$	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O1D
23	с	509	CLA	CHA-CBD-CGD-O1D
23	с	509	CLA	CHA-CBD-CGD-O2D
23	С	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	С	510	CLA	CHA-CBD-CGD-O2D
23	С	509	CLA	CHA-CBD-CGD-O1D
23	С	503	CLA	CHA-CBD-CGD-O1D
23	С	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	с	504	CLA	CHA-CBD-CGD-O1D
23	С	507	CLA	C3-C5-C6-C7
23	В	605	CLA	O1A-CGA-O2A-C1
23	С	512	CLA	O1A-CGA-O2A-C1
31	d	407	LHG	O10-C23-O8-C6
34	Z	101	LMG	O1-C7-C8-O7
34	a	417	LMG	07-C8-C9-O8
31	Е	101	LHG	O7-C5-C6-O8
26	f	101	SQD	O47-C45-C46-O48
34	m	101	LMG	O1-C7-C8-O7
37	h	103	DGD	01G-C1G-C2G-O2G
37	С	519	DGD	C2A-C1A-O1G-C1G
23	С	503	CLA	C10-C11-C12-C13
31	А	415	LHG	O1-C1-C2-O2
26	a	411	SQD	C35-C36-C37-C38
31	D	409	LHG	C15-C16-C17-C18
36	В	630	HTG	S1-C1'-C2'-C3'
35	Е	102	LMT	C3-C4-C5-C6
34	В	622	LMG	C33-C34-C35-C36
23	b	611	CLA	C6-C7-C8-C9
23	В	602	CLA	C11-C10-C8-C9
23	С	513	CLA	C14-C13-C15-C16
23	С	508	CLA	O1D-CGD-O2D-CED
23	С	512	CLA	O1D-CGD-O2D-CED
26	A	411	SQD	C29-C30-C31-C32
26	В	621	SQD	C5-C6-S-O8
37	Н	102	DGD	CCA-CDA-CEA-CFA
34	с	519	LMG	C31-C32-C33-C34
31	b	630	LHG	C13-C14-C15-C16
37	С	519	DGD	O1A-C1A-O1G-C1G
23	b	609	CLA	O1A-CGA-O2A-C1
34	m	101	LMG	C30-C31-C32-C33
27	В	628	GOL	O1-C1-C2-C3
34	J	101	LMG	C36-C37-C38-C39
31	D	409	LHG	C29-C30-C31-C32
23	С	507	CLA	C16-C17-C18-C20

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NT-1		Dee	Lan	• • • • • • • • • • • • • • • • • • •
MOI	Chain	Res	Type	Atoms
23	b	609	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O3
36	В	625	HTG	O5-C5-C6-O6
34	С	520	LMG	C40-C41-C42-C43
29	d	405	PL9	C45-C44-C46-C47
23	В	605	CLA	C2-C3-C5-C6
23	В	610	CLA	C2-C3-C5-C6
35	В	632	LMT	C4-C5-C6-C7
35	В	632	LMT	C5-C6-C7-C8
31	d	406	LHG	C3-O3-P-O5
31	D	408	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O5
24	D	402	PHO	C16-C17-C18-C19
34	Z	101	LMG	C10-C11-C12-C13
23	В	605	CLA	C13-C15-C16-C17
23	b	602	CLA	C10-C11-C12-C13
34	С	501	LMG	C29-C28-O8-C9
29	D	407	PL9	C29-C31-C32-C33
35	М	103	LMT	C6-C7-C8-C9
35	М	103	LMT	C9-C10-C11-C12
31	L	101	LHG	C13-C14-C15-C16
23	В	609	CLA	C13-C15-C16-C17
23	В	608	CLA	C3-C5-C6-C7
26	a	411	SQD	C26-C27-C28-C29
31	D	408	LHG	C26-C27-C28-C29
34	С	520	LMG	C32-C33-C34-C35
23	с	502	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	В	606	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CAD-CBD-CGD-O1D
26	A	411	SOD	C5-C6-S-O9
23	c	506	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
$\frac{-3}{26}$	B	621	SOD	C5-C6-S-O9
23	b	601	CLA	CAD-CBD-CGD-O1D
$\frac{-3}{23}$	C C	504	CLA	CAD-CBD-CGD-01D
23	<u>я</u>	406	CLA	C10-C11-C12-C13
35	M	103	LMT	<u>C1-C2-C3-C4</u>
$\frac{30}{23}$	C	510	CLA	<u>C16-C17-C18-C20</u>
23	R	606		<u>C6-C7-C8-C10</u>
20	<u> </u>	000	L ODU	

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Mol	Chain	Res	Type	Atoms
31	b	630	LHG	O6-C4-C5-O7
23	В	605	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	с	501	CLA	C11-C12-C13-C15
31	Е	101	LHG	C23-C24-C25-C26
36	с	521	HTG	C2-C1-S1-C1'
23	с	510	CLA	C6-C7-C8-C10
23	С	513	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C12-C13-C15
23	a	409	CLA	C11-C10-C8-C7
23	В	611	CLA	C12-C13-C15-C16
23	В	617	CLA	C12-C13-C15-C16
23	С	506	CLA	C12-C13-C15-C16
23	с	504	CLA	C11-C10-C8-C7
37	h	103	DGD	C9A-CAA-CBA-CCA
34	С	501	LMG	C13-C14-C15-C16
23	b	613	CLA	O1A-CGA-O2A-C1
23	В	610	CLA	O1A-CGA-O2A-C1
35	В	634	LMT	C4-C5-C6-C7
26	В	621	SQD	C33-C34-C35-C36
35	е	102	LMT	O5B-C1B-O1B-C4'
31	b	630	LHG	C16-C17-C18-C19
31	d	407	LHG	C9-C10-C11-C12
23	С	512	CLA	C3-C5-C6-C7
31	b	630	LHG	C25-C26-C27-C28
26	f	101	SQD	C44-C45-C46-O48
34	С	501	LMG	O10-C28-O8-C9
26	L	102	SQD	O47-C45-C46-O48
26	В	621	SQD	O47-C45-C46-O48
26	a	411	SQD	C16-C17-C18-C19
31	D	409	LHG	C14-C15-C16-C17
31	d	407	LHG	C16-C17-C18-C19
34	C	520	LMG	C35-C36-C37-C38
37	C	518	DGD	C8A-C9A-CAA-CBA
37	c	517	DGD	C2G-C3G-O3G-C1D
23	D	401	CLA	C16-C17-C18-C19
34	С	520	LMG	C11-C12-C13-C14
23	с	508	CLA	C11-C10-C8-C9
23	d	402	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	с	-507	\vdash CLA \vdash	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	В	617	CLA	C14-C13-C15-C16
37	h	103	DGD	CBB-CCB-CDB-CEB
23	С	503	CLA	C3-C5-C6-C7
34	С	520	LMG	C34-C35-C36-C37
34	В	622	LMG	C10-C11-C12-C13
31	d	406	LHG	O10-C23-O8-C6
27	В	628	GOL	O1-C1-C2-O2
31	D	408	LHG	C11-C10-C9-C8
37	с	517	DGD	C7B-C8B-C9B-CAB
35	В	623	LMT	C5-C6-C7-C8
24	a	408	PHO	C8-C10-C11-C12
31	d	406	LHG	C24-C25-C26-C27
34	С	501	LMG	C17-C18-C19-C20
35	D	403	LMT	C5-C6-C7-C8
34	В	622	LMG	C13-C14-C15-C16
23	С	507	CLA	C5-C6-C7-C8
31	D	408	LHG	C11-C12-C13-C14
34	a	417	LMG	C20-C21-C22-C23
35	Е	102	LMT	O1'-C1-C2-C3
23	b	616	CLA	O1A-CGA-O2A-C1
35	D	403	LMT	O5B-C5B-C6B-O6B
31	d	406	LHG	C24-C23-O8-C6
26	L	102	SQD	C31-C32-C33-C34
31	d	406	LHG	C34-C35-C36-C37
34	m	101	LMG	C37-C38-C39-C40
26	В	621	SQD	C46-C45-O47-C7
23	b	602	CLA	C2A-CAA-CBA-CGA
23	с	501	CLA	C2A-CAA-CBA-CGA
23	С	514	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
23	В	614	CLA	C2-C1-O2A-CGA
26	L	102	SQD	C26-C27-C28-C29
31	d	408	LHG	C29-C30-C31-C32
26	L	102	SQD	C11-C10-C9-C8
34	a	417	LMG	C29-C30-C31-C32
26	a	413	SQD	C18-C19-C20-C21
23	b	616	CLA	CBA-CGA-O2A-C1
31	d	407	LHG	O6-C4-C5-O7
25	d	404	BCR	C5-C6-C7-C8
25	В	618	BCR	C5-C6-C7-C8
25	с	514	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	с	514	BCR	C23-C24-C25-C30
29	d	405	PL9	C43-C44-C46-C47
34	с	519	LMG	O10-C28-O8-C9
26	a	413	SQD	C24-C23-O48-C46
23	с	512	CLA	C2A-CAA-CBA-CGA
26	a	413	SQD	O10-C23-O48-C46
31	Е	101	LHG	C4-O6-P-O3
26	В	621	SQD	C9-C10-C11-C12
34	m	101	LMG	C21-C22-C23-C24
26	f	101	SQD	O6-C44-C45-C46
35	М	103	LMT	C11-C10-C9-C8
23	с	508	CLA	C11-C10-C8-C7
23	с	506	CLA	C11-C12-C13-C15
23	с	506	CLA	C12-C13-C15-C16
23	С	510	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C10-C8-C7
26	А	411	SQD	C7-C8-C9-C10
23	А	405	CLA	C11-C10-C8-C9
23	А	405	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	с	501	CLA	C11-C12-C13-C14
23	В	616	CLA	C11-C12-C13-C14
23	а	409	CLA	C11-C10-C8-C9
25	k	101	BCR	C9-C10-C11-C12
23	а	404	CLA	C16-C17-C18-C19
34	В	622	LMG	O6-C5-C6-O5
37	с	517	DGD	CCB-CDB-CEB-CFB
34	Z	101	LMG	C4-C5-C6-O5
31	Ε	101	LHG	C15-C16-C17-C18
35	С	522	LMT	C4-C5-C6-C7
23	В	610	CLA	CBA-CGA-O2A-C1
23	A	407	CLA	C4-C3-C5-C6
23	В	610	CLA	C4-C3-C5-C6
31	d	406	LHG	С7-С8-С9-С10
31	D	408	LHG	C34-C35-C36-C37
23	В	604	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
34	Z	101	LMG	C12-C13-C14-C15
34	z	101	LMG	C18-C19-C20-C21
31	d	407	LHG	C31-C32-C33-C34
34	с	519	LMG	C29-C28-O8-C9
23	С	507	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	С	510	CLA	CBD-CGD-O2D-CED
23	с	513	CLA	C10-C11-C12-C13
35	В	633	LMT	C4-C5-C6-C7
23	D	401	CLA	C2C-C3C-CAC-CBC
23	С	509	CLA	C5-C6-C7-C8
23	В	609	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
23	С	505	CLA	C8-C10-C11-C12
34	a	417	LMG	C36-C37-C38-C39
23	В	614	CLA	C13-C15-C16-C17
31	L	101	LHG	C28-C29-C30-C31
23	D	404	CLA	C11-C10-C8-C9
23	с	509	CLA	C11-C12-C13-C14
23	С	514	CLA	C14-C13-C15-C16
23	b	607	CLA	C11-C12-C13-C14
23	С	503	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	В	611	CLA	C11-C12-C13-C14
23	В	611	CLA	C14-C13-C15-C16
23	В	612	CLA	C11-C12-C13-C14
24	D	402	PHO	C16-C17-C18-C20
23	b	601	CLA	C16-C17-C18-C19
31	d	408	LHG	C34-C35-C36-C37
31	b	630	LHG	C18-C19-C20-C21
24	А	406	PHO	O2A-C1-C2-C3
29	a	415	PL9	C2-C3-C7-C8
23	B	604	CLA	O1A-CGA-O2A-C1
34	j	101	LMG	C36-C37-C38-C39
35	b	620	LMT	C2-C3-C4-C5
26	L	102	SQD	C16-C17-C18-C19
36	В	624	HTG	C3'-C4'-C5'-C6'
34	C	521	LMG	C18-C19-C20-C21
26	В	621	SQD	C11-C10-C9-C8
23	В	602	CLA	C13-C15-C16-C17
29	a	415	PL9	C20-C19-C21-C22
23	b	601	CLA	CAA-CBA-CGA-O1A
23	с	511	CLA	C1A-C2A-CAA-CBA
37	с	516	DGD	CDB-CEB-CFB-CGB
24	А	406	PHO	C2-C3-C5-C6
23	С	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C12-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C15
23	D	405	CLA	C12-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C7
23	С	509	CLA	C13-C15-C16-C17
34	Ζ	101	LMG	C29-C28-O8-C9
37	с	516	DGD	CCB-CDB-CEB-CFB
37	Н	102	DGD	C9B-CAB-CBB-CCB
35	D	403	LMT	C4'-C5'-C6'-O6'
23	В	603	CLA	C2A-CAA-CBA-CGA
23	С	504	CLA	C15-C16-C17-C18
23	А	407	CLA	C8-C10-C11-C12
23	с	507	CLA	C5-C6-C7-C8
31	L	101	LHG	С11-С10-С9-С8
34	Z	101	LMG	C28-C29-C30-C31
37	h	103	DGD	CDA-CEA-CFA-CGA
23	b	611	CLA	C13-C15-C16-C17
23	с	509	CLA	C10-C11-C12-C13
35	b	628	LMT	C6-C7-C8-C9
35	D	403	LMT	C2B-C1B-O1B-C4'
31	d	408	LHG	O7-C5-C6-O8
34	С	521	LMG	07-C8-C9-O8
31	d	407	LHG	O7-C5-C6-O8
31	А	415	LHG	C29-C30-C31-C32
25	у	101	BCR	C9-C10-C11-C12
23	С	502	CLA	O1D-CGD-O2D-CED
23	с	503	CLA	C8-C10-C11-C12
34	a	417	LMG	C34-C35-C36-C37
29	А	413	PL9	C30-C29-C31-C32
23	b	614	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
29	a	415	PL9	C18-C19-C21-C22
26	A	409	SQD	C14-C15-C16-C17
23	C	503	CLA	C16-C17-C18-C20
23	с	506	CLA	C11-C10-C8-C9
31	D	409	LHG	C10-C11-C12-C13
29	A	413	PL9	C2-C3-C7-C8
37	h	103	DGD	O1B-C1B-C2B-C3B
34	C	521	LMG	C10-C11-C12-C13
31	е	101	LHG	C14-C15-C16-C17
26	D	413	SQD	O10-C23-O48-C46
25	A	408	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	С	516	BCR	C1-C6-C7-C8
25	С	515	BCR	C1-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C30
35	М	101	LMT	C9-C10-C11-C12
31	L	101	LHG	C33-C34-C35-C36
31	е	101	LHG	C25-C26-C27-C28
37	С	518	DGD	C2G-C3G-O3G-C1D
34	J	101	LMG	C8-C7-O1-C1
26	В	621	SQD	C45-C44-O6-C1
37	с	517	DGD	C8A-C9A-CAA-CBA
31	d	408	LHG	O6-C4-C5-O7
36	с	521	HTG	C4-C5-C6-O6
35	m	103	LMT	O5'-C5'-C6'-O6'
26	D	413	SQD	C24-C23-O48-C46
34	j	101	LMG	C28-C29-C30-C31
34	С	501	LMG	C18-C19-C20-C21
35	В	623	LMT	O5B-C1B-O1B-C4'
26	a	411	SQD	C19-C20-C21-C22
26	В	621	SQD	C34-C35-C36-C37
23	с	513	CLA	C4-C3-C5-C6
29	a	415	PL9	C9-C11-C12-C13
29	А	413	PL9	C28-C29-C31-C32
26	L	102	SQD	O48-C23-C24-C25
31	А	415	LHG	O8-C23-C24-C25
23	b	613	CLA	CAA-CBA-CGA-O2A
34	Ζ	101	LMG	C11-C12-C13-C14
36	D	412	HTG	C1'-C2'-C3'-C4'
37	с	518	DGD	CCB-CDB-CEB-CFB
37	С	519	DGD	C6B-C7B-C8B-C9B
34	Z	101	LMG	C18-C19-C20-C21
31	d	407	LHG	C11-C10-C9-C8
34	Z	101	LMG	O7-C10-C11-C12
29	a	415	PL9	C45-C44-C46-C47
24	D	402	PHO	C5-C6-C7-C8
37	С	519	DGD	C1B-C2B-C3B-C4B
31	b	630	LHG	O7-C7-C8-C9
26	f	101	SQD	O47-C7-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	с	509	CLA	C6-C7-C8-C9
23	с	506	CLA	C11-C12-C13-C14
23	С	510	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	В	605	CLA	C11-C12-C13-C14
23	с	510	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C12-C13-C14
23	D	405	CLA	C14-C13-C15-C16
23	С	506	CLA	C14-C13-C15-C16
23	с	504	CLA	C11-C10-C8-C9
23	В	602	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
31	d	406	LHG	C11-C10-C9-C8
26	В	621	SQD	O48-C23-C24-C25
23	В	605	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	С	511	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	с	510	CLA	CAD-CBD-CGD-O2D
23	А	404	CLA	CAD-CBD-CGD-O2D
23	С	509	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	С	513	CLA	CAD-CBD-CGD-O2D
23	С	506	CLA	CAD-CBD-CGD-O2D
31	D	409	LHG	C9-C10-C11-C12
37	с	516	DGD	CCA-CDA-CEA-CFA
23	b	601	CLA	C13-C15-C16-C17
37	С	517	DGD	CCB-CDB-CEB-CFB
23	В	602	CLA	C2-C1-O2A-CGA
35	е	102	LMT	C5-C6-C7-C8
23	b	616	CLA	C4-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
23	В	614	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	O7-C7-C8-C9
37	h	103	DGD	C8A-C9A-CAA-CBA
25	С	527	BCR	C7-C8-C9-C10
23	В	604	CLA	CBD-CGD-O2D-CED
34	c	519	LMG	O7-C10-C11-C12
34	C	520	LMG	O8-C28-C29-C30
23	C	511	CLA	CAA-CBA-CGA-O2A
37	H	102	DGD	O1B-C1B-C2B-C3B
35	B	633	LMT	C5-C6-C7-C8
34	В	622	LMG	C22-C23-C24-C25
36	В	625	HTG	C4'-C5'-C6'-C7'
24	a	407	PHO	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C15-C16-C17-C18
31	D	409	LHG	C28-C29-C30-C31
23	А	405	CLA	C3-C5-C6-C7
34	j	101	LMG	C19-C20-C21-C22
23	В	606	CLA	CHA-CBD-CGD-O1D
23	В	606	CLA	CHA-CBD-CGD-O2D
23	В	602	CLA	CHA-CBD-CGD-O2D
24	D	402	PHO	CHA-CBD-CGD-O2D
23	с	503	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	С	508	CLA	CHA-CBD-CGD-O1D
23	С	508	CLA	CHA-CBD-CGD-O2D
23	С	509	CLA	CHA-CBD-CGD-O2D
23	с	507	CLA	CHA-CBD-CGD-O1D
23	с	507	CLA	CHA-CBD-CGD-O2D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	В	615	CLA	CHA-CBD-CGD-O1D
23	В	615	CLA	CHA-CBD-CGD-O2D
23	с	504	CLA	CHA-CBD-CGD-O2D
29	А	413	PL9	C45-C44-C46-C47
24	А	406	PHO	C4-C3-C5-C6
29	a	415	PL9	C43-C44-C46-C47
23	В	613	CLA	CAA-CBA-CGA-O2A
34	J	101	LMG	O7-C10-C11-C12
23	А	405	CLA	C2C-C3C-CAC-CBC
34	Z	101	LMG	C22-C23-C24-C25
37	С	518	DGD	CDB-CEB-CFB-CGB
35	Е	102	LMT	C4B-C5B-C6B-O6B
27	A	410	GOL	O2-C2-C3-O3
29	D	407	PL9	C45-C44-C46-C47
35	D	403	LMT	O5B-C1B-O1B-C4'
23	В	616	CLA	C13-C15-C16-C17
23	C	507	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	С	513	CLA	C6-C7-C8-C10
23	b	602	CLA	CAA-CBA-CGA-O2A
37	С	518	DGD	O2G-C1B-C2B-C3B
23	С	510	CLA	CAA-CBA-CGA-O2A
23	С	507	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	А	409	SQD	C30-C31-C32-C33
23	b	612	CLA	CAA-CBA-CGA-O2A
34	Z	101	LMG	C13-C14-C15-C16
24	D	402	PHO	C4C-C3C-CAC-CBC
34	с	519	LMG	O9-C10-C11-C12
23	a	404	CLA	C16-C17-C18-C20
23	с	508	CLA	C4-C3-C5-C6
23	с	513	CLA	C2-C3-C5-C6
31	е	101	LHG	O8-C23-C24-C25
26	f	101	SQD	O49-C7-C8-C9
25	У	101	BCR	C21-C22-C23-C24
23	С	507	CLA	C1A-C2A-CAA-CBA
35	В	632	LMT	C11-C10-C9-C8
31	b	630	LHG	O9-C7-C8-C9
34	С	520	LMG	O10-C28-C29-C30
23	с	511	CLA	C2-C1-O2A-CGA
26	L	102	SQD	O10-C23-C24-C25
31	А	415	LHG	O10-C23-C24-C25
23	В	614	CLA	CAA-CBA-CGA-O1A
26	а	411	SQD	C11-C10-C9-C8
36	с	522	HTG	C4-C5-C6-O6
34	m	101	LMG	O7-C10-C11-C12
31	b	630	LHG	C19-C20-C21-C22
37	Н	102	DGD	C7B-C8B-C9B-CAB
23	А	404	CLA	C2A-CAA-CBA-CGA
23	D	404	CLA	C2C-C3C-CAC-CBC
26	В	621	SQD	C35-C36-C37-C38
23	с	513	CLA	C16-C17-C18-C20
26	В	621	SQD	O10-C23-C24-C25
23	с	512	CLA	C15-C16-C17-C18
31	b	630	LHG	C11-C12-C13-C14
37	С	517	DGD	CDB-CEB-CFB-CGB
31	E	101	LHG	C4-O6-P-O5
31	d	408	LHG	C4-O6-P-O5
23	b	613	CLA	CAA-CBA-CGA-O1A
24	a	408	PHO	C2C-C3C-CAC-CBC
37	С	519	DGD	C9B-CAB-CBB-CCB
35	M	103	LMT	C4-C5-C6-C7
25	b	618	BCR	C23-C24-C25-C26
25	D	406	BCR	C1-C6-C7-C8
23	D	401	CLA	C4C-C3C-CAC-CBC
34	z	101	LMG	C15-C16-C17-C18

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	Chain	Daa	Trees	Atoma
		nes	<u>rype</u>	ALOIIIS
	Z	101	LMG	<u>09-C10-C11-C12</u>
23	b	612	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A
34	a	417	LMG	C37-C38-C39-C40
31	d	408	LHG	C28-C29-C30-C31
36	b	621	HTG	C2'-C3'-C4'-C5'
23	В	614	CLA	C15-C16-C17-C18
31	е	101	LHG	O10-C23-C24-C25
23	с	510	CLA	CAA-CBA-CGA-O1A
31	L	101	LHG	O9-C7-C8-C9
23	с	503	CLA	C15-C16-C17-C18
23	В	608	CLA	CAD-CBD-CGD-O1D
23	b	611	CLA	CAD-CBD-CGD-O1D
23	с	505	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	С	505	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	a	405	CLA	CAD-CBD-CGD-O1D
23	В	610	CLA	CAD-CBD-CGD-O1D
34	a	417	LMG	C21-C22-C23-C24
24	a	408	PHO	NC-C1C-CHC-C4B
37	с	516	DGD	O2G-C1B-C2B-C3B
23	a	406	CLA	C11-C10-C8-C9
23	a	405	CLA	C11-C10-C8-C9
34	J	101	LMG	O9-C10-C11-C12
23	с	505	CLA	CAA-CBA-CGA-O2A
26	A	409	SQD	O47-C7-C8-C9
23	D	405	CLA	C8-C10-C11-C12
26	f	101	SQD	C24-C25-C26-C27
36	b	625	HTG	C1'-C2'-C3'-C4'
23	с	505	CLA	CAA-CBA-CGA-O1A
34	С	520	LMG	C31-C32-C33-C34
23	В	606	CLA	C4-C3-C5-C6
23	с	506	CLA	C4-C3-C5-C6
23	a	406	CLA	C11-C10-C8-C7
23	A	407	CLA	C2-C3-C5-C6
23	b	614	CLA	C12-C13-C15-C16
23	В	617	CLA	C11-C12-C13-C15
31	Е	101	LHG	07-C7-C8-C9
26	A	409	SQD	C13-C14-C15-C16
23	b	612	CLA	C8-C10-C11-C12

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Mol	Chain	\mathbf{Res}	Type	Atoms
23	b	604	CLA	C13-C15-C16-C17
25	Y	101	BCR	C21-C22-C23-C24
37	С	518	DGD	O1B-C1B-C2B-C3B
23	В	613	CLA	CAA-CBA-CGA-O1A
34	m	101	LMG	O9-C10-C11-C12
26	a	411	SQD	C10-C11-C12-C13
35	b	628	LMT	C2-C1-O1'-C1'
35	В	632	LMT	C2-C1-O1'-C1'
31	d	408	LHG	O8-C23-C24-C25
23	С	506	CLA	CAA-CBA-CGA-O2A
29	А	413	PL9	C19-C21-C22-C23
37	С	518	DGD	CBB-CCB-CDB-CEB
31	d	408	LHG	C25-C26-C27-C28
31	L	101	LHG	C16-C17-C18-C19
23	В	613	CLA	C13-C15-C16-C17
23	В	608	CLA	C2A-CAA-CBA-CGA
36	b	622	HTG	C4'-C5'-C6'-C7'
26	А	409	SQD	O49-C7-C8-C9
37	с	516	DGD	O1B-C1B-C2B-C3B
26	a	411	SQD	O47-C7-C8-C9
34	С	501	LMG	O8-C28-C29-C30

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There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









































































































































































































































































































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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 >	$\# RSRZ {>}2$	$OWAB(A^2)$	Q<0.9
1	А	334/344~(97%)	0.05	11 (3%) 46 50	22,33,58,97	0
1	а	334/344~(97%)	0.20	14 (4%) 36 39	24,36,65,113	0
2	В	504/505~(99%)	0.31	58 (11%) 4 4	24, 38, 68, 118	0
2	b	504/505~(99%)	0.47	70~(13%) 2 2	25, 40, 77, 122	0
3	C	451/455~(99%)	0.64	71 (15%) 2 1	27, 48, 70, 108	0
3	с	455/455~(100%)	0.45	61 (13%) 3 2	32, 52, 72, 118	0
4	D	342/342~(100%)	0.08	18 (5%) 26 28	22, 35, 58, 113	0
4	d	341/342~(99%)	0.28	26 (7%) 13 14	24, 39, 59, 124	0
5	E	81/84~(96%)	0.34	7 (8%) 10 10	40, 59, 90, 125	0
5	е	79/84~(94%)	0.95	19 (24%) 0 0	45, 62, 100, 125	0
6	F	34/44~(77%)	-0.09	1 (2%) 51 55	41, 51, 81, 96	0
6	f	31/44~(70%)	-0.07	4 (12%) 3 3	48, 53, 84, 128	0
7	Н	64/65~(98%)	0.37	8 (12%) 3 3	37, 51, 72, 104	0
7	h	65/65~(100%)	1.14	19 (29%) 0 0	40, 54, 79, 152	0
8	Ι	37/38~(97%)	0.42	7(18%) 1 1	36, 48, 98, 129	0
8	i	37/38~(97%)	0.24	3 (8%) 12 12	38, 49, 107, 137	0
9	J	38/39~(97%)	0.29	6 (15%) 2 1	37, 55, 113, 156	0
9	j	39/39~(100%)	0.84	10 (25%) 0 0	46, 56, 109, 137	0
10	K	37/37~(100%)	0.15	4 (10%) 5 5	49, 58, 81, 98	0
10	k	37/37~(100%)	0.40	3 (8%) 12 12	52, 60, 82, 99	0
11	L	36/37~(97%)	0.50	5 (13%) 2 2	23, 30, 98, 143	0
11	1	$\overline{36/37}\ (97\%)$	0.19	4(11%) 5 5	$\overline{24, 31, 97, 143}$	0
12	M	32/36~(88%)	-0.19	1 (3%) 49 52	24, 31, 53, 125	0
12	m	33/36~(91%)	-0.30	3 (9%) 9 9	$\overline{24, 32, 66, 126}$	0

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Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
13	Ο	243/244~(99%)	0.36	30 (12%) 4 3	22, 50, 103, 163	0
13	0	243/244~(99%)	0.57	45 (18%) 1 1	26, 50, 108, 151	0
14	Т	29/32~(90%)	0.28	1 (3%) 45 48	26, 31, 68, 97	0
14	t	29/32~(90%)	-0.03	0 100 100	26, 31, 69, 98	0
15	U	96/104~(92%)	0.57	13 (13%) 3 2	32, 44, 72, 86	0
15	u	97/104~(93%)	-0.10	4 (4%) 37 40	37, 47, 72, 105	0
16	V	137/137~(100%)	0.17	5 (3%) 42 46	30, 46, 75, 111	0
16	V	137/137~(100%)	0.45	21 (15%) 2 1	37, 54, 79, 112	0
17	X	38/40~(95%)	0.40	3 (7%) 12 12	49, 58, 80, 121	0
17	x	38/40~(95%)	1.08	9 (23%) 0 0	50, 60, 84, 123	0
18	Y	29/30~(96%)	1.71	12 (41%) 0 0	60, 76, 112, 120	0
18	У	29/30~(96%)	1.07	7 (24%) 0 0	63, 76, 107, 118	0
19	Z	62/62~(100%)	1.44	23 (37%) 0 0	57, 77, 127, 161	0
19	Z	62/62~(100%)	1.60	18 (29%) 0 0	61, 79, 127, 161	0
20	R	34/34~(100%)	6.37	34 (100%) 0 0	92, 116, 145, 149	0
All	All	5284/5384 (98%)	0.43	658 (12%) 3 3	22, 45, 88, 163	0

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All (658) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	11.0
20	R	20	VAL	10.3
2	b	495	PHE	9.2
20	R	35	LEU	8.9
1	А	11	ALA	8.3
20	R	14	LEU	8.3
20	R	6	LEU	8.1
20	R	15	ALA	8.1
20	R	19	ALA	8.0
20	R	8	VAL	7.9
20	R	23	ILE	7.8
17	Х	38	GLN	7.8
9	j	3	GLU	7.7
20	R	5	VAL	7.5
9	j	2	SER	7.1
20	R	3	TRP	7.1
20	R	31	VAL	6.8



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7		nes	<u>Type</u>	
7	h D	00	GLY	0.7
20	R I	4	ARG	6.6
8		38	GLU	6.6
2	b	486	LEU	6.5
20	R	24	LEU	6.5
20	R	7	VAL	6.5
19	Z	4	LEU	6.4
2	b	218	LEU	6.3
3	С	437	PHE	6.3
2	b	494	GLY	6.3
3	С	253	LEU	6.1
1	А	13	LEU	6.1
20	R	12	VAL	6.1
13	0	27	ARG	6.0
2	b	493	TRP	6.0
20	R	16	ALA	6.0
20	R	34	LEU	5.9
5	Е	84	LYS	5.9
2	b	488	PRO	5.9
3	С	181	PHE	5.9
20	R	13	LEU	5.9
8	i	37	LEU	5.8
2	В	496	TYR	5.8
19	Z	32	ASP	5.8
9	J	5	GLY	5.8
13	0	22	LEU	5.7
3	C	276	LEU	5.7
2	b	487	SER	5.7
20	R	17	GLY	5.6
20	R	27	ALA	5.6
$\frac{-2}{20}$	R	33	LYS	5.6
19	Z	33	TRP	5.6
7	h	6	TRP	5.5
$\frac{1}{20}$	R	21	ARG	5.5
20	R	10	LEU	5.5
<u></u>	D	238	THR	5.5
3	C	60	ILE	5.5
10	7	60	PHE	5.0
<u>-19</u> -00	P D	00 0		5.4
20 Q		$\frac{2}{27}$	I FII	5.4
0 	D I	01 96	TVP	5.4
20		20		0.4
19	I Y	18	VAL	ರಿ.ರ



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Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	5.3
19	Z	7	LEU	5.3
3	с	143	TYR	5.3
17	X	33	GLN	5.3
20	R	32	GLN	5.3
19	Z	61	VAL	5.2
7	h	65	LEU	5.2
20	R	11	PRO	5.2
19	Z	3	ILE	5.2
3	С	433	LEU	5.1
19	Z	5	PHE	5.1
19	Z	1	MET	5.1
18	у	19	ILE	5.1
3	с	60	ILE	5.0
19	Z	31	GLN	4.9
20	R	22	ASN	4.9
19	Z	2	THR	4.9
2	В	495	PHE	4.9
9	j	5	GLY	4.8
19	Z	57	LEU	4.8
17	X	37	VAL	4.8
3	С	279	LEU	4.7
13	0	25	THR	4.7
11	1	3	PRO	4.7
3	с	426	LEU	4.7
17	Х	2	THR	4.7
2	b	249	ALA	4.6
20	R	28	VAL	4.6
2	b	161	LEU	4.6
1	А	12	ASN	4.6
2	b	504	THR	4.6
17	X	2	THR	4.6
2	В	461	LEU	4.6
3	C	143	TYR	4.6
2	В	494	GLY	4.6
4	d	12	ARG	4.5
13	0	142	PHE	4.5
3	C	281	MET	4.5
4	d	17	ILE	4.5
13	0	243	ILE	4.5
19	Z	30	PRO	4.5
2	b	496	TYR	4.5



Mol	Chain	Res	Type	RSRZ
13	0	36	GLN	4.5
2	b	484	PRO	4.5
17	Х	34	ILE	4.5
9	j	7	ILE	4.4
17	Х	3	ILE	4.4
3	с	200	THR	4.4
2	b	503	THR	4.4
19	Ζ	34	ASP	4.4
3	С	23	ALA	4.4
2	b	491	VAL	4.4
3	С	438	LEU	4.4
15	U	58	VAL	4.4
13	0	38	TYR	4.3
3	С	280	SER	4.3
2	b	497	GLN	4.3
10	k	18	PHE	4.3
2	В	253	ALA	4.3
3	С	282	MET	4.3
13	0	32	ILE	4.3
11	L	2	GLU	4.3
2	b	489	GLU	4.2
3	С	283	GLY	4.2
3	с	279	LEU	4.2
13	0	25	THR	4.2
19	Z	56	VAL	4.2
11	1	2	GLU	4.1
3	с	63	TRP	4.1
2	b	492	GLU	4.1
16	V	21	LEU	4.1
20	R	30	GLN	4.1
2	b	245	VAL	4.1
1	А	15	GLU	4.1
13	0	35	SER	4.1
15	U	73	GLN	4.1
18	Y	21	GLN	4.1
3	С	61	VAL	4.1
3	с	198	VAL	4.1
3	С	155	ASN	4.1
2	В	488	PRO	4.0
2	b	246	PHE	4.0
2	В	251	VAL	4.0
2	b	502	VAL	4.0



Mol	Chain	Res	Type	RSRZ
2	В	458	PHE	4.0
5	Е	15	THR	4.0
3	С	198	VAL	4.0
3	С	204	LEU	4.0
13	0	87	VAL	4.0
2	b	248	ALA	3.9
7	h	22	ALA	3.9
3	с	430	HIS	3.9
9	j	9	LEU	3.9
17	X	36	LYS	3.9
18	Y	43	ARG	3.9
3	С	286	ALA	3.9
3	С	436	PHE	3.8
2	В	462	PHE	3.8
13	0	27	ARG	3.8
3	с	201	ASN	3.8
4	d	154	VAL	3.8
15	U	104	LYS	3.8
3	С	430	HIS	3.8
3	с	191	PRO	3.8
2	b	499	VAL	3.8
3	с	140	LEU	3.7
3	с	433	LEU	3.7
20	R	25	PRO	3.7
3	С	285	ILE	3.7
11	L	7	ARG	3.7
20	R	9	LEU	3.7
16	v	10	VAL	3.7
10	k	17	ILE	3.7
16	V	107	LEU	3.7
3	с	203	THR	3.7
2	b	498	LYS	3.7
3	С	429	SER	3.7
5	Е	17	VAL	3.7
13	0	246	ALA	3.7
9	J	7	ILE	3.7
19	Z	35	ARG	3.7
13	0	133	VAL	3.6
1	a	11	ALA	3.6
2	b	296	ALA	3.6
2	В	489	GLU	3.6
8	Ι	36	ASP	3.6

I36ASP3.6Continued on next page...



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Mol	Chain	Res	Type	RSRZ		
15	U	70	ARG	3.6		
3	С	277	GLY	3.6		
3	с	87	ILE	3.6		
5	Е	83	LEU	3.6		
2	b	250	PHE	3.6		
15	U	62	LEU	3.6		
2	В	505	ARG	3.6		
9	j	1	MET	3.6		
2	b	462	PHE	3.6		
3	С	435	PHE	3.6		
3	с	146	PHE	3.6		
13	0	26	ALA	3.5		
16	V	4	THR	3.5		
5	е	20	TRP	3.5		
13	0	134	THR	3.5		
2	В	252	VAL	3.5		
3	С	284	PHE	3.5		
2	b	294	SER	3.5		
3	с	202	PRO	3.5		
7	h	23	PRO	3.5		
2	b	295	GLY	3.5		
3	С	262	ARG	3.5		
13	0	26	ALA	3.5		
2	b	247	PHE	3.5		
3	С	147	PHE	3.5		
3	С	59	LEU	3.5		
3	С	434	ALA	3.5		
2	b	251	VAL	3.5		
13	0	135	SER	3.5		
3	С	440	GLY	3.5		
2	b	217	ILE	3.4		
15	U	79	LEU	3.4		
3	С	145	SER	3.4		
3	С	439	VAL	3.4		
19	Z	3	ILE	3.4		
3	С	278	ALA	3.4		
13	0	37	THR	3.4		
3	С	148	GLY	3.4		
2	b	485	GLU	3.4		
3	С	432	VAL	3.4		
19	Z	62	VAL	3.4		
4	D	12	ARG	3.4		



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	Unaim	70	_ туре	
0 10	e	19	TUD	3.4
13	0	4	THR	3.4
13	0	211		3.4
4	d	148	ALA	3.4
20	R	29		3.4
2	b	252	VAL	3.4
3	с	195	ASP	3.4
17	X	39	ARG	3.4
6	f	42	PHE	3.4
7	Н	6	TRP	3.4
16	V	19	ILE	3.4
19	Z	29	SER	3.4
16	v	17	LYS	3.4
12	m	33	GLN	3.3
17	X	3	ILE	3.3
13	0	33	ASP	3.3
2	b	288	VAL	3.3
3	с	155	ASN	3.3
3	с	283	GLY	3.3
4	d	157	PHE	3.3
2	В	248	ALA	3.3
2	В	249	ALA	3.3
2	В	502	VAL	3.3
13	0	204	VAL	3.3
13	0	24	ASP	3.3
3	С	431	PHE	3.3
2	b	244	ALA	3.3
13	0	245	PRO	3.3
2	В	296	ALA	3.3
2	b	293	ALA	3.3
3	C	252	ILE	3.3
18	v	37	PHE	3.3
2	b	298	LEU	3.3
18	Y	25	ILE	3.3
3	C C	282	MET	3.3
3	C C	$\frac{202}{427}$	ALA	3.2
1२		136		3.2
- 5 - то	C C	200	SEB	3.2
<u>ງ</u> ງ	R R	454		3.2
	D 7	404 26	SED	3.2
19		00 150		0.2 2.0
4	a	102	VAL	<u>).2</u>
19		9	L LEU	3.2



Mol	Chain	Res	Type	RSRZ
2	В	504	THR	3.2
3	С	63	TRP	3.2
19	Z	59	PHE	3.2
13	0	24	ASP	3.2
1	A	16	ARG	3.2
2	В	459	ALA	3.2
5	Е	11	SER	3.2
4	d	153	PHE	3.1
13	0	62	GLU	3.1
19	Ζ	39	LEU	3.1
12	m	34	LYS	3.1
7	Н	2	ALA	3.1
18	Y	46	LEU	3.1
3	с	437	PHE	3.1
5	е	25	ILE	3.1
4	d	155	SER	3.1
13	0	56	PRO	3.1
2	В	457	VAL	3.1
2	b	219	VAL	3.1
7	h	58	VAL	3.1
4	d	159	ILE	3.1
8	Ι	34	ARG	3.1
5	е	72	ALA	3.1
18	Y	20	ALA	3.1
4	D	11	GLU	3.0
2	В	451	PHE	3.0
9	j	4	GLY	3.0
3	С	275	SER	3.0
3	с	59	LEU	3.0
18	У	41	VAL	3.0
3	С	146	PHE	3.0
9	J	4	GLY	3.0
2	В	460	LEU	3.0
16	V	135	VAL	3.0
4	d	149	PRO	3.0
2	b	162	PHE	3.0
17	X	34	ILE	3.0
3	C	25	ASN	3.0
2	b	126	PRO	3.0
5	e	59	GLU	3.0
3	с	190	ALA	3.0
13	0	22	LEU	3.0



9011

	Chain	Res	Type	BSB7
12		28	- JPC	3.0
10	7	$\frac{20}{97}$	TVR	3.0
19		27 19		0.0 2.0
1 12	a	15		3.0 2.0
13	0	0 0 7	LEU	3.0
13	0	80		3.0
<u> </u>	h D	10		3.0
	В	290	ALA	3.0
4	d	13	GLY	3.0
13	0	133	VAL	2.9
3	C	57	ALA	2.9
3	с	192	GLY	2.9
2	b	291	SER	2.9
2	b	458	PHE	2.9
3	с	429	SER	2.9
2	b	292	LEU	2.9
3	с	260	ALA	2.9
4	d	151	ALA	2.9
11	L	10	VAL	2.9
3	С	180	MET	2.9
15	U	59	GLU	2.9
2	b	290	ALA	2.9
2	b	483	ASP	2.9
15	U	103	TYR	2.9
7	h	12	ARG	2.9
13	0	59	LYS	2.9
7	h	7	LEU	2.9
13	0	93	LEU	2.9
3	С	135	ARG	2.9
8	i	38	GLU	2.9
3	с	196	VAL	2.9
16	v	5	PRO	2.9
5	е	57	ALA	2.9
13	0	5	LEU	2.9
13	0	29	ALA	2.9
13	0	93	LEU	2.8
3	c	193	GLY	2.8
3	C C	280	SER	2.8
4	b d	147	SER	2.8
<u>+</u> 13		01	GLY	2.0
10		291		2.0
1 0	R A	2/24		2.0
2 		242		2.0
ა		200	ιπκ	2.ð



5GTI

Mol	Chain	Res	Type	RSRZ
19	Z	26	ALA	2.8
19	Z	42	LEU	2.8
19	Z	46	LEU	2.8
13	0	60	ARG	2.8
16	V	16	GLY	2.8
1	a	265	PHE	2.8
4	d	150	ILE	2.8
15	U	74	ILE	2.8
2	b	459	ALA	2.8
2	В	161	LEU	2.8
2	b	238	LEU	2.8
3	с	147	PHE	2.8
2	В	293	ALA	2.8
3	С	254	THR	2.8
2	В	487	SER	2.8
9	J	3	GLU	2.8
11	L	9	PRO	2.8
4	D	150	ILE	2.8
16	V	26	TYR	2.7
15	U	99	ASN	2.7
18	Y	45	ASN	2.7
3	с	64	ALA	2.7
2	В	294	SER	2.7
7	Н	46	LEU	2.7
13	0	139	SER	2.7
4	D	122	LEU	2.7
19	Z	38	GLN	2.7
2	В	85	GLY	2.7
2	b	127	ARG	2.7
13	Ο	204	VAL	2.7
16	v	22	THR	2.7
5	е	83	LEU	2.7
5	е	84	LYS	2.7
3	с	61	VAL	2.7
19	Z	56	VAL	2.7
2	В	297	THR	2.7
10	K	14	ALA	2.7
3	С	199	ILE	2.7
3	с	88	LEU	2.7
3	с	199	ILE	2.7
19	Z	7	LEU	2.7
13	0	207	ARG	2.7



$5 \mathrm{GTI}$

Mol	Chain	Res	Type	RSRZ
18	Y	42	ARG	2.7
3	С	201	ASN	2.7
13	0	132	ASN	2.7
13	0	57	LYS	2.7
11	L	8	GLN	2.7
2	В	284	ILE	2.7
3	с	257	PHE	2.7
4	d	123	ILE	2.7
18	Y	38	LEU	2.7
10	K	29	PRO	2.7
13	0	130	GLN	2.7
2	b	242	ILE	2.6
5	е	36	LEU	2.6
6	f	43	ILE	2.6
2	b	412	THR	2.6
3	С	56	HIS	2.6
13	0	23	ASP	2.6
1	А	14	TRP	2.6
2	b	457	VAL	2.6
3	с	22	PHE	2.6
16	V	136	TYR	2.6
7	h	64	ALA	2.6
13	0	83	GLY	2.6
2	В	250	PHE	2.6
2	b	123	PHE	2.6
3	С	257	PHE	2.6
2	b	121	GLU	2.6
15	u	103	TYR	2.6
7	h	8	GLY	2.6
3	С	182	PHE	2.6
3	с	265	ILE	2.6
19	Ζ	60	PHE	2.6
7	h	13	PRO	2.6
16	V	12	LEU	2.6
3	с	284	PHE	2.6
4	D	159	ILE	2.6
4	d	14	TRP	2.6
2	В	241	SER	2.6
5	е	21	VAL	2.5
19	Z	53	VAL	2.5
2	В	490	GLN	2.5
4	d	146	PHE	2.5



5C	TT	
JG	ΤT	

<u>р</u> и. 1		D -		
	Unain	Kes	Type	KSKZ
10	K	28	ILE	2.5
18	у	43	ARG	2.5
4	d	126	MET	2.5
12	m	31	SER	2.5
3	С	255	THR	2.5
4	d	156	VAL	2.5
3	с	317	PHE	2.5
2	b	172	TYR	2.5
3	C	55	ALA	2.5
3	С	287	THR	2.5
3	С	340	TYR	2.5
4	D	148	ALA	2.5
2	b	505	ARG	2.5
13	0	207	ARG	2.5
1	a	15	GLU	2.5
13	0	199	LEU	2.5
16	V	8	LEU	2.5
1	a	264	SER	2.5
1	a	225	ARG	2.5
2	В	304	ALA	2.5
2	В	350	GLU	2.5
4	D	351	ALA	2.5
3	с	56	HIS	2.5
2	b	482	ILE	2.5
19	Z	6	GLN	2.5
2	В	245	VAL	2.5
16	v	25	GLN	2.5
9	J	6	ARG	2.5
19	Z	59	PHE	2.5
2	В	126	PRO	2.5
4	d	119	ALA	2.5
7	h	9	ASP	2.5
1	A	19	ASN	2.5
13	0	4	THR	2.5
13	0	58	ASN	2.5
16	v	7	VAL	2.5
15	Ū	76	ARG	2.5
1	a	285	PHE	2.5
2	B	200	PHE	2.5
$\frac{2}{2}$	R	452	THR	2.5
2		255	THR	2.0 2.5
5 7	ц Ц	00 	LEII	2.0
1	11	44	L L L U	∠.4



5GTI

Mol	Chain	Res	Type	RSRZ
1	a	262	TYR	2.4
4	D	147	SER	2.4
3	С	154 LYS		2.4
3	С	272	LEU	2.4
10	k	38	VAL	2.4
19	Z	62	VAL	2.4
2	В	463 PHE		2.4
18	Y	22 LEU		2.4
8	Ι	26	GLY	2.4
16	V	50	PRO	2.4
3	с	144	SER	2.4
5	е	14	ILE	2.4
2	b	414	PRO	2.4
3	C	288	CYS	2.4
3	с	259	TRP	2.4
2	b	301	ALA	2.4
13	0	138	THR	2.4
3	С	442	LEU	2.4
18	у	22	LEU	2.4
13	0	39 ARG		2.4
2	b	223	GLN	2.4
15	U	101	GLY	2.4
1	a	340	PRO	2.4
1	a	14	TRP	2.4
2	b	501	ASP	2.4
8	Ι	29	ALA	2.4
3	С	26	ARG	2.4
16	V	132	GLY	2.4
4	D	123	ILE	2.4
14	Т	29	ILE	2.4
7	h	3	ARG	2.4
13	0	208	THR	2.4
19	Z	33	TRP	2.4
2	b	289	GLN	2.3
5	е	42	LEU	2.3
9	J	9	LEU	2.3
13	0	15	LEU	2.3
3	C	196	VAL	2.3
2	В	162	PHE	2.3
3	С	58	GLY	2.3
4	d	158	LEU	2.3
7	Н	43	LEU	2.3



5GTI

Mol	Chain	Res Type		RSRZ
4	D	154	VAL	2.3
6	f	15 ILE		2.3
5	е	15 THR		2.3
5	е	39 SER		2.3
2	В	455 HIS		2.3
13	0	86	LYS	2.3
3	с	425	TRP	2.3
13	0	87	VAL	2.3
3	С	459	ILE	2.3
2	В	411	PHE	2.3
2	В	214	LEU	2.3
2	В	501	ASP	2.3
2	b	490	GLN	2.3
3	с	204	LEU	2.3
4	d	37	LEU	2.3
1	А	249	VAL	2.3
2	В	219	VAL	2.3
4	D	280	TRP	2.3
3	С	183 GLY		2.3
3	с	184	GLY	2.3
8	Ι	6	ILE	2.3
2	b	243	ALA	2.3
4	D	151	ALA	2.3
6	f	16	PHE	2.3
16	V	110	LYS	2.3
16	V	95	LEU	2.3
3	с	58	GLY	2.3
1	А	152	ALA	2.3
5	Е	74	GLN	2.3
13	0	40	ILE	2.3
13	0	63	ALA	2.3
3	С	426	LEU	2.3
5	е	7	GLU	2.3
6	F	13	TYR	2.3
7	h	42	LEU	2.3
2	В	180	PRO	2.2
19	Z	38	GLN	2.2
3	с	97	TRP	2.2
4	d	279	LEU	2.2
13	0	131	PRO	2.2
13	0	155	ASN	2.2
3	с	183	GLY	2.2



Mol	Chain	Res	Type	RSRZ	
2	B	503	THR	2.2	
	0	140	THR	2.2	
4	D	149	PRO	2.2	
2	b	241	SER.	2.2	
7	h	20	LYS	2.2	
16	v	1 ALA		2.2	
4	d	127 LEU		2.2	
5	e	81	GLU	2.2	
3	С	64	ALA	2.2	
2	B	464	PHE	2.2	
7	Н	8	GLY	2.2	
3	С	266	TRP	2.2	
9	i	6	ARG	2.2	
2	b	155	ALA	2.2	
3	с	55	ALA	2.2	
3	с	256	PRO	2.2	
4	d	122	LEU	2.2	
13	0	209	GLY	2.2	
7	h	16	SER	2.2	
13	0	30 TYR		2.2	
3	с	67 MET		2.2	
7	Н	10	ILE	2.2	
2	В	286	ARG	2.1	
15	u	101	GLY	2.1	
1	A	339	PHE	2.1	
4	D	273	PHE	2.1	
2	В	298	LEU	2.1	
1	a	330	VAL	2.1	
2	b	456	ALA	2.1	
16	V	6	GLU	2.1	
18	Y	40	ALA	2.1	
18	У	20	ALA	2.1	
2	b	463	PHE	2.1	
12	М	33	GLN	2.1	
19	Z	57	LEU	2.1	
2	В	456	ALA	2.1	
2	В	491	VAL	2.1	
13	Ο	30	TYR	2.1	
19	Z	28	ALA	2.1	
3	с	24	THR	2.1	
16	v	9	THR	2.1	
7	h	55	LEU	2.1	



Mol	Chain	ResType		RSRZ	
13	0	34	34 SER 2		
15	U	94	4 GLY 2.1		
9	j	14	14 THR 2.		
13	0	23	ASP	2.1	
19	Ζ	4	4 LEU		
4	D	350	ASN	2.1	
13	0	91	GLY	2.1	
5	е	82	GLN	2.1	
3	с	428	THR	2.1	
1	a	120	LEU	2.1	
1	a	297	LEU	2.1	
2	b	466	HIS	2.1	
3	с	230	LEU	2.1	
2	b	224	ARG	2.1	
3	С	206	PRO	2.1	
3	С	144	SER	2.1	
17	Х	7	LEU	2.1	
11	1	8	GLN	2.1	
13	Ο	196	GLN	2.1	
19	Ζ	1	MET	2.0	
9	j	8	PRO	2.0	
10	K	30	VAL	2.0	
1	А	38	ILE	2.0	
2	b	239	SER	2.0	
4	D	343	GLU	2.0	
5	е	24	SER	2.0	
15	u	70	ARG	2.0	
2	В	256	MET	2.0	
3	с	281	MET	2.0	
3	с	66	ALA	2.0	
13	0	241	ALA	2.0	
2	В	288	VAL	2.0	
4	D	277	THR	2.0	
7	Н	5	THR	2.0	
16	V	2	GLU	2.0	
16	V	18	THR	2.0	
3	С	339	LYS	2.0	
2	В	254	GLY	2.0	
18	У	38	LEU	2.0	
8	i	2	GLU	2.0	
4	d	40	CYS	2.0	
7	h	5	THR	2.0	



Mol	Chain	Res Type		RSRZ
13	0	61	GLN	2.0
5	е	17	VAL	2.0
16	V	135	VAL	2.0
13	0	226	GLY	2.0
2	В	292	LEU	2.0
3	с	21	ILE	2.0
13	0	10	ILE	2.0
15	u	102	LEU	2.0
3	с	187	ASP	2.0
5	Е	82	GLN	2.0
11	1	9	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
8	FME	i	1	10/11	0.96	0.11	$38,\!50,\!63,\!74$	0
12	FME	m	1	10/11	0.96	0.11	$26,\!43,\!69,\!74$	0
12	FME	М	1	10/11	0.97	0.17	33,41,72,72	0
8	FME	Ι	1	10/11	0.97	0.17	29,49,53,54	0
14	FME	t	1	10/11	0.97	0.10	22,34,47,66	0
14	FME	Т	1	10/11	0.98	0.09	19,37,45,52	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
30	UNL	А	414	28/-	0.27	0.57	$66,\!93,\!121,\!126$	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
36	HTG	В	626	19/19	0.48	0.70	$51,\!135,\!163,\!189$	0
36	HTG	D	412	16/19	0.48	0.40	43,118,136,138	0
34	LMG	С	521	51/55	0.52	0.51	50,107,149,153	0
30	UNL	a	416	30/-	0.54	0.50	86,102,121,129	0
36	HTG	С	524	9/19	0.57	1.21	70,90,106,139	0
35	LMT	В	633	35/35	0.58	0.45	$39,\!117,\!133,\!139$	0
30	UNL	b	627	33/-	0.59	0.45	53,80,145,147	0
36	HTG	b	623	19/19	0.59	0.61	73,116,140,180	0
35	LMT	D	403	35/35	0.60	0.40	40,112,125,126	0
35	LMT	С	522	35/35	0.60	0.64	83,119,141,151	0
34	LMG	с	520	51/55	0.64	0.43	62,104,135,147	0
35	LMT	е	102	35/35	0.64	0.80	75,139,161,171	0
35	LMT	m	103	35/35	0.65	0.50	40,85,113,117	0
30	UNL	J	102	10/-	0.66	0.45	59,66,85,90	0
35	LMT	М	103	35/35	0.68	0.34	37,128,152,157	0
35	LMT	М	101	35/35	0.68	0.34	40,85,105,107	0
30	UNL	В	631	33/-	0.68	0.26	36,92,134,151	0
30	UNL	Ι	101	40/-	0.70	0.32	39,89,141,148	0
36	HTG	с	522	19/19	0.70	0.82	83,139,149,158	0
25	BCR	h	102	40/40	0.71	0.29	42,57,71,74	0
36	HTG	В	625	19/19	0.72	0.43	$43,\!101,\!109,\!111$	0
34	LMG	Z	101	37/55	0.72	0.40	57,103,134,149	0
30	UNL	j	102	10/-	0.73	0.32	57,81,94,94	0
35	LMT	Е	102	35/35	0.73	0.56	$91,\!129,\!157,\!163$	0
31	LHG	е	101	42/49	0.73	0.43	$63,\!119,\!140,\!150$	0
30	UNL	с	525	32/-	0.73	0.33	74,104,124,132	0
30	UNL	K	101	34/-	0.74	0.32	62,102,116,137	0
30	UNL	m	102	10/-	0.75	0.32	36,47,64,66	0
30	UNL	i	101	40/-	0.75	0.38	56,91,147,151	0
29	PL9	a	415	55/55	0.75	0.34	56,82,108,115	0
27	GOL	d	401	6/6	0.76	0.68	36,51,76,77	0
36	HTG	b	622	19/19	0.76	0.83	77,105,127,134	0
36	HTG	b	621	19/19	0.78	0.26	33,91,127,144	0
29	PL9	A	413		0.78	0.34	44,83,100,110	0
35	LMT	b	628	$\frac{25/35}{12/54}$	0.78	0.28	37,63,135,142	0
26	SQD	t	101	43/54	0.78	0.32	86,117,154,157	0
35	LMT	b	620		0.79	0.24	55,88,143,147	0
	HTG	h T	101	10/19	0.79	0.38	71,110,125,143	
20	SQD		102	<u> </u>	0.79	0.26	39,73,114,123	
33	UA	B	601		0.79	0.12	144,144,144,144	
30	HTG		523	19/19	0.80	0.43	95,107,121,133	
30	UNL	a a	029	30/-	0.81	0.33	40,80,130,141	U



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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	Q < 0.9	
36	HTG	с	521	19/19	0.81	0.37	$71,\!125,\!137,\!163$	0	
36	HTG	b	626	19/19	0.81	0.25	$66,\!114,\!151,\!181$	0	
31	LHG	Ε	101	42/49	0.81	0.26	$47,\!95,\!114,\!121$	0	
36	HTG	В	630	19/19	0.82	0.27	$67,\!116,\!145,\!154$	0	
26	SQD	В	621	54/54	0.82	0.24	44,82,109,118	0	
35	LMT	В	632	25/35	0.82	0.26	$41,\!68,\!135,\!136$	0	
25	BCR	Н	101	40/40	0.82	0.23	$35,\!46,\!66,\!73$	0	
34	LMG	С	520	51/55	0.83	0.28	43,75,125,134	0	
34	LMG	С	501	51/55	0.83	0.29	40,81,110,113	0	
27	GOL	0	302	6/6	0.83	0.27	$63,\!68,\!72,\!78$	0	
30	UNL	Х	101	18/-	0.84	0.32	$47,\!66,\!104,\!105$	0	
35	LMT	В	623	35/35	0.84	0.26	$50,\!95,\!120,\!122$	0	
26	SQD	А	411	54/54	0.85	0.25	41,71,114,129	0	
30	UNL	М	102	10/-	0.85	0.27	38,51,60,60	0	
30	UNL	D	411	40/-	0.85	0.28	49,76,125,128	0	
35	LMT	a	418	35/35	0.86	0.53	$97,\!118,\!139,\!139$	0	
27	GOL	В	628	6/6	0.86	0.26	47,58,65,72	0	
36	HTG	V	203	11/19	0.86	0.61	88,101,107,108	0	
34	LMG	Z	101	39/55	0.86	0.24	$69,\!117,\!144,\!151$	0	
33	CA	0	301	1/1	0.87	0.12	101,101,101,101	0	
30	UNL	D	410	17/-	0.87	0.37	46,64,94,102	0	
34	LMG	с	519	51/55	0.87	0.28	47,78,122,143	0	
34	LMG	a	417	51/55	0.87	0.22	42,79,99,115	0	
36	HTG	В	624	19/19	0.88	0.21	33,71,128,130	0	
35	LMT	В	634	26/35	0.88	0.18	$48,\!90,\!109,\!115$	0	
27	GOL	a	412	6/6	0.88	0.24	56,70,85,86	0	
34	LMG	В	622	51/55	0.88	0.23	$35,\!53,\!83,\!101$	0	
37	DGD	h	103	62/66	0.88	0.29	34,46,67,76	0	
23	CLA	С	513	65/65	0.88	0.22	46,60,106,112	0	
23	CLA	С	514	65/65	0.89	0.25	$50,\!65,\!100,\!107$	0	
30	UNL	Х	101	18/-	0.89	0.20	39,66,83,87	0	
26	SQD	a	413	54/54	0.89	0.22	37,73,134,146	0	
37	DGD	С	518	62/66	0.89	0.23	35,51,111,119	0	
23	CLA	b	602	65/65	0.89	0.25	$36,\!48,\!68,\!77$	0	
23	CLA	с	512	65/65	0.89	0.22	$53,\!66,\!96,\!104$	0	
25	BCR	у	101	40/40	0.89	0.17	48,60,74,77	0	
34	LMG	m	101	51/55	0.90	0.20	33,52,85,99	0	
23	CLA	с	507	65/65	0.90	0.19	43,57,70,72	0	
36	HTG	В	629	19/19	0.90	0.20	47,59,78,83	0	
23	CLA	В	603	65/65	0.90	0.23	31,41,57,69	0	
23	CLA	с	513	65/65	0.90	0.22	58,74,112,119	0	
23	CLA	b	616	65/65	0.90	0.20	34,51,101,111	0	



Mol Type Chain Res Atoms RSCC RSR B-factors(A ²)) Q < 0.9
23 CLA C 512 65/65 0.90 0.18 39,54,77,85	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0
37 DGD H 102 62/66 0.90 0.29 29,42,64,68	0
34 LMG J 101 51/55 0.91 0.20 33,54,96,105	0
23 CLA C 504 65/65 0.91 0.29 37,47,66,75	0
23 CLA b 609 65/65 0.91 0.17 39,48,63,74	0
23 CLA b 615 65/65 0.91 0.18 33,43,65,87	0
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37 DGD C 517 62/66 0.92 0.26 30,41,77,88	0
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23 CLA C 502 65/65 0.92 0.23 36,45,67,70	0
23 CLA c 511 65/65 0.92 0.19 47,56,78,89	0
23 CLA B 612 65/65 0.92 0.26 24,32,49,54	0
25 BCR D 406 40/40 0.92 0.19 35,46,78,84	0
23 CLA C 507 65/65 0.93 0.16 42,57,106,115	0
36 HTG b 625 19/19 0.93 0.11 40,60,90,94	0
23 CLA c 503 65/65 0.93 0.44 44,55,67,84	0
23 CLA B 616 65/65 0.93 0.15 29,38,60,67	0
33 CA V 201 1/1 0.93 0.11 94,94,94,94	0
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23 CLA C 505 65/65 0.93 0.23 32,46,91,111	0
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23 CLA B 615 65/65 0.93 0.17 23,32,86,95	0
25 BCR C 527 40/40 0.93 0.17 43,55,71,72	0
23 CLA C 503 65/65 0.93 0.36 33,43,60,67	0
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23 CLA D 405 65/65 0.93 0.18 33,48,111,119	0
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33 CA o 301 1/1 0.93 0.11 89,89,89,89	0
23 CLA b 612 65/65 0.93 0.28 28,35,48,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\frac{B-factors(A^2)}{40.55,105,111}$	Q<0.9
31	LHG	d	408	49/49	0.94	0.21	40,55,105,111	0
37	DGD	с	516	$\frac{62/66}{10/10}$	0.94	0.23	35,47,74,93	0
25	BCR	с	514	$\frac{40}{40}$	0.94	0.14	58,68,80,83	0
23	CLA	С	508	65/65	0.94	0.20	39,53,121,131	0
25	BCR	Y	101	40/40	0.94	0.15	40,51,62,71	0
23	CLA	В	617	65/65	0.94	0.21	33,45,121,132	0
23	CLA	В	613	65/65	0.94	0.25	$26,\!33,\!45,\!65$	0
23	CLA	D	404	65/65	0.94	0.18	21,29,50,56	0
23	CLA	В	605	65/65	0.94	0.31	$22,\!31,\!101,\!111$	0
31	LHG	L	101	49/49	0.94	0.25	$26,\!39,\!54,\!75$	0
23	CLA	С	510	65/65	0.94	0.32	$39,\!53,\!71,\!79$	0
31	LHG	d	406	49/49	0.94	0.23	27,48,81,84	0
23	CLA	С	509	65/65	0.94	0.32	$33,\!46,\!93,\!103$	0
25	BCR	k	101	40/40	0.94	0.17	50,60,84,87	0
25	BCR	С	515	40/40	0.94	0.17	49,60,74,82	0
25	BCR	d	404	40/40	0.94	0.15	43,55,79,81	0
25	BCR	b	619	40/40	0.94	0.15	33,46,69,80	0
23	CLA	В	602	65/65	0.94	0.21	$39,\!61,\!93,\!123$	0
23	CLA	b	606	65/65	0.94	0.14	29,42,91,110	0
31	LHG	D	409	49/49	0.94	0.21	$32,\!50,\!107,\!117$	0
23	CLA	В	607	65/65	0.94	0.14	28,37,76,93	0
26	SQD	A	409	54/54	0.94	0.16	41,66,99,109	0
23	CLA	с	501	65/65	0.94	0.23	43,53,67,72	0
23	CLA	b	610	65/65	0.95	0.22	35,44,56,61	0
29	PL9	d	405	55/55	0.95	0.20	24,33,49,66	0
23	CLA	с	510	65/65	0.95	0.34	39,51,67,71	0
37	DGD	с	518	62/66	0.95	0.20	39,50,74,97	0
23	CLA	b	608	65/65	0.95	0.29	34,44,67,72	0
23	CLA	С	506	65/65	0.95	0.28	33,44,75,82	0
23	CLA	b	604	65/65	0.95	0.33	$24,\!33,\!95,\!101$	0
23	CLA	b	614	65/65	0.95	0.15	$25,\!35,\!93,\!107$	0
23	CLA	b	605	65/65	0.95	0.26	26, 34, 51, 76	0
30	UNL	d	409	17/-	0.95	0.38	48,58,94,99	0
29	PL9	D	407	55/55	0.95	0.24	20,30,44,53	0
23	CLA	b	603	65/65	0.95	0.27	32,44,61,70	0
27	GOL	В	627	6/6	0.95	0.36	60,77,93,95	0
23	CLA	с	504	65/65	0.95	0.29	41,52,94,117	0
25	BCR	b	617	40/40	0.95	0.16	21,35,45,51	0
23	CLA	a	405	65/65	0.96	0.15	23,29,52,60	0
25	BCR	с	515	40/40	0.96	0.14	41,54,66,70	0
31	LHG	D	408	49/49	0.96	0.26	25,37,56,78	0
25	BCR	В	618	40/40	0.96	0.18	24,37,48,49	0
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
23	CLA	d	402	65/65	0.96	0.22	$27,\!32,\!58,\!72$	0
25	BCR	b	618	40/40	0.96	0.22	$22,\!36,\!51,\!56$	0
23	CLA	С	511	65/65	0.96	0.48	$36,\!48,\!61,\!67$	0
23	CLA	с	506	65/65	0.96	0.15	47,65,98,117	0
23	CLA	В	606	65/65	0.96	0.21	$24,\!33,\!46,\!51$	0
23	CLA	В	608	65/65	0.96	0.22	$20,\!28,\!59,\!67$	0
23	CLA	b	613	65/65	0.96	0.26	24,36,79,89	0
23	CLA	b	611	65/65	0.96	0.21	$27,\!35,\!57,\!62$	0
23	CLA	b	607	65/65	0.96	0.18	$21,\!30,\!58,\!67$	0
33	CA	с	523	1/1	0.96	0.17	$68,\!68,\!68,\!68$	0
23	CLA	А	405	65/65	0.96	0.15	$24,\!33,\!85,\!94$	0
25	BCR	t	101	40/40	0.96	0.24	$23,\!43,\!64,\!68$	0
24	PHO	a	408	64/64	0.96	0.28	$30,\!40,\!53,\!60$	0
23	CLA	a	409	65/65	0.96	0.18	$30,\!44,\!124,\!130$	0
39	MG	j	103	1/1	0.96	0.13	48,48,48,48	0
27	GOL	А	410	6/6	0.96	0.12	$45,\!57,\!60,\!90$	0
25	BCR	a	410	40/40	0.96	0.15	$28,\!38,\!55,\!58$	0
23	CLA	a	404	65/65	0.96	0.19	$27,\!33,\!52,\!66$	0
25	BCR	В	619	40/40	0.96	0.23	$21,\!36,\!52,\!60$	0
23	CLA	А	404	65/65	0.96	0.17	$22,\!25,\!39,\!58$	0
23	CLA	А	407	65/65	0.97	0.15	28,38,98,117	0
39	MG	J	103	1/1	0.97	0.17	43,43,43,43	0
38	HEM	е	103	43/43	0.97	0.20	52,78,106,116	0
23	CLA	В	604	65/65	0.97	0.27	$30,\!43,\!56,\!67$	0
25	BCR	Т	101	40/40	0.97	0.24	$21,\!37,\!55,\!60$	0
23	CLA	D	401	65/65	0.97	0.16	$21,\!28,\!43,\!47$	0
24	PHO	А	406	64/64	0.97	0.20	$22,\!29,\!39,\!46$	0
24	PHO	D	402	64/64	0.97	0.24	$25,\!31,\!44,\!55$	0
23	CLA	В	611	65/65	0.97	0.23	$29,\!41,\!55,\!70$	0
25	BCR	А	408	40/40	0.97	0.17	$23,\!34,\!48,\!56$	0
23	CLA	В	609	65/65	0.97	0.24	$30,\!42,\!56,\!66$	0
23	CLA	В	614	65/65	0.97	0.32	$23,\!31,\!72,\!87$	0
23	CLA	a	406	65/65	0.97	0.20	$30,\!38,\!98,\!103$	0
33	CA	С	526	1/1	0.98	0.26	59, 59, 59, 59, 59	0
40	HEC	V	201	43/43	0.98	0.14	$44,\!53,\!63,\!82$	0
40	HEC	V	202	43/43	0.98	0.12	$33,\!36,\!48,\!70$	0
38	HEM	E	103	$43\overline{/43}$	0.98	0.09	43,56,69,83	0
24	PHO	a	407	64/64	0.98	0.20	$24,\!31,\!45,\!50$	0
$\overline{32}$	BCT	a	419	4/4	0.98	0.07	$41,\!45,\!48,\!58$	0
33	CA	с	524	1/1	0.98	0.08	$66,\!66,\!66,\!66$	0
32	BCT	A	416	4/4	0.98	0.08	$32,\!45,\!46,\!51$	0
$\overline{22}$	CL	a	403	1/1	0.98	0.27	41,41,41,41	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
22	CL	А	402	1/1	0.99	0.10	24, 24, 24, 24	0
28	OEX	А	412	10/10	0.99	0.10	$23,\!32,\!46,\!47$	0
21	FE2	a	401	1/1	0.99	0.04	$47,\!47,\!47,\!47$	0
21	FE2	А	401	1/1	0.99	0.05	46, 46, 46, 46	0
28	OEX	a	414	10/10	0.99	0.09	$29,\!36,\!46,\!48$	0
22	CL	А	403	1/1	0.99	0.25	27,27,27,27	0
22	CL	a	402	1/1	1.00	0.13	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.




































































































































































































































































































































































































































































6.5 Other polymers (i)

There are no such residues in this entry.

